BACHELOR THESIS

CONFIDENTIAL COMPUTING VIA HARDWARE TRUSTED EXECUTION ENVIRONMENTS BY AN OPENSTACK HPC CAPABLE CLOUD

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There is a great difference between discoveries and inventions. With discoveries, one can always be skeptical, and many surprises can take place. In the case of inventions, surprises can really only occur for people who have not had anything to do with it.

— WERNER HEISENBERG

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ABSTRACT

Confidential computing protects data in use by using secure and isolated hardware trusted execution environments. These environments prevent unauthorized access or modification of applications and data in use. Organizations that manage sensitive and regulated data rely on enhanced security assurances provided by this technology. Across industries and institutions, computing is used on multiple platforms which can span from private, hybrid or public cloud and also, to the edge. In some cases, organizations also require high-performance computing to process big and sensitive data in the cloud.

DigiMed Bayern is a research project with more than 24.5 million Euros in funding from the Bavarian State Ministry of Health and Care. It combines comprehensive datasets of patients diagnosed with atherosclerotic diseases or with genetic risk factors. The multidimensional molecular characterization will further enhance the sample material. The analysis of big and sensitive data is required to be ethical- and legally compliant, highly secure and sustainable. This is to be ensured by the underlying information technology infrastructure which uses OpenStack for its confidential cloud and high-performance computing capabilities.

In the first place, we provide details about the used hardware and software, including the virtualization and cloud services and how the implementation of Advanced Micro Devices hardware-based trusted execution environments functions.
Secondly, we investigate the security attestation of trusted execution environments and show the correlation of concept and implementation of the system, from hard- and software perspectives. Furthermore, the front- and backend will show the usability as the complexity of usage can be relevant.
Finally, concrete use cases in different setups of high-performance computing components in the DigiMed cloud will illustrate the impacts of security and scalability on the computation units and their performances.

CONTENTS

1 INTRODUCTION

Confidential computing and confidential high-performance computing [30] (HPC) is a frequently demanded service as the number of security threats to IT infrastructures has increased over the last years [11]. According to the Forrester study [10], IT infrastructure has been modernized after security issues and vulnerabilities have been found respectively by half of IT decision-makers. Refreshing on-premises hardware can be a challenge resulting in delays considering IT projects and priorities of the IT department. In comparison, modernization attracts less attention than new projects. Especially high expenses like these need to be properly addressed and justified. Reinvestment into the already existing infrastructure seems costly and lavish. However, in this case, it is crucial to modernize on-premise infrastructure to minimize security targets.

Another approach is to reconsider strategic decisions considering dynamic outsourcing as a beneficial tool to save money and effort. It is crucial to distinguish the need for computing and data transfer. With the proper security concept in place, information is classified and needs to be properly handled. Each class of information needs its respective set of security measures implemented on the network. Depending on the requirements, it might be worth outsourcing sensitive data to the cloud service provider because otherwise, the whole infrastructure for sensitive data processing needs to be in place.

Therefore, there are solutions in the public cloud [32] available. For example Infrastructure as a Service (IaaS) is a public cloud solution that provides a platform to generate and interconnect virtual machines and respectively, their services. These machines can be prepared and scaled to solve large problems. Furthermore, a wide set of security features can be implemented on them.

As a consequence, users do not have to invest in on-premise infrastructure to carry out their projects.
Generally, cloud platforms on the Internet are considered untrusted. Sensitive data processing is not per se to be considered feasible on the Internet as it is the responsibility of the cloud provider to provide the respective service. The key issue for the users was and still is to ensure trust between the service provider and the users themselves. The provider is believed to ensure sufficient security measures to protect from all kinds of attacks and prevent failures of the IT operation.

To approach the privacy concerns with the recent developments, new security features have been introduced to the latest processor generations. Trusted execution environments (TEE) such as Intel Software Guard Extensions (Intel SGX) and AMD Secure Encrypted Virtualiza-

tion (AMD SEV) are the key technologies to ensure data integrity and confidentiality on the hardware level, concluding that trust already begins with the production of the CPUs. These features face several challenges regarding their usability, security and performance. For example, Intel SGX requires specific code implementations to ensure the confidential execution of workloads. During runtime, it is not possible to use OS programs APIs to access the file system or the user interface to ensure a strong security guarantee. When OS API is accessed, data will be exchanged in the untrusted memory. Another example is the performance as TEE comes with performance penalties depending on the tasks and processing units [20].

Besides, there are several challenges regarding single- and multiuser computing. Speaking of single-user cases, users may execute confidential computation jobs on the Internet. Either the hypervisor or the OS of the system can be compromised. Preservation of data and program integrity and confidentiality are crucial while availability has lower priority. On the other side, HPC workloads often require collaborative workflows. TEE implementations increase the attack surface, but not explicitly due to its HPC nature, but its mechanisms and weaknesses which leads to the first research question.

RQ1: How does the security attestation of TEEs work?

In Chapter 5.3, we discuss the concept and the implementation of TEEs in AMD CPUs. There, we also present the results of the investigation of the interaction with the trusted execution environments on the physical and logical systems of the DigiMed prototype infrastructure.

The Confidential Computing Consortium (CCC) defined the term TEE and describes it briefly as an environment that provides a level of assurance of data confidentiality, data integrity and code integrity.

AMD presents its implementation of TEE with its AMD Secure Encrypted Virtualization (SEV) technologies. This realization is based on virtual machines and fully encrypts them.

Computers in the DigiMed prototype infrastructure with their AMD-based CPU architecture make use of AMD SEV technologies and by providing insights about the implementation, we sheer light on rising issues implementing advanced security measures. In most cases, the usability is affected, too. This leads to the second research question.

RQ2: How is Usability affected when TEEs are implemented in a confidential HPCaaS?

In Chapter 5.4, when analyzing the usability of TEEs, we consider the perspectives of the front- and backend and how they fulfill the standards of usability.

ISO 9241-11:2018 [6] defines the term ergonomics of human-system interaction and introduces its concept. The framework describes where interactive systems or other types of systems are being used, e.g. in built environments, industrial and consumer products and technical and personal services. In this case, TEEs are part of central processing units (CPU) as an industrial product. In software engineering, the front- and backend describe the separation between the presentation and the data access layer of software.

Firstly, we present the results about how user interaction is affected when using TEEs. This means, which stages need to be stepped through to enable TEEs while operating on the user interfaces or which and how other user operations are impacted.

Secondly, we report on the impacts on the underlying components, their configuration and data flow. The usage of TEE also limits the usability of virtualization technologies. These limitations were briefly illustrated, too. Security measures not only and regularly affect the usability, but also have impacts on the performance of the involved systems which leads to the third and last research question.

RQ3: How is Performance affected when TEEs are implemented in a confidential HPCaaS?

In Chapter 5.5, we present the results of the performance impacts on several benchmark setups when using TEEs. As the aspects of High-performance computing are also of interest, clusters from one to more than one hundred virtual machines have been created. Also, each involved computer is referenced as an HPC component as their technical parts are of a performant and industrial configuration.

With each of these scenarios, the impacts of security and scalability were examined. Parameters were the status of TEE, number of CPUs, number of CPU cores, the size of random-access memory (RAM), type and bandwidth of network interface controller (NIC) and number of nodes.

Furthermore, regarding the DigiMed use cases, standard benchmarks in molecular dynamics (MD) analysis were used to measure the performance of the virtual nodes. The GROningen MAchine for Chemical Simulations (GROMACS) - benchmarks are typical simulation systems to cover a wide range of system sizes from 6k to 12M atoms. Here, they fit well as the DigiMed project covers the analysis of proteomics, DNA and RNA sequencing and genotyping.

2 BACKGROUND

2.1 CONFIDENTIAL COMPUTING

Isolation of sensitive data in a protected Central Processing Unit (CPU) enclave during processing is called Confidential Computing [4]. It is a cloud computing technology. The protected area is only accessible to the authorized program. To anything else, including the service provider, the secured domain is unreachable. The protection includes contents such as the processed data and the code itself.
As the management of companies wants to rely more and more on flexible cloud solutions, data privacy is imperative. The idea of Confidential Computing is to assure leaders that their data in the cloud is protected and confidential while data integrity is ensured. Ideally, the successful implementation of this technology encourages them to move sensitive data and workloads to the public cloud [12] [9].
Traditional services of cloud providers are encryption services to protect static data, for example in storage and database systems. Also possible is the protection of dynamic data, e.g. while being transferred over the network. There is a security gap that needs to be addressed: data in use. For that, Confidential Computing has been developed which protects the data during processing.
The first state of data before being confidentially processed is unencrypted in the memory. This state leaves several threats open. Therefore it is possible to impose memory dumps just before, during and directly after the operation. Furthermore, root user exploits and other attacks are feasible.
Trusted Execution Environments (TEEs) address these issues by adding a hardware-based security layer to the CPU. This secured domain is identified as a secure enclave. The concept ensures protection by embedded mechanisms to authorize only privileged applications. This includes the usage of encryption keys and attestation mechanisms. The CPU recognizes if malicious or hacked software is used to get credentials or to access security components. Then, it denies access and cancels further processing of the program [21].
The following Figures 2.1, 2.2 and 2.3 further explain the nature of Trusted Execution Environments. There are three states regarding data: in transit, at rest and in use. Trusted Execution Environments are allocated to the data in use components and additionally, to be distinguished from the other ones. Within the data in use concept, TEEs coexists with Homomorphic Encryption (HE) and Trusted Platform Modules (TPM).

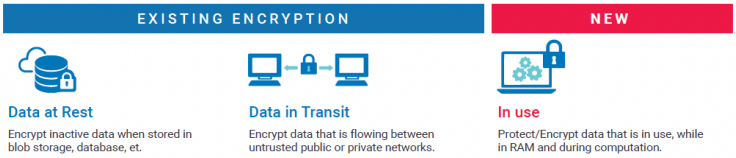

Figure 2.1: **States of data [21]**

In Figure 2.2, isolation is differenced between CPU Addressability Isolation and Memory Isolation. Further, their components as Access Control Validation, Address Translation, Paging Control and RAM Encryption are being used by some example platforms. These are acknowledged by the CCC and show how they ensure isolation and confidentiality.

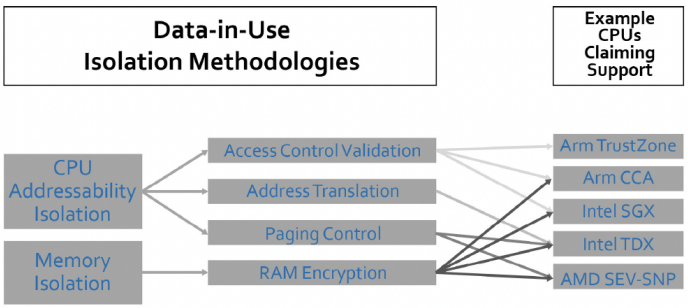

Figure 2.2: **Data in use [21]**

In Figure 2.3, the characteristics of the data in use technologies are shown. Essential categories are confidentiality, integrity and usability. Each of those has its specifics and is divided into further details listed in the matrix. Programmability means the requirement of modification or the possibility of customization.
The concept of TEE ensures the protection of sensitive data in memory

	HW TEE	Homomorphic Encryption	Secure Element e.g., TPM
Data Integrity	Y	Y (subject to code integrity)	Keys only
Data confidentiality	Y	Y	Keys only
Code integrity	Y	No	Y
Code confidentiality	Y (may require work)	No	Y
Programmability	Y	Partial (“circuits”)	No
Unspoofability/Recoverability	Y	No	Y
Attestability	Y	No	Y

Figure 2.3: **Comparison data in use technologies [21]**

until the program tells the CPU and its TEE to reveal the data. During runtime, the data is decrypted and not reachable by any other potential stakeholder, such as the operating system or hypervisor, other services and the cloud service provider.

The ultimate goal of Confidential Computing is to enable sensitive workloads on the cloud, not explicitly HPC ones. It helps to protect these sensitive workloads while in use. In combination with static and dynamic data encryption with key monitoring, Confidential Computing dismantles the only blocking point to transferring and processing sensitive and highly regulated Big Data and program workloads from a static and inefficient on-premise IT network to a modern, dynamically scalable public cloud platform [20].
To achieve this, several aspects need to be covered: *Protection of intellectual property*, *Secure Multiparty Computation*, *Elimination of cloud service provider concerns*, *Protection of Edge Computing* [17].
Protection of intellectual property is crucial to keep business intelligence (BI) as proprietary logic, algorithms and entire programs private.
Secure Multiparty Computation enables collaboration between stakeholders to process sensitive data and to create new solutions without exposing unwanted information.
Elimination of cloud service provider concerns encourages organizations to choose Confidential Computing over the cloud as a service as the best solution for one's technical and business needs. Worries about storing and processing business-related and proprietary data, technology and other sensitive assets need to be stopped. It further alleviates any concerns about competition if the service provider also provides competing services.
Protection of Edge Computing is a technology that moves enterprise software to embedded systems or edge servers as this framework uses distributed cloud technology. Confidential computing protects data and software at edge nodes.
The Confidential Computing Consortium [21] (CCC) was formed by a group of CPU manufacturers, cloud providers and software companies in 2019. These companies include Alibaba, AMD, Baidu, Fortanix, Google, IBM/Red Hat, Intel, Microsoft, Oracle, Swisscom, Tencent and VMware. Its intention is the definition of industry standards for Confidential Computing and the promotion of the development of open-source tools. TEE implementations are complex as programs have to be modified to benefit from their security features. Open-source projects such as Enclave SDK and Red Hat Enarx are the first projects of the Consortium.
Nonetheless, Confidential Computing technologies have already been used before the organization of the CCC. One of these key technologies is the Intel SGX which enables TEEs not only on the Intel Xeon CPU architecture but also on the Intel Core CPU family. However, its inception had been on workstations- and accordingly, server systems. Intel introduced its TEE implementation in 2015. IBM for example has introduced Confidential Computing in its product line since 2018.

2.2 TRUSTED EXECUTION ENVIRONMENTS

Over the years, Digital Rights Management (DRM), mobile financial services, authentication, secure modular programming, organizations and their cloud emerged with the further need for confidentiality. Furthermore, the EU General Data Protection Regulation (GDPR) has put stricter legal policies in place when organizations process and transmit data from their clients. Privacy has been increased with concepts such as homomorphic encryption. Unfortunately, these come with significant performance overhead [15] [20].
Trusted Execution Environments (TEEs) have been introduced to address the aspects of privacy, performance and practicability, considering a wider range of use cases at lower costs than pure software approaches. To consolidate findings about the definition, the CCC is quoted as follows:

> "A Trusted Execution Environment (TEE) is commonly defined as an environment that provides a level of assurance of data integrity, data confidentiality, and code integrity. A hardware-based TEE uses hardware-backed techniques to provide increased security guarantees for the execution of code and protection of data within that environment."
>
> Confidential Computing Consortium. (2021). Confidential Computing: Hardware-Based Trusted Execution for Applications and Data [21].

However, challenges such as security issues will be treated later in the thesis. In our daily life, there are many examples given as Apple's Secure Enclave [19] uses the concept of TEEs for its Secure Enclave Processor (SEP). It is one of Apple's key security features as it is implemented in their current SoC-based products such as their handhelds and accessory devices. Their iOS and Apps make use of encryption keys which are kept secure by the SEP.
Furthermore, business computers are regularly equipped with a Trusted Platform Module (TPM) which represents a form of TEE. The principle is to ensure the integrity of the hardware and software involved during boot. Occasionally, it is also used for other cases such as in the prevention of cheating on games. However, this technology lacks performance as it can not be used for large workloads. Newer Trusted Execution Environments enable organizations to securely process their data on the internet. Hardware and software developers hope that this technology is a long-term solution for Confidential Computing on mobile devices, computers and cloud systems while having security threats minimized.
Standard groups such as the Internet Engineering Task Force (IETF) and its Trusted Execution Environment Provisioning working group develop standards to ensure interoperability between systems, software and workloads. For example, with Open-TEE, the use of virtual

trusted execution environments is possible. This enables developers to build trusted programs while respecting GlobalPlatform's TEE specifications. Cloud service providers did not hesitate to expand their services through confidential cloud computing. Amazon Web Services (AWS) introduced AWS Nitro Enclaves to minimize targets for their software by the provisioning of a secured computing environment. It is hardened, highly isolated and trusted according to AWS. Most Intel- and AMD-based Amazon EC2 instance types built on the AWS Nitro System provide those enclaves. In contrast, Microsoft also rolled out its service for Confidential Computing with the offer of DCsv2-series virtual machines. The Intel Software Guard Extensions (SGX) are enabled on their Intel servers and by that, their security is enhanced. Azure confidential computing does not permit access to the data within the virtualized hardware-based TEEs to any unprivileged persons, including the cloud provider.
The concept of a Trusted Execution Environment makes it unique as hardware and software components are combined to establish a secure area within the memory. As illustrated in Figure 2.4, those components are built upon two distinct models for cloud computing. The whole system memory of a virtual machine is encrypted in the virtual machine-based model (A). Only an encrypted memory area within the virtual machine is established in the process-based model. In comparison, in A, the whole VM is encrypted. In contrast, in B, the confidential code has to be destined by its software developer to be run in a Secure Enclave. It further means that in B it is needed to distinguish between encrypted and unencrypted sections of the system memory [15] [14].

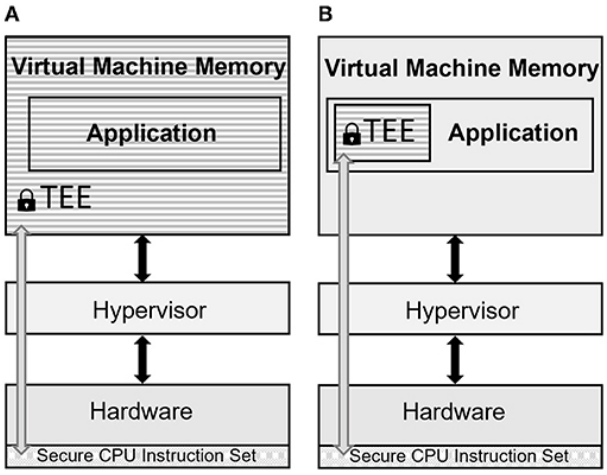

Figure 2.4: **TEE cloud computing [15]**
A: **Virtual machine-based model**, the whole memory of the virtual machine is encrypted.
B: **Process-based model**, only the memory of the enclave is encrypted.

The certification of CPUs is an important step to ensure the integrity of their TEEs. To obtain a certificate, the hardware producer needs to prove that the TEE is implemented by conforming to the hardware and software standards of the TEE specification.
It is crucial to know that the hardware vendor, e.g. Intel or AMD represents the certificate authority (CA) as the CA provides the pair of private and public keys to identify the unique hardware. During production, the private key is installed into the hardware. This constitutes the so-called root of trust. In contrast, the CA signs with its private key the public key of the hardware. This ensures the reverse lookup to the CA while building trust [3].
TEE is implemented via platform-specific microcode instructions that come with the hardware.

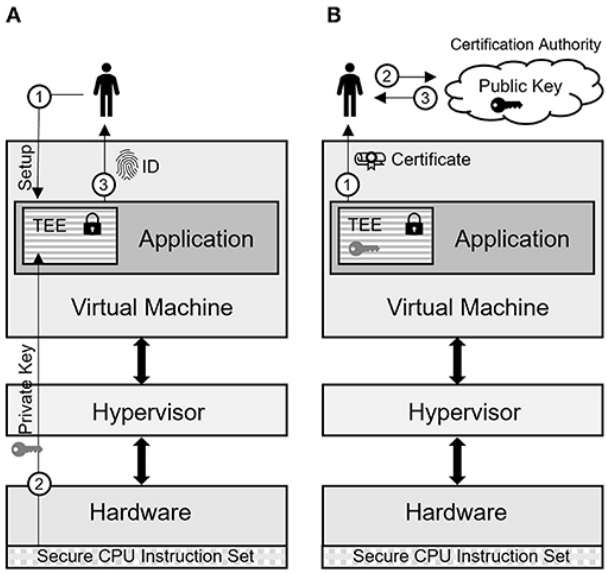

Figure 2.5: **Process-based model - TEE creation and validation [15]**
A: **Creation**, system memory is encrypted using a symmetric encryption schema.
B: **Validation**, a remote CA validation service uses the private validation key with metadata to send a certificate for validation to the CA.

As shown in Figure 2.5 (A), the system memory is user-defined and only for this encryption process, access to the private key is granted. This is the crucial part where confidentiality over the cloud service provider or other stakeholders is built up. After encryption, a portion of the application is loaded into the encrypted memory and finally, a unique identifier of the TEE is determined and sent to the user for validation. As shown in Figure 2.5 (B), validation needs to be done as the user responsible for the TEE on a cloud system does not have access to

the physical hardware. There is a necessity of trust that the TEE source is the vendor's infrastructure as only this guarantees the integrity of encryption and the expected program code lies in the secure area. The remote CA validation service is responsible for this procedure. Firstly, with the private key and the metadata, a certificate will be generated which will be retrieved by the user. Then, the certificate is signed by the TEE corresponding private validation key. This key contains the unique ID from A, and supplementary details about the considered program code and its underlying hardware. The anticipation of the user concerning the software can then be confirmed as the certificate is sent to the CA. With successful validation, the promise of privacy is fulfilled.

In contrast, the virtual machine-based model is being used by AMD with their AMD Secure Encrypted Virtualization (SEV) technologies. These technologies were introduced in 2016 for x86 architecture to enable isolation between VMs and corresponding hypervisors. Originally, hypervisors had been trusted components in the virtualization security model. However, it has its limits when it comes to Confidential Computing as the cloud service provider manages the hypervisor and has access to the machines. This fact leaves users to desire further isolation of their VMs at a hardware level from the hypervisor and other software [18].
To counter the issue, AMD implemented Secure Memory Encryption (SME). VMs can be assigned a unique AES encryption key to automatically encrypt the in-use data. Hypervisors have only access to the encrypted bytes.
Furthermore, in 2017, Encrypted State (ES) was added to the SEV portfolio. Before, the CPU register state had been exposed to the hypervisors. Now, with this feature, it is possible to encrypt these on each hypervisor transition so that the hypervisor can not read data while being processed within the VM. This feature enhances VM protection as the data in memory is additionally protected.
In 2020, Secure Nested Paging (SNP) has been introduced as the next-generation SEV technology. It adds supplementary hardware-level security features. Known threats on that level are data replay, memory remapping and more to have an isolated execution environment. To counter those malicious hypervisor-based attacks, SEV-SNP ensures strong memory integrity. Further virtualization-based use cases are supported and the protection around interrupt behavior has been fortified. SNP faces current threats by side-channel attacks. They will be discussed later [18].
AES ensures encryption and provides trust by protecting the memory. Without the corresponding key, for unprivileged individuals, it is not possible to decrypt the in-use data of the VM as it makes use of SME. A hardware random number generator creates the key stores in dedicated hardware registers. Software is not permitted to read it. Furthermore, by design, identical plaintext at different memory locations is encrypted differently by the hardware [18].
Besides, attempts to change memory values can not be excluded, even

without the encryption secret. Those attacks are called integrity attacks as RAM is manipulated. Without the secret, proper data placement seems difficult. However, the VM could see random values which might throw exceptions. Also, replay attacks could be conducted. In such a case, an attacker records ciphertext at one point in time and later replaces memory with the earlier captured data. The impact would be much higher if the attacker knew the semantics of the data [18].
In contrast, attacks that impact the integrity of the VM do not directly control a VM as the VM is treated as a black box. Patterns of behavior are being interpreted, as incorrect data shall compromise the VM or disclose information. Success is determined by how well the machine and its behavior had been analyzed and malicious data accurately implanted.
With AMD SEV-SNP in place, the risk associated with integrity attacks is significantly reduced. The main principle of SNP is the virtual machines' only permission to read a private and encrypted page of memory is given when it reads the last value it wrote. Assumed that a value A to RAM location was written by the VM. Whenever it later reads it, it sees either the value or the process throws an exception which indicates an access failure. By design, the VM can not see a different value at that location [16].
These technologies impede default virtualization features as an integrity guarantee has to hold in any case. So features and hardware need to be designed around. If memory pages are being transferred between disks or entire virtual machines migrated to new hosts or clusters, this guarantee has to be upheld. This requires state-of-the-art hardware. Within and without virtual machines need to run their jobs, in the latter with their corresponding interfaces. This might involve network communication, storage systems or other components. For external communication, unencrypted memory is used. Outgoing information is moved to a shared page of memory, respectively for incoming data. It is recommended to use at least secure communication protocols to transfer the information.

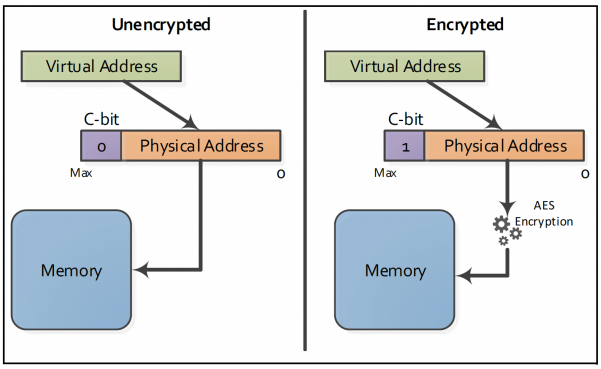

Figure 2.6: **Virtual machine-based model - Encryption Control [18]**
Unencrypted: **Shared memory**, C-bit is 0. Encryption is deactivated.
Encrypted: **Private memory**, C-bit 1. AES Encryption is active.

AMD SEV-enabled virtual machines have control over the state of being private or shared using the enCrypted bit (C-bit) in the guest page tables. The location of this bit depends on the implementation. It may be the top physical address as shown in Figure 2.6 [18].
Shared memory needs to be unencrypted, so the C-bit is 0 and encryption is deactivated. Private memory needs to be encrypted, so the C-bit is 1 and AES encryption is activated. In most cases, the majority of memory pages are marked private and only a careful selection needs external communication which then, needs to be marked as shared. SEV-SNP integrity guarantees come only into effect when private memory is used.
As mentioned before, there are many use cases for Trusted Execution Environments such as artificial intelligence, Secure Multiparty Computation (SMPC), Internet of Things (IoT) and cloud computing. Currently, the principal one is cloud computing. It is especially promising regarding its capability to add the same security properties to mobile and cloud systems that organizations strive for their on-premises environments. It fulfills the requirements regarding security and trust and with that, it shall also allow cloud computing in sensitive areas [20].
Speaking of HPC use cases, TEE enhances Confidential HPC in the public cloud. It enables secure data processing, the establishment of Secure Enclaves for processes and collaboration with stakeholders. Although not perfectly secured, Trusted Execution Environments enable a high level of security that is not accessible by the hardware producers and software developers. Big Data processing and intensive workloads with the need for split-second response latencies signify the difference between ordinary cloud computing and high-performance computing in the cloud. Furthermore, MPC is being done on HPC infrastructures, also with the need for enough security to process sensitive data. Data analysis on sensitive data, as mentioned before, of financial services can be a use case. MPC faces the challenge that it often relies on trusted third parties or legal contracts. There, data exploits are still possible [3].
Trusted Execution Environments can increase the trust in MPC as they offer sufficient security and efficiency. Those analytics can be run within the TEE. Each stakeholder can validate the code run within the TEE. The benefit is by putting raw data in and collecting aggregated output data.

2.3 CLOUD COMPUTING

Cloud computing is a term and paradigm that is approximately defined by national authority institutes of standards and technologies. Furthermore, the ISO has also published several parts to define it. In this case, the definition of the National Institute of Standards and Technology (NIST) of the United States took a pragmatic approach to the definition and defined it in 2011 as follows [22] [23] [24] [2]:

Cloud computing is a model for enabling ubiquitous, convenient, on-demand network access to a shared pool of configurable computing resources (e.g., networks, servers, storage, applications, and services) that can be rapidly provisioned and released with minimal management effort or service provider interaction. This cloud model is composed of five essential *characteristics*, three *service models*, and four *deployment models*.

According to the definition, the following *characteristics*, *service models* and *deployment models* will be further described as they are the pillars of cloud computing.
The *characteristics* are represented by the aspects of *on-demand self-service*, *broad network access*, *resource pooling*, *rapid elasticity* and *measured service* [2].

- *On-demand self-service* is the case when a customer requests computing services without the involvement of any stakeholders when it is needed. These services can be server time and network storage.
- *Broad network access* describes the possibility of using resources over the network by a variety of client platforms. Those can be handhelds, notebooks and PCs.
- *Resource pooling* occurs when service providers' resources are being pooled and offered to their customers in a multi-tenant environment. These can be physical and virtual resources (e.g. storage, processing, memory and network bandwidth) that can be requested and allocated flexibly. While the exact location of resources in most cases remains protected, it can be at least specified to a higher level of abstraction, e.g. country, state or data center.
- *Rapid elasticity* is the dynamic allocation of resources. This allocation can be of an automated nature and happens on demand. Furthermore, one further characteristic is the in- and outward scalability which seems to be unlimited as any quantity of resources can be acquired.
- *Measured service* is the usage of a metering measure which is implemented in a higher level of abstraction depending on the type of service, e.g. user accounts, CPU, storage and network

bandwidth. Those resources are managed by monitoring, controlling and reporting systems. They provide full control over these resources for the provider and user of the demanded services.

The *service models* are represented by the terms of *Software as a Service (SaaS)*, *Platform as a Service (PaaS)* and *Infrastructure as a Service (IaaS)*. A cloud infrastructure is a set of hardware and software that fulfill the characteristics of cloud computing. Physical components are servers, persistent storage and networking equipment. In some cases, organizations establish partnerships with the manufacturers to design custom and optimized components specific to their needs. Current demands are especially power efficiency and big data and AI processing [2].

- *Software as a Service* describes the provisioning of applications over the infrastructure of a cloud provider. Those applications can be addressed via web browsers or program interfaces of a diversity of client systems, such as thin clients, notebooks, smartphones et cetera. The actual user does not administer the cloud infrastructure components. Only user-specifics can be modified in the application configuration.

- *Platform as a Service* describes the capability of the user to upload his self-created or acquired programs. The provider supports these components which are based on programming languages, libraries, services and tools. The actual user does not administer the cloud infrastructure components. Although, the user has control over deployed applications and respectively, their configuration regarding the hosting platform.

- *Infrastructure as a Service* describes the provisioning of cloud infrastructure by the user. He can freely install and run software, including programs, but also operating systems. He does not have access to the underlying components of the cloud infrastructure. Further, the user potentially has additional control over storage, applied software and related networks, including security components (e.g. firewalls).

Further, there are different ways to make a cloud system accessible to its stakeholders. These are called *Deployment Models* which differentiate in source and target group, but also in ownership, management, operation and location. They are represented by the terms of *Private cloud*, *Community cloud*, *Public cloud* and *Hybrid cloud* [2].

- *Private cloud* describes a cloud infrastructure that is exclusively destined for a single organization with multiple user groups, analogous to business units. Ownership, management and operation can be handled by a third party, the organization itself or a combination of them. The Private Cloud may exist on- or off-site. The DigiMed prototype contains a private cloud infrastructure that is only reachable via a virtual private network (VPN).

- *Community cloud* describes a cloud infrastructure that is exclusively destined for a specific target group of organizations. They

have common interests in goals, requirements, policies et cetera. Ownership, management and operation can be handled by a third party, one or more of these organizations themselves or a combination of them. The Community Cloud may exist on- or off-site.

- *Public cloud* describes a cloud infrastructure that is open to the public. Ownership, management and operation can be handled by a company, an academic or a public institution or a combination of them. The Public Cloud exists on-site the cloud provider. Microsoft Azure contains a public cloud infrastructure that is reachable via the Internet.

- *Hybrid cloud* describes a cloud infrastructure that is a composition of many dedicated cloud private, community or public infrastructures. They are self-sufficient but combined with standardized or individual technology to enable flexibility in application and data. For instance, it is possible to make use of cloud bursting. In that context, the processing capabilities of a Private Cloud can be combined with a portion of the public one to handle a demanding workload [7].

2.4 LARGE PROBLEM-SOLVING

High-Performance Computing [38] (HPC) is a technology that uses a cluster of powerful Central Processing Units. They are parallelly used to process large and multidimensional data sets (Big Data) and to solve complex problems at extremely high speeds. In comparison to default desktops, laptops or servers, HPC systems are significantly faster.
For decades, a supercomputer has been the typical model of an HPC system. It holds a huge amount of processors and their cores. However, this idea has not changed. According to IBM, with a processing speed of 1.102 Exaflops or 1 Trillion floating point operations per second (FLOPS), the US-based Frontier is the fastest supercomputer in the world. HPC solutions as clusters of HPC systems are available on-premise or in the cloud while being used by enterprises or institutions [31].
The computers in this context handle large problems in scientific environments. HPC supports significantly the development of human knowledge and establishes competitive advantage. There are many domains where HPC is being used, e.g. in the sequencing of DNA, stock trade, algorithm and simulations and processing of artificial intelligence (AI). In the context of automated automobiles, embedded systems such as IoT sensors, radars and GPS generate Big Data that is processed in real time to induce split-second decisions [13] [25] [38].
HPC differs from common computing. Problems are divided and parallelly processed on two or more processing units of the HPC systems while default computers process them on their only multi-core processor. Distinctive characteristics of HPC are: *Massively Parallel Computing*, *Clustering* and *High-Performance Components* [8].

Parallel Computing describes the parallel processing of tasks on two or more servers or CPUs simultaneously. *Massively Parallel Computing* differs via the usage of thousands to millions of CPUs and respective cores.
Clustering is used to interconnect High-Performance computers. A central scheduler manages the HPC workload to be executed in parallel. The computer as a component of these clusters is called *node*. They consist of high-performance components such as CPUs with several cores or graphics processing units (GPUs). GPUs are especially beneficial for massively parallelized and accurate mathematical operations, models for machine learning and graphic-intensive tasks. One cluster potentially consists of more than 100.000 nodes [40].
High-Performance Components are provisioned to optimize the throughput of the cluster. Every component such as network-, memory-, storage- and file systems has high throughput with minimized latencies.
Until the last decade, for many companies, it had been difficult to access HPC. The reason was its costs. The scope covers ownership and leasing of either a supercomputer or an HPC cluster in a local data center. Nowadays, HPC becomes more and more accessible as cloud providers have extended their product range with another service: HPC as a Service (HPCaaS). For institutions and companies, it is a much faster, scalable and cost-efficient possibility to benefit from its characteristics. The service covers access to the HPC infrastructure of a cloud service provider, but also services such as analysis of AI or data and HPC knowledge [15].
HPC in the cloud engages with the following converging developments: *Increasing demand*, *Adoption of remote direct memory access (RDMA) with better performance*, *Wide adoption of HPCaaS*.
Increasing demand is determined as organizations of all kinds are getting more dependent on real-time analysis and competitive advantages resulting from large problem-solving via HPC. The detection of credit card fraud relies more and more on HPC to accelerate its recognition and minimize false alarms while fraudulent activities increase and tactics change. In this context, also collaborative workflows accelerate the search for findings in Big Data within HPC environments as Multi-party Computing accelerates this job.
Remote direct memory access enables an interconnected computer to access the memory of another networking computer without involving its operating system or halting its processes. It contributes to minimizing latencies and maximizing throughput. Existing performant RDMA implementations, including Infiniband, Virtual Interface Architecture and RDMA over Converged Ethernet (RoCE) makes cloud-based HPC possible.
Wide adoption of HPCaaS is nowadays given as every leading public cloud service provider provides HPC services. Because a portion of institutions still has to locally work with HPC workloads, there are also private cloud HPC solutions available. The reasons might be strong regulations or a certain degree of data sensitivity.

2.5 RELATED WORK

Other scientists have already dealt with the topic of TEEs in the domain of HPC to investigate their performance impacts in virtualized environments. Most of our aspects were represented, but the OpenStack cloud platform was not used in their research. Furthermore, there is much research in progress to further investigate the usage of TEEs in collaborative workflows as their implementation comes with constraints. Therefore, the interaction of stakeholders with the HPC systems for Confidential Computing is relevant and needs to be further examined while security threats need to be identified and minimized.
In the following section, the findings of the scientists regarding the performance impacts of TEEs will be presented and evaluated:
Firstly, Intel Software Guard Extensions (Intel SGX) are also a Trusted Execution environment as AMD Secure Encrypted Virtualization. Intel SGX requires specific code implementations to ensure the confidential execution of workloads. During runtime, it is not possible to use OS functions and routines APIs used to access the file system or the user interface to ensure a strong security guarantee [20].
Regarding AMD SEV and Intel Software Guard Extensions, performance-related data of HPC applications could be collected. Ordinary HPC workloads as well as modern applications were used. NAS Parallel Benchmark (NPB) is a software suite that provides different pseudo applications and kernels to test the performance of parallel supercomputers. It is an established suite and still up-to-date. Different data sizes were configured and profiled as classes for the benchmarks. NPB Class C was used for SEV and SGX to solve standard test problems. NPB Class D was only for SEV to solve large test problems. Here, relevant statistics and characteristics will be shown and evaluated. Only core issues will be further treated either still in this or the following sections depending on the use case. Apart from this software suite, modern HPC workloads had been used. Each of them has its characteristics:

- *GAPBS:* Graph workloads, with the input of a graph of road networks in the US.
- *Kripke:* Particle transport simulation.
- *Livermore Unstructured Lagrange Explicit Shock Hydro (LULESH):* Solves "Full-featured" hydrodynamics simulation problem.
- *LightGBM:* Machine learning training, decision tree workload, characterized by irregular memory accesses, using Microsoft's Learning to Rank (MSLR) data set.
- *Mobiliti:* Transportation system simulator (based on parallel discrete event simulation).
- *Basic Local Alignment Search Tool Nucleotide (BLASTN):* Bio-informatics tool to search sequence similarities, more specifically BLASTN

was used to search a nucleotide sequence against a nucleotide database.

Concerning the following findings, the relevant architectures and system configurations are illustrated in Figures 2.7 and 2.8. The evaluations had been done without hyperthreading. The number of cores corresponds to the number of threads on each system. Significant performance issues of Confidential Computing is minimized because cache contention is reduced. This affects threads with large jobs.

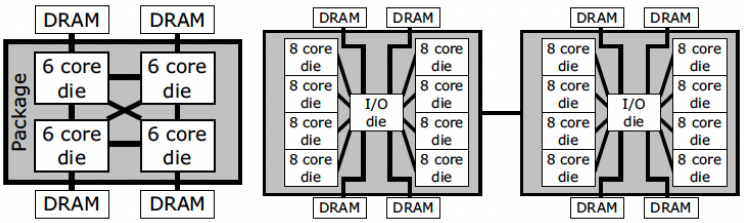

Figure 2.7: **AMD - NUMA-architecture [37]**
Left: **AMD EPYC 7401P (Naples)**
Right: **AMD EPYC 7702 (Rome)**

Three AMD-based servers were used to test SEV. The CPU scheme of AMD EPYC 7401P (Naples) and AMD EPYC 7702 (Rome) are shown in Figure 2.7. The Naples system consists of 24 CPU cores with 6 cores on each of 4 dies in a single CPU. It is single-socketed but has 4 NUMA nodes in total. A multi-chip CPU behaves similarly to a multi-socket system considering latency and bandwidth between separate dies. Depending on the location management of non-uniform memory access (NUMA) nodes, memory performance varies highly.
This technology is a memory design that is used in multiprocessing. Its access latencies depend on the memory location and its distance to the CPU. The closer the memory is to the CPU, the faster the access.
The system with the Rome architecture had a more uniform memory design, so it was also evaluated. It had 64 cores with 8 cores on each of 8 dies. It constitutes a multi-chip package. The dual-socket system consists of a total of 128 cores. It has more chips per package. The memory design is more uniform because each die has the same distance to the corresponding I/O die with the memory controllers. Per socket, there is only one NUMA node. In this case, considering the 2 sockets, there are 2 NUMA nodes in total.
Considering the Intel platform, a desktop-class CPU with 6 cores and 1 NUMA node was used to perform SGX simulations. In many cases, the size of secure memory was still significantly smaller than the job units of most studied HPC workloads, e.g. only the benchmark ep has a job unit smaller than 256 MB. It generates independent Gaussian random variates using the Marsaglia polar method. QEMU was used as a hypervisor for virtualization and performance could be improved by interleaving which is discussed later [37] [1].

Feature	AMD SEV 1	AMD SEV 2	AMD SEV 3	Intel SGX
CPU	EPYC 7401P	EPYC 7702	EPYC 7402P	Core i7-8700
Sockets	1	2	1	1
Cores	24	128	24	6
NUMA	4 Nodes	2 Nodes	1 Node	1 Node
RAM	64GB	1TB	64GB	32GB

Figure 2.8: **AMD EPYC - System configuration [37]**

Concerning the performance penalties of HPC workloads in Trusted Execution Environments, the following core reasons could be extracted by Akram et. al [37]:

1. Correct NUMA allocation policy implies small overhead with SEV enabled.

2. Virtualization dependencies (e.g. QEMU) imply significant performance cuts regarding irregular workloads, intensive I/O and CPU usage where a significant number of CPU threads are involved.

3. Initialization of SEV implies poor performance depending on the memory characteristics of the application.

4. Limited secure memory pages and partially, scalability and programming challenges in the usage of SGX imply high-performance overhead.

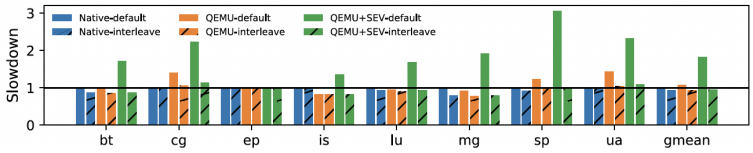

Figure 2.9: **AMD Naples (24 Threads) - SEV for NPB C [37]**
Evaluation: SEV performance overhead caused by default NUMA memory allocation. Solved by interleaving.

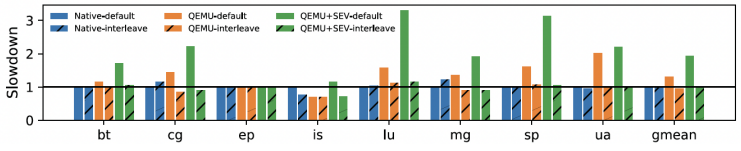

Figure 2.10: **AMD Naples (24 Threads) - SEV for NPB D [37]**
Evaluation: SEV performance overhead caused by default NUMA memory allocation. Solved by interleaving.

The following observations could be made regarding the results of Figures 2.9 and 2.10:

1. SEV activation causes performance penalties beyond virtualization.
2. SEV performance depends on NUMA design.

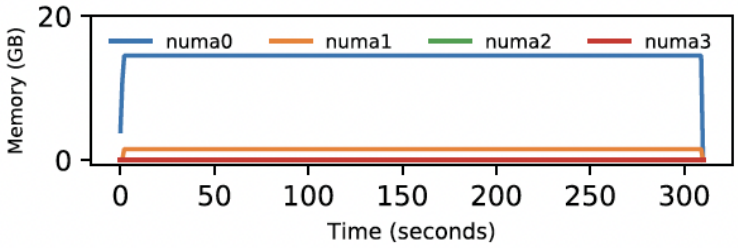

Figure 2.11: **AMD SEV1 (Figure 2.8) - SEV Default Allocation [37]**
Evaluation: VM (16 GB RAM) launch. Performance throttling by data allocation to one only NUMA node.

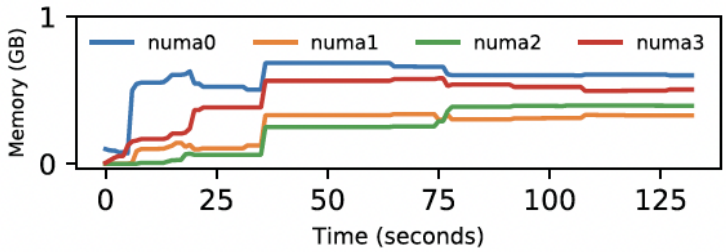

Figure 2.12: **AMD SEV1 (Figure 2.8) - No SEV Default Allocation [37]**
Evaluation: VM (16 GB RAM) launch. Data allocation to all four NUMA nodes following the on-demand paging scheme.

After the observations of the NUMA placement correlation, the assumptions were further compacted after the usage of the AMD SEV3-configuration. There, the NUMA design issues did not occur as the platform has a uniform memory architecture.
The conclusion was that the penalties came with the NUMA configurable allocation policy.

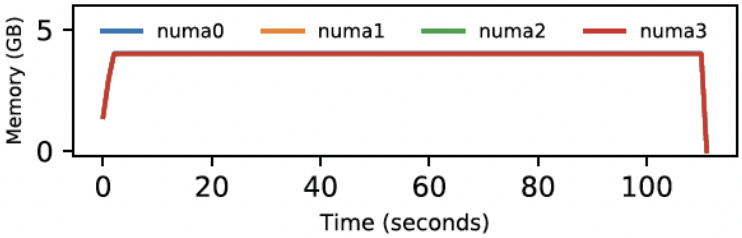

Figure 2.13: **AMD SEV1 (Figure 2.8) - SEV Interleaved Allocation [37]**
Evaluation: VM (16 GB RAM) launch. Data allocation to all four NUMA nodes with significantly increased performance.

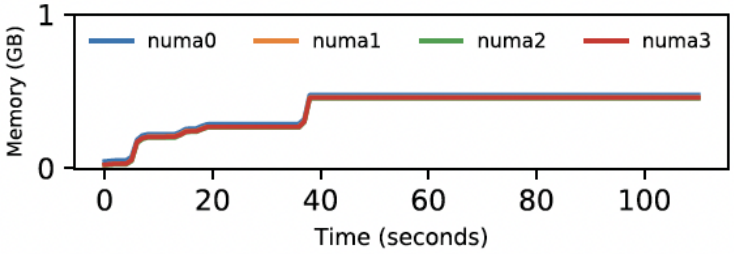

Figure 2.14: **AMD SEV1 (Figure 2.8) - No SEV Interleaved Allocation [37]**
Evaluation: VM (16 GB RAM) launch. Data allocation to all four NUMA nodes with poor performance.

Regarding the results of Figures 2.13 and 2.14, it showed that performance penalty mitigation was achieved by explicit interleaving of data across NUMA nodes using numactl. Numactl is a NUMA policy control of Linux and allows running processes with a specific NUMA scheduling or memory placement policy. It was used to assign memory pages across NUMA nodes. In that context, AMD SEV2 (Figure 2.8) was used to find out whether the improved uniformity regarding its NUMA design improves performance. It was found out that NUMA design has still a significant role as memory management is crucial for the overall performance while running benchmarks.

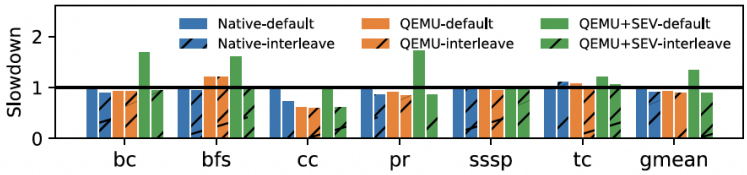

Figure 2.15: **AMD SEV1 (Figure 2.8) - SEV for GAPBS (road network) [37]**
Evaluation: Interleaving works for graph and other HPC workloads except for BLASTN.

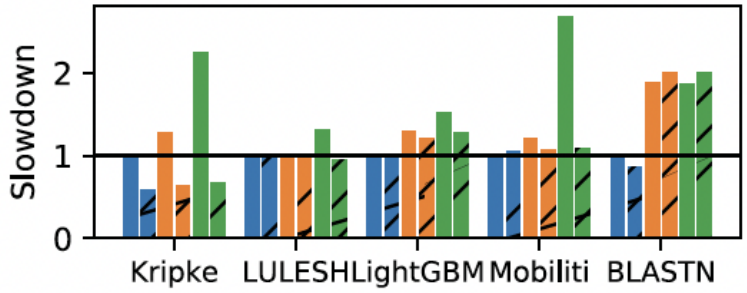

Figure 2.16: **AMD SEV1 (Figure 2.8) - SEV for Real world HPC workloads [37]**
Evaluation: Interleaving works for graph and other HPC workloads except for BLASTN.

BLASTN shows a significant slowdown mainly due to virtualized disk I/O operations. It uses a nucleotide database of approximately 245 GB in size which is larger than the memory size of 64 GB of the used system. This caused the slowdown under virtualization. In contrast, Figures 2.18 and 2.19 show that there is insignificant overhead due to virtualization with SEV enabled.

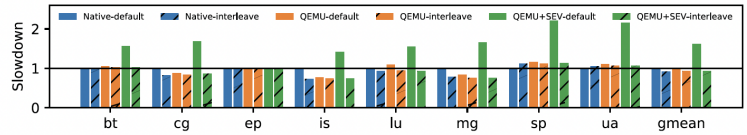

Figure 2.17: **AMD SEV2 (Figure 2.8) - SEV for NPB D [37]**

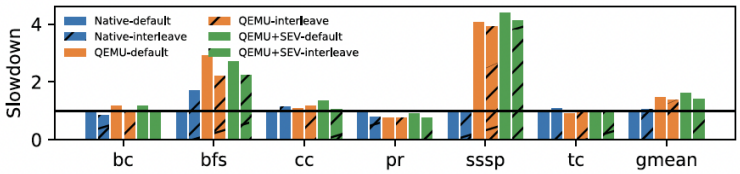

Figure 2.18: **AMD SEV2 (Figure 2.8) - SEV for GAPBS (road network) [37]**
Evaluation: NUMA placement still matters on more uniform memory designs.

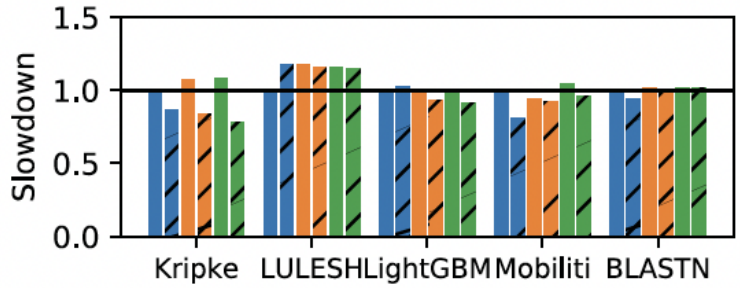

Figure 2.19: **AMD SEV2 (Figure 2.8) - SEV for Real world HPC workloads [37]** newline *Evaluation*: NUMA placement still matters on more uniform memory designs.

In summary, with SEV activation comes performance penalty within and without the virtualization nature. Modification of the interleave policy is the key to optimization depending on NUMA design. In the following, other, but for the scope of this paper less relevant findings will be summarized as follows [37]:

1. Remaining performance penalties with SEV activated due to virtualization overheads.
2. VM bootup time: Poor performance due to SEV and memory footprint of VM.
3. SGX: Poor performance and compatibility are only given by modified scientific software.

3 VIRTUALIZATION AND CLOUD-SERVICES

3.1 BACKGROUND

Virtualization is a technology to virtualize physical resources such as servers, storage-, network- and other physical computing devices. The virtualization software reproduces the behavior of physical hardware to provide parallelly running virtual machines[22]. These virtual machines are called guests and are isolated from each other. The virtualization software is called hypervisor[22]. It is installed on the physical hardware and manages the virtual machines. Companies and institutions use this technology to optimize the efficiency and return on investment of their IT. The technology also enhances computing services such as cloud computing by its advantages.
The interaction with any hardware resource is more flexible by using virtualization. In general, physical components consume electrical power, reserve storage capacities and need regular maintenance. Access to those systems is determined by location and network design. All of these limiting aspects are lifted by virtualization as management, maintenance and operation of the infrastructure are simplified and comparable with the interaction of applications on the web.

Example

Company A has the following business and service needs:

1. Confidential mail service for general business communication
2. Web service for public business representation and general business interaction
3. Business Application for internal business interaction

Each of the requirements has its specifics as the following:

1. The mail service needs to be confidential and secure. It is used by the employees of the company to communicate with each other and with external stakeholders. It specifically requires more storage capacity and a Microsoft Windows OS.
2. The web service is used by the public for general business interaction and specifically requires a Linux OS and high CPU capacities to handle large loads of web traffic.
3. The business application is used by the employees of the company. It requires iOS and more internal RAM.

Company A sets up the three different dedicated and physical servers for each application. Each of them has its own OS and hardware resources. The servers are located in the company's data center. The

maintenance and operation of the servers are done by the company's IT department. The servers are connected to the company's network. The employees of the company can access the servers via the company's network. The public can access the web service via the internet. It takes a high initial investment and pays the whole server's operation and maintenance costs.
Efficiency can be reached by consolidating the three servers into one physical server. The three applications are virtualized and run on the same physical server. The hypervisor software is installed on the physical server and manages the three virtual machines. The hypervisor provides the guests with virtual hardware resources. The guests are configured with the required OS and hardware resources. They run the demanded services, resulting in company A now having less hardware and minimized related costs.
Company A can consider going with IaaS one step further to benefit from virtualization technology used in cloud computing. The cloud provider uses the technology to virtualize the physical hardware resources and to provide virtual machines to its customers. Customers can use the virtual machines to run their applications. The cloud provider manages the virtual machines and the underlying physical hardware. The customers can access the virtual machines via the internet. The cloud provider charges the customers for the used virtual machines. The customers do not have to invest in physical hardware and its maintenance. They can focus on their business and pay only for the used virtual machines.

Virtualization allows a computer to share its hardware resources with multiple isolated computing instances that are called virtual machines. Each instance has its configuration and limits of resources such as CPU, memory, storage and network. This allows organizations to switch between different digital systems on the same server without administrative tasks such as shutdown, re- or conventional boot routines.
Virtual machines, also called guest machines, are software-defined and run on a physical computer that is also called a host machine. The guest nodes are logically separated from the host system hardware by its hypervisor software.
A hypervisor is a program that enables a computer to run multiple virtual instances of machines. It is also called a virtual machine monitor[22] (VMM). The hypervisor is installed on the host machine and manages the guest machines. It provides the guests with virtual hardware resources. The guests are configured with the required OS and hardware resources. They run the demanded services. The hypervisor is responsible for the isolation of the guests from each other and the host machine. It also manages the access to the physical hardware resources. The hypervisor is the core component of virtualization technology.
Type 1 hypervisors are installed directly on the host machine instead of the operating system. The hypervisor is the only software that runs on the host machine. They are also called bare-metal hypervisors. Therefore, this type of hypervisor is more efficient than type 2 hypervisors.

Type 1 hypervisors are used in data centers and cloud computing environments for enterprise needs.
Type 2 hypervisors are installed on top of the operating system. The hypervisor is software that runs on the OS. Therefore, this type of hypervisor is less efficient than type 1 hypervisors. Type 2 hypervisors are used on desktops and laptops for personal needs.

The major advantages of virtualization to any organization affect different aspects of IT management.
The load factor of hardware resources in a data center can be optimized by virtualization. Instead of running one service on a dedicated computer system, you can create virtual server instances on the same physical hardware. These can be created, used and deleted as demanded. This results in a higher utilization of the physical hardware resources. The number of physical hardware resources can be reduced. This frees up space and reduces the costs of electricity, generators and cooling appliances.
By migrating physical to virtual solutions, the infrastructure can be more controlled by using software tools. Deployment and configuration scripts and templates can be used to automate the setup of virtual machines. Infrastructure can be repeatedly, consistently and elastically set up and scaled. It also minimizes error-prone manual and distributed configurations.
Events such as natural disasters or cyberattacks can cause the loss of data or services. The impacts harm business operations and their recovery can take hours or even days. The recovery of access to the IT infrastructure and the replacement or repair of physical servers can be recovery tasks. However, virtualization can help to minimize the impacts of such events. Virtual machines can be backed up and restored more easily than physical servers. They can be migrated to other physical servers in case of a failure. This facilitates business continuity as higher availability of services and improved resiliency is achieved.

Hypervisor are specialized software to create multiple virtual nodes or cloud instances on a single physical server.
When the hypervisor is installed, one or many virtual machines can be created. They can be accessed the same way as a user interacts with other applications on a computer system. The computer is called the host while the virtual instances are called guests. Multiple guests can be created on one host. Each guest node has its proper OS that can be a different one from the one from the host.
For a user, a virtual machine behaves like a physical computer. The user can install software and run applications on it while being isolated from the host system. Virtual machines can be configured with the required hardware resources such as CPU, memory, storage and network that appear the same as on a physical computer. The user can access the virtual machine via the console of the hypervisor or remotely from an internal or external network.
The hypervisor is the intermediary software on the physical machine

that acts between the virtual machines and the underlying hardware or host OS. This depends on the type of hypervisor. The program coordinates the components of its hardware in a way that each virtual machine has its share of physical resources.
Virtual machines can request resources such as processing power and memory from the hypervisor. The hypervisor then passes the requests to the underlying hardware components to handle the job.
Type 1 hypervisors run directly on the computer hardware. They have limited sets of typical OS functions. Because they directly interact with the underlying hardware elements, they are highly efficient.
Type 2 hypervisors run as software within the OS of a computer system. They are less efficient than type 1 hypervisors because they have to interact with the OS of the host system. However, they are easier to install and use. Therefore, it is recommended to use them for running multiple OSs on a single system.

Different types of physical infrastructure can be virtualized. The following sections describe the different types of virtualization of *server*, *storage*, *network*, *data*, *application* and *desktop* and their benefits.
Server virtualization[23] is the most common form of virtualization that partitions a physical server into multiple virtual ones to use server resources and to deploy IT services efficiently and cost-effectively. Otherwise, only a portion of the performance of dedicated physical servers would be called.
Storage virtualization[23] is the pooling of physical storage from multiple network and direct storage devices into what appears to be a single storage device that is managed from a central console. These storage systems can be from different vendors and different types. This single storage can then be a large unit of virtual storage that you can allocate and control by using the management software. Storage virtualization is used to improve storage utilization, simplify management and increase flexibility and scalability. Archiving, backup and recovery activities can be streamlined by that technology.
Network virtualization[23] is the process of combining all networks and their resources of multiple geographic locations into one software-defined and administrative entity. Those network resources can be hardware elements such as switches, routers and firewalls. Network virtualization is used to improve network speed, efficiency, security, management and scalability. It is also used to reduce the time and costs of network administration. *Software-defined networking (SDN)* and *network function virtualization (NFV)* are two types of network virtualization.
Software-defined networking manages traffic routing from data routing in the physical environment. One benefit can be that the quality of service can be optimized as it allows the network administrator to manage traffic loads flexibly. It also allows the administrator to quickly respond to changing business requirements.
Network function virtualization bundles the functions of network appliances such as firewalls, load balancers and intrusion detection systems to improve network performance.

Data virtualization collects data from multiple sources and formats it in a way that appears to be in one place. Without it, it can be in different places, such as in a cloud infrastructure or an on-premises data center and also, in different formats. The technology sets up a software layer between the data and the application that needs it. It then processes the requests of an application and returns the output in a suitable format. This improves the flexibility in data integration and enables cross-functional data analysis.
Application virtualization is the process of decoupling the application layer from the OS layer. This allows the application to run on different OSs without being installed on them. There are three different modes to achieve application virtualization:

- Application streaming: The application is delivered to the client device on-demand and is executed locally.
- Server-based application virtualization: The application is executed on a server. The user interacts with the software via a web browser or a client interface.
- Local application virtualization: The application is delivered with a fully integrated cross-platform compatible environment.

Desktop virtualization is being used to create virtual desktops on a central server. The virtual desktops are then delivered to the client devices. The client devices can be thin clients, laptops, tablets or smartphones. The virtual desktops are hosted on a remote server. The client devices can access the virtual desktops via a web browser or a client interface. Virtual desktop infrastructure (VDI) is used to host and manage virtual desktops on a central server. The virtual desktops are then delivered to the client devices.
Local desktop virtualization is used to host and manage virtual desktops on the client device itself. The hypervisor is run on the client device. The software can be used to locally create virtual computers with different OSs. The user can switch between the local and virtual environment analogous to switching between different applications.

Virtualization and cloud computing are different technologies. Virtualization is the core technology of cloud computing[24]. It is used to create virtual machines on a physical server. Cloud computing is the delivery of computing services such as servers, storage, databases, networking, software, analytics and intelligence over different networks and to different target groups. It is used to provide on-demand access to these services. The services are provided by a cloud provider. The cloud provider manages the underlying physical hardware and the virtual machines. The cloud provider charges the customers for the used services. The customers do not have to invest in physical hardware and its maintenance. They can focus on their business and pay only for the used services. Containerization is a technology to create containers[22] on a host machine. Containers are isolated environments that run on a host machine. They are similar to virtual machines but do not

contain an OS. They are smaller than virtual machines and use fewer resources. They are used to run applications in a portable and isolated environment. They are also used to deploy applications in a fast and consistent way. Containers are created from images[22]. Images are templates that contain the application and its dependencies. They are used to create containers. Images are stored in a registry. The registry is a repository for images. It is used to store and distribute images. The registry can be public or private. The public registry is used to store and distribute public images. The private registry is used to store and distribute private images. The images can be created by the user or by the cloud provider. The cloud provider can provide a registry for the user to store and distribute images. The user can then create containers from the images and run them on the host machine. The user can access the containers via the console of the host machine or remotely from an internal or external network.
In contrast, server virtualization builds up an entire virtual environment by including an OS and then runs the application on it.

3.2 QUICK EMULATOR

Quick Emulator[28] (QEMU) is a generic and open-source machine emulator and virtualizer. It offers full-system and user-mode emulation, but also virtualization features.
As a machine emulator, QEMU can run OSs and programs made for one machine on a different machine. They can differentiate in system architecture and OS. QEMU also uses dynamic translation to improve significantly performance. When it encounters code, it transforms it to the host instruction set. Dynamic translators are complex and depend highly on the CPU. The CPU is always emulated. This mode is called *User Mode Emulation*.
As a virtualizer, QEMU can be used to launch different OSs without rebooting the host system or debugging system code. It can also be used to provide virtual hardware to run and test software. It can be used to run programs for one architecture on a different architecture. The achieved performance is nearly native by executing the guest software directly on the host CPU. The Xen hypervisor or KVM kernel module in Linux can be used to run QEMU as a virtualizer. With KVM, QEMU can virtualize the following architectures: x86, server and embedded PowerPC, 64-bit POWER, S390, 32- and 64-bit ARM and MIPS. By virtualization, it can provide a complete virtual model of an entire machine, including CPU, memory and emulated devices. This mode is called *System Emulation*.
QEMU also provides a set of command line utilities for disk image management and conversion.

Multiple host OS platforms are supported. The following matrix will give further details about the principal build targets. These are essential for 3rd party dependencies of QEMU. These platforms are included in automated tests of the QEMU project whenever patches are pushed for review and testing before or after merge.

CPU Architecture	Accelerators
Arm	kvm (64 bit only), tcg, xen
MIPS (little endian only)	kvm, tcg
PPC	kvm, tcg
RISC-V	kvm, tcg
s390x	kvm, tcg
SPARC	tcg
x86	hvf (64 bit only), kvm, nvmm, tcg, whpx (64 bit only), xen

Table 3.1: **QEMU - Supported host architectures**

System Emulation provides virtual instances to run a guest OS. This mode supports just-in-time (JIT) compilation, also called dynamic translation, for the emulation of CPUs. For this, it uses its Tiny Code Generator (TCG). Also, it supports a set of hypervisors that are called accelerators. In the following, the most important ones are described. For the investigation of the DigiMed prototype, a significant point of

Accelerator	Host OS	Host Architectures
KVM	Linux	Arm (64 bit only), MIPS, PPC, RISC-V, s390x, x86
Xen	Linux (as dom0)	Arm, x86
Hypervisor Framework (hvf)	MacOS	x86 (64 bit only), Arm (64 bit only)
Windows Hypervisor Platform (whpx)	Windows	x86
NetBSD Virtual Machine Monitor (nvmm)	NetBSD	x86
Tiny Code Generator (tcg)	Linux, other POSIX, Windows, MacOS	Arm, x86, Loongarch64, MIPS, PPC, s390x, Sparc64

Table 3.2: **QEMU - Supported Accelerators**

interest is the support of AMD SEV. The QEMU project describes it as an extension to the AMD-V architecture that enables running fully encrypted virtual machines under the control of KVM. The set of hardware extensions for virtualization support by the x86-CPU-architecture of AMD is called AMD-V. An extensive description of the security concept follows in Chapter 5.3.
Briefly, each encrypted VM has its code and data confidential in a way that only the VM itself has access to them. A unique encryption key is allocated to each VM. If the data of the VM is being accessed by another system, the attempt fails as it leads to unintelligible data that is incorrectly decrypted.
This unique encryption key is being managed by a co-processor called AMD Secure Processor (AMD-SP). It is a dedicated ARM Cortex-A5 processor that is integrated into the AMD SoCs. It is responsible for the encryption and decryption of the VM memory. It also manages the encryption keys and the VM state. The AMD Secure Processor is also called (PSP). The firmware of the AMD-SEP provides commands to manage a VM lifecycle, including commands for launching, snapshotting, migrating and debugging the encrypted guest. The ioctls of KVM_MEMORY_ENCRYPT_OP can be used to submit the commands.
To build upon AMD SEV, AMD SEV-ES can be used to enhance the protection of the guest system by encrypting its register state. To control the guest as a guest, the hypervisor supports notifying a guest's

OS when VMEXIT-events occur. This allows the guest to selectively fulfill the hypervisor's requested actions.
During the launch, boot images such as BIOS have to be in an encrypted state before a virtual machine can be started. The ioctls of MEMORY_ENCRYPT_OP provides a set of commands to cipher the images: LAUNCH_START, LAUNCH_UPDATE_DATA, LAUNCH_MEASURE and LAUNCH_FINISH. All of them generate a fresh memory encryption key for the VM, cipher the boot images and provide indicators to attest to the success of a launch. A virtual machine with SEV-ES activated can use the command LAUNCH_UPDATE_VMSA to encrypt its register state or VM save area (VMSA) for all its virtual CPUs.
A VM with SEV-ES activated has restrictions in comparison to a SEV guest. Because the register state is ciphered and can not be changed by the hypervisor, the SEV-ES has the following characteristics:

- Does not support System Management Mode (SMM) - SMM requires alternating the guest register state.
- Does not support reboot - reboot requires alternating the guest register state.
- Requires in-kernel interrupt controller (irqchip) - the load is placed on the hypervisor to manage Applications Processors (APs)

The verification of the VM launch measurement has to be computed by its owner according to the AMD-SP and its respective SEV API specifications. Therefore, the following operations will be further described:

- **GCTXL.LD**

  - Creates a hash code of cleartext data imported into the VM memory.

- **HMAC(0x04** || **API_MAJOR** || **API_MINOR** || **BUILD** || **GCTX.POLICY** || **GCTX.LD** || **MNONCE; GCTX.TIK)**

  - Calculates launch measurement, "||" is the concatenation operator.

  AMD. (2021). AMD Memory Encryption [18].

With the QEMU Machine Protocol (QMP) command query-sev, the values of API_MAJOR, API_MINOR, BUILD and GCTX.POLICY can be called.
The response message of query-sev-launch-measure contains the value MNONCE. It is part of the last 16 bytes of the base64-decoded data field.

The value of GCTX.LD is a SHA-256 of firmware_blob || kernel_hashes_blob || vmsas_blob. They have the following characteristics:

- firmware_blob contains the data of the entire firmware flash file, e.g. 0VMF.fd. The used firmware must be stateless and does not use any NVRAM. The NVRAM is not being measured, concluding that it is not secure to use firmware that uses states from an NVRAM memory.

- kernel_hashes_blob is part of the PaddedSevHashTable that includes zero padding when the kernel is being used and kernel-hashes=on. It contains the hashes of the kernel, initrd and cmdline that are applied by the VM. The struct of PaddedSevHashTable can be found in target/i386/sev.c.

- vmsas_blob is the concatenation of the entire collection of virtual CPUs of the VM when SEV-ES is activated. Each VMSA contains 4096 bytes and is part of the Linux kernel code as struct vmcb_save_area or in AMD APM Volume 2 Table B-2, including VMCB Layout and State Save Area.

If the kernel hashes are not applied or SEV-ES is deactivated, empty blobs for kernel_hashes_blob and vmsas_blob shall be used.
If the VM provides the capability of debugging, the hypervisor can make use of that functionality. Beforehand it needs to be considered that the VM with SEV enabled has its memory fully encrypted which results in cipher text that will be returned to the hypervisor when it accesses the guest memory. With the commands DEBUG_DECRYPT and DEBUG_ENCRYPT it can selectively access the VMs' memory for debugging. This is generally possible but has not been supported by Quick Emulator itself.
Aspects of Snapshot, Restoration and Live Migration are limited in the SEV environment as QEMU does currently not implement them in that context.

3.3 OPENSTACK

OpenStack is one of the most popular open-source platforms for Infrastructure as a Service. It empowers many notable companies, and science or research organizations. Interestingly, the domains of research and science cover most of the relevant use cases regarding OpenStack clouds. These clouds fulfill the needs by provisioning flexible infrastructure for research computing.
Figure 3.1 shows its concept by presenting different layers of the system. OpenStack orchestrates shared networking and storage resources. It is important to mention that it does not host by itself, it only controls its resources via APIs. Those resources can contain bare metal nodes, virtual machines and containers.

The OpenStack services are being managed by built-in tools or third-party services. The OpenStack dashboard, OpenStackClient or OpenStack SDK count to the built-in tools. Services such as Kubernetes, CloudFoundry and Terraform are third-party tools. They are used to manage the OpenStack cloud. Considering Chapter 5 of this paper, OpenStack dashboard, OpenStackClient and Terraform have been used to manage the OpenStack Cloud.

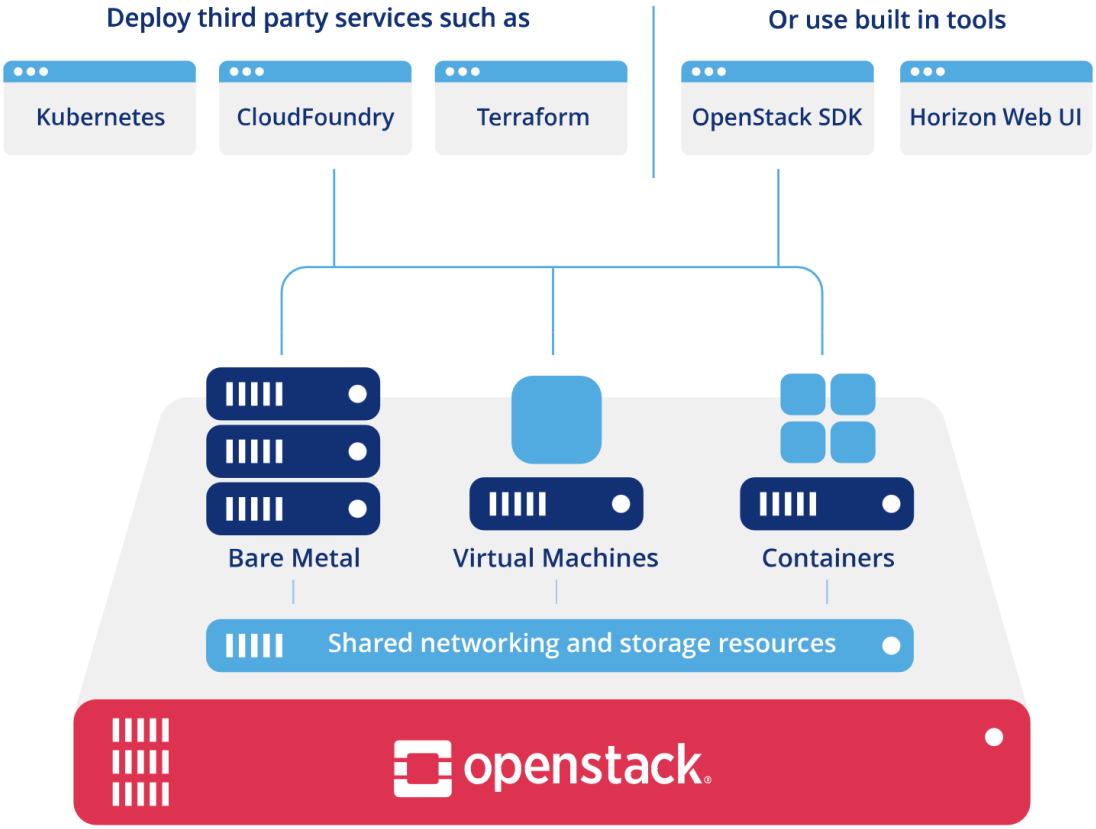

Figure 3.1: **OpenStack - Concept [27]**

Figure 3.2 shows a detailed model of the OpenStack architecture. In the following, some of the components will be explained as they were actively or passively used within the DigiMed prototype infrastructure. Here, especially the management and compute nodes are considered.

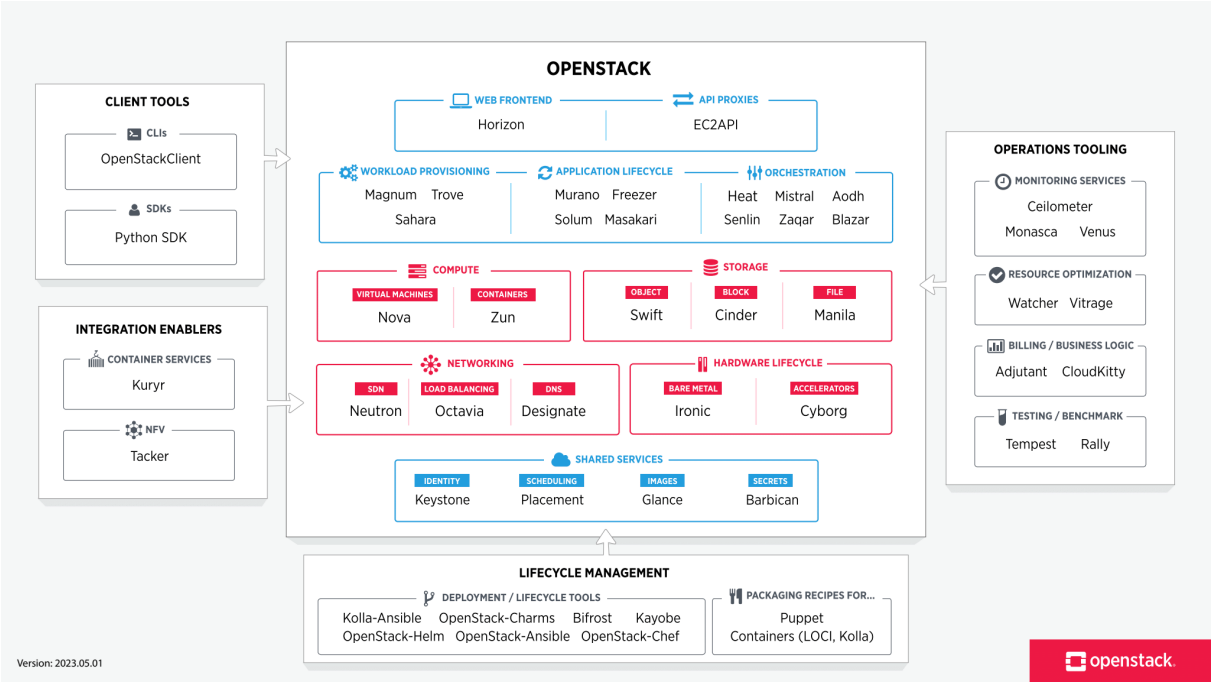

Figure 3.2: **OpenStack - Architecture [27]**

- **Web frontend and client tools:** Horizon is a web interface and OpenStackClient a command-line interface to manage the OpenStack cloud. They are used to manage the OpenStack cloud.
- **Compute:** Nova is a service to manage and automate the provisioning of computing resources. It is used to manage the virtual nodes.
- **Storage:** Cinder is a service to manage and automate the provisioning of block storage. It is used to manage the storage nodes.
- **Networking:** Neutron is a service to manage and automate the provisioning of networking resources. It is used to manage the network nodes as it contributes to the SDN concept. Octavia is a service to manage and automate the provisioning of load balancing. It is used to manage the load balancer nodes. Designate is a service to manage and automate the provisioning of Domain Name System (DNS). It is used to manage the DNS nodes.
- **Shared services:** Keystone is a service to manage and automate the provisioning of identity services. It is used to manage client authentication, service discovery and distributed multi-tenant authorization by using OpenStack's Identity API. Glance is a service to manage and automate the provisioning of image services. It is used to manage the image assets. It includes discovering, registering and retrieving VM images. Barbican is a service to manage OpenStack keys, certificates and secrets. It is used to manage the encryption keys that can be symmetric, asymmetric, certificates or binary data.

- **Lifecycle management:** Kolla-Ansible is a service to manage the lifecycle of OpenStack services. It is used to deploy and upgrade OpenStack services in Docker containers. It is also used to manage the configuration of OpenStack services. Its goal is to provide production-ready containers and deployment tools for operating OpenStack clouds. OpenStack-Ansible is also a service to manage the lifecycle of OpenStack services. It contains playbooks and roles for the deployment and configuration of OpenStack.

- **Packaging recipes for:** Kolla-toolbox is used for production-ready Docker containers and deployment tools for OpenStack environments.

High-performance computing HPC and high-throughput computing HTC need for Big Data computing a suitable cluster network that provides massive scaling capabilities for its resources such as storage, computing and network access to large volumes of data. Furthermore, the cluster also needs workload and infrastructure manageability, e. g. by the SLURM workload manager, OpenStack Horizon service or a combination of both. The development community fills the gaps by expanding its services to extend the features of OpenStack. Researcher can use the resources of an OpenStack private cloud to work in IT networks tailored to their needs. The effective time of research is enhanced by cutting setup processes as the dynamic, automated SDN infrastructure is deployed more efficiently.
In the following, OpenStack [27] will be further investigated in the aspects of HPC. Here, especially *Virtualization*, *Network Fabrics*, *High-Performance Data*, *Workload Management* and *Infrastructure Management* will be covered [39].
Statistics over the performance of virtualization for applications show that the overhead of the technology usage regarding CPU driven tasks is marginal. Furthermore, the overhead of guest applications that use the passed-through non-uniform memory access NUMA configuration of the hypervisor regarding memory-intensive tasks is low. Analogously, software with high transfer volumes, depending on network communication or high-bandwidth I/O, can achieve almost bare metal setups. Wherever a significant penalty occurs, it can be often identified as overcommitment of hardware resources or interfering neighbors. These effects also occur in non-virtualized setups.
Nonetheless, there remains a collection of applications whose performance receives a virtualization penalty.
HPC software that is sensitive to factors such as storage IOPs and network latencies experience critical impacts on its performance. Those applications are especially worse in their performance when being used in conventional virtual infrastructures. Fully virtual infrastructures imply additional overhead in their I/O traffic and can impact the performance of software considering their respective access patterns.
Paravirtualization counters these challenges by providing support for virtualized environments. Enhanced cooperation between host and

guest system reduces the overhead of hardware device management. Direct operations are being executed by the host system that keeps the micro-management of hardware close to the physical device. The hypervisor then works more efficiently by providing an improved software interface to a simplified driver for the virtual machine. Interactions between guest and host system are then more streamlined which results in improved performance.

Modern Ethernet NICs establish hardware offload with a set of protocols, e.g. IP, TCP et cetera. NICs free up CPU cycles when transformations between data in user buffers and packets on the wire, including the other way around, is being done.
With virtualization, the hypervisor provides a SDN which contains the network traffic of a guest VM. Therefore, packet computing is more complex than in a typical HPC constellation. Hardware offload functionalities are often practically unusable or ineffective in this context. In a virtualized environment, this can lead to a worse network- and CPU performance compared to an equivalent bare metal environment. Virtual environments also generate a variance of jitter that results in latency distribution for interrupts and I/O interactions.
Massive parallel and synchronous tasks that iterate in lock-step, are being processed at the speed of the slowest working node. In a virtual environment, if jitter effects occur and result in the determination of the slowest worker, then the overall application progress will also be affected.

As virtualization is a well-established technology, its development is continuous on all levels: CPU architecture, hypervisor, OS and cloud orchestration. Therefore, OpenStack can deliver virtualized HPC.
Biannually, OpenStack software is being released with new features to improve performance and flexibility.
The OpenStack community contributes via continual and collaborative testing and optimization to the efficiency of the hypervisor. Empirical studies with different setups, including various tuning parameters are frequently enclosed and reviewed. Outstanding improvements are summarized as a guide on hypervisor performance tuning best practices.
OpenStack Nova compute service supports the extraction of many hypervisor features to improve performance.

- Activates CPU extensions for virtualization.

- Controls hypervisor features to efficiently manage multiple VMs, e. g. Kernel Same-page Merging (KSM). It adds CPU overhead while having memory usage improved by the de-duplication of identical pages. To further improve memory-intensive tasks, KSM can be modified to prevent merging between NUMA nodes. Every attribute can be deactivated to maximize the performance for performance-critical HPC.

- Allocates virtual cores to physical ones.

- Passes through the NUMA topology of the host system to the VM to benefit from NUMA-aware memory allocation and job scheduling optimizations.
- Passes through the CPU model of the host system to the VM to benefit from the architecture-dependent extensions and runtime microarchitectural optimizations in HPC scientific libraries.
- Backes the VM memory with huge pages to minimize the impact of Translation Lookaside Buffer (TLB)

These functionalities optimize the performance as CPU and memory-related workloads typically result in one to two percent overhead in comparison to bare metal setups.
In contrast, with further limitations referred to virtual architectures, these measures can make migrations of VM instances more difficult in a cloud infrastructure while having a diversity of hypervisor hardware. Particularly live migration may be precluded.
Hardware that supports Single-Rooted I/O Virtualization (SR-IOV) establishes the capability of passing through functions of hardware resources as many virtual functions. Each of these virtual functions can be individually adjusted and allocated to different VMs. This technology can provide performance almost without overhead while serving the needs of many virtual instances.
By the nature of its direct access to physical components, SR-IOV limits software-defined infrastructures. Security group policies of OpenStack can not be allocated to a network interface that is mapped to a SR-IOV virtual function. Therefore, the VM is not protected by the security group policies. This can be an issue in multi-tenant environments or externally accessible networks. Anyway, it should not prevent the usage of SR-IOV in HPC setups when an OpenStack-hosted parallel workload is being handled between its processes.
As different HPC applications exist, so do their respective hardware requirements, e. g. types of GPU, CPU et cetera.
Software-defined infrastructure can enable the usage of dedicated compute hardware resources such as Peripheral Component Interconnect PCI devices by pass-through. The device can be directly allocated to the device management of a VM in such a manner that the VM has exclusive access to that hardware resource.
Demands of guest machines for hardware accelerators can be scheduled to a hypervisor with the resources available and the guest machine is assembled by the allocation of resources of the underlying hardware. The resource management model of graphics processing units does not support SR-IOV. Therefore, whenever a GPU is attached to a guest machine, it is passed through entirely. A hypervisor can allocate multiple GPUs to multiple different machines. It is also possible to attach multiple GPUs to a single virtual instance. Peer-to-peer data transfers can occur between GPU devices and also RDMA enabled NICs.
The usage of device pass-through can have impacts on the performance of virtualized memory management. This technology requires the configuration of Input/Output Memory Management Unit (IOMMU)

which limits the use of transparent huge pages. Memory needs to be pinned in a guest machine when using pass-through devices. The flexibility of software-defined infrastructure can be reduced to overcommit virtualized resources. This issue is uncommon in HPC use cases. To enhance virtual memory performance, static huge pages can still be used.
In scientific workloads, the performance overhead of virtualized GPU-intensive is negligible. The performance of GPU pass-through is comparable to bare metal setups.
Figure 3.3 shows different approaches to hardware device management in OpenStack setups, e.g. *paravirtualization*, *PCI pass-through* and *SR-IOV*.
Paravirtualization creates a virtual network device that is designed to be an efficient software interface.
PCI pass-through transfers exclusively a physical device of the host to the guest machine.

SR-IOV creates virtual functions to share physical resources. These can be passed through to a guest machine while the physical device stays behind in the hypervisor.

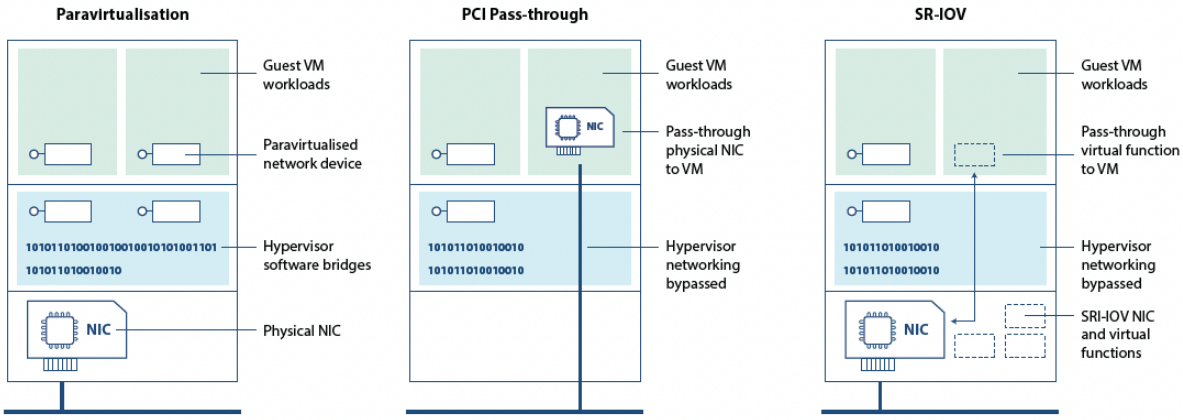

Figure 3.3: **OpenStack - Strategies for efficient handling of hardware devices, e. g. NIC [27]**

Containers are a virtualization technology that adds another model of compute abstraction on the OS-level. It comes with the benefit of almost eliminating the overhead of virtualization. Especially popularised by Docker, Containers contain an application and its requirements as a minimized and self-contained execution environment in contrast to a whole virtual machine resulting in optimized memory usage and reduced I/O-overhead.
In HPC setups, containers can be used with RDMA capabilities, but are limited. The OpenFabrics Enterprise Distribution OFED software stack does not recognize network namespaces and cgroups. That prevents per-container control and isolation of RDMA resources. Containers with host networking enabled can use RDMA devices.
Furthermore, Ironic is an OpenStack project that provides bare metal provisioning. It is a driver for virtualization and presents bare metal compute nodes by abstraction, although they were virtual compute ones. Its concept results in zero overhead to the performance of compute nodes. It also brings the benefits of software-defined infrastructure management.
With Ironic it is possible to retain bare metal performance and to achieve the flexibility of using any software image for the deployment of a compute node.

The latest OpenStack release offers new functionalities such as serial consoles, volume attachments and multi-tenant networking. The deployment of more complex images, e.g. over a collection of disks, is evolving.
Ironic has limitations regarding the following aspects:

- Its bare metal machines can not be mixed with virtual machines. But they can be used parallelly in separate cells or regions within the same cloud.

- Standard virtualization features such as overcommitment and migration could never be supported.

The expression "Time to Paper" is being used as a metric of the scientists and should be considered when OpenStack is being evaluated as a candidate for HPC infrastructure for research computing.
Whenever criticism regarding the usage of OpenStack is raised, the various overheads of virtualization are pointed out. As OpenStack is rapidly developing, these arguments might already be outdated. While the number of trade-offs of cloud infrastructure is diminishing, the number of convincing new capabilities is increasing.
The following aspects streamline the benefits of OpenStack in comparison to conventional HPC system management:

- Standardisation: Users use user-friendly interfaces such as web- and command line interface or software API.
- Flexibility and agility: Users use compute resources on demand and have only use of virtual resources. Access to physical resources is being controlled in a detailed manner.
- Self-service: Users can self-serve and boot software images without the need for the operator. They also create their ones which contributes to efficiency as the interaction with administrators is not needed and further delays can be prevented.
- Security: Users are separated to a higher degree and cannot observe other ones. Furthermore, their networks are isolated from each other.

HPC-aware configuration and optimization of OpenStack realizes the benefits of software-defined infrastructure while minimizing the various overheads. By its variety, virtualization strikes a balance between new features and resulting overhead [27].

4 INFRASTRUCTURE

4.1 HARDWARE

The prototype infrastructure of the DigiMed project is deployed in the double cube of the LRZ.

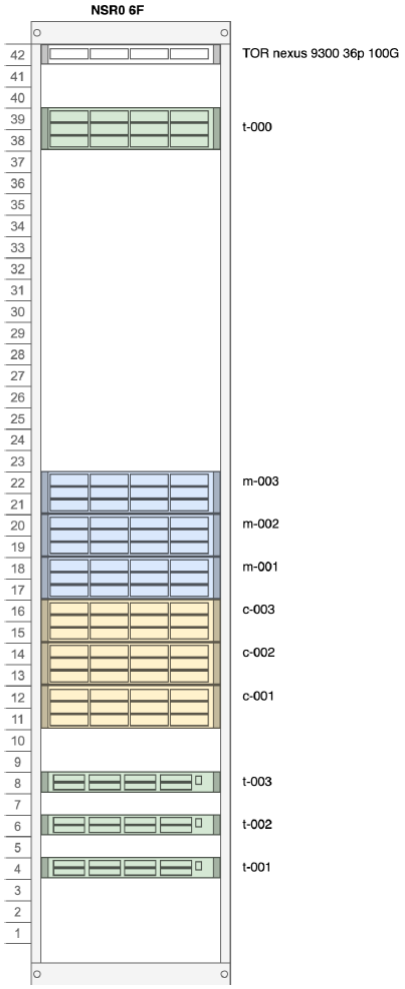

Figure 4.1: **LRZ double cube - Rack NSR0 6F**

The referred rack hoards a computer cluster with a total amount of ten servers. All of them are high-performance components. Three of them are used as management servers and the other three are used as compute nodes. The management servers are used to manage the compute nodes and to provide the OpenStack services. The compute nodes are the hosts used to run the virtual machines. They operate the hypervisor on top of which the VMs can run. The last servers are intended to be used as test nodes. They are no further considered. The

rack also has one multilayer switch installed.
The following enumerations shows the nomenclature regarding this rack:

- *c-xxx* is the term for the compute node and its following ID.
- *m-xxx* is the term for the management node and its following ID.
- *t-xxx* is the term for the test node and its following ID.
- *TOR nexus 9300 36p 100G* is the description for the switch.

Management servers

Count	Description	CPU	RAM	Storage	Network
m-001	Lenovo ThinkSystem SR665	1x AMD EPYC 75F3 32 cores @2.95GHz up to 4.0GHz, 8 Memory Channels	4x 64 GB DDR 4	2x 3.84TB SATA SSD RAID 1	1x 100GbE 1x 40GbE 1x 1GbE
m-002	Lenovo ThinkSystem SR665	1x AMD EPYC 75F3 32 cores @2.95GHz up to 4.0GHz, 8 Memory Channels	4x 64 GB DDR 4	2x 3.84TB SATA SSD RAID 1	1x 100GbE 1x 40GbE 1x 1GbE
m-003	Lenovo ThinkSystem SR665	1x AMD EPYC 75F3 32 cores @2.95GHz up to 4.0GHz, 8 Memory Channels	4x 64 GB DDR 4	2x 3.84TB SATA SSD RAID 1	1x 100GbE 1x 40GbE 1x 1GbE

Table 4.1: DigiMed - Prototype

As shown in Table 4.1, the management servers are Lenovo ThinkSystem SR665 with one AMD EPYC 75F3 CPU each. Deriving from Table 3.2, the compute servers are Lenovo ThinkSystem SR665 with two AMD EPYC 75F3 CPU each. These CPUs belong to the Epyc 7003 'Milan' series and are based on the Zen 3 microarchitecture. Among other things, supported key features are AMD Infinity Guard and AMD Infinity Architecture. AMD Secure Encrypted Virtualization is part of the AMD Infinity Guard concept. These CPU technologies contribute to the security concept of the project in a significant way as they provide the core capabilities for applied Confidential Computing, especially in the cloud.

Compute servers

Count	Description	CPU	RAM	Storage	Network
c-001	Lenovo ThinkSystem SR665	2x AMD EPYC 75F3 32 cores @2.95GHz up to 4.0GHz, 8 Memory Channels	16x 64 GB DDR 4	1x 800GB NVMe SSD	1x 100GbE 1x 40GbE 1x 1GbE
c-002	Lenovo ThinkSystem SR665	2x AMD EPYC 75F3 32 cores @2.95GHz up to 4.0GHz, 8 Memory Channels	16x 64 GB DDR 4	1x 800GB NVMe SSD	1x 100GbE 1x 40GbE 1x 1GbE
c-003	Lenovo ThinkSystem SR665	2x AMD EPYC 75F3 32 cores @2.95GHz up to 4.0GHz, 8 Memory Channels	16x 64 GB DDR 4	1x 800GB NVMe SSD	1x 100GbE 1x 40GbE 1x 1GbE

Table 4.2: DigiMed - Prototype

Furthermore, the setup additionally consists of storage hardware as a distributed file system (DFS) of four Servers. These provide Quobyte file services and their storage capabilities to the OpenStack environment. Currently, as an important element of data at rest, the mentioned storage system is out of scope as it still needs to be integrated into the current infrastructure environment.

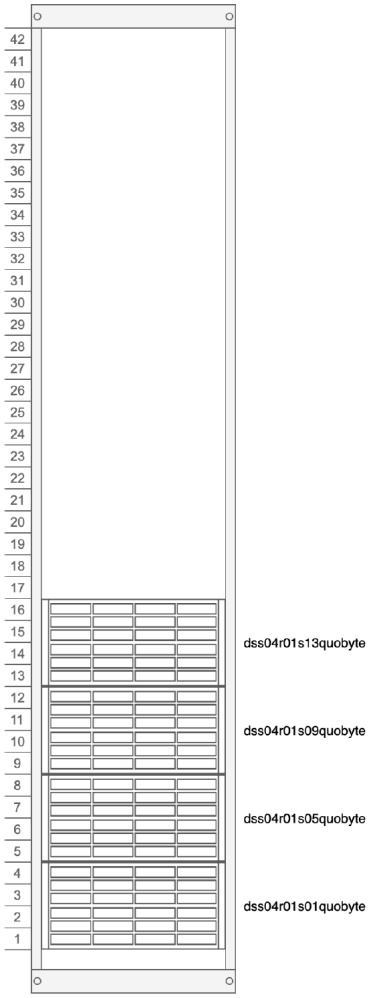

Figure 4.2: **LRZ double cube - Rack NSR1 DSS04R01**

Storage servers					
Count	Description	OS	RAM	Storage	Network
dss04r01s01quobyte	Supermicro Server CSE-848X	RedHat 8.3	8x 24 GB DDR 4	16x 12TB HDD 2x 1TB NVMe SSD 4x 7,6TB NVMe SSD	1x 100GbE 1x 1GbE
dss04r01s05quobyte	Supermicro Server CSE-848X	RedHat 8.3	8x 24 GB DDR 4	16x 12TB HDD 2x 1TB NVMe SSD 4x 7,6TB NVMe SSD	1x 100GbE 1x 1GbE
dss04r01s09quobyte	Supermicro Server CSE-848X	RedHat 8.3	8x 24 GB DDR 4	16x 12TB HDD 2x 1TB NVMe SSD 4x 7,6TB NVMe SSD	1x 100GbE 1x 1GbE
dss04r01s13quobyte	Supermicro Server CSE-848X	RedHat 8.3	8x 24 GB DDR 4	16x 12TB HDD 2x 1TB NVMe SSD 4x 7,6TB NVMe SSD	1x 100GbE 1x 1GbE

Table 4.3: **DigiMed - Prototype**

In the following, the network will be further described. The networking devices are one multilayer switch which is a Cisco Nexus 9300 Series 36P and one HPE multilayer switch. The first one is equipped with 40 GbE and 100 GbE QSFP28 modules and interconnects the compute nodes, the management servers and the storage server. Its two further uplinks lead to Rack 6A which then connects to other internal networks and the internet.

The second one is equipped with 1 GbE ports and interconnects all management components and servers with the management network. XClarity software of Lenovo enhances this network with its automated provisioning and operations management. Furthermore, it is only accessible through highly secure login nodes.
Out-of-band management elements such as lights-out management (LOM) are being used to manage the servers. The LOM is a hardware management component that is integrated into the server. It provides the ability to monitor, control and manage the server remotely. The LOM is independent of the server's OS and runs on its processor. Baseboard management controller (BMC) are also being used to remotely monitor the physical state of a node such as a server. It is a specialized microcontroller embedded in the motherboard of a computer system. It is used to manage the interface between system management software and platform hardware. Both, LOM and BMC are used to manage the servers remotely and connected to the management network.

		Networking device			
Count	Description	RU	Bandwith	Used Ports	Purpose
TOR	Cisco Nexus 9336C-FX2-E	1	7.2 Tbps	6x 100GbE 6x 40GbE	HPC cluster
SWU1-2WR	HPE Switch	1		10x 1GbE	Management network

Table 4.4: **DigiMed - Prototype**

4.2 SOFTWARE

4.2.1 *Background*

Red Hat Quay focuses on security and offers a private registry platform for building, storing and distributing content across decentralized data centers and cloud systems. It provides a hardened container registry that contains software based on containers to develop around Red Hat OpenShift and Kubernetes. Red Hat OpenShift is a software stack for containerization. Its core product is OpenShift Container Platform which is a hybrid cloud platform. It contains Linux containers that are managed by Kubernetes upon Red Hat Enterprise Linux. Kubernetes is open-source and orchestrates containers for software deployment automation, scaling and management.
OSISM is a German company developing solutions for the management of sustainable and software-defined cloud infrastructures. It builds and packages OpenStack services into docker containers to disclose them on quai.io. In the following, the aforementioned management and compute nodes will be further described while referring to the OSISM software family.

4.2.2 *Management Nodes*

Regarding the management servers, the operating system is Ubuntu 22.04. The following services are installed on the management nodes:

- quay.io/osism/ovn-northd:23.6.1.20230919
- quay.io/osism/ovn-sb-db-server:23.6.1.20230919
- quay.io/osism/ovn-nb-db-server:23.6.1.20230919
- quay.io/osism/ovn-controller:23.6.1.20230919
- quay.io/osism/dnsdist:1.8.0
- quay.io/osism/horizon:23.1.1.20230919
- quay.io/osism/keystone:23.0.1.20230919
- quay.io/osism/keystone-fernet:23.0.1.20230919
- quay.io/osism/keystone-ssh:23.0.1.20230919
- mariadb:10.11.5quay.io/osism/mariadb-server:10.6.15.20230919
- quay.io/osism/mariadb-clustercheck:10.6.15.20230919
- quay.io/osism/keepalived:2.2.4.20230919
- quay.io/osism/haproxy:2.4.22.20230919
- quay.io/osism/osism-ansible:6.0.1
- quay.io/osism/kolla-ansible:6.0.1
- quay.io/osism/ara-server:1.7.0
- quay.io/osism/inventory-reconciler:6.0.1
- quay.io/osism/osism:0.20230919.0
- quay.io/osism/osism:0.20230919.0
- quay.io/osism/osism:0.20230919.0
- quay.io/osism/osism:0.20230919.0
- redis:7.2.0-alpinequay.io/osism/osism:0.20230919.0
- gitlab.lrz.de:1337/digimed/infrastructure/digimed_cfg_openstack/cinder-volume:21.3.1.20230615.quobyte
- gitlab.lrz.de:1337/digimed/infrastructure/digimed_cfg_openstack/nova-compute:26.2.1.20230615.quobyte
- quay.io/osism/nova-libvirt:8.0.0.20230615
- quay.io/osism/nova-ssh:26.2.1.20230615

- quay.io/osism/nova-novncproxy:26.2.1.20230615
- quay.io/osism/nova-conductor:26.2.1.20230615
- quay.io/osism/nova-api:26.2.1.20230615
- quay.io/osism/nova-scheduler:26.2.1.20230615
- quay.io/osism/designate-sink:15.0.1.20230615
- quay.io/osism/designate-worker:15.0.1.20230615
- quay.io/osism/designate-mdns:15.0.1.20230615
- quay.io/osism/designate-producer:15.0.1.20230615
- quay.io/osism/designate-central:15.0.1.20230615
- quay.io/osism/designate-api:15.0.1.20230615
- quay.io/osism/designate-backend-bind9:15.0.1.20230615
- quay.io/osism/barbican-worker:15.0.1.20230615
- quay.io/osism/barbican-keystone-listener:15.0.1.20230615
- quay.io/osism/barbican-api:15.0.1.20230615
- quay.io/osism/octavia-worker:11.0.1.20230615
- quay.io/osism/octavia-housekeeping:11.0.1.20230615
- quay.io/osism/octavia-health-manager:11.0.1.20230615
- quay.io/osism/octavia-driver-agent:11.0.1.20230615
- quay.io/osism/octavia-api:11.0.1.20230615
- quay.io/osism/cinder-backup:21.3.1.20230615
- quay.io/osism/cinder-scheduler:21.3.1.20230615
- quay.io/osism/cinder-api:21.3.1.20230615
- quay.io/osism/neutron-metadata-agent:21.1.2.20230615
- quay.io/osism/neutron-server:21.1.2.20230615
- quay.io/osism/glance-api:25.1.1.20230615
- quay.io/osism/openvswitch-vswitchd:3.1.1.20230615
- quay.io/osism/openvswitch-db-server:3.1.1.20230615
- quay.io/osism/redis-sentinel:6.0.16.20230615
- quay.io/osism/redis:6.0.16.20230615
- quay.io/osism/rabbitmq:3.11.18.20230615

- quay.io/osism/opensearch-dashboards:16.20.0.20230615
- quay.io/osism/memcached:1.6.14.20230615
- quay.io/osism/opensearch:2.8.0.20230615
- quay.io/osism/cron:3.0.20230615
- quay.io/osism/kolla-toolbox:15.1.1.20230615
- quay.io/osism/fluentd:4.5.0.20230615
- quay.io/keycloak/keycloak:19.0.1-legacy
- postgres:14-alpinequay.io/osism/patchman:2.0.3
- postgres:14.2-alpine
- memcached:1.6.14-alpinequay.io/osism/openstackclient:6.2.0

4.2.3 *Compute Nodes*

Regarding the compute servers, the operating system is Ubuntu 22.04.
The following services are installed on the management nodes:

- quay.io/osism/ovn-controller:23.6.1.20230919
- gitlab.lrz.de:1337/digimed/infrastructure/digimed_cfg_openstack/nova-compute:26.2.1.20230615.quobyte
- quay.io/osism/nova-libvirt:8.0.0.20230615
- quay.io/osism/nova-ssh:26.2.1.20230615
- quay.io/osism/openvswitch-vswitchd:3.1.1.20230615
- quay.io/osism/openvswitch-db-server:3.1.1.20230615
- quay.io/osism/cron:3.0.20230615
- quay.io/osism/kolla-toolbox:15.1.1.20230615
- quay.io/osism/fluentd:4.5.0.20230615
- quay.io/osism/neutron-metadata-agent:21.1.2.20230615

Furthermore, QEMU and KVM are installed on the compute nodes.
This has the following implications:

- QEMU emulator version 6.2.0 (Debian 1:6.2+dfsg-2ubuntu6.9)
- Kernel 6.6-rc1-snp-host-XXX

To check the availability of AMD SEV-SNP, sevctl from VirTEE on GitHub is used. VirTEE is an open community that builds components for virtualization-based TEEs. Sevctl is one of the disclosed tools to use for the management of AMD SEV-SNP. This tool can be used to manage the certificates and keys of the TEE and to check the availability of its services on the host. The following figure shows the output of sevctl on the compute nodes [36].

```
dragon@digimed-compute-003:~/virtee/snphost/target/release$ sudo ./snphost ok
[ PASS ] - AMD CPU
[ PASS ]   - Microcode support
[ PASS ]   - Secure Memory Encryption (SME)
[ PASS ]   - Secure Encrypted Virtualization (SEV)
[ PASS ]     - Encrypted State (SEV-ES)
[ PASS ]     - Secure Nested Paging (SEV-SNP)
[ PASS ]       - VM Permission Levels
[ PASS ]         - Number of VMPLs: 4
[ PASS ]     - Physical address bit reduction: 5
[ PASS ]     - C-bit location: 51
[ PASS ]     - Number of encrypted guests supported simultaneously: 509
[ PASS ]     - Minimum ASID value for SEV-enabled, SEV-ES disabled guest: 1
[ PASS ]     - Reading /dev/sev: /dev/sev readable
[ PASS ]     - Writing /dev/sev: /dev/sev writable
[ PASS ]   - Page flush MSR: ENABLED
[ PASS ] - KVM supported: API version: 12
[ PASS ]   - SEV enabled in KVM: enabled
[ FAIL ]   - SEV-ES enabled in KVM: Error - contents read from /sys/module/kvm_amd/parameters/sev_es: N
[ FAIL ]   - SEV-SNP enabled in KVM: Error - contents read from /sys/module/kvm_amd/parameters/sev_snp: N
[ PASS ] - Memlock resource limit: Soft: 134453796864 | Hard: 134453796864
ERROR: One or more tests in sevctl-ok reported a failure
Error: One or more tests in sevctl-ok reported a failure
```

Figure 4.3: **VirTEE - sevctl - c-003**

It can be already seen that AMD SEV-SNP is available on the compute nodes, but probably not to its full extent. Its implications are further investigated in the following chapter.

4.2.4 *OpenStack*

The OpenStack prototype infrastructure was preinstalled and configured by the LRZ. This includes all OpenStack services, the available flavors, images, et cetera. This affects also available networks, and security groups for software-defined networking, e.g. for Secure Shell Protocol (SSH) access. SSH is being used for secure and remote control of a computer system.
Node flavors are used to define the composition of a VM. This includes name, image, volume size, security groups, attached network interfaces, et cetera. The images include the operating system and the software that is being used on the VM. When a VM is being deployed, the image is being deployed on a once-created volume. The volume is then attached to the VM and the VM is being booted. The VM is then ready to use.
In the following, an instance is created and shows the available flavors: 6C-8-50 is the default flavor that is used for the planned cluster. It has 6 vCPUs, 8 GB RAM and 50 GB disk space.

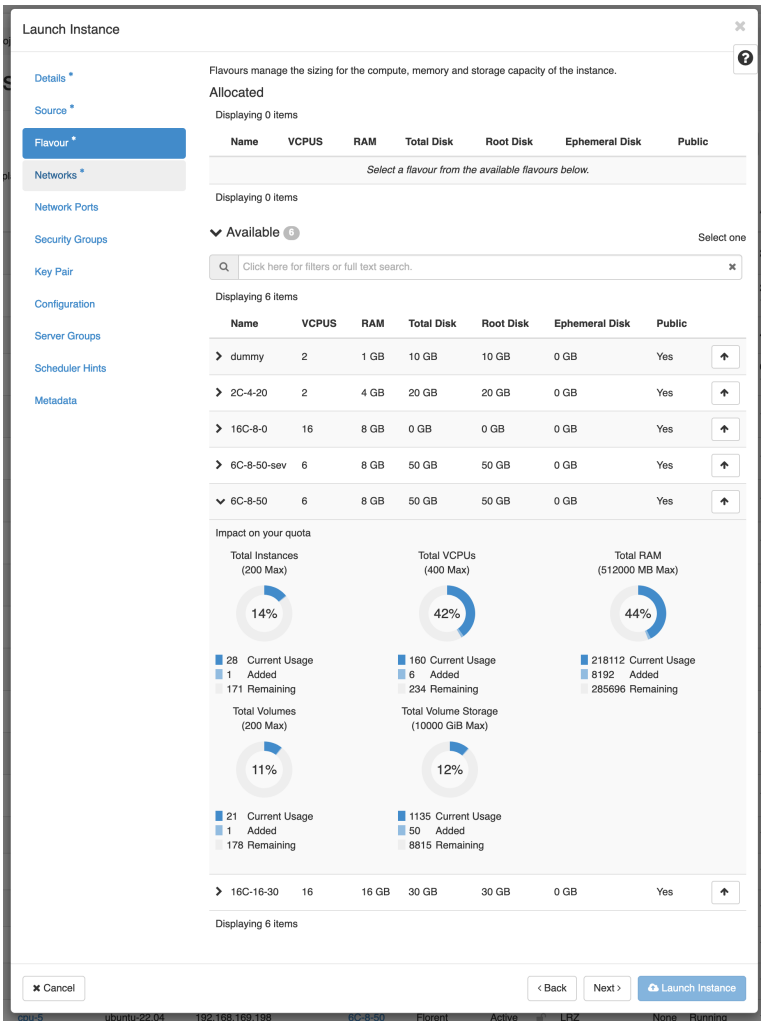

Figure 4.4: **DigiMed - OpenStack Cloud - Launch instance**

There are images with Ubuntu 22.04 and implementing the cloud-init service. Cloud-init is a package that is used to configure and initialize VMs in the cloud. It is being used to configure the network, the hostname, the SSH keys, et cetera. It is also used to install packages and to run scripts.
The images are provided by the LRZ and are distinguished between Ubuntu 22.04 and Ubuntu 22.04 with SEV. The latter one is used to deploy VMs with AMD SEV enabled.

5 DEPLOYMENT

5.1 BACKGROUND

For the interactions of the user with the OpenStack cloud infrastructure, the following tools are used:

- OpenStackClient
- Terraform
- Ansible

OpenStackClient is a command-line client for OpenStack that provides a user-friendly interface for OpenStack services. It is used to authenticate the user and to gain access to the OpenStack environment via CLI. For that, a user account was created.
Initially, a secure web login via username and password is necessary to continue with further steps to enhance access to the systems. OpenRC files are used to connect via OpenStackClient, authenticate the user only by password and gain access to the OpenStack environment via CLI. The OpenRC file is a shell script that contains the credentials to access the OpenStack environment. It is used to set the environment variables for the OpenStack CLI to authenticate the user.
Terraform is an open-source infrastructure as a code software tool that provides a declarative language to define and create infrastructure. It is used to deploy the control node and/or the cluster. Terraform can be configured to use the OpenStackClient or SSH. In this case, the OpenStackClient is used [35].
Ansible is an open-source software provisioning, configuration management and application-deployment tool. It is used to configure the control node and/or configure the HPC cluster [34].
Slurm Workload Manager(SLURM) is an open-source workload manager designed for Linux clusters of all sizes. It provides three key functions. First, it allocates exclusive and/or non-exclusive access to resources (computer nodes) to users for some duration of time so they can perform work. Second, it provides a framework for starting, executing, and monitoring work (typically a parallel job) on a set of allocated nodes. Finally, it arbitrates contention for resources by managing a queue of pending work [29].
GROningen MAchine for Chemical Simulations (GROMACS) is a molecular dynamics package mainly designed for simulations of proteins, lipids, and nucleic acids. It was originally developed in the Biophysical Chemistry department of University of Groningen, and is now maintained by contributors in universities and research centers worldwide. GROMACS is one of the fastest and most popular software packages available and can run on CPUs as well as GPUs [26].

5.2 CONCEPT

To find answers to the research questions, there are several approaches to be considered.
Regarding the **RQ1** and its security attestation, one node with AMD SEV capabilities can be deployed to investigate its components. The most important ones are at least to check the availability of security features and certificate verification.
Regarding the **RQ2** and its usability, the OpenStack environment can be used to deploy, configure and operate HPC cluster. While doing so, the usability of the OpenStack environment can be evaluated.
Regarding the **RQ3** and its performance, the HPC cluster can be used to run GROMACS benchmarks that are scheduled via SLURM over OpenMPI. As GROMACS is a widely used HPC application for biomedical simulation, it is a good choice to evaluate the performance of the HPC cluster. It also delivers embedded performance measurement tools.

Therefore, the following deployment approach is chosen to cover all aspects:

- The control node is deployed via Terraform and configured via Ansible. Only the control node is equipped with SLURM. The instance count is one.
- The cluster is deployed via Terraform and configured via Ansible. The instance count is ten for each partition. There is one for the SEV partition and one for the non-SEV partition.
- All nodes are equipped with OpenMPI and GROMACS.
- All instances are configured with the 6C-8-50 flavor.
- Each partition has its proper Ubuntu 22.04 - image.
- The control node uses the Ubuntu 22.04 - image without SEV.

5.3 SECURITY ATTESTATION

5.3.1 *Model*

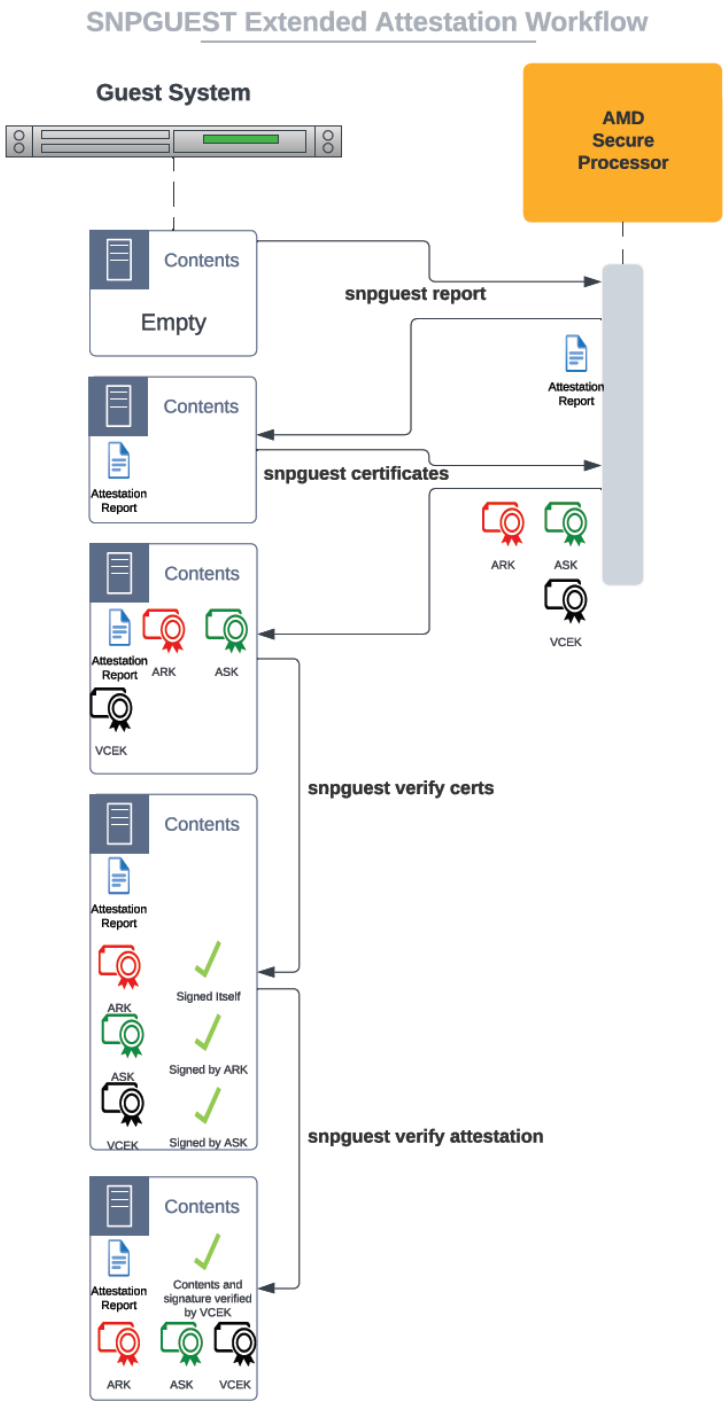

Figure 5.1: **VirTEE - SNP Extended Attestation Workflow [36]**

The following figure shows efficiently the workflow of the security attestation. With this procedure, it is possible to verify that a

virtual machine is running encrypted in a trusted and confidential environment.

1. **snpguest report:** The guest sends a report request to the hypervisor.
2. **ACK:** The hypervisor acknowledges the request and sends back the attestation report.
3. **snpguest certificates:** The guest sends a certificate request to the hypervisor.
4. **ACK:** The hypervisor acknowledges the request and sends back the certificate chain.
5. **snpguest verify certs:** The guest verifies the certificate chain.
6. **snpguest verify attestation:** The guest verifies the attestation report.

5.3.2 *Certification Process Inspection*

To check the availability of AMD SEV-SNP, sevctl is used on one only node of the cpu-sev partition cluster. The figure shows that AMD SEV

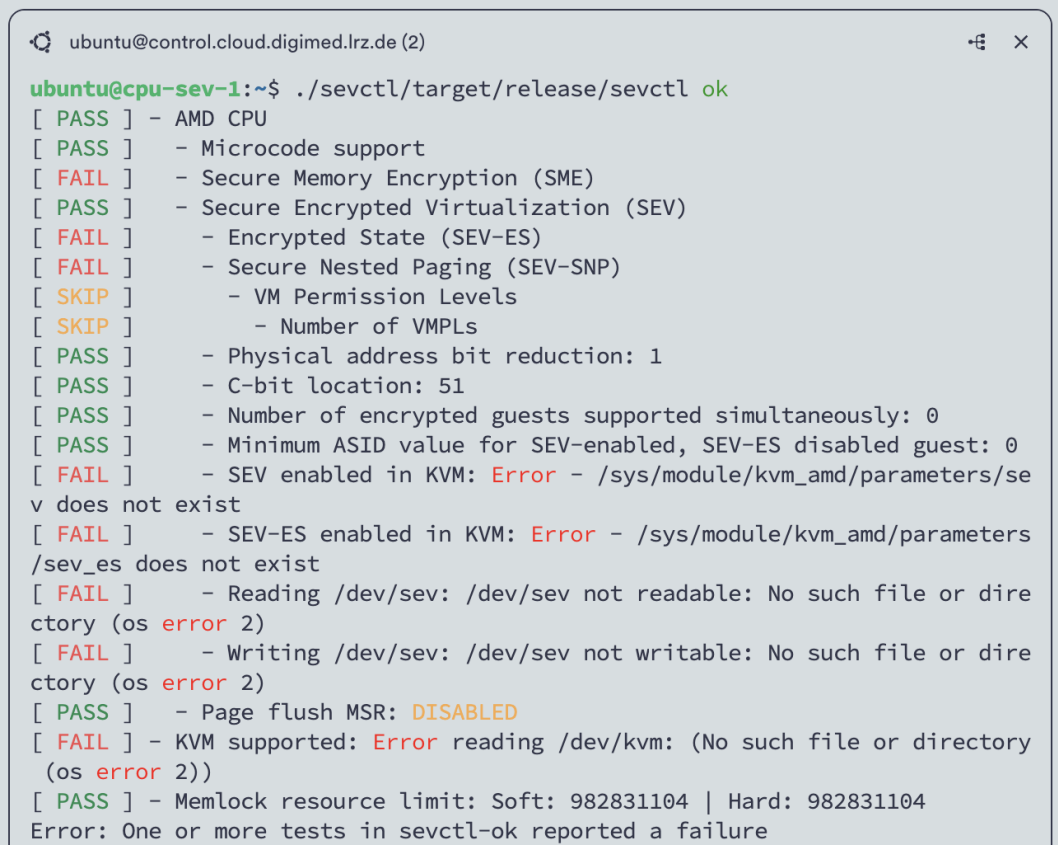

Figure 5.2: **VirTEE - sevctl - cpu-sev-1**

is available, but very likely not to its full extent. Further investigation

is needed to find out why, although the AMD CPU is not only capable of SEV but also SEV-ES and SEV-SNP. Furthermore, snpguest is a CLI tool for managing AMD SEV-SNP guests and is used for various operations such as attestation, certificate, management, derived key fetching, et cetera. As AMD SEV is not available to its full extent, the operation to quest the certificate chain to initialize the security attestation fails.

5.4 USABILITY

5.4.1 *ISO standard*

The EN ISO 9241-11:2018 - Usability in a Use Case Context is used to evaluate the usability of the OpenStack environment. It is a standard for software and systems engineering. It provides a process for measuring the usability of software and systems and is in this case more to be understood as a guideline for achieving a sufficient level of quality while measuring the usability. The goal of this standard is to ensure that the usability of the referring entity is sufficient for the intended use.
In the middle of usability is an entity, e. g. system, product or service. Around that entity is the context of use, the users and their tasks. The context of use is the environment in which the entity is used. The users are the people who use the entity. The tasks are the activities that the users perform with the entity. Usability is the extent to which the entity can be used by the users to achieve specified goals with effectiveness, efficiency and satisfaction in a specified context of use. It also can describe the availability, user experience, et cetera [6].

5.4.2 *Frontend*

Users who deal with a confidential OpenStack environment will not recognize much of a difference from a non-confidential OpenStack environment. The only difference is that the user needs to choose the right image to deploy a VM with SEV enabled. This is done by choosing the image with SEV in its name. Furthermore, depending on the scalability of the HPC cluster, the user may notice a difference in the performance of the HPC cluster. This is because the SEV partition is limited to 15 guests per host. This is a limitation of the first generation of AMD CPUs and is expected to be resolved in the future. Furthermore, there are further performance penalties to be considered which are not in the scope of this thesis. This is related to the fact, that the impacts of SEV behave differently when the HPC cluster is scaled up and a heavy or quiet specific workload is applied.

5.4.3 *Backend*

Administrators that deal with the implementation of Confidential Computing and AMDCPUs in an OpenStack cloud, should be capable of implementing AMD SEV. It comes with a lot of challenges and requires a lot of knowledge as the implications need to be considered on every layer of hardware- and software.
Firstly, SEV is only supported when using the libvirt compute driver with a libvirt.virt_type of KVM or QEMU. Secondly, at least one host machine needs to have AMD SEV capable hardware.
The operator also needs to perform the following steps:

- Reservation of sufficient memory on the SEV compute hosts for host-level services, because SEV-enabled guest pin pages in RAM, preventing any memory overcommitment.
- Definition of SEV-enabled flavors or images needed.
- Depending on the generation of used AMD CPU, the operator needs to configure the number of guests an AMD SEV can host with memory encrypted because that varies depending on CPU, e. g. only 15 are possible with earlier generations.
- libvirt version 8.0.0 exposes the maximum number of these guests, so the limit is automatically detected using this feature.
- ram_allocation_ration needs to be set to 1.0 to prevent overcommitment of memory on all SEV compute hosts.
- libvirt.hw_machine_type on all SEV-enabled compute hosts need to include x86_64=q35 so that all those images implement the q35 machine by default.
- Configuration of a flavor or image needs further steps to be considered. The flavor needs to be configured with hw:mem_encryption to True and an image with hw_mem_encryption set to True. In all cases, SEV instances can only be booted from images with UEFI firmware.

Furthermore, there are impermanent and permanent limitations to be considered. The impermanent limitations are:

- Encrypted guests cannot be live migrated or suspended. They need to be shut down first, e.g. if maintenance is required on the host.
- Encrypted guests have no PCI pass-through support. E. g. virtual GPU support is currently not supported. Virtio-vhost-user are supported and let guests act as backends so that virtual network devices can be used and can provide devices to other guests.
- Encrypted guest can only have virtio-boot disks (virtio-blk). These are default for libvirt disks on x86.

These impermanent limitations are expected to be resolved in the future.
The permanent limitations are:

- The number of encrypted hosts will always be limited by the number of AMD SEV capable hosts. The current number with the first generation of AMD CPUs is 15 guests.
- The OS running in an encrypted guest must support AMD SEV. This is currently only the case for Linux.

5.5 PERFORMANCE

5.5.1 *ISO standard*

The ISO/IEC/IEEE 15939:2017 - Measurement process model is used to measure the performance of the OpenStack cluster. It is a standard for software and systems engineering. It provides a process for measuring the performance of software and systems and is in this case more to be understood as a guideline for achieving a sufficient level of quality while measuring the performance. The goal of this standard is to describe the measurement process as a method to collect, analyze and report information to support effective management and demonstrate the quality of the referring entity. As shown in the measurement process

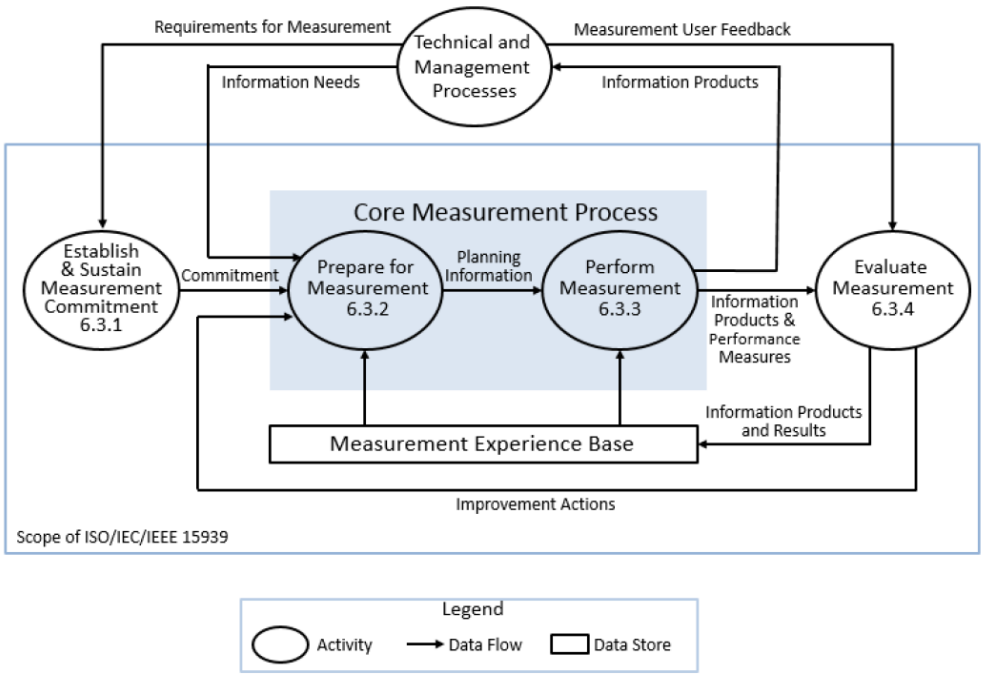

Figure 5.3: **ISO/IEC/IEEE 15939:2017 - Measurement process model [5]**

model, only 6.3.2, 6.3.3 and 6.3.4 are briefly discussed.

In 6.3.2, the measurement strategy needs to be determined. The needed information needs to be identified and prioritized. Further, data needs to be collected, analyzed, accessed and reported. The included systems need to be enabled. According to the concept, the deployment cluster was installed and configured regarding affected instances, used software and workload. They are accessible and generate operational, but also measurement output files.
In 6.3.3, procedures for data generation, collection and analysis need to be determined. This data needs also to be collected, stored and verified. The results need to be recorded. GROMACS uses internal tools to cover all of this. It includes also mega-flops accounting and time accounting, so the performance of the cluster can be measured. The Mega-Flops Accounting tool is used to measure the performance of the cluster in terms of MFLOPS. The Time Accounting tool is used to measure the performance of the cluster in terms of time.
In 6.4.4, the information needs to be evaluated against the specified evaluation criteria. In this case, the measurement metrics such as MFLOPS and time are used. After the figures are shown, the measurements are evaluated and compared to each other. The results are then discussed and conclusions are drawn.

5.5.2 *Single Node*

During the following benchmarks, only a single node is used.

cpu			
	benchRIB	**cmet_eq**	**benchBFC**
M-Flops	925205908.230	14527316278.663	34223340.327

Table 5.1: **Partition cpu - Single Node - Mega-Flops Accounting**

cpu-sev			
	benchRIB	**cmet_eq**	**benchBFC**
M-Flops	925063918.719	14542858037.511	34287275.083

Table 5.2: **Partition cpu-sev - Single Node - Mega-Flops Accounting**

The MFLOPS of the SEV partition are slightly higher than the MFLOPS of the non-SEV partition. This is a good, but unexpected result as the performance is impacted positively. To clarify the origins of these facts, further investigation is needed.

cpu			
	benchRIB	**cmet_eq**	**benchBFC**
Wall t (s)	3208.421	53174.533	214.008
Core t (s)	19250.521	319047.194	1284.048
Effective t (mm:ss)	53:28	14h46:14	3:40

Table 5.3: **Partition cpu - Single Node - Time Accounting**

cpu-sev			
	benchRIB	**cmet_eq**	**benchBFC**
Wall t (s)	2697.893	60848.689	151.757
Core t (s)	16187.353	365092.133	910.543
Effective t (mm:ss)	44:57	16h54:08	2:31

Table 5.4: **Partition cpu-sev - Single Node - Time Accounting**

The effective time of the SEV partition is approximately 15% shorter than the effective time of the non-SEV partition. This is a good, but unexpected result as the performance is impacted positively. To clarify the origins of these facts, further investigation is needed. Much more demanding workloads such as cmet_eq-benchmark can show the performance penalty of 13% due to the SEV technology on the performance of the single node.

5.5.3 *Three-Node Cluster*

During the following benchmarks, a cluster of three nodes is used.

	cpu		
	benchRIB	**cmet_eq**	**benchBFC**
M-Flops	938244867.570	15230958917.053	35912739.227

Table 5.5: **Partition cpu - Three-Node Cluster - Mega-Flops Accounting**

	cpu-sev		
	benchRIB	**cmet_eq**	**benchBFC**
M-Flops	938197070.312	15228015556.021	35903490.594

Table 5.6: **Partition cpu-sev - Three-Node Cluster - Mega-Flops Accounting**

The MFLOPS of the SEV partition are slightly lower than the MFLOPS of the non-SEV partition. This is a good result as the performance penalty is low.

	cpu		
	benchRIB	**cmet_eq**	**benchBFC**
Wall t (s)	2278.896	37748.322	106.490
Core t (s)	41020.113	679469.783	1916.798
Effective t (mm:ss)	37:58	10h29:08	1:46

Table 5.7: **Partition cpu - Three-Node Cluster - Time Accounting**

	cpu-sev		
	benchRIB	**cmet_eq**	**benchBFC**
Wall t (s)	2300.233	37748.322	107.563
Core t (s)	41403.986	679469.783	1936.119
Effective t (mm:ss)	38:20	11h19:57	1:48

Table 5.8: **Partition cpu-sev - Three-Node Cluster - Time Accounting**

The effective time of the SEV partition is slightly slower than the effective time of the non-SEV partition. This is a good result as the performance penalty is low.
Regarding the scalability effects between the single node and the three-node cluster of the partition cpu, the performance of three-node cluster is better than the performance of the single node. This is an expected result. The benefits are between 29 and 47%. The same comparison of the same amount of the partition cpu-sev shows benefits between 15 and 33 %.

5.5.4 *Small Cluster*

During the following benchmarks, a cluster of ten nodes is used.

cpu			
	benchRIB	**cmet_eq**	**benchBFC**
M-Flops	1071630614.665	15299855815.791	58838419.978

Table 5.9: **Partition cpu - Small Cluster - Mega-Flops Accounting**

cpu-sev			
	benchRIB	**cmet_eq**	**benchBFC**
M-Flops	1104463557.104	19590361804.160	47120266.026

Table 5.10: **Partition cpu-sev - Small Cluster - Mega-Flops Accounting**

The MFLOPS of the SEV partition are slightly lower than the MFLOPS of the non-SEV partition. This is a good result as the performance penalty is low. Occasionally, the performance of the SEV partition is even better than the performance of the non-SEV partition. To clarify the origins of these facts, further investigation is needed.

cpu			
	benchRIB	**cmet_eq**	**benchBFC**
Wall t (s)	1153.569	21768.311	86.232
Core t (s)	69212.669	1306098.487	5173.522
Effective t (mm:ss)	19:16	6h02:48	1:26

Table 5.11: **Partition cpu - Small Cluster - Time Accounting**

cpu-sev			
	benchRIB	**cmet_eq**	**benchBFC**
Wall t (s)	665.509	22587.554	87.012
Core t (s)	39919.275	1355252.592	5219.928
Effective t (mm:ss)	11:05	6h16:27	1:27

Table 5.12: **Partition cpu-sev - Small Cluster - Time Accounting**

The effective time of the SEV partition is slightly slower than the effective time of the non-SEV partition. This is a good result as the performance penalty is low. Occasionally, the performance of the SEV partition is even much better than the performance of the non-SEV partition. To clarify the origins of these facts, further investigation is needed.

Regarding the scalability effects between the three-node and the small cluster of the partition cpu, the performance of the small cluster is better than the performance of the three-node cluster. This is an expected result. The benefits are between 19 and 57%. The same comparison of the same amount of the partition cpu-sev shows benefits between 19 and 71%.

6 CONCLUSION AND OUTLOOK

With the accomplished investigation, the research questions could be partially answered.

RQ1: How does the security attestation of TEEs work?

As discussed, there is a simple workflow for the security attestation of TEEs. The guest sends a report request to the hypervisor. The hypervisor acknowledges the request and sends back the attestation report. The guest sends a certificate request to the hypervisor. The hypervisor acknowledges the request and sends back the certificate chain. The guest verifies the certificate chain. The guest verifies the attestation report. Furthermore, additional tools of VirTEE are used to execute the security attestation and to build trust between the guest and the hypervisor.
Unfortunately, with the current status of the DigiMed project, it is not possible to fully implement the security attestation. This is because the AMD CPU is not capable of SEV to its full extent. This issue needs to be further investigated as the required hardware and software are given.

RQ2: How is Usability affected when TEEs are implemented in a confidential HPCaaS?

While excluding aspects of multi-tenant systems, the usability of the HPC cluster is not affected by the implementation of TEEs. The user does not recognize any difference from a non-confidential HPC cluster. The only difference is that the user needs to choose the right image to deploy a VM with SEV enabled. This is done by choosing the image with SEV in its name. Furthermore, depending on the scalability of the HPC cluster, the user may notice a difference in the performance of the HPC cluster. This is because the SEV partition is limited to 15 guests per host. This is a limitation of the first generation of AMD CPUs and is expected to be resolved in the future. Furthermore, there are further performance penalties to be considered which are not in the scope of this thesis. This is related to the fact, that the impacts of SEV behave differently when the HPC cluster is scaled up and a heavy or quiet specific workload is applied.
This might drastically change as multiple users are using the HPC cluster at the same time. The DigiMed project is aimed to process Big Data in an automated way. Furthermore, many stakeholders would like to operate with the system. This is why usability needs also to be considered in terms of multi-tenancy while the project is further developed.

RQ3: How is Performance affected when TEEs are implemented in a confidential HPCaaS?

Considering the performance of the HPC cluster, the performance of the SEV partition is slightly lower than the performance of the non-SEV partition. This is a good result as the performance penalty is low. Occasionally, the performance of the SEV partition is even better than the performance of the non-SEV partition. To clarify the origins of these facts, further investigation is needed. Furthermore, although the performance seems satisfying, the number of nodes was still limited to ten nodes. This is why the performance needs to be further investigated as the quantity of nodes massively increases in the context of HPC. This is related to the fact, that the impacts of SEV behave differently when the HPC cluster is scaled up and a heavy or quiet specific workload is applied.

Confidential Computing in the cloud is with the DigiMed prototype still at its early stages. Therefore, there are still many bugs that need to be fixed and many features that need to be implemented. This is why the project needs to be further investigated and developed. The following list shows some of the next steps that need to be considered: The full implementation of AMD SEV-SNP, the migration of real use cases and the capacities of up-scale HPC cluster.

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ACRONYMS

AES Advanced Encryption Standard. 11–13

AI Artificial intelligence. 15–17

AMD Advanced Micro Devices, Inc.. 1, 2, 7, 9–11, 18, 31–33, 44, 57–59, 65

AMD SEV AMD Secure Encrypted Virtualization. 2, 13, 18, 31, 51, 54, 56–59

AMD SEV-ES AMD Secure Encrypted Virtualization - Encrypted State. 31

AMD SEV-SNP AMD Secure Encrypted Virtualization - Secure Nested Paging. 12, 50, 56, 57, 66

AMD-SEP AMD Secure Encrypted Processor. 31

AMD-SP AMD Secure Processor. 31, 32

AMD-V AMD Virtualization. 31

AP Application Processor. 32

API Application programming interface. 2, 18, 32, 33, 35, 41

APM Authenticated Page Mapping. 33

ARM Advanced RISC Machines. 31

AWS Amazon Web Services. 9

BI Business intelligence. 7

BIOS Basic Input/Output System. 32

BLASTN Basic Local Alignment Search Tool for nucleotides. 18, 23

BMC Baseboard management controller. 46

C-bit EnCrypted bit. 12, 13

CA Certificate authority. 10, 11

CCC Confidential Computing Consortium. 2, 6–8

CLI Command-line interface. 53, 57

CPU Central Processing Unit. 2, 3, 5–7, 10, 11, 17, 19, 20, 25–27, 30–33, 36–38, 44, 57–59, 65, 95

DCsv2 Azure Virtual Machines DCsv2-series. 9

DNA Deoxyribonucleic acid. 3, 16

DNS Domain Name System. 35

DRM Digital rights management. 8

EC2 Amazon Elastic Compute Cloud. 9

ES AMD Secure Encrypted Virtualization - Encrypted State. 11

EU European Union. 8

FLOPS Floating point operations per second. 16

GAPBS Graph Algorithm Platform Benchmark Suite. 18, 23, 24

GDPR General Data Protection Regulation. 8

GPS Global Positioning System. 16

GPU Graphics processing unit. 17, 38, 39, 58, 95

GROMACS GROningen MAchine for Chemical Simulations. 3, 53, 54, 60, 95

HE Homomorphic encryption. 5

HPC High-performance computing. 1–3, 7, 13, 16–20, 23, 24, 36–41, 53, 54, 57, 65, 66

HPCaaS High-performance computing as a service. 2, 3, 17, 65, 66

HTC High-throughput computing. 36

I/O Input/Output. 19, 20, 23, 36, 37, 40

IaaS Infrastructure as a service. 1, 15, 26

IBM International Business Machines Corporation. 7, 16

ID Identifier. 11

IETF Internet Engineering Task Force. 8

Intel SGX Intel Software Guard Extensions. 1, 2, 7, 18

IOMMU Input/Output Memory Management Unit. 38

IOP Input/Output 36

iOS Apple iOS. 8, 25

IoT Internet of Things. 13, 16

IP Internet Protocol. 37

ISO International Organization for Standardization. 3, 14

IT Information technology. 1, 7, 25, 26, 36

JIT Just-in-time compilation. 31

KSM Kernel Same-page Merging. 37

KVM Kernel-based Virtual Machine. 30, 31, 49, 58

LightGBM Light Gradient Boosting Machine. 18

LOM Lights-out management. 46

LRZ Leibniz Supercomputing Centre. 50, 51

LULESH Livermore Unstructured Lagrangian Explicit Shock Hydrodynamics. 18

MD Molecular dynamics. 3

MFLOPS Mega floating point operations per second. 60–63

MPC Multi-party computation. 13

MSLR Microsoft's Learning to Rank. 18

NFV Network function virtualization. 28

NIC Network interface controller. 3, 37, 38, 40

NIST National Institute of Standards and Technology. 14

NPB NAS Parallel Benchmarks. 18, 20, 23

NUMA Non-unified Memory Access. 19–22, 24, 36–38

NVRAM Non-Volatile RAM. 33

OFED OpenFabrics Enterprise Distribution. 40

OpenMPI Open MPI. 54, 81, 82

OS Operating system. 2, 18, 25–32, 37, 40, 46, 59

OS API Operating system application programming interface. 2

PaaS Platform as a Service. 15

PC Personal computer. 14

PCI Peripheral Component Interconnect. 38, 39, 58

PSP AMD Platform Security Processor. 31

QEMU Quick Emulator. 19, 20, 30, 31, 33, 49, 58

QMP QEMU Machine Protocol. 32

RAM Random-access memory. 3, 6, 12, 21, 22, 25, 58

RDMA Remote direct memory access. 17, 38, 40

RNA Ribonucleic acid. 3

RoCE RDMA over Converged Ethernet. 17

SaaS Software as a Service. 15

SDK Software development kit. 7, 34

SDN Software-defined networking. 28, 35–37

SEP Apple Secure Enclave Processor. 8

SEV AMD Secure Encrypted Virtualization. 2, 11, 18–24, 32, 33, 54, 57, 58, 61–63, 65, 66

SEV-ES AMD Secure Encrypted Virtualization - Encrypted State. 32, 33, 57

SEV-SNP AMD Secure Encrypted Virtualization - Secure Nested Paging. 11, 13

SGX Intel Software Guard Extensions. 9, 18–20, 24

SHA-256 Secure Hash Algorithm 2, hash value 256. 33

SLURM Slurm Workload Manager. 53, 54

SME AMD Secure Memory Encryption. 11

SMM System Management Mode. 32

SMPC Secure multi-party computation. 13

SNP AMD Secure Nested Paging. 11, 12

SoC System on a chip. 8, 31

SR-IOV Single Root I/O Virtualization. 38–40

SSH Secure Shell Protocol. 50, 51, 53

TCG Tiny Code Generator. 31

TCP Transport Control Protocol. 37

TEE Trusted execution environment. 1–3, 5–11, 13, 18, 50, 65, 66

TLB Translation Lookaside Buffer. 38

TPM Trusted Platform Module. 5, 8

UEFI Unified Extensible Firmware Interface. 58

US United States. 16, 18

VDI Virtual desktop infrastructure. 29

VM Virtual machine. 9, 11, 12, 21, 22, 24, 31–33, 35, 37, 38, 43, 50, 51, 57, 65

VMCB Virtual Machine Control Block. 33

VMM Virtual machine monitor. 26

VMSA Virtual Machine save area. 32, 33

VPN Virtual private network. 15

APPENDIX - HANDS-ON: MISCELLEANEOUS

DEPLOYMENT AUTOMATION WITH TERRAFORM

Terraform - Cluster Deployment

```
# https://registry.terraform.io/providers
    /terraform-provider-openstack/
    openstack/latest/docs
terraform {
  required_providers {
    openstack = {
      source = "terraform-provider-
          openstack/openstack"
      version = "1.52.1"
    }
  }
}

// How many compute nodes do you want to
    create?
variable "instance_count" {
  default = "100"
}

// Security group: Allow SSH
resource "openstack_compute_secgroup_v2"
    "ssh" {
  name = "ssh-security-group"
  description = "security␣group␣for␣
      opening␣the␣port␣22"
  rule {
    from_port = 22
    to_port = 22
    ip_protocol = "tcp"
    cidr = "0.0.0.0/0"
  }
}

// Security group: Open ports required by
    SLURM, OpenMPI etc.
resource "openstack_compute_secgroup_v2"
    "slurm" {
    name = "slurm"
    description = "security␣group␣for␣
        slurm␣and␣and␣the␣benchmarks"
```

```
    rule {
      from_port = 6817
    to_port = 6817
    ip_protocol = "tcp"
    cidr = "0.0.0.0/0"
    }
    rule {
      from_port = 6818
    to_port = 6818
    ip_protocol = "tcp"
    cidr = "0.0.0.0/0"
    }
}

// The VM
resource "openstack_compute_instance_v2"
   "cpu-sev" {
  count        = var.instance_count
  name         = "cpu-sev"
  flavor_name = "6C-8-50" // 6 cores, 8
     GB RAM, 50 GB disk
  key_pair     = "Florent"
  security_groups = ["default",
     openstack_compute_secgroup_v2.ssh.id
     , openstack_compute_secgroup_v2.
     slurm.id]

  // The block device
  block_device {
    uuid                  = "52ea7c42-
       bbe9-43b6-bf2f-0c45585a0c40" // An
        SEV image
    source_type           = "image"
    volume_size           = 50
    boot_index            = 0
    destination_type      = "volume"
    delete_on_termination = true
  }

  // The MWN network
  network {
    uuid = "4b872f7e-abf5-42fe-9bb0
       -0741118a979e"
  }
}
```

CONFIGURATION AUTOMATION WITH ANSIBLE

Ansible - Inventory file

```
[control]
10.156.170.42

[cpu]
192.168.42.128
192.168.42.129
192.168.42.130
192.168.42.131
192.168.42.132
192.168.42.133
192.168.42.134
192.168.42.135
192.168.42.136
192.168.42.137
192.168.42.138

[cpu-sev]
192.168.42.192
192.168.42.193
192.168.42.194
192.168.42.195
192.168.42.196
192.168.42.197
192.168.42.198
192.168.42.199
192.168.42.200
192.168.42.201

[filesystem]
10.156.70.190
```

Ansible - Configuration file

```
[defaults]
inventory   = ./inventory.ini
remote_user = ubuntu
host_key_checking = False
private_key_file = ~/V-MACBOOK.pem
```

Ansible Playbook - Install GROMACS on the cluster

```
- name: Install GROMACS on the cluster
  hosts: cpu,cpu-sev
  become: true

  tasks:
    - name: Install GROMACS on the
        cluster
      ansible.builtin.shell: |
        sudo apt update
        sudo apt upgrade -y
        sudo apt install cmake -y
        wget https://ftp.gromacs.org/
            gromacs/gromacs-2023.3.tar.
            gz
        tar xfz gromacs-2023.3.tar.gz
        cd gromacs-2023.3
        mkdir build
        cd build
        cmake .. -DGMX_MPI=on -
            DGMX_BUILD_OWN_FFTW=ON -
            DREGRESSIONTEST_DOWNLOAD=ON
        make
        make check
        sudo make install
        echo "#Add␣GROMACS␣to␣PATH" |
            sudo tee -a ../.bashrc
        echo "export␣PATH="$PATH:/usr/
            local/gromacs/bin/GMX_MPI""
            | sudo tee -a ../.bashrc
        echo "export␣PATH="$PATH:/usr/
            local/gromacs/bin/GMXRC"" |
            sudo tee -a ../.bashrc
        echo "export␣PATH="$PATH:/usr/
            local/gromacs/bin/"" | sudo
            tee -a ../.bashrc
```

Ansible Playbook - Install openMPI on the cluster

```
- name: Install openMPI on the cluster
hosts: cpu,cpu-sev
become: true

tasks:
  - name: Install gcc on the cluster
    ansible.builtin.apt: name={{ item
        }} state=present
```

```
  with_items:
  - gcc
  - openmpi-bin
  - openmpi-common
  - libopenmpi-dev
  - libgtk2.0-dev

- name: Download and decompress file
   openmpi on the cluster
  ansible.builtin.get_url:
    url: https://download.open-mpi.
       org/release/open-mpi/v5.0/
       openmpi-5.0.1.tar.gz
    dest: /home/ubuntu/openmpi-5.0.1.
       tar.gz
    mode: '0440'

- name: Install OpenMPI on the
   cluster
  ansible.builtin.shell: |
    sudo tar  -xvzf /home/ubuntu/
       openmpi-5.0.1.tar.gz
    cd /home/ubuntu/openmpi-5.0.1
      sudo ./configure --prefix="/
         home/ubuntu/.openmpi"
      sudo make
      sudo make install

- name: Export PATH on the cluster
  ansible.builtin.shell: |
    echo "export PATH="$PATH:/home/
       ubuntu/.openmpi/bin"" | sudo
       tee -a ../.bashrc
    echo "export LD_LIBRARY_PATH="
       $LD_LIBRARY_PATH:/home/ubuntu
       /.openmpi/lib"" | sudo tee -a
       ../.bashrc
```

C-program for Prime Number Calculation

```
# include <math.h>
# include <mpi.h>
# include <stdio.h>
# include <stdlib.h>
# include <time.h>

int main ( int argc, char *argv[] );
int prime_number ( int n, int id, int p )
   ;
void timestamp ( );

/*
   ******************************************************
   */

int main ( int argc, char *argv[] )

/*
   ******************************************************
   */
/*
  Purpose:

    MAIN is the main program for
       PRIME_MPI.

  Discussion:

    This program calls a version of
       PRIME_NUMBER that includes
    MPI calls for parallel processing.

  Licensing:

    This code is distributed under the
       GNU LGPL license.

  Modified:

    07 August 2009

  Author:

    John Burkardt
*/
```

```
{
  int i;
  int id;
  int ierr;
  int n;
  int n_factor;
  int n_hi;
  int n_lo;
  int p;
  int primes;
  int primes_part;
  double wtime;

  n_lo = 1;
  n_hi = 1048576;
  n_factor = 2;
/*
  Initialize MPI.
*/
  ierr = MPI_Init ( &argc, &argv );
/*
  Get the number of processes.
*/
  ierr = MPI_Comm_size ( MPI_COMM_WORLD,
    &p );
/*
  Determine this processes's rank.
*/
  ierr = MPI_Comm_rank ( MPI_COMM_WORLD,
    &id );

  if ( id == 0 )
  {
    timestamp ( );
    printf ( "\n" );
    printf ( "PRIME_MPI\n" );
    printf ( "  C/MPI version\n" );
    printf ( "\n" );
    printf ( "  An MPI example program to
      count the number of primes.\n" );
    printf ( "  The number of processes
      is %d\n", p );
    printf ( "\n" );
    printf ( "         N        Pi
      Time\n" );
    printf ( "\n" );
  }

  n = n_lo;
```

```
  while ( n <= n_hi )
  {
    if ( id == 0 )
    {
      wtime = MPI_Wtime ( );
    }
    ierr = MPI_Bcast ( &n, 1, MPI_INT, 0,
        MPI_COMM_WORLD );

    primes_part = prime_number ( n, id, p
        );

    ierr = MPI_Reduce ( &primes_part, &
       primes, 1, MPI_INT, MPI_SUM, 0,
      MPI_COMM_WORLD );

    if ( id == 0 )
    {
      wtime = MPI_Wtime ( ) - wtime;
      printf ( "  %8d  %8d  %14f\n", n,
         primes, wtime );
    }
    n = n * n_factor;
  }
/*
  Terminate MPI.
*/
  ierr = MPI_Finalize ( );
/*
  Terminate.
*/
  if ( id == 0 )
  {
    printf ( "\n");
    printf ( "PRIME_MPI - Master process
       :\n");
    printf ( "  Normal end of execution.\
       n");
    printf ( "\n" );
    timestamp ( );
  }

  return 0;
}
/*
    **********************************************************
    */

int prime_number ( int n, int id, int p )
```

```
/*
  ****************************************************************************
  */
/*
  Purpose:

    PRIME_NUMBER returns the number of
    primes between 1 and N.

  Discussion:

    In order to divide the work up evenly
    among P processors, processor
  ID starts at 2+ID and skips by P.

    A naive algorithm is used.

    Mathematica can return the number of
    primes less than or equal to N
  by the command PrimePi[N].

                N   PRIME_NUMBER

                1             0
               10             4
              100            25
            1,000           168
           10,000         1,229
          100,000         9,592
        1,000,000        78,498
       10,000,000       664,579
      100,000,000     5,761,455
    1,000,000,000    50,847,534

  Licensing:

    This code is distributed under the
    GNU LGPL license.

  Modified:

    21 May 2009

  Author:

    John Burkardt

  Parameters:

    Input, int N, the maximum number to
```

```
        check.

    Input, int ID, the ID of this process
        ,
    between 0 and P-1.

    Input, int P, the number of processes
        .

    Output, int PRIME_NUMBER, the number
        of prime numbers up to N.
*/
{
  int i;
  int j;
  int prime;
  int total;

  total = 0;

  for ( i = 2 + id; i <= n; i = i + p )
  {
    prime = 1;
    for ( j = 2; j < i; j++ )
    {
      if ( ( i % j ) == 0 )
      {
        prime = 0;
        break;
      }
    }
    total = total + prime;
  }
  return total;
}
/*
    ****************************************************
    */

void timestamp ( void )

/*
    ****************************************************
    */
/*
  Purpose:

    TIMESTAMP prints the current YMDHMS
        date as a time stamp.
```

```
  Example:

    31 May 2001 09:45:54 AM

  Licensing:

    This code is distributed under the
      GNU LGPL license.

  Modified:

    24 September 2003

  Author:

    John Burkardt

  Parameters:

    None
*/
{
# define TIME_SIZE 40

  static char time_buffer[TIME_SIZE];
  const struct tm *tm;
  size_t len;
  time_t now;

  now = time ( NULL );
  tm = localtime ( &now );

  len = strftime ( time_buffer, TIME_SIZE
      , "%d %B %Y %I:%M:%S %p", tm );

  printf ( "%s\n", time_buffer );

  return;
# undef TIME_SIZE
}
```

Compilation for OpenMPI-processing

```
mpicc mpi-prime.c -o ./outputfile
```

Execution of OpenMPI-job

```
ubuntu@control-2:~$ mpirun --H "cpu-sev-5:22""cpu-sev-6:22" -np 5 /mnt/shared/home/ubuntu/openmpi/outputfile
13 January 2024 08:50:09 PM

PRIME_MPI
  C/MPI version

  An MPI example program to count the number of primes.
  The number of processes is 5

         N        Pi          Time

         1         0        0.003960
         2         1        0.000033
         4         2        0.000218
         8         4        0.000021
        16         6        0.000178
        32        11        0.000019
        64        18        0.000148
       128        31        0.000022
       256        54        0.000123
       512        97        0.000041
      1024       172        0.000066
      2048       309        0.000193
      4096       564        0.000635
      8192      1028        0.002230
     16384      1900        0.008550
     32768      3512        0.046055
     65536      6542        0.121924
    131072     12251        0.435356
    262144     23000        1.674015
    524288     43390        6.353576
   1048576     82025       24.289235

PRIME_MPI - Master process:
  Normal end of execution.

13 January 2024 08:50:42 PM
```

Figure 1: **mpirun of outputfile**
Successful execution of the OpenMPI-job

JOB SCHEDULING WITH SLURM

SBATCH - benchRIB_cpu-cluster_1n

```
#!/bin/bash
#
#SBATCH --partition=cpu           ###
    Partition (you may need to change this
    )
#SBATCH --job-name=benchBFC
#SBATCH --time=1:00:00        ### WallTime
     - set it accordningly

#SBATCH --nodes               1     # May vary
#SBATCH --ntasks-per-core 1     # Bind one
     MPI tasks to one CPU core
#SBATCH --ntasks-per-node 6  # Must be
    less/equal to the number of CPU cores
#SBATCH --cpus-per-task    1     # Must be
    2, unless you have a better guess

#SBATCH -o slurm.%j.out           # STDOUT
#SBATCH -e slurm.%j.err           # STDERR

module purge
module load gromacs/2023/2023.3

export OMP_NUM_THREADS=${
   SLURM_CPUS_PER_TASK}
export OMP_PLACES=cores
export OMP_PROC_BIND=spread
export UCX_NET_DEVICES=mlx5_0:1

cd $SLURM_SUBMIT_DIR

mpirun /usr/local/gromacs/bin/gmx_mpi
    mdrun -v -s /mnt/shared/home/ubuntu/
    mpinat-gromacs/mpinat-gromacs-free-
    energy-bench/benchBFC.tpr
```

SBATCH - cmet_eq_cpu-sev-cluster_10n

```
#!/bin/bash
#
#SBATCH --partition=cpu-sev          ### Partition (you may need to change this)
#SBATCH --job-name=cmet_eq
#SBATCH --time=10:00:00          ### WallTime - set it accordningly

#SBATCH --nodes              10     # May vary
#SBATCH --ntasks-per-core 1     # Bind one MPI tasks to one CPU core
#SBATCH --ntasks-per-node 6  # Must be less/equal to the number of CPU cores
#SBATCH --cpus-per-task    1     # Must be 2, unless you have a better guess

#SBATCH -o slurm.%j.out          # STDOUT
#SBATCH -e slurm.%j.err          # STDERR

module purge
module load gromacs/2023/2023.3

export OMP_NUM_THREADS=${SLURM_CPUS_PER_TASK}
export OMP_PLACES=cores
export OMP_PROC_BIND=spread
export UCX_NET_DEVICES=mlx5_0:1

cd $SLURM_SUBMIT_DIR

mpirun /usr/local/gromacs/bin/gmx_mpi mdrun -v -s /mnt/shared/home/ubuntu/mpinat-gromacs/mpinat-gromacs-binding-affinity-study-bench/cmet_eq.tpr
```

SIMULATION OF BIOMEDICAL DATA WITH GROMACS/SLURM

benchRIB_cpu-cluster_3n

```
Protein
2136412
    1NALA   MN1    1  18.818  24.238   7.941 -0.4151  0.2248 -0.3300
    1NALA   MN2    2  18.809  24.252   7.862  0.1694  0.0271 -0.4387
    1NALA     N    3  18.817  24.241   7.900 -0.1328  0.1068 -0.3459
    1NALA    H1    4  18.807  24.250   8.000 -0.7700  0.4493 -0.4337
    1NALA    H2    5  18.856  24.326   7.863  0.4791 -0.1472 -0.3448
    1NALA    H3    6  18.727  24.224   7.858  0.0616  0.3419 -0.9094
    1NALA    CA    7  18.907  24.128   7.870 -0.3787 -0.3637  0.5997
    1NALA    HA    8  18.876  24.043   7.931 -0.5137 -0.1551  0.8236
    1NALA  MCB1    9  18.931  24.054   7.727 -0.5089 -0.4126  0.6045
    1NALA  MCB2   10  18.867  24.119   7.712  0.0187  0.0947  0.4645
    1NALA    CB   11  18.899  24.087   7.723 -0.2488 -0.1646  0.5363
    1NALA   HB1   12  18.968  24.005   7.705 -0.8060 -0.6825  0.6772
    1NALA   HB2   13  18.797  24.055   7.700 -0.4388  0.6254  0.1993
    1NALA   HB3   14  18.925  24.172   7.660  0.5914 -0.2940  0.6869
    1NALA     C   15  19.049  24.166   7.910 -0.2473 -0.1405 -0.0517
    1NALA     O   16  19.089  24.282   7.917  0.5115 -0.3974  0.1131
    2VAL      N   17  19.137  24.067   7.928  0.2104  0.2668 -0.0059
    2VAL      H   18  19.103  23.973   7.922  0.6191  0.1191 -0.0212
    2VAL     CA   19  19.279  24.080   7.955  0.1533  0.8083  0.0579
    2VAL     HA   20  19.312  24.183   7.940  0.3121  0.8226  0.4896
    2VAL     CB   21  19.300  24.037   8.100 -0.5978 -0.5161 -0.1879
    2VAL     HB   22  19.312  23.929   8.102 -0.3912 -0.5033 -0.6714
    2VAL   MCG1   23  19.412  24.144   8.154 -0.9461  0.0138 -0.5018
    2VAL   MCG2   24  19.453  24.061   8.155 -0.4945  0.2265 -0.7757
    2VAL    CG1   25  19.429  24.101   8.153 -0.7170  0.1028 -0.6264
    2VAL   HG11   26  19.414  24.208   8.165 -1.2489  0.0132 -0.4256
    2VAL   HG12   27  19.454  24.057   8.249 -0.0857  0.1086 -0.7770
    2VAL   HG13   28  19.510  24.083   8.082 -0.9016  0.6291 -0.9903
    2VAL   MCG1   29  19.161  24.042   8.186 -0.2488 -0.1239  0.3718
    2VAL   MCG2   30  19.214  24.111   8.218  0.4018 -0.7715  0.7369
    2VAL    CG2   31  19.191  24.075   8.199  0.0581 -0.4496  0.5340
    2VAL   HG21   32  19.106  24.008   8.187 -0.5109  0.2883  0.2991
    2VAL   HG22   33  19.229  24.067   8.301  0.3821 -1.5624  0.3555
    2VAL   HG23   34  19.159  24.178   8.181  0.7723 -0.0269  1.4639
    2VAL      C   35  19.357  23.983   7.868 -0.1424  0.3137  0.3336
    2VAL      O   36  19.313  23.874   7.834  0.7273 -0.0937  0.4569
    3VAL      N   37  19.482  24.016   7.834 -0.1003 -0.0527  0.1230
    3VAL      H   38  19.522  24.099   7.876  0.1782 -0.2383  0.2234
    3VAL     CA   39  19.568  23.944   7.742 -0.3051  0.0174 -0.1242
    3VAL     HA   40  19.529  23.843   7.732 -0.2438  0.0068 -0.2591
    3VAL     CB   41  19.570  24.007   7.603 -0.0759  0.3203  0.0137
    3VAL     HB   42  19.592  24.113   7.615 -0.2394  0.3427  0.1265
    3VAL   MCG1   43  19.670  23.902   7.528  0.3297  0.2814  0.6043
    3VAL   MCG2   44  19.691  23.986   7.496  0.1740  0.2104  0.3158
    3VAL    CG1   45  19.678  23.946   7.514  0.2429  0.2479  0.4478
    3VAL   HG11   46  19.681  23.838   7.530  0.4924  0.3099  0.8729
    3VAL   HG12   47  19.656  23.967   7.410  0.3749 -0.2162  0.3212
    3VAL   HG13   48  19.775  23.989   7.540  0.0893  0.5984  0.4598
    3VAL   MCG1   49  19.432  23.950   7.536 -0.1180  0.0007  0.3679
    3VAL   MCG2   50  19.431  24.041   7.523  0.1149 -0.1110 -0.5102
    3VAL    CG2   51  19.435  23.996   7.531 -0.0035 -0.0449 -0.0688
    3VAL   HG21   52  19.404  23.892   7.529 -0.2459 -0.0074  0.8903
    3VAL   HG22   53  19.361  24.055   7.584  0.0527  0.6512 -0.7302
    3VAL   HG23   54  19.445  24.033   7.429  0.2344 -1.0396 -0.4256
    3VAL      C   55  19.704  23.937   7.809 -0.0557  0.1829 -0.5984
    3VAL      O   56  19.766  24.032   7.856  0.0952 -0.2538  0.1277
```

4LYP	N	57	19.764	23.818	7.815	0.4373	0.4527	0.2142
4LYP	H	58	19.711	23.737	7.788	0.3236	0.3154	0.8411
4LYP	CA	59	19.900	23.793	7.857	0.4200	-0.1524	-0.0735
4LYP	HA	60	19.928	23.867	7.932	0.8675	-0.5395	0.1487
4LYP	CB	61	19.922	23.654	7.917	0.3924	-0.5290	-0.9012
4LYP	HB1	62	19.846	23.637	7.985	-0.1262	-1.2793	-1.6463
4LYP	HB2	63	19.919	23.586	7.840	1.2729	0.0194	-1.4382
4LYP	CG	64	20.054	23.633	7.991	-0.1410	-0.6233	0.0621
4LYP	HG1	65	20.137	23.652	7.923	0.1958	-0.8451	0.6259
4LYP	HG2	66	20.060	23.702	8.075	-0.7269	-0.5694	-0.1186
4LYP	CD	67	20.063	23.490	8.043	-0.3263	-0.4831	0.4905
4LYP	HD1	68	19.970	23.464	8.096	-0.2686	-0.2310	1.3255
4LYP	HD2	69	20.077	23.421	7.959	-1.0432	-1.1533	0.5413
4LYP	CE	70	20.182	23.481	8.138	0.4093	0.2410	-0.3188
4LYP	HE1	71	20.271	23.532	8.095	0.5638	-0.0397	-1.3338
4LYP	HE2	72	20.159	23.533	8.235	1.3302	1.1369	-0.1329
4LYP	MNZ1	73	20.219	23.328	8.124	-0.3059	0.0298	-0.0046
4LYP	MNZ2	74	20.204	23.338	8.203	-0.2882	0.2528	-0.0296
4LYP	NZ	75	20.210	23.339	8.162	-0.2694	0.1452	-0.0289
4LYP	HZ1	76	20.234	23.294	8.075	-0.4460	-0.1414	0.0672
4LYP	HZ2	77	20.288	23.330	8.227	-0.3285	-0.0937	0.0194
4LYP	HZ3	78	20.129	23.294	8.202	-0.5004	0.6049	0.0261
4LYP	C	79	19.990	23.811	7.736	0.3181	-0.2877	-0.1696
4LYP	O	80	19.961	23.769	7.624	0.4446	-0.0591	-0.2898
5CYN	N	81	20.109	23.870	7.751	0.1470	0.0408	-0.1104
5CYN	H	82	20.130	23.906	7.843	-0.2917	0.4979	-0.1860
5CYN	CA	83	20.213	23.891	7.652	0.5665	-0.0699	0.3028
5CYN	HA	84	20.167	23.916	7.556	0.8301	-0.1141	0.1658
5CYN	CB	85	20.298	24.009	7.699	0.1206	0.1965	0.4621
5CYN	HB1	86	20.235	24.098	7.713	-0.1442	0.2566	0.2439
5CYN	HB2	87	20.347	23.983	7.794	0.0287	0.4868	0.7893
5CYN	SG	88	20.423	24.040	7.572	0.1960	-0.0812	0.4665
5CYN	HG	89	20.514	23.955	7.620	-0.8395	-2.0438	-0.8068
5CYN	C	90	20.287	23.759	7.640	0.4593	-0.1380	0.3845
5CYN	O	91	20.311	23.689	7.738	0.3304	0.1017	0.5892
6LYP	N	92	20.338	23.734	7.519	0.1929	-0.5808	0.3587
6LYP	H	93	20.317	23.797	7.442	-0.2915	-0.8286	0.2894
6LYP	CA	94	20.423	23.621	7.491	0.4244	-0.3014	-0.0962
6LYP	HA	95	20.375	23.535	7.537	0.8205	-0.4915	-0.0400
6LYP	CB	96	20.428	23.591	7.341	-0.3427	0.0319	-0.1983
6LYP	HB1	97	20.331	23.595	7.304	-0.9818	-0.5229	-0.0134
6LYP	HB2	98	20.489	23.663	7.296	-0.8133	0.7130	-0.9064
6LYP	CG	99	20.486	23.454	7.307	0.4406	0.1887	0.4307
6LYP	HG1	100	20.580	23.456	7.334	0.8541	0.6736	0.4818
6LYP	HG2	101	20.434	23.389	7.359	0.6792	-0.2948	0.8682
6LYP	CD	102	20.485	23.403	7.163	0.3128	0.3437	0.3773
6LYP	HD1	103	20.390	23.423	7.123	0.5523	0.9853	0.3681
6LYP	HD2	104	20.559	23.455	7.110	0.6532	-0.0785	0.6281
6LYP	CE	105	20.513	23.254	7.148	-0.6251	0.1923	-0.0135
6LYP	HE1	106	20.614	23.228	7.189	-1.1810	-0.3834	0.3228
6LYP	HE2	107	20.438	23.193	7.207	-1.2421	0.7920	-0.6391
6LYP	MNZ1	108	20.465	23.233	6.999	-0.1597	-0.5117	-0.0692
6LYP	MNZ2	109	20.542	23.210	6.999	0.1779	0.5281	0.0349
6LYP	NZ	110	20.504	23.222	7.005	-0.0157	0.0154	-0.0170
6LYP	HZ1	111	20.411	23.242	6.971	-0.2766	-1.2589	-0.1413
6LYP	HZ2	112	20.570	23.279	6.954	-0.6932	0.9271	0.0343
6LYP	HZ3	113	20.525	23.125	6.991	1.3418	0.2565	0.0535
6LYP	C	114	20.559	23.635	7.558	0.5478	0.0631	-0.4165

6LYP	O	115	20.595	23.751	7.577	-0.0667	0.1800	0.0717
7PRO	N	116	20.631	23.534	7.606	0.1705	-0.2022	-0.4060
7PRO	CD	117	20.593	23.394	7.603	-0.3139	-0.0918	0.1560
7PRO	HD1	118	20.479	23.380	7.611	-0.2532	0.3592	1.1418
7PRO	HD2	119	20.625	23.342	7.505	-1.2896	-0.2911	-0.0069
7PRO	CG	120	20.666	23.337	7.724	0.4481	-0.3252	-0.3963
7PRO	HG1	121	20.607	23.355	7.819	0.5872	-1.2362	-0.3876
7PRO	HG2	122	20.682	23.226	7.714	1.0625	0.0519	-1.2728
7PRO	CB	123	20.799	23.412	7.727	0.1573	0.1872	0.2639
7PRO	HB1	124	20.836	23.429	7.834	-0.5735	0.5728	0.4657
7PRO	HB2	125	20.881	23.355	7.671	0.7222	0.3643	0.8991
7PRO	CA	126	20.766	23.545	7.658	0.0984	-0.0865	-0.2450
7PRO	HA	127	20.762	23.619	7.737	-0.1344	0.0867	-0.4215
7PRO	C	128	20.886	23.582	7.572	0.0681	0.1647	-0.1823
7PRO	O	129	20.998	23.554	7.612	-0.1263	-0.0286	0.2360
8THR	N	130	20.866	23.659	7.464	-0.6260	0.0805	-0.1252
8THR	H	131	20.772	23.688	7.444	-0.7024	-0.2792	-0.2921
8THR	CA	132	20.968	23.705	7.373	-0.1490	0.1013	0.4081
8THR	HA	133	21.042	23.624	7.367	-0.1918	0.0573	0.4786
8THR	CB	134	20.911	23.719	7.232	-0.1231	0.2518	0.4123
8THR	HB	135	20.994	23.730	7.162	-0.0773	0.2493	0.4662
8THR	MCG1	136	20.819	23.611	7.150	-0.3341	0.2726	0.6193
8THR	MCG2	137	20.836	23.574	7.232	0.5185	-0.0876	0.3044
8THR	CG2	138	20.830	23.596	7.192	0.0863	0.0969	0.4605
8THR	HG21	139	20.792	23.609	7.091	-0.8142	0.4615	0.8232
8THR	HG22	140	20.893	23.508	7.196	0.5259	0.3386	-0.5187
8THR	HG23	141	20.746	23.584	7.261	0.6971	-0.6204	1.1115
8THR	OG1	142	20.826	23.830	7.216	-0.3288	0.0374	-0.0258
8THR	HG1	143	20.879	23.908	7.202	-0.4710	0.0887	-0.2951
8THR	C	144	21.045	23.828	7.420	-0.2604	0.1581	0.4419
8THR	O	145	20.979	23.924	7.459	-0.4505	0.1907	0.0594
9SER	N	146	21.178	23.822	7.418	-0.2600	0.2594	-0.0935
9SER	H	147	21.220	23.757	7.354	-0.5339	0.6503	-0.6690
9SER	CA	148	21.273	23.898	7.497	0.1746	-0.2596	-0.1029
9SER	HA	149	21.372	23.859	7.476	0.1033	-0.3547	-0.2641
9SER	CB	150	21.274	24.047	7.462	-0.0014	-0.1527	0.3302
9SER	HB1	151	21.175	24.089	7.480	-0.0361	0.0659	1.0897
9SER	HB2	152	21.347	24.098	7.524	0.5482	-0.1103	0.0719
9SER	OG	153	21.308	24.063	7.326	-0.8288	-0.3909	0.0835
9SER	HG	154	21.289	24.154	7.300	0.6712	0.1216	0.5667
9SER	C	155	21.245	23.879	7.645	0.3655	0.6161	0.0582
9SER	O	156	21.132	23.857	7.687	0.3868	-0.2112	-0.2747
10PRO	N	157	21.348	23.895	7.729	0.6776	-0.7379	-0.0153
10PRO	CD	158	21.491	23.910	7.711	0.6467	-0.2908	0.0698
10PRO	HD1	159	21.538	23.811	7.697	1.0823	-0.2094	0.1884
10PRO	HD2	160	21.512	23.971	7.621	0.5950	-0.2681	-0.0462
10PRO	CG	161	21.548	23.978	7.835	0.0807	0.0352	0.1557
10PRO	HG1	162	21.664	23.960	7.852	0.1477	0.5708	0.4356
10PRO	HG2	163	21.536	24.096	7.835	-0.4398	0.0066	0.0853
10PRO	CB	164	21.458	23.907	7.936	0.1481	-0.3469	-0.0513
10PRO	HB1	165	21.495	23.801	7.956	-0.0190	-0.6484	-0.5572
10PRO	HB2	166	21.456	23.962	8.035	0.3316	-0.8623	0.3949
10PRO	CA	167	21.320	23.906	7.871	0.1926	0.4123	-0.1748
10PRO	HA	168	21.269	23.815	7.902	0.2787	0.3717	-0.1513
10PRO	C	169	21.235	24.025	7.913	-0.8400	-0.1958	-0.4629
10PRO	O	170	21.232	24.123	7.839	-0.0351	0.3249	0.1585
11GLY	N	171	21.183	24.027	8.036	-0.2157	-0.1620	-0.1880
11GLY	H	172	21.190	23.945	8.094	0.4078	-0.0379	-0.0938

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11GLY     CA  173  21.114  24.142   8.092 -0.3741 -0.3626  0.0351
11GLY    HA1  174  21.131  24.143   8.195 -0.3083 -0.6268 -0.1918
11GLY    HA2  175  21.154  24.229   8.047 -0.5232 -0.4752  0.1950
11GLY      C  176  20.964  24.142   8.068 -0.4263 -0.0562  0.3617
11GLY      O  177  20.897  24.225   8.131 -1.1263 -0.2604 -0.0916
12ARG      N  178  20.916  24.060   7.974 -0.2560  0.0537  0.1780
12ARG      H  179  20.975  23.985   7.942 -0.2481  0.0211  0.2676
12ARG     CA  180  20.785  24.070   7.913 -0.0995  0.2455 -0.1328
12ARG     HA  181  20.740  24.160   7.954 -0.1892  0.3250 -0.4094
12ARG     CB  182  20.797  24.093   7.763 -0.0165 -0.4472 -0.2400
12ARG    HB1  183  20.856  24.012   7.717  0.9683 -0.2666  0.0342
12ARG    HB2  184  20.697  24.096   7.717 -0.1170 -1.6025 -0.7363
12ARG     CG  185  20.868  24.227   7.742 -1.1691  0.2219 -0.0366
12ARG    HG1  186  20.798  24.303   7.759 -2.1665 -0.2007 -0.9415
12ARG    HG2  187  20.947  24.233   7.811 -1.6819  1.3631  0.7748
12ARG     CD  188  20.926  24.246   7.602 -0.2118 -0.1131  0.2971
12ARG    HD1  189  21.011  24.315   7.606  0.3821 -0.1609  0.4831
12ARG    HD2  190  20.964  24.149   7.564 -0.0732 -0.5272  0.2194
12ARG     NE  191  20.822  24.298   7.513 -0.2342  0.1585  0.4781
12ARG     HE  192  20.810  24.398   7.517 -0.5932  0.0898  1.1298
12ARG     CZ  193  20.742  24.232   7.428  0.1580  0.4030 -0.0939
12ARG    NH1  194  20.738  24.100   7.406  0.5343  0.3743 -0.0033
12ARG   HH11  195  20.800  24.038   7.456  0.3509  0.5331  0.4198
12ARG   HH12  196  20.672  24.062   7.339  1.0014  0.1954 -0.3577
12ARG    NH2  197  20.658  24.307   7.356 -0.2019  0.1083  0.0084
12ARG   HH21  198  20.658  24.408   7.367 -0.9003  0.0667  0.3777
12ARG   HH22  199  20.595  24.264   7.290  0.2269 -0.0738 -0.2822
12ARG      C  200  20.689  23.956   7.947 -0.0058  0.1343 -0.2391
12ARG      O  201  20.570  23.980   7.932 -0.0422 -0.0196 -0.1927
13ARG      N  202  20.741  23.840   7.988  0.2067  0.2642 -0.1383
13ARG      H  203  20.841  23.841   8.001  0.2170  0.3261 -0.2203
13ARG     CA  204  20.683  23.711   8.018  0.1361  0.3343  0.0282
13ARG     HA  205  20.651  23.664   7.925 -0.0704  0.4929  0.0202
13ARG     CB  206  20.798  23.629   8.077 -0.0735 -0.2140 -0.3109
13ARG    HB1  207  20.861  23.605   7.999 -0.7882 -0.4885 -0.4003
13ARG    HB2  208  20.846  23.688   8.146  0.2555 -0.4358 -0.7981
13ARG     CG  209  20.758  23.500   8.146  0.2559 -0.0687  0.1556
13ARG    HG1  210  20.679  23.520   8.212  0.3658  0.0666 -0.3021
13ARG    HG2  211  20.729  23.430   8.073  0.7132 -0.0912  0.4804
13ARG     CD  212  20.872  23.437   8.228 -0.2073 -0.0811  0.8078
13ARG    HD1  213  20.899  23.505   8.306 -0.0044  0.2341  1.1074
13ARG    HD2  214  20.836  23.346   8.273 -0.5104 -0.2700  1.3101
13ARG     NE  215  20.990  23.407   8.147 -0.5229 -0.2550  0.4037
13ARG     HE  216  21.061  23.478   8.157 -0.7778  0.0018  0.4075
13ARG     CZ  217  21.023  23.308   8.063  0.3570  0.2197  0.1644
13ARG    NH1  218  20.938  23.207   8.040  0.4498  0.1634  0.0636
13ARG   HH11  219  20.848  23.206   8.086  0.4451  0.0422  0.0505
13ARG   HH12  220  20.964  23.132   7.977  0.5249  0.2425  0.0008
13ARG    NH2  221  21.142  23.294   8.003 -0.1753 -0.0612 -0.8671
13ARG   HH21  222  21.215  23.361   8.019  0.0326 -0.0859 -1.7074
13ARG   HH22  223  21.158  23.215   7.942 -0.7986 -0.2467 -0.7973
13ARG      C  224  20.564  23.719   8.112  0.2721 -0.2570  0.2618
13ARG      O  225  20.468  23.645   8.090 -0.0047  0.0676  0.3574
14HIE      N  226  20.563  23.797   8.221  0.1475 -0.3738  0.3454
14HIE      H  227  20.645  23.853   8.241  0.1656 -0.4634  0.5188
14HIE     CA  228  20.452  23.810   8.314  0.0467 -0.3421  0.2216
14HIE     HA  229  20.396  23.716   8.310 -0.0203 -0.2982  0.1327
14HIE     CB  230  20.498  23.829   8.458 -0.5312 -0.1310  0.3849
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   14HIE     HB1  231  20.540  23.932   8.473 -1.0805  0.2676  0.7353
   14HIE     HB2  232  20.411  23.823   8.529 -0.8017 -0.6598  0.3470
   14HIE      CG  233  20.601  23.724   8.490 -0.0712  0.2406  0.1534
   14HIE     ND1  234  20.583  23.586   8.500  0.1711  0.1677 -0.3369
   14HIE     CE1  235  20.701  23.526   8.508  0.0794  0.0567  0.2787
   14HIE     HE1  236  20.718  23.421   8.524 -0.0378  0.1281  0.8757
   14HIE     NE2  237  20.797  23.620   8.493  0.1407 -0.0474  0.0097
   14HIE     HE2  238  20.896  23.602   8.485  0.1135 -0.0426 -0.3408
   14HIE     CD2  239  20.737  23.744   8.491 -0.0170 -0.1146  0.3116
   14HIE     HD2  240  20.788  23.840   8.489  0.0484 -0.1439  0.6110
   14HIE       C  241  20.355  23.922   8.279  0.2133 -0.2477  0.0624
   14HIE       O  242  20.260  23.930   8.356 -0.0526  0.6353 -0.3303
   15VAL       N  243  20.370  23.999   8.171 -0.3726 -0.2455 -0.0229
   15VAL       H  244  20.440  23.976   8.102 -0.7906 -0.4954 -0.3636
   15VAL      CA  245  20.290  24.117   8.146 -0.0577 -0.0308 -0.0287
   15VAL      HA  246  20.280  24.174   8.239 -0.1053 -0.0951  0.0051
   15VAL      CB  247  20.363  24.204   8.043 -0.2200  0.1011 -0.0344
   15VAL      HB  248  20.380  24.145   7.953  0.0492  0.1036  0.0168
   15VAL    MCG1  249  20.250  24.305   7.983  0.0158  0.1801 -0.3472
   15VAL    MCG2  250  20.311  24.358   8.027 -0.0831  0.1347 -0.1513
   15VAL     CG1  251  20.283  24.328   8.006 -0.0387  0.1559 -0.2434
   15VAL    HG11  252  20.195  24.299   7.948  0.1147  0.2195 -0.5116
   15VAL    HG12  253  20.251  24.380   8.096 -0.2791  0.1527 -0.3241
   15VAL    HG13  254  20.345  24.395   7.946  0.1778  0.1346 -0.0440
   15VAL    MCG1  255  20.513  24.212   8.106 -0.4155  0.1736  0.4307
   15VAL    MCG2  256  20.487  24.299   8.090 -0.4000  0.1599  0.3316
   15VAL     CG2  257  20.497  24.254   8.097 -0.4026  0.1649  0.3698
   15VAL    HG21  258  20.557  24.169   8.128 -0.4635  0.1954  0.5767
   15VAL    HG22  259  20.549  24.309   8.019 -0.1819  0.1686  0.5174
   15VAL    HG23  260  20.479  24.319   8.182 -0.6931  0.1765  0.3045
   15VAL       C  261  20.151  24.075   8.099 -0.0085 -0.1149 -0.0994
   15VAL       O  262  20.142  24.000   8.002  0.3527 -0.1033 -0.1440
   16VAL       N  263  20.050  24.118   8.174 -0.1726 -0.3090 -0.2088
   16VAL       H  264  20.073  24.180   8.250 -0.4048 -0.5624  0.0666
   16VAL      CA  265  19.908  24.090   8.162 -0.1200 -0.3464 -0.8362
   16VAL      HA  266  19.889  24.043   8.066 -0.1523 -0.1125 -0.9447
   16VAL      CB  267  19.843  24.007   8.273 -0.0057 -0.1342 -0.6063
   16VAL      HB  268  19.736  24.003   8.251 -0.0007 -0.1245 -0.6331
   16VAL    MCG1  269  19.879  23.853   8.232 -0.3420 -0.3893  0.0430
   16VAL    MCG2  270  19.912  23.866   8.317 -0.3602 -0.1189  0.0106
   16VAL     CG1  271  19.894  23.863   8.275 -0.3417 -0.2508  0.0095
   16VAL    HG11  272  19.869  23.815   8.180 -0.4016 -0.5801  0.1924
   16VAL    HG12  273  20.002  23.863   8.288 -0.3451 -0.4485  0.0707
   16VAL    HG13  274  19.847  23.809   8.357 -0.5186  0.1926  0.2059
   16VAL    MCG1  275  19.842  24.108   8.402 -0.7365 -0.4785 -0.3323
   16VAL    MCG2  276  19.876  24.027   8.432  0.2092 -0.2131 -0.6410
   16VAL     CG2  277  19.859  24.066   8.413 -0.2566 -0.3400 -0.4899
   16VAL    HG21  278  19.824  24.169   8.413 -1.3708 -0.6849 -0.1180
   16VAL    HG22  279  19.800  24.008   8.483  0.5403 -1.1820 -0.4813
   16VAL    HG23  280  19.964  24.063   8.442 -0.1187  0.6997 -0.7872
   16VAL       C  281  19.848  24.230   8.162  0.4163 -0.1001 -0.0447
   16VAL       O  282  19.890  24.316   8.239  0.0374  0.3520 -0.3296
   17LYP       N  283  19.771  24.260   8.057  0.1048  0.3136  0.2946

[...]

  31.01850  31.01850  21.93340   0.00000   0.00000   0.00000   0.00000
15.50925  15.50925
```

benchRIB_cpu-cluster_3n

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simulation system in water
67291
    1LEU      N    1   6.676   8.307   5.218 -0.0021  0.2320  0.3734
    1LEU     H1    2   6.628   8.383   5.170  0.2022  1.0936  1.4869
    1LEU     H2    3   6.754   8.279   5.160 -0.5346  1.9381 -1.2836
    1LEU     H3    4   6.707   8.345   5.306 -1.2838  0.7273  0.6310
    1LEU     CA    5   6.577   8.200   5.236  0.0149  0.2382  0.5116
    1LEU     HA    6   6.509   8.227   5.317  1.5597  1.7079  1.4059
    1LEU     CB    7   6.490   8.179   5.113  0.2767  0.3929  0.2988
    1LEU    HB1    8   6.526   8.100   5.046 -0.1229  0.2690  0.2300
    1LEU    HB2    9   6.481   8.272   5.056 -2.2664  1.4961  2.2916
    1LEU     CG   10   6.348   8.149   5.160  0.3299  0.0771  0.2632
    1LEU     HG   11   6.313   8.232   5.222 -1.6791 -1.0963  0.7993
    1LEU    CD1   12   6.261   8.148   5.035 -0.1730  0.1152  0.6084
    1LEU   HD11   13   6.286   8.070   4.963 -1.4504 -1.5029  1.8549
    1LEU   HD12   14   6.156   8.138   5.064 -0.7241 -0.8285 -1.5230
    1LEU   HD13   15   6.269   8.240   4.977  2.5567  0.0101  0.7211
    1LEU    CD2   16   6.331   8.021   5.242  0.4724 -0.4599 -0.5311
    1LEU   HD21   17   6.225   8.000   5.247  0.0952  1.0427 -1.4632
    1LEU   HD22   18   6.374   7.928   5.206 -1.5759 -2.3507  1.6337
    1LEU   HD23   19   6.366   8.042   5.343 -0.2712  0.0354 -0.3660
    1LEU      C   20   6.645   8.077   5.292 -0.4084 -0.3012 -0.1438
    1LEU      O   21   6.612   8.047   5.407 -0.0462  0.4095  0.1540
    2VAL      N   22   6.745   8.017   5.227  0.0692 -0.2689  0.5394
    2VAL      H   23   6.751   8.048   5.130 -1.4857  0.2933  0.6025
    2VAL     CA   24   6.823   7.902   5.266 -0.0882 -0.4541  0.3109
    2VAL     HA   25   6.820   7.895   5.374  0.7069  2.3873  0.5837
    2VAL     CB   26   6.776   7.773   5.198 -0.6673 -0.1747  0.1825
    2VAL     HB   27   6.838   7.686   5.218  1.0639  1.1361  0.7455
    2VAL    CG1   28   6.631   7.743   5.234 -0.8224 -0.1232 -0.3858
    2VAL   HG11   29   6.563   7.826   5.214 -0.4515  0.0343 -0.9883
    2VAL   HG12   30   6.598   7.652   5.184 -1.2555 -0.0914 -0.1698
    2VAL   HG13   31   6.627   7.732   5.343 -0.3692  1.0998 -0.2268
    2VAL    CG2   32   6.777   7.785   5.046 -0.0669 -0.1960  0.1841
    2VAL   HG21   33   6.704   7.860   5.017 -1.2035 -2.0675 -2.1356
    2VAL   HG22   34   6.869   7.830   5.007 -0.2276 -0.5204 -0.5901
    2VAL   HG23   35   6.739   7.693   5.001  1.6827 -1.8427  1.8530
    2VAL      C   36   6.972   7.916   5.236 -0.1893 -0.1121 -0.0306
    2VAL      O   37   7.013   8.005   5.161  0.3586 -0.3279  0.0134
    3GLN      N   38   7.057   7.825   5.284 -0.0223  0.0025 -0.1095
    3GLN      H   39   7.023   7.747   5.338 -0.1999  0.1886  0.0474
    3GLN     CA   40   7.196   7.806   5.248 -0.0595 -0.1751 -0.1582
    3GLN     HA   41   7.216   7.876   5.167 -1.2834  1.7235  1.1028
    3GLN     CB   42   7.285   7.841   5.367 -0.1017  0.2400 -0.2480
    3GLN    HB1   43   7.389   7.851   5.335  0.8701 -2.7055  1.5738
    3GLN    HB2   44   7.276   7.767   5.447  0.6695 -0.3157 -0.6575
    3GLN     CG   45   7.261   7.969   5.446 -0.2982 -0.3392  0.6420
    3GLN    HG1   46   7.335   7.961   5.525  0.0316 -2.8528  0.1616
    3GLN    HG2   47   7.158   7.969   5.483 -1.3995 -1.0156 -2.1908
    3GLN     CD   48   7.283   8.104   5.380 -0.4388 -0.4558  0.3504
    3GLN    OE1   49   7.370   8.122   5.295 -0.2227 -0.0765  0.6451
    3GLN    NE2   50   7.196   8.204   5.400  0.4908  0.4224  0.0928
    3GLN   HE21   51   7.127   8.195   5.473  0.2798 -0.2019 -0.1775
    3GLN   HE22   52   7.217   8.299   5.374 -2.0940  1.6728  2.1539
    3GLN      C   53   7.223   7.677   5.174 -0.0859 -0.1037 -0.2908
    3GLN      O   54   7.337   7.648   5.138 -0.2887 -0.6338 -0.5223
    4ALA      N   55   7.123   7.594   5.143 -0.0962 -0.1552 -0.1157
    4ALA      H   56   7.034   7.634   5.170  0.7895  1.6078  0.3257
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    4ALA     CA   57   7.126   7.461   5.085 -0.0083 -0.3026  0.2239
    4ALA     HA   58   7.168   7.388   5.154 -0.1360 -0.4844  0.1053
    4ALA     CB   59   6.979   7.419   5.086 -0.0977  0.0035  0.3830
    4ALA    HB1   60   6.925   7.458   5.000  1.0513  0.8878  0.0243
    4ALA    HB2   61   6.958   7.313   5.076 -1.9159  0.5323 -2.3603
    4ALA    HB3   62   6.926   7.450   5.176  0.3036 -0.3296  0.7383
    4ALA      C   63   7.187   7.446   4.946 -0.4610 -0.0365 -0.0034
    4ALA      O   64   7.241   7.339   4.920  0.1882  0.1590  0.5108
    5VAL      N   65   7.196   7.550   4.863  0.1246 -0.2606 -0.2225
    5VAL      H   66   7.157   7.638   4.892 -0.8686  0.0333 -2.2857
    5VAL     CA   67   7.264   7.545   4.735  0.5068  0.0495 -0.0312
[...]
21250ClJ    ClJ67284  12.949   5.209   5.064  0.5256  0.1989  0.3175
21251ClJ    ClJ67285   7.547   5.588   5.235 -0.1682 -0.0014  0.1189
21252ClJ    ClJ67286   6.451   3.525   5.970 -0.2570 -0.4948 -0.2313
21253ClJ    ClJ67287   9.163   9.410   4.132  0.1440  0.3170  0.2095
21254ClJ    ClJ67288   5.741   7.649   2.457 -0.4625  0.1306 -0.3416
21255ClJ    ClJ67289  11.510   4.863   4.494  0.3226 -0.2051 -0.1277
21256ClJ    ClJ67290   4.837   1.999   5.864  0.2453 -0.0636 -0.2043
21257ClJ    ClJ67291   9.423   0.031   3.015  0.2124 -0.1384 -0.3437
[...]
   9.85491   9.85491   6.96847   0.00000   0.00000   0.00000   0.00000
4.92746   4.92746
```

APPENDIX - PERFORMANCE BENCHMARKS: GROMACS

ABOUT

The Max Planck Institute for Multidisciplinary Sciences released an open GROMACS benchmark set with a collection of input files for GROMACS performance evaluation. The given benchmarks are common simulations used in the research projects of the referred institute. They cover wide ranges of atom systems with dimensions of 6k and 12M atoms. In the following description, some of these input files are further technically explained. In most of the cases, excluding benchPEP-h, all standard benchmarks use bond constraints. Therefore, the update step has to be done on the CPU. Benchmarks covering the GPU-performance are not covered [33].

Benchmark characteristics

Standard MD benchmarks

Tab. 1: Specifications of the "standard" benchmarks.

MD system	MEM	RIB	PEP
# atoms	81,743	2,136,412	12,495,503
system size / nm	$10.8 \times 10.2 \times 9.6$	31.2^3	50.0^3
time step / fs	2	4	2
cutoff radii / nm	1.0	1.0	1.2
PME grid spacing / nm	0.12	0.135	0.16

Useful command line arguments for benchmarking

Run the MEM benchmark for 10,000 steps, reset cycle counters after half of the steps:
`mdrun -s MEM.tpr -nsteps 10000 -resethway`

Run the MEM benchmark for 4,000 steps, reset cycle counters at 3,000 steps:
`mdrun -s MEM.tpr -nsteps 4000 -resetstep 3000`

Run the MEM benchmark for an hour, reset cycle counters after 30 minutes:
`mdrun -s MEM.tpr -nsteps -1 -maxh 1.0 -resethway`

Same as above, but suppress output of the last configuration (which we don't need anyway):
`mdrun -s MEM.tpr -nsteps -1 -maxh 1.0 -resethway -noconfout`

Free energy benchmarks

Tab. 2: Specifications of the "solvation free energy" benchmarks.

MD system	SFI	SFC	STI	STC	SNI	SNC
# atoms			3,363			
# perturbed atoms			48			
system size / nm			$3.65 \times 3.65 \times 2.58$			
time step / fs			2			
cutoff radii / nm			1.2			
PME grid spacing / nm			0.1			
nstcalcenergy	1	100	1	100	1	100
free-energy	yes	yes	slow-growth	slow-growth	no	no

Three letter code for the free energy benchmarks:

- first letter: S = solvation free energy, B = binding free energy MD system, N = no free energy

Tab. 3: Specifications of the "binding free energy" benchmarks.

MD system	BFI	BFC	BTI	BTC	BNI	BNC
# atoms			43,952			
# perturbed atoms			48			
system size / nm			$8.55 \times 8.55 \times 6.04$			
time step / fs			2			
cutoff radii / nm			1.2			
PME grid spacing / nm			0.1			
nstcalcenergy	1	100	1	100	1	100
free-energy	yes	yes	slow-growth	slow-growth	no	no

- second letter: T = TI, F = FEP
- third letter: value of nstcalcenergy, I = 1 step, C = 100 steps

The following two different simulation systems are part of the free energy benchmark suite:

S **solvation** – bromosporine solvation in water

B **binding** – absolute binding affinity of bromosporine to bromodomain

Simulation modes:

NI `noFreeEnergy_nstcalcenergy1` – no free energy, energy evaluations done every step

NC `noFreeEnergy_nstcalcenergy100` – no free energy, energy evaluations done every 100 steps

TI `ti_constLambda_nstcalcenergy1` – free energy is controlled with init-lambda, (delta-lambda set to 0.0 to allow for longer running benchmarks as well), energy evaluations done every step

TC `ti_constLambda_nstcalcenergy100` – free energy is controlled with init-lambda, (delta-lambda set to 0.0 to allow for longer running benchmarks as well), energy evaluations done every 100 steps

FI `fep_nstcalcenergy1` – free energy is controlled with init-lambda-state, coul-lambdas and vdw-lambdas vectors, all 20 lambda neighbors are calculated, energy evaluations done every step

FC `fep_nstcalcenergy100` – free energy is controlled with init-lambda-state, coul-lambdas and vdw-lambdas vectors, all 20 lambda neighbors are calculated, energy evaluations done every 100 steps

Free energy benchmark results

Tab. 9: Solvation free energy benchmarks (48 of 3,363 atoms are perturbed). Single-node performances for CUDA 8.0 and GROMACS 2018.

processor Intel	sockets × cores	clock (GHz)	GPUs GTX	SFI (ns/d)	SFC (ns/d)	STI (ns/d)	STC (ns/d)	SNI (ns/d)	SNC (ns/d)
E3-1240v6	1 × 4	3.7	–	6.1	62.9	59.4	70.3	148.1	208.4
E3-1240v6	1 × 4	3.7	1080	6.7	85.1	87.6	94.2	701	912.1
E3-1240v6	1 × 4	3.7	1080			PME on CPU:		645.7	799.9

Tab. 10: Binding free energy benchmarks (48 of 43,952 atoms are perturbed). Single-node performances for CUDA 8.0 and GROMACS 2018.

processor Intel	sockets × cores	clock (GHz)	GPUs GTX	BFI (ns/d)	BFC (ns/d)	BTI (ns/d)	BTC (ns/d)	BNI (ns/d)	BNC (ns/d)
E3-1240v6	1 × 4	3.7	–	3.2	9	7.1	9	9.9	13.3
E3-1240v6	1 × 4	3.7	1080	4.4	22.4	21.2	22.7	74.7	95.9
E3-1240v6	1 × 4	3.7	1080			PME on CPU:		58.4	73.5

STANDARD MD BENCHMARKS

benchRIB_cpu-cluster_1n

```
                :-) GROMACS - gmx mdrun, 2023.3 (-:

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under the terms of the GNU Lesser General Public License
as published by the Free Software Foundation; either version 2.1
of the License, or (at your option) any later version.

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Wennberg
       Maarten Wolf

                    Coordinated by the GROMACS project leaders:
                      Paul Bauer, Berk Hess, and Erik Lindahl

GROMACS:      gmx mdrun, version 2023.3
Executable:   /usr/local/gromacs/bin/gmx_mpi
Data prefix:  /usr/local/gromacs
Working dir:  /home/ubuntu
Process ID:   10162
Command line:
  gmx_mpi mdrun -v -s /mnt/shared/home/ubuntu/mpinat-gromacs/mpinat-
gromacs-standard-md-bench/benchRIB.tpr

GROMACS version:    2023.3
Precision:          mixed
Memory model:       64 bit
MPI library:        MPI
OpenMP support:     enabled (GMX_OPENMP_MAX_THREADS = 128)
GPU support:        disabled
SIMD instructions:  AVX2_256
```

```
CPU FFT library:    fftw-3.3.8-sse2-avx-avx2-avx2_128
GPU FFT library:    none
Multi-GPU FFT:      none
RDTSCP usage:       enabled
TNG support:        enabled
Hwloc support:      disabled
Tracing support:    disabled
C compiler:         /usr/bin/cc GNU 11.4.0
C compiler flags:   -fexcess-precision=fast -funroll-all-loops -mavx2 -
mfma -Wno-missing-field-initializers -O3 -DNDEBUG
C++ compiler:       /usr/bin/c++ GNU 11.4.0
C++ compiler flags: -fexcess-precision=fast -funroll-all-loops -mavx2 -
mfma -Wno-missing-field-initializers -Wno-cast-function-type-strict -
fopenmp -O3 -DNDEBUG
BLAS library:       Internal
LAPACK library:     Internal


Running on 1 node with total 6 cores, 6 processing units
Hardware detected on host cpu-5 (the node of MPI rank 0):
  CPU info:
    Vendor: AMD
    Brand:  AMD EPYC-Milan Processor
    Family: 25   Model: 1   Stepping: 1
    Features: aes amd apic avx avx2 clfsh cmov cx8 cx16 f16c fma lahf
misalignsse mmx msr pcid pclmuldq pdpe1gb popcnt pse rdrnd rdtscp sha
sse2 sse3 sse4a sse4.1 sse4.2 ssse3 tdt x2apic
  Hardware topology: Basic
    Packages, cores, and logical processors:
    [indices refer to OS logical processors]
      Package  0: [   0]
      Package  1: [   1]
      Package  2: [   2]
      Package  3: [   3]
      Package  4: [   4]
      Package  5: [   5]
    CPU limit set by OS: -1   Recommended max number of threads: 6


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
M. J. Abraham, T. Murtola, R. Schulz, S. P√°ll, J. C. Smith, B. Hess, E.
Lindahl
GROMACS: High performance molecular simulations through multi-level
parallelism from laptops to supercomputers
SoftwareX 1 (2015) pp. 19-25
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. P√°ll, M. J. Abraham, C. Kutzner, B. Hess, E. Lindahl
Tackling Exascale Software Challenges in Molecular Dynamics Simulations
with
GROMACS
In S. Markidis & E. Laure (Eds.), Solving Software Challenges for
Exascale 8759 (2015) pp. 3-27
-------- -------- --- Thank You --- -------- --------
```

```
++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. Pronk, S. P√°ll, R. Schulz, P. Larsson, P. Bjelkmar, R. Apostolov, M.
R.
Shirts, J. C. Smith, P. M. Kasson, D. van der Spoel, B. Hess, and E.
Lindahl
GROMACS 4.5: a high-throughput and highly parallel open source molecular
simulation toolkit
Bioinformatics 29 (2013) pp. 845-54
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
B. Hess and C. Kutzner and D. van der Spoel and E. Lindahl
GROMACS 4: Algorithms for highly efficient, load-balanced, and scalable
molecular simulation
J. Chem. Theory Comput. 4 (2008) pp. 435-447
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
D. van der Spoel, E. Lindahl, B. Hess, G. Groenhof, A. E. Mark and H. J.
C.
Berendsen
GROMACS: Fast, Flexible and Free
J. Comp. Chem. 26 (2005) pp. 1701-1719
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
E. Lindahl and B. Hess and D. van der Spoel
GROMACS 3.0: A package for molecular simulation and trajectory analysis
J. Mol. Mod. 7 (2001) pp. 306-317
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
H. J. C. Berendsen, D. van der Spoel and R. van Drunen
GROMACS: A message-passing parallel molecular dynamics implementation
Comp. Phys. Comm. 91 (1995) pp. 43-56
-------- -------- --- Thank You --- -------- --------


++++ PLEASE CITE THE DOI FOR THIS VERSION OF GROMACS ++++
https://doi.org/10.5281/zenodo.10017686
-------- -------- --- Thank You --- -------- --------


The number of OpenMP threads was set by environment variable
OMP_NUM_THREADS to 1

Input Parameters:
   integrator                     = md
   tinit                          = 0
   dt                             = 0.004
   nsteps                         = 10000
   init-step                      = 0
   simulation-part                = 1
   mts                            = false
```

```
comm-mode                       = Linear
nstcomm                         = 100
bd-fric                         = 0
ld-seed                         = 14771
emtol                           = 1e-05
emstep                          = 0.01
niter                           = 20
fcstep                          = 0
nstcgsteep                      = 1000
nbfgscorr                       = 10
rtpi                            = 0.05
nstxout                         = 0
nstvout                         = 0
nstfout                         = 0
nstlog                          = 0
nstcalcenergy                   = 100
nstenergy                       = 500
nstxout-compressed              = 0
compressed-x-precision          = 1000
cutoff-scheme                   = Verlet
nstlist                         = 25
pbc                             = xyz
periodic-molecules              = false
verlet-buffer-tolerance         = 0.005
rlist                           = 1.041
coulombtype                     = PME
coulomb-modifier                = Potential-shift
rcoulomb-switch                 = 0
rcoulomb                        = 1
epsilon-r                       = 1
epsilon-rf                      = inf
vdw-type                        = Cut-off
vdw-modifier                    = Potential-shift
rvdw-switch                     = 0
rvdw                            = 1
DispCorr                        = No
table-extension                 = 1
fourierspacing                  = 0.135
fourier-nx                      = 240
fourier-ny                      = 240
fourier-nz                      = 240
pme-order                       = 4
ewald-rtol                      = 1e-06
ewald-rtol-lj                   = 1e-06
lj-pme-comb-rule                = Geometric
ewald-geometry                  = 3d
epsilon-surface                 = 0
ensemble-temperature-setting    = constant
ensemble-temperature            = 300
tcoupl                          = V-rescale
nsttcouple                      = 25
nh-chain-length                 = 0
print-nose-hoover-chain-variables = false
pcoupl                          = Berendsen
pcoupltype                      = Isotropic
nstpcouple                      = 25
tau-p                           = 1
compressibility (3x3):
```

```
      compressibility[    0]={ 4.50000e-05,  0.00000e+00,  0.00000e+00}
      compressibility[    1]={ 0.00000e+00,  4.50000e-05,  0.00000e+00}
      compressibility[    2]={ 0.00000e+00,  0.00000e+00,  4.50000e-05}
   ref-p (3x3):
      ref-p[    0]={ 1.00000e+00,  0.00000e+00,  0.00000e+00}
      ref-p[    1]={ 0.00000e+00,  1.00000e+00,  0.00000e+00}
      ref-p[    2]={ 0.00000e+00,  0.00000e+00,  1.00000e+00}
   refcoord-scaling               = No
   posres-com (3):
      posres-com[0]= 0.00000e+00
      posres-com[1]= 0.00000e+00
      posres-com[2]= 0.00000e+00
   posres-comB (3):
      posres-comB[0]= 0.00000e+00
      posres-comB[1]= 0.00000e+00
      posres-comB[2]= 0.00000e+00
   QMMM                           = false
qm-opts:
   ngQM                           = 0
   constraint-algorithm           = Lincs
   continuation                   = false
   Shake-SOR                      = false
   shake-tol                      = 0.0001
   lincs-order                    = 6
   lincs-iter                     = 2
   lincs-warnangle                = 30
   nwall                          = 0
   wall-type                      = 9-3
   wall-r-linpot                  = -1
   wall-atomtype[0]               = -1
   wall-atomtype[1]               = -1
   wall-density[0]                = 0
   wall-density[1]                = 0
   wall-ewald-zfac                = 3
   pull                           = false
   awh                            = false
   rotation                       = false
   interactiveMD                  = false
   disre                          = No
   disre-weighting                = Equal
   disre-mixed                    = false
   dr-fc                          = 1000
   dr-tau                         = 0
   nstdisreout                    = 100
   orire-fc                       = 0
   orire-tau                      = 0
   nstorireout                    = 100
   free-energy                    = no
   cos-acceleration               = 0
   deform (3x3):
      deform[    0]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
      deform[    1]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
      deform[    2]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
   simulated-tempering            = false
   swapcoords                     = no
   userint1                       = 0
   userint2                       = 0
   userint3                       = 0
```

```
   userint4                       = 0
   userreal1                      = 0
   userreal2                      = 0
   userreal3                      = 0
   userreal4                      = 0
   applied-forces:
     electric-field:
grpopts:
   nrdf:      292326  3.76895e+06
   ref-t:         300         300
   tau-t:         0.1         0.1
annealing:          No          No
annealing-npoints:           0           0
   acc:               0           0           0
   nfreeze:           N           N           N
   energygrp-flags[  0]: 0


Changing rlist from 1.041 to 1 for non-bonded 4x4 atom kernels

Changing nstlist from 25 to 80, rlist from 1 to 1.124

Update groups can not be used for this system because an incompatible
virtual site type is used

Initializing Domain Decomposition on 6 ranks
Dynamic load balancing: auto
Minimum cell size due to atom displacement: 2.155 nm
Initial maximum distances in bonded interactions:
    two-body bonded interactions: 0.433 nm, LJ-14, atoms 176875 176884
  multi-body bonded interactions: 0.433 nm, Ryckaert-Bell., atoms 176875
176884
Minimum cell size due to bonded interactions: 0.476 nm
Maximum distance for 7 constraints, at 120 deg. angles, all-trans: 1.166
nm
Estimated maximum distance required for P-LINCS: 1.166 nm
Scaling the initial minimum size with 1/0.8 (option -dds) = 1.25
Using 0 separate PME ranks because: there are too few total ranks for
efficient splitting
Optimizing the DD grid for 6 cells with a minimum initial size of 2.694
nm
The maximum allowed number of cells is: X 9 Y 9 Z 8
Domain decomposition grid 6 x 1 x 1, separate PME ranks 0
PME domain decomposition: 6 x 1 x 1
Domain decomposition rank 0, coordinates 0 0 0

The initial number of communication pulses is: X 1
The initial domain decomposition cell size is: X 4.25 nm

The maximum allowed distance for atoms involved in interactions is:
                 non-bonded interactions           1.124 nm
(the following are initial values, they could change due to box
deformation)
            two-body bonded interactions  (-rdd)   1.124 nm
          multi-body bonded interactions  (-rdd)   1.124 nm
              virtual site constructions  (-rcon)  4.252 nm
  atoms separated by up to 7 constraints  (-rcon)  4.252 nm
```

```
When dynamic load balancing gets turned on, these settings will change
to:
The maximum number of communication pulses is: X 1
The minimum size for domain decomposition cells is 2.155 nm
The requested allowed shrink of DD cells (option -dds) is: 0.80
The allowed shrink of domain decomposition cells is: X 0.51
The maximum allowed distance for atoms involved in interactions is:
                 non-bonded interactions           1.124 nm
            two-body bonded interactions  (-rdd)   1.124 nm
          multi-body bonded interactions  (-rdd)   1.124 nm
              virtual site constructions  (-rcon)  2.155 nm
  atoms separated by up to 7 constraints  (-rcon)  2.155 nm

Using 6 MPI processes

Non-default thread affinity set, disabling internal thread affinity

Using 1 OpenMP thread per MPI process

System total charge: -0.000
Will do PME sum in reciprocal space for electrostatic interactions.

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
U. Essmann, L. Perera, M. L. Berkowitz, T. Darden, H. Lee and L. G.
Pedersen
A smooth particle mesh Ewald method
J. Chem. Phys. 103 (1995) pp. 8577-8592
-------- -------- --- Thank You --- -------- --------

Using a Gaussian width (1/beta) of 0.289108 nm for Ewald
Potential shift: LJ r^-12: -1.000e+00 r^-6: -1.000e+00, Ewald -1.000e-06
Initialized non-bonded Coulomb Ewald tables, spacing: 8.87e-04 size: 1129

Generated table with 1062 data points for 1-4 COUL.
Tabscale = 500 points/nm
Generated table with 1062 data points for 1-4 LJ6.
Tabscale = 500 points/nm
Generated table with 1062 data points for 1-4 LJ12.
Tabscale = 500 points/nm


Using SIMD 4x8 nonbonded short-range kernels

Using a dual 4x8 pair-list setup updated with dynamic pruning:
  outer list: updated every 80 steps, buffer 0.124 nm, rlist 1.124 nm
  inner list: updated every 30 steps, buffer 0.002 nm, rlist 1.002 nm
At tolerance 0.005 kJ/mol/ps per atom, equivalent classical 1x1 list
would be:
  outer list: updated every 80 steps, buffer 0.330 nm, rlist 1.330 nm
  inner list: updated every 30 steps, buffer 0.144 nm, rlist 1.144 nm

The non-bonded pair calculation algorithm tolerates a few missing pair
interactions close to the cut-off. This can lead to a systematic
overestimation of the pressure due to missing LJ interactions. The error
in the average pressure due to missing LJ interactions is at most 7.54
bar.
```

```
The pressure error can be controlled by setting the environment variable
GMX_VERLET_BUFFER_PRESSURE_TOLERANCE to the allowed error in units of
bar.

Using Lorentz-Berthelot Lennard-Jones combination rule
Removing pbc first time

Linking all bonded interactions to atoms
There are 98588 inter update-group virtual sites,
will perform an extra communication step for selected coordinates and
forces


Initializing Parallel LINear Constraint Solver

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
B. Hess
P-LINCS: A Parallel Linear Constraint Solver for molecular simulation
J. Chem. Theory Comput. 4 (2008) pp. 116-122
-------- -------- --- Thank You --- -------- --------

The number of constraints is 179952
There are constraints between atoms in different decomposition domains,
will communicate selected coordinates each lincs iteration
29316 constraints are involved in constraint triangles,
will apply an additional matrix expansion of order 6 for couplings
between constraints inside triangles

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. Miyamoto and P. A. Kollman
SETTLE: An Analytical Version of the SHAKE and RATTLE Algorithms for
Rigid
Water Models
J. Comp. Chem. 13 (1992) pp. 952-962
-------- -------- --- Thank You --- -------- --------


Intra-simulation communication will occur every 25 steps.

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
G. Bussi, D. Donadio and M. Parrinello
Canonical sampling through velocity rescaling
J. Chem. Phys. 126 (2007) pp. 014101
-------- -------- --- Thank You --- -------- --------

There are: 2037824 Atoms
There are: 98588 VSites
Atom distribution over 6 domains: av 356068 stddev 5247 min 348611 max
361668

Constraining the starting coordinates (step 0)

Constraining the coordinates at t0-dt (step 0)
Center of mass motion removal mode is Linear
We have the following groups for center of mass motion removal:
  0:  rest
RMS relative constraint deviation after constraining: 9.79e-06
Initial temperature: 302.726 K
```

```
Started mdrun on rank 0 Sat Jan 13 08:50:14 2024

           Step           Time
              0        0.00000

   Energies (kJ/mol)
  Connect Bonds          Angle    Proper Dih. Ryckaert-Bell.          LJ-
14
    0.00000e+00    3.47953e+05    1.20867e+04    7.60968e+05
2.87075e+05
     Coulomb-14        LJ (SR)   Coulomb (SR)   Coul. recip.
Potential
   -1.18824e+06    5.05955e+06   -4.35305e+07    3.60665e+05   -
3.78905e+07
    Kinetic En.   Total Energy  Conserved En.    Temperature Pressure
(bar)
    5.39060e+06   -3.24999e+07   -3.24896e+07    3.19279e+02   -
5.32617e+02
   Constr. rmsd
    9.62942e-06


DD  step 79 load imb.: force  8.4%

step 160 Turning on dynamic load balancing, because the performance loss
due to load imbalance is 4.2 %.
Writing checkpoint, step 2880 at Sat Jan 13 09:05:33 2024


Writing checkpoint, step 5680 at Sat Jan 13 09:20:24 2024


Writing checkpoint, step 8480 at Sat Jan 13 09:35:25 2024



DD  step 9999  vol min/aver 0.920  load imb.: force  4.3%
           Step           Time
          10000       40.00000

Writing checkpoint, step 10000 at Sat Jan 13 09:43:38 2024


   Energies (kJ/mol)
  Connect Bonds          Angle    Proper Dih. Ryckaert-Bell.          LJ-
14
    0.00000e+00    3.47697e+05    1.18373e+04    7.61276e+05
2.87082e+05
     Coulomb-14        LJ (SR)   Coulomb (SR)   Coul. recip.
Potential
   -1.18805e+06    5.16286e+06   -4.37264e+07    3.53883e+05   -
3.79899e+07
    Kinetic En.   Total Energy  Conserved En.    Temperature Pressure
(bar)
    5.06863e+06   -3.29212e+07   -3.25295e+07    3.00209e+02
1.72497e+01
   Constr. rmsd
```

```
    9.04413e-06


Energy conservation over simulation part #1 of length 40 ps, time 0 to 40
ps
  Conserved energy drift: -4.68e-04 kJ/mol/ps per atom


      <======  ###############  ==>
      <====  A V E R A G E S  ====>
      <==  ###############  ======>

      Statistics over 10001 steps using 101 frames

   Energies (kJ/mol)
  Connect Bonds          Angle    Proper Dih. Ryckaert-Bell.          LJ-
14
    0.00000e+00    3.47793e+05    1.19263e+04    7.61199e+05
2.87413e+05
     Coulomb-14        LJ (SR)   Coulomb (SR)   Coul. recip.
Potential
   -1.18730e+06    5.15997e+06   -4.37252e+07    3.52939e+05   -
3.79913e+07
    Kinetic En.   Total Energy  Conserved En.    Temperature Pressure
(bar)
    5.06782e+06   -3.29235e+07   -3.25092e+07    3.00161e+02   -
1.34673e+01
   Constr. rmsd
    0.00000e+00

          Box-X          Box-Y          Box-Z
    3.10288e+01    3.10288e+01    2.19407e+01

   Total Virial (kJ/mol)
    1.69704e+06   -2.40899e+03   -1.06758e+03
   -2.40745e+03    1.69773e+06   -2.09351e+02
   -1.16295e+03   -2.12509e+02    1.69911e+06

   Pressure (bar)
   -1.07882e+01    2.88854e+00    3.48047e-01
    2.88614e+00   -1.43253e+01    1.41306e+00
    4.97970e-01    1.41802e+00   -1.52884e+01

          T-mol      T-solvent
    3.00185e+02    3.00159e+02


     M E G A - F L O P S   A C C O U N T I N G

 NB=Group-cutoff nonbonded kernels    NxN=N-by-N cluster Verlet kernels
 RF=Reaction-Field  VdW=Van der Waals  QSTab=quadratic-spline table
 W3=SPC/TIP3p  W4=TIP4p (single or pairs)
 V&F=Potential and force  V=Potential only  F=Force only

 Computing:                                M-Number         M-Flops  %
Flops
-----------------------------------------------------------------------
----
```

```
 Pair Search distance check          128323.217362     1154908.956
0.1
 NxN Ewald Elec. + LJ [F]           7476227.546368   493431018.060
53.3
 NxN Ewald Elec. + LJ [V&F]           76268.739744     8160755.153
0.9
 NxN Ewald Elec. [F]                5668210.664448   345760850.531
37.4
 NxN Ewald Elec. [V&F]                57824.310080     4857242.047
0.5
 1,4 nonbonded interactions            6369.046841      573214.216
0.1
 Calc Weights                         64098.769236     2307555.692
0.2
 Spread Q Bspline                   1367440.410368     2734880.821
0.3
 Gather F Bspline                   1367440.410368     8204642.462
0.9
 3D-FFT                             6558947.569174    52471580.553
5.7
 Solve PME                              576.057600       36867.686
0.0
 Reset In Box                           269.187912         807.564
0.0
 CG-CoM                                 271.324324         813.973
0.0
 Angles                                4258.985856      715509.624
0.1
 Propers                                212.081206       48566.596
0.0
 RB-Dihedrals                          6469.816917     1598044.778
0.2
 Virial                                 856.809482       15422.571
0.0
 Stop-CM                                217.914024        2179.140
0.0
 P-Coupling                             856.701212        5140.207
0.0
 Calc-Ekin                             1713.402424       46261.865
0.0
 Lincs                                 2133.158012      127989.481
0.0
 Lincs-Mat                            58659.035540      234636.142
0.0
 Constraint-V                         23392.528955      210532.761
0.0
 Constraint-Vir                         852.335961       20456.063
0.0
 Settle                                6376.182605     2359187.564
0.3
 Virtual Site 3                          91.227450        3375.416
0.0
 Virtual Site 3fd                       193.227552       18356.617
0.0
 Virtual Site 3fad                      110.344416       19420.617
0.0
 Virtual Site 3out                      361.968796       31491.285
0.0
```

```
 Virtual Site 4fd                      100.036034       11003.964
0.0
 Virtual Site 4fdn                     170.062298       43195.824
0.0
-----------------------------------------------------------------------
----
 Total                                                925205908.230
100.0
-----------------------------------------------------------------------
----
```

D O M A I N D E C O M P O S I T I O N S T A T I S T I C S

```
 av. #atoms communicated per step for force:  2 x 569045.3
 av. #atoms communicated per step for vsites: 3 x 5144.3
 av. #atoms communicated per step for LINCS:  3 x 70429.8


Dynamic load balancing report:
 DLB was turned on during the run due to measured imbalance.
 Average load imbalance: 3.2%.
 The balanceable part of the MD step is 59%, load imbalance is computed
from this.
 Part of the total run time spent waiting due to load imbalance: 1.9%.
 Steps where the load balancing was limited by -rdd, -rcon and/or -dds: X
0 %
```

R E A L C Y C L E A N D T I M E A C C O U N T I N G

On 6 MPI ranks

```
 Activity:              Num   Num      Call    Wall time         Giga-
Cycles
                       Ranks Threads  Count      (s)         total sum
%
-----------------------------------------------------------------------
-------
 Domain decomp.            6    1        126      21.093        372.634
0.7
 DD comm. load             6    1        125       0.046          0.811
0.0
 DD comm. bounds           6    1        124       0.061          1.075
0.0
 Vsite constr.             6    1      10001      16.510        291.670
0.5
 Neighbor search           6    1        126      58.460       1032.797
1.8
 Comm. coord.              6    1       9875      10.906        192.668
0.3
 Force                     6    1      10001    1788.273      31592.717
55.7
 Wait + Comm. F            6    1      10001      12.604        222.678
0.4
 PME mesh                  6    1      10001    1069.069      18886.828
33.3
```

```
 NB X/F buffer ops.        6    1      29751      17.293        305.508
0.5
 Vsite spread              6    1      10402      18.447        325.895
0.6
 Write traj.               6    1          4       1.142         20.181
0.0
 Update                    6    1      10001      12.634        223.191
0.4
 Constraints               6    1      10003     176.833       3124.031
5.5
 Comm. energies            6    1        401       0.665         11.748
0.0
 Rest                                             4.385         77.474
0.1
-----------------------------------------------------------------------
-------
 Total                                         3208.421      56681.907
100.0
-----------------------------------------------------------------------
-------
 Breakdown of PME mesh activities
-----------------------------------------------------------------------
-------
 PME redist. X/F           6    1      20002     208.613       3685.489
6.5
 PME spread                6    1      10001     274.792       4854.635
8.6
 PME gather                6    1      10001     244.531       4320.035
7.6
 PME 3D-FFT                6    1      20002     252.648       4463.424
7.9
 PME 3D-FFT Comm.          6    1      20002      75.645       1336.395
2.4
 PME solve Elec            6    1      10001      12.741        225.091
0.4
-----------------------------------------------------------------------
-------

               Core t (s)   Wall t (s)        (%)
       Time:    19250.521     3208.421      600.0
                         53:28
                 (ns/day)    (hour/ns)
Performance:        1.077       22.278
Finished mdrun on rank 0 Sat Jan 13 09:43:42 2024
```

benchRIB_cpu-cluster_3n

```
                    :-) GROMACS - gmx mdrun, 2023.3 (-:

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   Christoph Junghans         Prashanth Kanduri          Sebastian Keller
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                    Coordinated by the GROMACS project leaders:
                      Paul Bauer, Berk Hess, and Erik Lindahl

GROMACS:      gmx mdrun, version 2023.3
Executable:   /usr/local/gromacs/bin/gmx_mpi
Data prefix:  /usr/local/gromacs
Working dir:  /home/ubuntu
Process ID:   4508
Command line:
  gmx_mpi mdrun -v -s /mnt/shared/home/ubuntu/mpinat-gromacs/mpinat-
gromacs-standard-md-bench/benchRIB.tpr

GROMACS version:    2023.3
Precision:          mixed
Memory model:       64 bit
MPI library:        MPI
OpenMP support:     enabled (GMX_OPENMP_MAX_THREADS = 128)
GPU support:        disabled
SIMD instructions:  AVX2_256
```

```
CPU FFT library:    fftw-3.3.8-sse2-avx-avx2-avx2_128
GPU FFT library:    none
Multi-GPU FFT:      none
RDTSCP usage:       enabled
TNG support:        enabled
Hwloc support:      disabled
Tracing support:    disabled
C compiler:         /usr/bin/cc GNU 11.4.0
C compiler flags:   -fexcess-precision=fast -funroll-all-loops -mavx2 -
mfma -Wno-missing-field-initializers -O3 -DNDEBUG
C++ compiler:       /usr/bin/c++ GNU 11.4.0
C++ compiler flags: -fexcess-precision=fast -funroll-all-loops -mavx2 -
mfma -Wno-missing-field-initializers -Wno-cast-function-type-strict -
fopenmp -O3 -DNDEBUG
BLAS library:
LAPACK library:


Running on 3 nodes with total 18 cores, 18 processing units
  Cores per node:            6
  Logical processing units per node:    6
  OS CPU Limit / recommended threads to start per node:    6
Hardware detected on host cpu-2 (the node of MPI rank 0):
  CPU info:
    Vendor: AMD
    Brand:  AMD EPYC-Milan Processor
    Family: 25   Model: 1   Stepping: 1
    Features: aes amd apic avx avx2 clfsh cmov cx8 cx16 f16c fma lahf
misalignsse mmx msr pcid pclmuldq pdpe1gb popcnt pse rdrnd rdtscp sha
sse2 sse3 sse4a sse4.1 sse4.2 ssse3 tdt x2apic
  Hardware topology: Basic
    Packages, cores, and logical processors:
    [indices refer to OS logical processors]
      Package  0: [   0]
      Package  1: [   1]
      Package  2: [   2]
      Package  3: [   3]
      Package  4: [   4]
      Package  5: [   5]
    CPU limit set by OS: -1   Recommended max number of threads: 6


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
M. J. Abraham, T. Murtola, R. Schulz, S. P√°ll, J. C. Smith, B. Hess, E.
Lindahl
GROMACS: High performance molecular simulations through multi-level
parallelism from laptops to supercomputers
SoftwareX 1 (2015) pp. 19-25
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. P√°ll, M. J. Abraham, C. Kutzner, B. Hess, E. Lindahl
Tackling Exascale Software Challenges in Molecular Dynamics Simulations
with
GROMACS
In S. Markidis & E. Laure (Eds.), Solving Software Challenges for
Exascale 8759 (2015) pp. 3-27
```

```
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. Pronk, S. P√°ll, R. Schulz, P. Larsson, P. Bjelkmar, R. Apostolov, M.
R.
Shirts, J. C. Smith, P. M. Kasson, D. van der Spoel, B. Hess, and E.
Lindahl
GROMACS 4.5: a high-throughput and highly parallel open source molecular
simulation toolkit
Bioinformatics 29 (2013) pp. 845-54
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
B. Hess and C. Kutzner and D. van der Spoel and E. Lindahl
GROMACS 4: Algorithms for highly efficient, load-balanced, and scalable
molecular simulation
J. Chem. Theory Comput. 4 (2008) pp. 435-447
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
D. van der Spoel, E. Lindahl, B. Hess, G. Groenhof, A. E. Mark and H. J.
C.
Berendsen
GROMACS: Fast, Flexible and Free
J. Comp. Chem. 26 (2005) pp. 1701-1719
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
E. Lindahl and B. Hess and D. van der Spoel
GROMACS 3.0: A package for molecular simulation and trajectory analysis
J. Mol. Mod. 7 (2001) pp. 306-317
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
H. J. C. Berendsen, D. van der Spoel and R. van Drunen
GROMACS: A message-passing parallel molecular dynamics implementation
Comp. Phys. Comm. 91 (1995) pp. 43-56
-------- -------- --- Thank You --- -------- --------


++++ PLEASE CITE THE DOI FOR THIS VERSION OF GROMACS ++++
https://doi.org/10.5281/zenodo.10017686
-------- -------- --- Thank You --- -------- --------


The number of OpenMP threads was set by environment variable
OMP_NUM_THREADS to 1

Input Parameters:
   integrator                   = md
   tinit                        = 0
   dt                           = 0.004
   nsteps                       = 10000
```

```
init-step                       = 0
simulation-part                 = 1
mts                             = false
comm-mode                       = Linear
nstcomm                         = 100
bd-fric                         = 0
ld-seed                         = 14771
emtol                           = 1e-05
emstep                          = 0.01
niter                           = 20
fcstep                          = 0
nstcgsteep                      = 1000
nbfgscorr                       = 10
rtpi                            = 0.05
nstxout                         = 0
nstvout                         = 0
nstfout                         = 0
nstlog                          = 0
nstcalcenergy                   = 100
nstenergy                       = 500
nstxout-compressed              = 0
compressed-x-precision          = 1000
cutoff-scheme                   = Verlet
nstlist                         = 25
pbc                             = xyz
periodic-molecules              = false
verlet-buffer-tolerance         = 0.005
rlist                           = 1.041
coulombtype                     = PME
coulomb-modifier                = Potential-shift
rcoulomb-switch                 = 0
rcoulomb                        = 1
epsilon-r                       = 1
epsilon-rf                      = inf
vdw-type                        = Cut-off
vdw-modifier                    = Potential-shift
rvdw-switch                     = 0
rvdw                            = 1
DispCorr                        = No
table-extension                 = 1
fourierspacing                  = 0.135
fourier-nx                      = 240
fourier-ny                      = 240
fourier-nz                      = 240
pme-order                       = 4
ewald-rtol                      = 1e-06
ewald-rtol-lj                   = 1e-06
lj-pme-comb-rule                = Geometric
ewald-geometry                  = 3d
epsilon-surface                 = 0
ensemble-temperature-setting    = constant
ensemble-temperature            = 300
tcoupl                          = V-rescale
nsttcouple                      = 25
nh-chain-length                 = 0
print-nose-hoover-chain-variables = false
pcoupl                          = Berendsen
pcoupltype                      = Isotropic
```

```
   nstpcouple                     = 25
   tau-p                          = 1
   compressibility (3x3):
      compressibility[    0]={ 4.50000e-05,  0.00000e+00,  0.00000e+00}
      compressibility[    1]={ 0.00000e+00,  4.50000e-05,  0.00000e+00}
      compressibility[    2]={ 0.00000e+00,  0.00000e+00,  4.50000e-05}
   ref-p (3x3):
      ref-p[    0]={ 1.00000e+00,  0.00000e+00,  0.00000e+00}
      ref-p[    1]={ 0.00000e+00,  1.00000e+00,  0.00000e+00}
      ref-p[    2]={ 0.00000e+00,  0.00000e+00,  1.00000e+00}
   refcoord-scaling               = No
   posres-com (3):
      posres-com[0]= 0.00000e+00
      posres-com[1]= 0.00000e+00
      posres-com[2]= 0.00000e+00
   posres-comB (3):
      posres-comB[0]= 0.00000e+00
      posres-comB[1]= 0.00000e+00
      posres-comB[2]= 0.00000e+00
   QMMM                           = false
qm-opts:
   ngQM                           = 0
   constraint-algorithm           = Lincs
   continuation                   = false
   Shake-SOR                      = false
   shake-tol                      = 0.0001
   lincs-order                    = 6
   lincs-iter                     = 2
   lincs-warnangle                = 30
   nwall                          = 0
   wall-type                      = 9-3
   wall-r-linpot                  = -1
   wall-atomtype[0]               = -1
   wall-atomtype[1]               = -1
   wall-density[0]                = 0
   wall-density[1]                = 0
   wall-ewald-zfac                = 3
   pull                           = false
   awh                            = false
   rotation                       = false
   interactiveMD                  = false
   disre                          = No
   disre-weighting                = Equal
   disre-mixed                    = false
   dr-fc                          = 1000
   dr-tau                         = 0
   nstdisreout                    = 100
   orire-fc                       = 0
   orire-tau                      = 0
   nstorireout                    = 100
   free-energy                    = no
   cos-acceleration               = 0
   deform (3x3):
      deform[    0]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
      deform[    1]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
      deform[    2]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
   simulated-tempering            = false
   swapcoords                     = no
```

```
   userint1                       = 0
   userint2                       = 0
   userint3                       = 0
   userint4                       = 0
   userreal1                      = 0
   userreal2                      = 0
   userreal3                      = 0
   userreal4                      = 0
   applied-forces:
     electric-field:
grpopts:
   nrdf:      292326  3.76895e+06
   ref-t:         300         300
   tau-t:         0.1         0.1
annealing:          No          No
annealing-npoints:           0           0
   acc:               0           0           0
   nfreeze:           N           N           N
   energygrp-flags[  0]: 0


Changing rlist from 1.041 to 1 for non-bonded 4x4 atom kernels

Changing nstlist from 25 to 80, rlist from 1 to 1.124

Update groups can not be used for this system because an incompatible
virtual site type is used

Initializing Domain Decomposition on 18 ranks
Dynamic load balancing: auto
Minimum cell size due to atom displacement: 2.155 nm
Initial maximum distances in bonded interactions:
    two-body bonded interactions: 0.433 nm, LJ-14, atoms 176875 176884
  multi-body bonded interactions: 0.433 nm, Ryckaert-Bell., atoms 176875
176884
Minimum cell size due to bonded interactions: 0.476 nm
Maximum distance for 7 constraints, at 120 deg. angles, all-trans: 1.166
nm
Estimated maximum distance required for P-LINCS: 1.166 nm
Scaling the initial minimum size with 1/0.8 (option -dds) = 1.25
Using 0 separate PME ranks because: there are too few total ranks for
efficient splitting
Optimizing the DD grid for 18 cells with a minimum initial size of 2.694
nm
The maximum allowed number of cells is: X 9 Y 9 Z 8
Domain decomposition grid 6 x 3 x 1, separate PME ranks 0
PME domain decomposition: 6 x 3 x 1
Domain decomposition rank 0, coordinates 0 0 0

The initial number of communication pulses is: X 1 Y 1
The initial domain decomposition cell size is: X 4.25 nm Y 8.50 nm

The maximum allowed distance for atoms involved in interactions is:
                 non-bonded interactions           1.124 nm
(the following are initial values, they could change due to box
deformation)
            two-body bonded interactions  (-rdd)   1.124 nm
          multi-body bonded interactions  (-rdd)   1.124 nm
```

```
              virtual site constructions  (-rcon)  4.252 nm
  atoms separated by up to 7 constraints  (-rcon)  4.252 nm

When dynamic load balancing gets turned on, these settings will change
to:
The maximum number of communication pulses is: X 1 Y 1
The minimum size for domain decomposition cells is 2.155 nm
The requested allowed shrink of DD cells (option -dds) is: 0.80
The allowed shrink of domain decomposition cells is: X 0.51 Y 0.25
The maximum allowed distance for atoms involved in interactions is:
                 non-bonded interactions           1.124 nm
            two-body bonded interactions  (-rdd)   1.124 nm
          multi-body bonded interactions  (-rdd)   1.124 nm
              virtual site constructions  (-rcon)  2.155 nm
  atoms separated by up to 7 constraints  (-rcon)  2.155 nm
Using two step summing over 3 groups of on average 6.0 ranks


Using 18 MPI processes

Non-default thread affinity set, disabling internal thread affinity

Using 1 OpenMP thread per MPI process

System total charge: -0.000
Will do PME sum in reciprocal space for electrostatic interactions.

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
U. Essmann, L. Perera, M. L. Berkowitz, T. Darden, H. Lee and L. G.
Pedersen
A smooth particle mesh Ewald method
J. Chem. Phys. 103 (1995) pp. 8577-8592
-------- -------- --- Thank You --- -------- --------

Using a Gaussian width (1/beta) of 0.289108 nm for Ewald
Potential shift: LJ r^-12: -1.000e+00 r^-6: -1.000e+00, Ewald -1.000e-06
Initialized non-bonded Coulomb Ewald tables, spacing: 8.87e-04 size: 1129

Generated table with 1062 data points for 1-4 COUL.
Tabscale = 500 points/nm
Generated table with 1062 data points for 1-4 LJ6.
Tabscale = 500 points/nm
Generated table with 1062 data points for 1-4 LJ12.
Tabscale = 500 points/nm


Using SIMD 4x8 nonbonded short-range kernels

Using a dual 4x8 pair-list setup updated with dynamic pruning:
  outer list: updated every 80 steps, buffer 0.124 nm, rlist 1.124 nm
  inner list: updated every 30 steps, buffer 0.002 nm, rlist 1.002 nm
At tolerance 0.005 kJ/mol/ps per atom, equivalent classical 1x1 list
would be:
  outer list: updated every 80 steps, buffer 0.330 nm, rlist 1.330 nm
  inner list: updated every 30 steps, buffer 0.144 nm, rlist 1.144 nm

The non-bonded pair calculation algorithm tolerates a few missing pair
interactions close to the cut-off. This can lead to a systematic
```

```
overestimation of the pressure due to missing LJ interactions. The error
in the average pressure due to missing LJ interactions is at most 7.54
bar.
The pressure error can be controlled by setting the environment variable
GMX_VERLET_BUFFER_PRESSURE_TOLERANCE to the allowed error in units of
bar.

Using Lorentz-Berthelot Lennard-Jones combination rule
Removing pbc first time

Linking all bonded interactions to atoms
There are 98588 inter update-group virtual sites,
will perform an extra communication step for selected coordinates and
forces


Initializing Parallel LINear Constraint Solver

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
B. Hess
P-LINCS: A Parallel Linear Constraint Solver for molecular simulation
J. Chem. Theory Comput. 4 (2008) pp. 116-122
-------- -------- --- Thank You --- -------- --------

The number of constraints is 179952
There are constraints between atoms in different decomposition domains,
will communicate selected coordinates each lincs iteration
29316 constraints are involved in constraint triangles,
will apply an additional matrix expansion of order 6 for couplings
between constraints inside triangles

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. Miyamoto and P. A. Kollman
SETTLE: An Analytical Version of the SHAKE and RATTLE Algorithms for
Rigid
Water Models
J. Comp. Chem. 13 (1992) pp. 952-962
-------- -------- --- Thank You --- -------- --------


Intra-simulation communication will occur every 25 steps.

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
G. Bussi, D. Donadio and M. Parrinello
Canonical sampling through velocity rescaling
J. Chem. Phys. 126 (2007) pp. 014101
-------- -------- --- Thank You --- -------- --------

There are: 2037824 Atoms
There are: 98588 VSites
Atom distribution over 18 domains: av 118689 stddev 2667 min 115469 max
123890

Constraining the starting coordinates (step 0)

Constraining the coordinates at t0-dt (step 0)
Center of mass motion removal mode is Linear
We have the following groups for center of mass motion removal:
```

```
  0:  rest
RMS relative constraint deviation after constraining: 1.01e-05
Initial temperature: 302.747 K

Started mdrun on rank 0 Fri Jan 12 00:02:05 2024

           Step           Time
              0        0.00000

   Energies (kJ/mol)
  Connect Bonds          Angle    Proper Dih. Ryckaert-Bell.          LJ-
14
    0.00000e+00    3.47960e+05    1.20867e+04    7.60989e+05
2.87074e+05
     Coulomb-14        LJ (SR)   Coulomb (SR)   Coul. recip.
Potential
   -1.18825e+06    5.05954e+06   -4.35900e+07    3.60933e+05   -
3.79497e+07
    Kinetic En.   Total Energy  Conserved En.    Temperature Pressure
(bar)
    5.39098e+06   -3.25587e+07   -3.25484e+07    3.19301e+02   -
5.32615e+02
   Constr. rmsd
    9.95022e-06


DD  step 79 load imb.: force 11.3%

step 160 Turning on dynamic load balancing, because the performance loss
due to load imbalance is 4.9 %.
step 1600 Turning off dynamic load balancing, because it is degrading
performance.
Atom distribution over 18 domains: av 118689 stddev 2114 min 116371 max
122762
Writing checkpoint, step 4080 at Fri Jan 12 00:17:13 2024


step 8000 Turning on dynamic load balancing, because the performance loss
due to load imbalance is 11.3 %.
Writing checkpoint, step 8080 at Fri Jan 12 00:32:29 2024



DD  step 9999  vol min/aver 0.851  load imb.: force 22.5%
           Step           Time
          10000       40.00000

Writing checkpoint, step 10000 at Fri Jan 12 00:39:58 2024


   Energies (kJ/mol)
  Connect Bonds          Angle    Proper Dih. Ryckaert-Bell.          LJ-
14
    0.00000e+00    3.48927e+05    1.18221e+04    7.61099e+05
2.87777e+05
     Coulomb-14        LJ (SR)   Coulomb (SR)   Coul. recip.
Potential
```

```
   -1.18669e+06    5.16683e+06   -4.38011e+07    3.53096e+05   -
3.80583e+07
    Kinetic En.   Total Energy  Conserved En.    Temperature Pressure
(bar)
    5.07111e+06   -3.29872e+07   -3.25894e+07    3.00356e+02
8.74662e+00
   Constr. rmsd
    9.42370e-06


Energy conservation over simulation part #1 of length 40 ps, time 0 to 40
ps
  Conserved energy drift: -4.80e-04 kJ/mol/ps per atom


      <======  ###############  ==>
      <====  A V E R A G E S  ====>
      <==  ###############  ======>

      Statistics over 10001 steps using 101 frames

   Energies (kJ/mol)
  Connect Bonds          Angle    Proper Dih. Ryckaert-Bell.          LJ-
14
    0.00000e+00    3.47884e+05    1.19011e+04    7.60921e+05
2.87448e+05
     Coulomb-14        LJ (SR)   Coulomb (SR)   Coul. recip.
Potential
   -1.18742e+06    5.16113e+06   -4.37869e+07    3.53198e+05   -
3.80518e+07
    Kinetic En.   Total Energy  Conserved En.    Temperature Pressure
(bar)
    5.06779e+06   -3.29840e+07   -3.25690e+07    3.00159e+02   -
1.34840e+01
   Constr. rmsd
    0.00000e+00

          Box-X          Box-Y          Box-Z
    3.10298e+01    3.10298e+01    2.19414e+01

   Total Virial (kJ/mol)
    1.69810e+06   -1.16324e+03   -3.02855e+03
   -1.16272e+03    1.69664e+06   -5.41878e+02
   -3.02179e+03   -5.38756e+02    1.69914e+06

   Pressure (bar)
   -1.25612e+01    9.22170e-01    2.82063e+00
    9.21359e-01   -1.27624e+01    1.62809e+00
    2.81000e+00    1.62317e+00   -1.51283e+01

          T-mol      T-solvent
    3.00102e+02    3.00164e+02


     M E G A - F L O P S   A C C O U N T I N G

 NB=Group-cutoff nonbonded kernels    NxN=N-by-N cluster Verlet kernels
 RF=Reaction-Field  VdW=Van der Waals  QSTab=quadratic-spline table
```

```
 W3=SPC/TIP3p  W4=TIP4p (single or pairs)
 V&F=Potential and force  V=Potential only  F=Force only

 Computing:                                M-Number         M-Flops  %
Flops
-----------------------------------------------------------------------
----
 Pair Search distance check          128541.629970     1156874.670
0.1
 NxN Ewald Elec. + LJ [F]           7581751.083888   500395571.537
53.3
 NxN Ewald Elec. + LJ [V&F]           77345.195856     8275935.957
0.9
 NxN Ewald Elec. [F]                5762429.404752   351508193.690
37.5
 NxN Ewald Elec. [V&F]                58783.583056     4937820.977
0.5
 1,4 nonbonded interactions            6369.046841      573214.216
0.1
 Calc Weights                         64098.769236     2307555.692
0.2
 Spread Q Bspline                   1367440.410368     2734880.821
0.3
 Gather F Bspline                   1367440.410368     8204642.462
0.9
 3D-FFT                             6558947.569174    52471580.553
5.6
 Solve PME                             1728.172800      110603.059
0.0
 Reset In Box                           267.051500         801.154
0.0
 CG-CoM                                 271.324324         813.973
0.0
 Angles                                4258.985856      715509.624
0.1
 Propers                                212.081206       48566.596
0.0
 RB-Dihedrals                          6469.816917     1598044.778
0.2
 Virial                                 857.026022       15426.468
0.0
 Stop-CM                                217.914024        2179.140
0.0
 P-Coupling                             856.701212        5140.207
0.0
 Calc-Ekin                             1713.402424       46261.865
0.0
 Lincs                                 2286.652635      137199.158
0.0
 Lincs-Mat                            62752.373360      251009.493
0.0
 Constraint-V                         23902.673041      215124.057
0.0
 Constraint-Vir                         866.639511       20799.348
0.0
 Settle                                6443.918089     2384249.693
0.3
```

```
 Virtual Site 3                          91.893851        3400.072
0.0
 Virtual Site 3fd                       193.227552       18356.617
0.0
 Virtual Site 3fad                      110.344416       19420.617
0.0
 Virtual Site 3out                      361.968796       31491.285
0.0
 Virtual Site 4fd                       100.036034       11003.964
0.0
 Virtual Site 4fdn                      170.062298       43195.824
0.0
-----------------------------------------------------------------------
----
 Total                                                938244867.570
100.0
-----------------------------------------------------------------------
----


    D O M A I N   D E C O M P O S I T I O N   S T A T I S T I C S

 av. #atoms communicated per step for force:  2 x 957617.7
 av. #atoms communicated per step for vsites: 3 x 7585.9
 av. #atoms communicated per step for LINCS:  3 x 106802.1


Dynamic load balancing report:
 DLB was turned on during the run due to measured imbalance.
 Average load imbalance: 27.3%.
 The balanceable part of the MD step is 44%, load imbalance is computed
from this.
 Part of the total run time spent waiting due to load imbalance: 11.9%.
 Steps where the load balancing was limited by -rdd, -rcon and/or -dds: X
0 % Y 0 %

NOTE: 11.9 % of the available CPU time was lost due to load imbalance
      in the domain decomposition.
      You can consider manually changing the decomposition (option -dd);
      e.g. by using fewer domains along the box dimension in which there
is
      considerable inhomogeneity in the simulated system.

      R E A L   C Y C L E   A N D   T I M E   A C C O U N T I N G

On 18 MPI ranks

 Activity:              Num   Num      Call    Wall time         Giga-
Cycles
                       Ranks Threads  Count      (s)         total sum
%
-----------------------------------------------------------------------
-------
 Domain decomp.           18    1        126      15.798        837.275
0.7
 DD comm. load            18    1         61       0.019          1.010
0.0
```

```
 DD comm. bounds          18     1          44       0.054          2.855
0.0
 Vsite constr.            18     1       10001      19.712       1044.729
0.9
 Neighbor search          18     1         126      28.307       1500.254
1.2
 Comm. coord.             18     1        9875      19.171       1016.073
0.8
 Force                    18     1       10001     927.012      49131.613
40.7
 Wait + Comm. F           18     1       10001      16.329        865.421
0.7
 PME mesh                 18     1       10001    1096.230      58100.194
48.1
 NB X/F buffer ops.       18     1       29751       9.409        498.674
0.4
 Vsite spread             18     1       10402      17.749        940.676
0.8
 Write traj.              18     1           3       0.620         32.879
0.0
 Update                   18     1       10001       5.663        300.152
0.2
 Constraints              18     1       10003     119.699       6344.030
5.3
 Comm. energies           18     1         401       1.076         57.003
0.0
 Rest                                                2.050        108.630
0.1
-----------------------------------------------------------------------------
-------
 Total                                           2278.896     120781.469
100.0
-----------------------------------------------------------------------------
-------
 Breakdown of PME mesh activities
-----------------------------------------------------------------------------
-------
 PME redist. X/F          18     1       20002     387.416      20533.021
17.0
 PME spread               18     1       10001     142.923       7574.907
6.3
 PME gather               18     1       10001     113.778       6030.254
5.0
 PME 3D-FFT               18     1       20002     123.558       6548.586
5.4
 PME 3D-FFT Comm.         18     1       40004     321.755      17053.018
14.1
 PME solve Elec           18     1       10001       6.684        354.226
0.3
-----------------------------------------------------------------------------
-------

               Core t (s)   Wall t (s)        (%)
       Time:    41020.113     2278.896     1800.0
                         37:58
                 (ns/day)    (hour/ns)
Performance:        1.517       15.824
Finished mdrun on rank 0 Fri Jan 12 00:40:04 2024
```

benchRIB_cpu-cluster_10n

```
                :-) GROMACS - gmx mdrun, 2023.3 (-:

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                    Coordinated by the GROMACS project leaders:
                      Paul Bauer, Berk Hess, and Erik Lindahl

GROMACS:      gmx mdrun, version 2023.3
Executable:   /usr/local/gromacs/bin/gmx_mpi
Data prefix:  /usr/local/gromacs
Working dir:  /home/ubuntu
Process ID:   7861
Command line:
  gmx_mpi mdrun -v -s /mnt/shared/home/ubuntu/mpinat-gromacs/mpinat-
gromacs-standard-md-bench/benchRIB.tpr

GROMACS version:    2023.3
Precision:          mixed
Memory model:       64 bit
MPI library:        MPI
OpenMP support:     enabled (GMX_OPENMP_MAX_THREADS = 128)
GPU support:        disabled
SIMD instructions:  AVX2_256
```

```
CPU FFT library:    fftw-3.3.8-sse2-avx-avx2-avx2_128
GPU FFT library:    none
Multi-GPU FFT:      none
RDTSCP usage:       enabled
TNG support:        enabled
Hwloc support:      disabled
Tracing support:    disabled
C compiler:         /usr/bin/cc GNU 11.4.0
C compiler flags:   -fexcess-precision=fast -funroll-all-loops -mavx2 -
mfma -Wno-missing-field-initializers -O3 -DNDEBUG
C++ compiler:       /usr/bin/c++ GNU 11.4.0
C++ compiler flags: -fexcess-precision=fast -funroll-all-loops -mavx2 -
mfma -Wno-missing-field-initializers -Wno-cast-function-type-strict -
fopenmp -O3 -DNDEBUG
BLAS library:       Internal
LAPACK library:     Internal


Running on 10 nodes with total 60 cores, 60 processing units
  Cores per node:            6
  Logical processing units per node:    6
  OS CPU Limit / recommended threads to start per node:    6
Hardware detected on host cpu-1 (the node of MPI rank 0):
  CPU info:
    Vendor: AMD
    Brand:  AMD EPYC-Milan Processor
    Family: 25   Model: 1   Stepping: 1
    Features: aes amd apic avx avx2 clfsh cmov cx8 cx16 f16c fma lahf
misalignsse mmx msr pcid pclmuldq pdpe1gb popcnt pse rdrnd rdtscp sha
sse2 sse3 sse4a sse4.1 sse4.2 ssse3 tdt x2apic
  Hardware topology: Basic
    Packages, cores, and logical processors:
    [indices refer to OS logical processors]
      Package  0: [   0]
      Package  1: [   1]
      Package  2: [   2]
      Package  3: [   3]
      Package  4: [   4]
      Package  5: [   5]
    CPU limit set by OS: -1   Recommended max number of threads: 6


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
M. J. Abraham, T. Murtola, R. Schulz, S. P√°ll, J. C. Smith, B. Hess, E.
Lindahl
GROMACS: High performance molecular simulations through multi-level
parallelism from laptops to supercomputers
SoftwareX 1 (2015) pp. 19-25
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. P√°ll, M. J. Abraham, C. Kutzner, B. Hess, E. Lindahl
Tackling Exascale Software Challenges in Molecular Dynamics Simulations
with
GROMACS
In S. Markidis & E. Laure (Eds.), Solving Software Challenges for
Exascale 8759 (2015) pp. 3-27
```

```
-------- -------- --- Thank You --- -------- --------


+++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. Pronk, S. P√°ll, R. Schulz, P. Larsson, P. Bjelkmar, R. Apostolov, M.
R.
Shirts, J. C. Smith, P. M. Kasson, D. van der Spoel, B. Hess, and E.
Lindahl
GROMACS 4.5: a high-throughput and highly parallel open source molecular
simulation toolkit
Bioinformatics 29 (2013) pp. 845-54
-------- -------- --- Thank You --- -------- --------


+++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
B. Hess and C. Kutzner and D. van der Spoel and E. Lindahl
GROMACS 4: Algorithms for highly efficient, load-balanced, and scalable
molecular simulation
J. Chem. Theory Comput. 4 (2008) pp. 435-447
-------- -------- --- Thank You --- -------- --------


+++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
D. van der Spoel, E. Lindahl, B. Hess, G. Groenhof, A. E. Mark and H. J.
C.
Berendsen
GROMACS: Fast, Flexible and Free
J. Comp. Chem. 26 (2005) pp. 1701-1719
-------- -------- --- Thank You --- -------- --------


+++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
E. Lindahl and B. Hess and D. van der Spoel
GROMACS 3.0: A package for molecular simulation and trajectory analysis
J. Mol. Mod. 7 (2001) pp. 306-317
-------- -------- --- Thank You --- -------- --------


+++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
H. J. C. Berendsen, D. van der Spoel and R. van Drunen
GROMACS: A message-passing parallel molecular dynamics implementation
Comp. Phys. Comm. 91 (1995) pp. 43-56
-------- -------- --- Thank You --- -------- --------


+++++ PLEASE CITE THE DOI FOR THIS VERSION OF GROMACS ++++
https://doi.org/10.5281/zenodo.10017686
-------- -------- --- Thank You --- -------- --------


The number of OpenMP threads was set by environment variable
OMP_NUM_THREADS to 1

Input Parameters:
   integrator                     = md
   tinit                          = 0
   dt                             = 0.004
   nsteps                         = 10000
```

```
init-step                      = 0
simulation-part                = 1
mts                            = false
comm-mode                      = Linear
nstcomm                        = 100
bd-fric                        = 0
ld-seed                        = 14771
emtol                          = 1e-05
emstep                         = 0.01
niter                          = 20
fcstep                         = 0
nstcgsteep                     = 1000
nbfgscorr                      = 10
rtpi                           = 0.05
nstxout                        = 0
nstvout                        = 0
nstfout                        = 0
nstlog                         = 0
nstcalcenergy                  = 100
nstenergy                      = 500
nstxout-compressed             = 0
compressed-x-precision         = 1000
cutoff-scheme                  = Verlet
nstlist                        = 25
pbc                            = xyz
periodic-molecules             = false
verlet-buffer-tolerance        = 0.005
rlist                          = 1.041
coulombtype                    = PME
coulomb-modifier               = Potential-shift
rcoulomb-switch                = 0
rcoulomb                       = 1
epsilon-r                      = 1
epsilon-rf                     = inf
vdw-type                       = Cut-off
vdw-modifier                   = Potential-shift
rvdw-switch                    = 0
rvdw                           = 1
DispCorr                       = No
table-extension                = 1
fourierspacing                 = 0.135
fourier-nx                     = 240
fourier-ny                     = 240
fourier-nz                     = 240
pme-order                      = 4
ewald-rtol                     = 1e-06
ewald-rtol-lj                  = 1e-06
lj-pme-comb-rule               = Geometric
ewald-geometry                 = 3d
epsilon-surface                = 0
ensemble-temperature-setting   = constant
ensemble-temperature           = 300
tcoupl                         = V-rescale
nsttcouple                     = 25
nh-chain-length                = 0
print-nose-hoover-chain-variables = false
pcoupl                         = Berendsen
pcoupltype                     = Isotropic
```

```
   nstpcouple                     = 25
   tau-p                          = 1
   compressibility (3x3):
      compressibility[    0]={ 4.50000e-05,  0.00000e+00,  0.00000e+00}
      compressibility[    1]={ 0.00000e+00,  4.50000e-05,  0.00000e+00}
      compressibility[    2]={ 0.00000e+00,  0.00000e+00,  4.50000e-05}
   ref-p (3x3):
      ref-p[    0]={ 1.00000e+00,  0.00000e+00,  0.00000e+00}
      ref-p[    1]={ 0.00000e+00,  1.00000e+00,  0.00000e+00}
      ref-p[    2]={ 0.00000e+00,  0.00000e+00,  1.00000e+00}
   refcoord-scaling               = No
   posres-com (3):
      posres-com[0]= 0.00000e+00
      posres-com[1]= 0.00000e+00
      posres-com[2]= 0.00000e+00
   posres-comB (3):
      posres-comB[0]= 0.00000e+00
      posres-comB[1]= 0.00000e+00
      posres-comB[2]= 0.00000e+00
   QMMM                           = false
qm-opts:
   ngQM                           = 0
   constraint-algorithm           = Lincs
   continuation                   = false
   Shake-SOR                      = false
   shake-tol                      = 0.0001
   lincs-order                    = 6
   lincs-iter                     = 2
   lincs-warnangle                = 30
   nwall                          = 0
   wall-type                      = 9-3
   wall-r-linpot                  = -1
   wall-atomtype[0]               = -1
   wall-atomtype[1]               = -1
   wall-density[0]                = 0
   wall-density[1]                = 0
   wall-ewald-zfac                = 3
   pull                           = false
   awh                            = false
   rotation                       = false
   interactiveMD                  = false
   disre                          = No
   disre-weighting                = Equal
   disre-mixed                    = false
   dr-fc                          = 1000
   dr-tau                         = 0
   nstdisreout                    = 100
   orire-fc                       = 0
   orire-tau                      = 0
   nstorireout                    = 100
   free-energy                    = no
   cos-acceleration               = 0
   deform (3x3):
      deform[    0]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
      deform[    1]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
      deform[    2]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
   simulated-tempering            = false
   swapcoords                     = no
```

```
   userint1                       = 0
   userint2                       = 0
   userint3                       = 0
   userint4                       = 0
   userreal1                      = 0
   userreal2                      = 0
   userreal3                      = 0
   userreal4                      = 0
   applied-forces:
     electric-field:
grpopts:
   nrdf:      292326  3.76895e+06
   ref-t:         300         300
   tau-t:         0.1         0.1
annealing:          No          No
annealing-npoints:           0           0
   acc:               0           0           0
   nfreeze:           N           N           N
   energygrp-flags[  0]: 0


Changing rlist from 1.041 to 1 for non-bonded 4x4 atom kernels

Changing nstlist from 25 to 80, rlist from 1 to 1.124

Update groups can not be used for this system because an incompatible
virtual site type is used

Initializing Domain Decomposition on 60 ranks
Dynamic load balancing: auto
Minimum cell size due to atom displacement: 2.155 nm
Initial maximum distances in bonded interactions:
    two-body bonded interactions: 0.433 nm, LJ-14, atoms 176875 176884
  multi-body bonded interactions: 0.433 nm, Ryckaert-Bell., atoms 176875
176884
Minimum cell size due to bonded interactions: 0.476 nm
Maximum distance for 7 constraints, at 120 deg. angles, all-trans: 1.166
nm
Estimated maximum distance required for P-LINCS: 1.166 nm
Scaling the initial minimum size with 1/0.8 (option -dds) = 1.25
Guess for relative PME load: 0.22
Will use 45 particle-particle and 15 PME only ranks
This is a guess, check the performance at the end of the log file
Using 15 separate PME ranks, as guessed by mdrun
Optimizing the DD grid for 45 cells with a minimum initial size of 2.694
nm
The maximum allowed number of cells is: X 9 Y 9 Z 8
Domain decomposition grid 9 x 5 x 1, separate PME ranks 15
PME domain decomposition: 15 x 1 x 1
Interleaving PP and PME ranks
This rank does only particle-particle work.
Domain decomposition rank 0, coordinates 0 0 0

The initial number of communication pulses is: X 1 Y 1
The initial domain decomposition cell size is: X 2.83 nm Y 5.10 nm

The maximum allowed distance for atoms involved in interactions is:
                 non-bonded interactions           1.124 nm
```

```
(the following are initial values, they could change due to box
deformation)
            two-body bonded interactions  (-rdd)   1.124 nm
          multi-body bonded interactions  (-rdd)   1.124 nm
              virtual site constructions  (-rcon)  2.835 nm
  atoms separated by up to 7 constraints  (-rcon)  2.835 nm

When dynamic load balancing gets turned on, these settings will change
to:
The maximum number of communication pulses is: X 1 Y 1
The minimum size for domain decomposition cells is 2.155 nm
The requested allowed shrink of DD cells (option -dds) is: 0.80
The allowed shrink of domain decomposition cells is: X 0.76 Y 0.42
The maximum allowed distance for atoms involved in interactions is:
                 non-bonded interactions           1.124 nm
            two-body bonded interactions  (-rdd)   1.124 nm
          multi-body bonded interactions  (-rdd)   1.124 nm
              virtual site constructions  (-rcon)  2.155 nm
  atoms separated by up to 7 constraints  (-rcon)  2.155 nm
Using two step summing over 10 groups of on average 4.5 ranks


Using 60 MPI processes

Non-default thread affinity set, disabling internal thread affinity

Using 1 OpenMP thread per MPI process

System total charge: -0.000
Will do PME sum in reciprocal space for electrostatic interactions.

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
U. Essmann, L. Perera, M. L. Berkowitz, T. Darden, H. Lee and L. G.
Pedersen
A smooth particle mesh Ewald method
J. Chem. Phys. 103 (1995) pp. 8577-8592
-------- -------- --- Thank You --- -------- --------

Using a Gaussian width (1/beta) of 0.289108 nm for Ewald
Potential shift: LJ r^-12: -1.000e+00 r^-6: -1.000e+00, Ewald -1.000e-06
Initialized non-bonded Coulomb Ewald tables, spacing: 8.87e-04 size: 1129

Generated table with 1062 data points for 1-4 COUL.
Tabscale = 500 points/nm
Generated table with 1062 data points for 1-4 LJ6.
Tabscale = 500 points/nm
Generated table with 1062 data points for 1-4 LJ12.
Tabscale = 500 points/nm


Using SIMD 4x8 nonbonded short-range kernels

Using a dual 4x8 pair-list setup updated with dynamic pruning:
  outer list: updated every 80 steps, buffer 0.124 nm, rlist 1.124 nm
  inner list: updated every 30 steps, buffer 0.002 nm, rlist 1.002 nm
At tolerance 0.005 kJ/mol/ps per atom, equivalent classical 1x1 list
would be:
  outer list: updated every 80 steps, buffer 0.330 nm, rlist 1.330 nm
```

```
  inner list: updated every 30 steps, buffer 0.144 nm, rlist 1.144 nm

The non-bonded pair calculation algorithm tolerates a few missing pair
interactions close to the cut-off. This can lead to a systematic
overestimation of the pressure due to missing LJ interactions. The error
in the average pressure due to missing LJ interactions is at most 7.54
bar.
The pressure error can be controlled by setting the environment variable
GMX_VERLET_BUFFER_PRESSURE_TOLERANCE to the allowed error in units of
bar.

Using Lorentz-Berthelot Lennard-Jones combination rule
Removing pbc first time

Linking all bonded interactions to atoms
There are 98588 inter update-group virtual sites,
will perform an extra communication step for selected coordinates and
forces


Initializing Parallel LINear Constraint Solver

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
B. Hess
P-LINCS: A Parallel Linear Constraint Solver for molecular simulation
J. Chem. Theory Comput. 4 (2008) pp. 116-122
-------- -------- --- Thank You --- -------- --------

The number of constraints is 179952
There are constraints between atoms in different decomposition domains,
will communicate selected coordinates each lincs iteration
29316 constraints are involved in constraint triangles,
will apply an additional matrix expansion of order 6 for couplings
between constraints inside triangles

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. Miyamoto and P. A. Kollman
SETTLE: An Analytical Version of the SHAKE and RATTLE Algorithms for
Rigid
Water Models
J. Comp. Chem. 13 (1992) pp. 952-962
-------- -------- --- Thank You --- -------- --------


Intra-simulation communication will occur every 25 steps.

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
G. Bussi, D. Donadio and M. Parrinello
Canonical sampling through velocity rescaling
J. Chem. Phys. 126 (2007) pp. 014101
-------- -------- --- Thank You --- -------- --------

There are: 2037824 Atoms
There are: 98588 VSites
Atom distribution over 45 domains: av 47475 stddev 1177 min 45929 max
49545

Constraining the starting coordinates (step 0)
```

```
Constraining the coordinates at t0-dt (step 0)
Center of mass motion removal mode is Linear
We have the following groups for center of mass motion removal:
  0:  rest
RMS relative constraint deviation after constraining: 1.01e-05
Initial temperature: 302.751 K

Started mdrun on rank 0 Fri Jan 12 07:59:12 2024

           Step           Time
              0        0.00000

   Energies (kJ/mol)
  Connect Bonds          Angle    Proper Dih. Ryckaert-Bell.          LJ-
14
    0.00000e+00    3.47961e+05    1.20867e+04    7.60995e+05
2.87071e+05
     Coulomb-14        LJ (SR)   Coulomb (SR)   Coul. recip.
Potential
   -1.18825e+06    5.05953e+06   -4.35657e+07    3.60894e+05   -
3.79254e+07
    Kinetic En.   Total Energy  Conserved En.    Temperature Pressure
(bar)
    5.39105e+06   -3.25344e+07   -3.25241e+07    3.19305e+02   -
5.32592e+02
   Constr. rmsd
    9.94959e-06


DD  step 79 load imb.: force 26.3%  pme mesh/force 1.180
step  480: timed with pme grid 240 240 240, coulomb cutoff 1.000: 19929.0
M-cycles
step  640: timed with pme grid 216 216 216, coulomb cutoff 1.072: 20110.8
M-cycles
step  800: timed with pme grid 200 200 200, coulomb cutoff 1.157: 20223.9
M-cycles
step  960: timed with pme grid 168 168 168, coulomb cutoff 1.378: 27075.5
M-cycles
step 1120: timed with pme grid 192 192 192, coulomb cutoff 1.206: 21058.4
M-cycles
step 1280: timed with pme grid 200 200 200, coulomb cutoff 1.157: 20984.0
M-cycles
step 1440: timed with pme grid 208 208 208, coulomb cutoff 1.113: 19531.5
M-cycles
step 1600: timed with pme grid 216 216 216, coulomb cutoff 1.072: 18447.4
M-cycles
step 1760: timed with pme grid 224 224 224, coulomb cutoff 1.033: 18947.5
M-cycles
step 1920: timed with pme grid 240 240 240, coulomb cutoff 1.000: 19983.9
M-cycles
step 2080: timed with pme grid 200 200 200, coulomb cutoff 1.157: 29322.3
M-cycles
step 2240: timed with pme grid 208 208 208, coulomb cutoff 1.113: 20275.2
M-cycles
step 2400: timed with pme grid 216 216 216, coulomb cutoff 1.072: 19605.6
M-cycles
```

```
step 2560: timed with pme grid 224 224 224, coulomb cutoff 1.033: 19562.2
M-cycles
step 2720: timed with pme grid 240 240 240, coulomb cutoff 1.000: 19161.6
M-cycles
step 2880: timed with pme grid 200 200 200, coulomb cutoff 1.157: 20885.3
M-cycles
step 3040: timed with pme grid 208 208 208, coulomb cutoff 1.113: 19786.2
M-cycles
step 3200: timed with pme grid 216 216 216, coulomb cutoff 1.072: 18956.9
M-cycles
step 3360: timed with pme grid 224 224 224, coulomb cutoff 1.033: 18093.3
M-cycles
step 3520: timed with pme grid 240 240 240, coulomb cutoff 1.000: 20610.0
M-cycles
step 3680: timed with pme grid 200 200 200, coulomb cutoff 1.157: 20641.3
M-cycles
step 3840: timed with pme grid 208 208 208, coulomb cutoff 1.113: 18972.8
M-cycles
step 4000: timed with pme grid 216 216 216, coulomb cutoff 1.072: 19120.3
M-cycles
step 4160: timed with pme grid 224 224 224, coulomb cutoff 1.033: 18491.1
M-cycles
step 4320: timed with pme grid 240 240 240, coulomb cutoff 1.000: 19073.8
M-cycles
step 4480: timed with pme grid 200 200 200, coulomb cutoff 1.157: 20871.4
M-cycles
step 4640: timed with pme grid 208 208 208, coulomb cutoff 1.113: 19881.3
M-cycles
step 4800: timed with pme grid 216 216 216, coulomb cutoff 1.072: 19746.3
M-cycles
step 4960: timed with pme grid 224 224 224, coulomb cutoff 1.033: 19278.9
M-cycles
step 5120: timed with pme grid 240 240 240, coulomb cutoff 1.000: 20641.7
M-cycles
              optimal pme grid 224 224 224, coulomb cutoff 1.033
Writing checkpoint, step 7840 at Fri Jan 12 08:14:16 2024



DD  step 9999 load imb.: force 20.1%  pme mesh/force 1.214
           Step           Time
          10000       40.00000

Writing checkpoint, step 10000 at Fri Jan 12 08:18:20 2024


   Energies (kJ/mol)
  Connect Bonds          Angle    Proper Dih. Ryckaert-Bell.          LJ-
14
    0.00000e+00    3.48742e+05    1.19408e+04    7.60727e+05
2.87806e+05
     Coulomb-14        LJ (SR)   Coulomb (SR)   Coul. recip.
Potential
   -1.18637e+06    5.16366e+06   -4.37253e+07    3.09192e+05   -
3.80296e+07
    Kinetic En.   Total Energy  Conserved En.    Temperature Pressure
(bar)
```

```
    5.06850e+06   -3.29611e+07   -3.25360e+07    3.00201e+02
1.54467e+01
   Constr. rmsd
    9.38751e-06


Energy conservation over simulation part #1 of length 40 ps, time 0 to 40
ps
  Conserved energy drift: -1.39e-04 kJ/mol/ps per atom


      <======  ###############  ==>
      <====  A V E R A G E S  ====>
      <==  ###############  ======>

      Statistics over 10001 steps using 101 frames

   Energies (kJ/mol)
  Connect Bonds          Angle    Proper Dih. Ryckaert-Bell.          LJ-
14
    0.00000e+00    3.47715e+05    1.19223e+04    7.61239e+05
2.87422e+05
     Coulomb-14        LJ (SR)   Coulomb (SR)   Coul. recip.
Potential
   -1.18698e+06    5.15917e+06   -4.36983e+07    2.91909e+05   -
3.80259e+07
    Kinetic En.   Total Energy  Conserved En.    Temperature Pressure
(bar)
    5.06783e+06   -3.29580e+07   -3.25276e+07    3.00161e+02   -
1.69430e+01
   Constr. rmsd
    0.00000e+00

          Box-X          Box-Y          Box-Z
    3.10270e+01    3.10270e+01    2.19394e+01

   Total Virial (kJ/mol)
    1.69862e+06   -1.83983e+03    1.48271e+03
   -1.83638e+03    1.70244e+06    6.25269e+02
    1.48600e+03    6.29594e+02    1.69945e+06

   Pressure (bar)
   -1.32057e+01    2.13575e+00   -4.13935e+00
    2.13033e+00   -2.16084e+01   -3.03440e-02
   -4.14451e+00   -3.71552e-02   -1.60149e+01

         T-mol      T-solvent
    3.00185e+02    3.00160e+02


      P P   -   P M E   L O A D   B A L A N C I N G

 PP/PME load balancing changed the cut-off and PME settings:
          particle-particle                    PME
           rcoulomb  rlist            grid      spacing   1/beta
  initial  1.000 nm  1.002 nm     240 240 240   0.130 nm  0.289 nm
  final    1.033 nm  1.035 nm     224 224 224   0.140 nm  0.299 nm
cost-ratio           1.10             0.81
```

(note that these numbers concern only part of the total PP and PME load)

M E G A - F L O P S A C C O U N T I N G

NB=Group-cutoff nonbonded kernels NxN=N-by-N cluster Verlet kernels
RF=Reaction-Field VdW=Van der Waals QSTab=quadratic-spline table
W3=SPC/TIP3p W4=TIP4p (single or pairs)
V&F=Potential and force V=Potential only F=Force only

Computing:	M-Number	M-Flops	% Flops
Pair Search distance check	138709.886678	1248388.980	0.1
NxN Ewald Elec. + LJ [F]	8845964.505888	583833657.389	54.5
NxN Ewald Elec. + LJ [V&F]	89757.790496	9604083.583	0.9
NxN Ewald Elec. [F]	6742216.427360	411275202.069	38.4
NxN Ewald Elec. [V&F]	68408.791808	5746338.512	0.5
1,4 nonbonded interactions	6369.046841	573214.216	0.1
Calc Weights	64098.769236	2307555.692	0.2
Spread Q Bspline	1367440.410368	2734880.821	0.3
Gather F Bspline	1367440.410368	8204642.462	0.8
3D-FFT	5050700.934126	40405607.473	3.8
Solve PME	486.992896	31167.545	0.0
Reset In Box	269.187912	807.564	0.0
CG-CoM	271.324324	813.973	0.0
Angles	4258.985856	715509.624	0.1
Propers	212.081206	48566.596	0.0
RB-Dihedrals	6469.816917	1598044.778	0.1
Virial	857.513237	15435.238	0.0
Stop-CM	217.914024	2179.140	0.0
P-Coupling	856.701212	5140.207	0.0
Calc-Ekin	1713.402424	46261.865	0.0
Lincs	2576.031399	154561.884	0.0
Lincs-Mat	70445.835016	281783.340	0.0

```
 Constraint-V                          24812.934362      223316.409
0.0
 Constraint-Vir                          891.532222       21396.773
0.0
 Settle                                 6554.450384     2425146.642
0.2
 Virtual Site 3                           93.069755        3443.581
0.0
 Virtual Site 3fd                        193.227552       18356.617
0.0
 Virtual Site 3fad                       110.344416       19420.617
0.0
 Virtual Site 3out                       361.968796       31491.285
0.0
 Virtual Site 4fd                        100.036034       11003.964
0.0
 Virtual Site 4fdn                       170.062298       43195.824
0.0
-----------------------------------------------------------------------
----
 Total                                                 1071630614.665
100.0
-----------------------------------------------------------------------
----


    D O M A I N   D E C O M P O S I T I O N   S T A T I S T I C S

 av. #atoms communicated per step for force:  2 x 1609842.7
 av. #atoms communicated per step for vsites: 3 x 11828.4
 av. #atoms communicated per step for LINCS:  3 x 165922.7


Dynamic load balancing report:
 DLB was off during the run due to low measured imbalance.
 Average load imbalance: 20.6%.
 The balanceable part of the MD step is 57%, load imbalance is computed
from this.
 Part of the total run time spent waiting due to load imbalance: 11.7%.
 Average PME mesh/force load: 1.193
 Part of the total run time spent waiting due to PP/PME imbalance: 10.1 %

NOTE: 11.7 % of the available CPU time was lost due to load imbalance
      in the domain decomposition.
      Dynamic load balancing was automatically disabled, but it might be
beneficial to manually turn it on (option -dlb yes.)
      You can also consider manually changing the decomposition (option -
dd);
      e.g. by using fewer domains along the box dimension in which there
is
      considerable inhomogeneity in the simulated system.
NOTE: 10.1 % performance was lost because the PME ranks
      had more work to do than the PP ranks.
      You might want to increase the number of PME ranks
      or increase the cut-off and the grid spacing.


     R E A L   C Y C L E   A N D   T I M E   A C C O U N T I N G
```

```
On 45 MPI ranks doing PP, and
on 15 MPI ranks doing PME

 Activity:              Num   Num      Call    Wall time         Giga-
Cycles
                       Ranks Threads  Count      (s)         total sum
%
-----------------------------------------------------------------------
-------
 Domain decomp.           45    1        126      21.964       2910.135
1.4
 DD comm. load            45    1         15       0.006          0.823
0.0
 Vsite constr.            45    1      10001      16.453       2179.932
1.1
 Send X to PME            45    1      10001       7.353        974.213
0.5
 Neighbor search          45    1        126      14.875       1970.881
1.0
 Comm. coord.             45    1       9875      39.677       5257.147
2.6
 Force                    45    1      10001     568.608      75339.035
37.0
 Wait + Comm. F           45    1      10001     159.931      21190.444
10.4
 PME mesh *               15    1      10001     869.264      38391.715
18.8
 PME wait for PP *                             284.262      12554.648
6.2
 Wait + Recv. PME F       45    1      10001     154.485      20468.806
10.0
 NB X/F buffer ops.       45    1      29751       7.091        939.524
0.5
 Vsite spread             45    1      10402      45.620       6044.475
3.0
 Write traj.              45    1          2       0.402         53.259
0.0
 Update                   45    1      10001       2.598        344.287
0.2
 Constraints              45    1      10003     110.522      14643.906
7.2
 Comm. energies           45    1        401       2.520        333.917
0.2
 Rest                                            1.464        194.033
0.1
-----------------------------------------------------------------------
-------
 Total                                        1153.569     203793.089
100.0
-----------------------------------------------------------------------
-------
(*) Note that with separate PME ranks, the walltime column actually sums
to
    twice the total reported, but the cycle count total and % are
correct.
-----------------------------------------------------------------------
-------
```

```
 Breakdown of PME mesh activities
-----------------------------------------------------------------------------
-------
 PME redist. X/F          15    1      20002     177.970       7860.171
3.9
 PME spread               15    1      10001     163.846       7236.380
3.6
 PME gather               15    1      10001     130.334       5756.320
2.8
 PME 3D-FFT               15    1      20002     146.447       6467.929
3.2
 PME 3D-FFT Comm.         15    1      20002     242.752      10721.321
5.3
 PME solve Elec           15    1      10001       7.752        342.363
0.2
-----------------------------------------------------------------------------
-------

               Core t (s)   Wall t (s)        (%)
       Time:    69212.669     1153.569     5999.9
                 (ns/day)    (hour/ns)
Performance:        2.996        8.010
Finished mdrun on rank 0 Fri Jan 12 08:18:25 2024
```

benchRIB_cpu-sev-cluster_1n

:-) GROMACS - gmx mdrun, 2023.3 (-:

Current GROMACS contributors:

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Coordinated by the GROMACS project leaders:
Paul Bauer, Berk Hess, and Erik Lindahl

```
GROMACS:      gmx mdrun, version 2023.3
Executable:   /usr/local/gromacs/bin/gmx_mpi
Data prefix:  /usr/local/gromacs
Working dir:  /home/ubuntu
Process ID:   20293
Command line:
  gmx_mpi mdrun -v -s /mnt/shared/home/ubuntu/mpinat-gromacs/mpinat-
gromacs-standard-md-bench/benchRIB.tpr

GROMACS version:    2023.3
Precision:          mixed
Memory model:       64 bit
MPI library:        MPI
OpenMP support:     enabled (GMX_OPENMP_MAX_THREADS = 128)
GPU support:        disabled
SIMD instructions:  AVX2_256
```

```
CPU FFT library:    fftw-3.3.8-sse2-avx-avx2-avx2_128
GPU FFT library:    none
Multi-GPU FFT:      none
RDTSCP usage:       enabled
TNG support:        enabled
Hwloc support:      disabled
Tracing support:    disabled
C compiler:         /usr/bin/cc GNU 11.4.0
C compiler flags:   -fexcess-precision=fast -funroll-all-loops -mavx2 -
mfma -Wno-missing-field-initializers -O3 -DNDEBUG
C++ compiler:       /usr/bin/c++ GNU 11.4.0
C++ compiler flags: -fexcess-precision=fast -funroll-all-loops -mavx2 -
mfma -Wno-missing-field-initializers -Wno-cast-function-type-strict -
fopenmp -O3 -DNDEBUG
BLAS library:       Internal
LAPACK library:     Internal


Running on 1 node with total 6 cores, 6 processing units
Hardware detected on host cpu-sev-1 (the node of MPI rank 0):
  CPU info:
    Vendor: AMD
    Brand:  AMD EPYC-Milan Processor
    Family: 25   Model: 1   Stepping: 1
    Features: aes amd apic avx avx2 clfsh cmov cx8 cx16 f16c fma lahf
misalignsse mmx msr pcid pclmuldq pdpe1gb popcnt pse rdrnd rdtscp sha
sse2 sse3 sse4a sse4.1 sse4.2 ssse3 tdt x2apic
  Hardware topology: Basic
    Packages, cores, and logical processors:
    [indices refer to OS logical processors]
      Package  0: [   0]
      Package  1: [   1]
      Package  2: [   2]
      Package  3: [   3]
      Package  4: [   4]
      Package  5: [   5]
    CPU limit set by OS: -1   Recommended max number of threads: 6


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
M. J. Abraham, T. Murtola, R. Schulz, S. P√°ll, J. C. Smith, B. Hess, E.
Lindahl
GROMACS: High performance molecular simulations through multi-level
parallelism from laptops to supercomputers
SoftwareX 1 (2015) pp. 19-25
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. P√°ll, M. J. Abraham, C. Kutzner, B. Hess, E. Lindahl
Tackling Exascale Software Challenges in Molecular Dynamics Simulations
with
GROMACS
In S. Markidis & E. Laure (Eds.), Solving Software Challenges for
Exascale 8759 (2015) pp. 3-27
-------- -------- --- Thank You --- -------- --------
```

```
++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. Pronk, S. P√°ll, R. Schulz, P. Larsson, P. Bjelkmar, R. Apostolov, M.
R.
Shirts, J. C. Smith, P. M. Kasson, D. van der Spoel, B. Hess, and E.
Lindahl
GROMACS 4.5: a high-throughput and highly parallel open source molecular
simulation toolkit
Bioinformatics 29 (2013) pp. 845-54
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
B. Hess and C. Kutzner and D. van der Spoel and E. Lindahl
GROMACS 4: Algorithms for highly efficient, load-balanced, and scalable
molecular simulation
J. Chem. Theory Comput. 4 (2008) pp. 435-447
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
D. van der Spoel, E. Lindahl, B. Hess, G. Groenhof, A. E. Mark and H. J.
C.
Berendsen
GROMACS: Fast, Flexible and Free
J. Comp. Chem. 26 (2005) pp. 1701-1719
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
E. Lindahl and B. Hess and D. van der Spoel
GROMACS 3.0: A package for molecular simulation and trajectory analysis
J. Mol. Mod. 7 (2001) pp. 306-317
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
H. J. C. Berendsen, D. van der Spoel and R. van Drunen
GROMACS: A message-passing parallel molecular dynamics implementation
Comp. Phys. Comm. 91 (1995) pp. 43-56
-------- -------- --- Thank You --- -------- --------


++++ PLEASE CITE THE DOI FOR THIS VERSION OF GROMACS ++++
https://doi.org/10.5281/zenodo.10017686
-------- -------- --- Thank You --- -------- --------


The number of OpenMP threads was set by environment variable
OMP_NUM_THREADS to 1

Input Parameters:
   integrator                     = md
   tinit                          = 0
   dt                             = 0.004
   nsteps                         = 10000
   init-step                      = 0
   simulation-part                = 1
   mts                            = false
```

```
comm-mode                       = Linear
nstcomm                         = 100
bd-fric                         = 0
ld-seed                         = 14771
emtol                           = 1e-05
emstep                          = 0.01
niter                           = 20
fcstep                          = 0
nstcgsteep                      = 1000
nbfgscorr                       = 10
rtpi                            = 0.05
nstxout                         = 0
nstvout                         = 0
nstfout                         = 0
nstlog                          = 0
nstcalcenergy                   = 100
nstenergy                       = 500
nstxout-compressed              = 0
compressed-x-precision          = 1000
cutoff-scheme                   = Verlet
nstlist                         = 25
pbc                             = xyz
periodic-molecules              = false
verlet-buffer-tolerance         = 0.005
rlist                           = 1.041
coulombtype                     = PME
coulomb-modifier                = Potential-shift
rcoulomb-switch                 = 0
rcoulomb                        = 1
epsilon-r                       = 1
epsilon-rf                      = inf
vdw-type                        = Cut-off
vdw-modifier                    = Potential-shift
rvdw-switch                     = 0
rvdw                            = 1
DispCorr                        = No
table-extension                 = 1
fourierspacing                  = 0.135
fourier-nx                      = 240
fourier-ny                      = 240
fourier-nz                      = 240
pme-order                       = 4
ewald-rtol                      = 1e-06
ewald-rtol-lj                   = 1e-06
lj-pme-comb-rule                = Geometric
ewald-geometry                  = 3d
epsilon-surface                 = 0
ensemble-temperature-setting    = constant
ensemble-temperature            = 300
tcoupl                          = V-rescale
nsttcouple                      = 25
nh-chain-length                 = 0
print-nose-hoover-chain-variables = false
pcoupl                          = Berendsen
pcoupltype                      = Isotropic
nstpcouple                      = 25
tau-p                           = 1
compressibility (3x3):
```

```
      compressibility[    0]={ 4.50000e-05,  0.00000e+00,  0.00000e+00}
      compressibility[    1]={ 0.00000e+00,  4.50000e-05,  0.00000e+00}
      compressibility[    2]={ 0.00000e+00,  0.00000e+00,  4.50000e-05}
   ref-p (3x3):
      ref-p[    0]={ 1.00000e+00,  0.00000e+00,  0.00000e+00}
      ref-p[    1]={ 0.00000e+00,  1.00000e+00,  0.00000e+00}
      ref-p[    2]={ 0.00000e+00,  0.00000e+00,  1.00000e+00}
   refcoord-scaling               = No
   posres-com (3):
      posres-com[0]= 0.00000e+00
      posres-com[1]= 0.00000e+00
      posres-com[2]= 0.00000e+00
   posres-comB (3):
      posres-comB[0]= 0.00000e+00
      posres-comB[1]= 0.00000e+00
      posres-comB[2]= 0.00000e+00
   QMMM                           = false
qm-opts:
   ngQM                           = 0
   constraint-algorithm           = Lincs
   continuation                   = false
   Shake-SOR                      = false
   shake-tol                      = 0.0001
   lincs-order                    = 6
   lincs-iter                     = 2
   lincs-warnangle                = 30
   nwall                          = 0
   wall-type                      = 9-3
   wall-r-linpot                  = -1
   wall-atomtype[0]               = -1
   wall-atomtype[1]               = -1
   wall-density[0]                = 0
   wall-density[1]                = 0
   wall-ewald-zfac                = 3
   pull                           = false
   awh                            = false
   rotation                       = false
   interactiveMD                  = false
   disre                          = No
   disre-weighting                = Equal
   disre-mixed                    = false
   dr-fc                          = 1000
   dr-tau                         = 0
   nstdisreout                    = 100
   orire-fc                       = 0
   orire-tau                      = 0
   nstorireout                    = 100
   free-energy                    = no
   cos-acceleration               = 0
   deform (3x3):
      deform[    0]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
      deform[    1]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
      deform[    2]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
   simulated-tempering            = false
   swapcoords                     = no
   userint1                       = 0
   userint2                       = 0
   userint3                       = 0
```

```
   userint4                       = 0
   userreal1                      = 0
   userreal2                      = 0
   userreal3                      = 0
   userreal4                      = 0
   applied-forces:
     electric-field:
grpopts:
   nrdf:      292326  3.76895e+06
   ref-t:         300         300
   tau-t:         0.1         0.1
annealing:          No          No
annealing-npoints:           0           0
   acc:               0           0           0
   nfreeze:           N           N           N
   energygrp-flags[  0]: 0


Changing rlist from 1.041 to 1 for non-bonded 4x4 atom kernels

Changing nstlist from 25 to 80, rlist from 1 to 1.124

Update groups can not be used for this system because an incompatible
virtual site type is used

Initializing Domain Decomposition on 6 ranks
Dynamic load balancing: auto
Minimum cell size due to atom displacement: 2.155 nm
Initial maximum distances in bonded interactions:
    two-body bonded interactions: 0.433 nm, LJ-14, atoms 176875 176884
  multi-body bonded interactions: 0.433 nm, Ryckaert-Bell., atoms 176875
176884
Minimum cell size due to bonded interactions: 0.476 nm
Maximum distance for 7 constraints, at 120 deg. angles, all-trans: 1.166
nm
Estimated maximum distance required for P-LINCS: 1.166 nm
Scaling the initial minimum size with 1/0.8 (option -dds) = 1.25
Using 0 separate PME ranks because: there are too few total ranks for
efficient splitting
Optimizing the DD grid for 6 cells with a minimum initial size of 2.694
nm
The maximum allowed number of cells is: X 9 Y 9 Z 8
Domain decomposition grid 6 x 1 x 1, separate PME ranks 0
PME domain decomposition: 6 x 1 x 1
Domain decomposition rank 0, coordinates 0 0 0

The initial number of communication pulses is: X 1
The initial domain decomposition cell size is: X 4.25 nm

The maximum allowed distance for atoms involved in interactions is:
                 non-bonded interactions           1.124 nm
(the following are initial values, they could change due to box
deformation)
            two-body bonded interactions  (-rdd)   1.124 nm
          multi-body bonded interactions  (-rdd)   1.124 nm
              virtual site constructions  (-rcon)  4.252 nm
  atoms separated by up to 7 constraints  (-rcon)  4.252 nm
```

```
When dynamic load balancing gets turned on, these settings will change
to:
The maximum number of communication pulses is: X 1
The minimum size for domain decomposition cells is 2.155 nm
The requested allowed shrink of DD cells (option -dds) is: 0.80
The allowed shrink of domain decomposition cells is: X 0.51
The maximum allowed distance for atoms involved in interactions is:
                 non-bonded interactions           1.124 nm
            two-body bonded interactions  (-rdd)   1.124 nm
          multi-body bonded interactions  (-rdd)   1.124 nm
              virtual site constructions  (-rcon)  2.155 nm
  atoms separated by up to 7 constraints  (-rcon)  2.155 nm

Using 6 MPI processes

Non-default thread affinity set, disabling internal thread affinity

Using 1 OpenMP thread per MPI process

System total charge: -0.000
Will do PME sum in reciprocal space for electrostatic interactions.

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
U. Essmann, L. Perera, M. L. Berkowitz, T. Darden, H. Lee and L. G.
Pedersen
A smooth particle mesh Ewald method
J. Chem. Phys. 103 (1995) pp. 8577-8592
-------- -------- --- Thank You --- -------- --------

Using a Gaussian width (1/beta) of 0.289108 nm for Ewald
Potential shift: LJ r^-12: -1.000e+00 r^-6: -1.000e+00, Ewald -1.000e-06
Initialized non-bonded Coulomb Ewald tables, spacing: 8.87e-04 size: 1129

Generated table with 1062 data points for 1-4 COUL.
Tabscale = 500 points/nm
Generated table with 1062 data points for 1-4 LJ6.
Tabscale = 500 points/nm
Generated table with 1062 data points for 1-4 LJ12.
Tabscale = 500 points/nm


Using SIMD 4x8 nonbonded short-range kernels

Using a dual 4x8 pair-list setup updated with dynamic pruning:
  outer list: updated every 80 steps, buffer 0.124 nm, rlist 1.124 nm
  inner list: updated every 30 steps, buffer 0.002 nm, rlist 1.002 nm
At tolerance 0.005 kJ/mol/ps per atom, equivalent classical 1x1 list
would be:
  outer list: updated every 80 steps, buffer 0.330 nm, rlist 1.330 nm
  inner list: updated every 30 steps, buffer 0.144 nm, rlist 1.144 nm

The non-bonded pair calculation algorithm tolerates a few missing pair
interactions close to the cut-off. This can lead to a systematic
overestimation of the pressure due to missing LJ interactions. The error
in the average pressure due to missing LJ interactions is at most 7.54
bar.
```

```
The pressure error can be controlled by setting the environment variable
GMX_VERLET_BUFFER_PRESSURE_TOLERANCE to the allowed error in units of
bar.

Using Lorentz-Berthelot Lennard-Jones combination rule
Removing pbc first time

Linking all bonded interactions to atoms
There are 98588 inter update-group virtual sites,
will perform an extra communication step for selected coordinates and
forces


Initializing Parallel LINear Constraint Solver

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
B. Hess
P-LINCS: A Parallel Linear Constraint Solver for molecular simulation
J. Chem. Theory Comput. 4 (2008) pp. 116-122
-------- -------- --- Thank You --- -------- --------

The number of constraints is 179952
There are constraints between atoms in different decomposition domains,
will communicate selected coordinates each lincs iteration
29316 constraints are involved in constraint triangles,
will apply an additional matrix expansion of order 6 for couplings
between constraints inside triangles

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. Miyamoto and P. A. Kollman
SETTLE: An Analytical Version of the SHAKE and RATTLE Algorithms for
Rigid
Water Models
J. Comp. Chem. 13 (1992) pp. 952-962
-------- -------- --- Thank You --- -------- --------


Intra-simulation communication will occur every 25 steps.

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
G. Bussi, D. Donadio and M. Parrinello
Canonical sampling through velocity rescaling
J. Chem. Phys. 126 (2007) pp. 014101
-------- -------- --- Thank You --- -------- --------

There are: 2037824 Atoms
There are: 98588 VSites
Atom distribution over 6 domains: av 356068 stddev 5247 min 348611 max
361668

Constraining the starting coordinates (step 0)

Constraining the coordinates at t0-dt (step 0)
Center of mass motion removal mode is Linear
We have the following groups for center of mass motion removal:
  0:  rest
RMS relative constraint deviation after constraining: 9.79e-06
Initial temperature: 302.726 K
```

```
Started mdrun on rank 0 Sat Jan 13 10:21:35 2024

           Step           Time
              0        0.00000

   Energies (kJ/mol)
  Connect Bonds          Angle    Proper Dih. Ryckaert-Bell.          LJ-
14
    0.00000e+00    3.47953e+05    1.20867e+04    7.60968e+05
2.87075e+05
     Coulomb-14        LJ (SR)   Coulomb (SR)   Coul. recip.
Potential
   -1.18824e+06    5.05955e+06   -4.35305e+07    3.60665e+05   -
3.78905e+07
    Kinetic En.   Total Energy  Conserved En.    Temperature Pressure
(bar)
    5.39060e+06   -3.24999e+07   -3.24896e+07    3.19279e+02   -
5.32618e+02
   Constr. rmsd
    9.62972e-06


DD  step 79 load imb.: force  5.1%

step 160 Turning on dynamic load balancing, because the performance loss
due to load imbalance is 3.2 %.
Writing checkpoint, step 3360 at Sat Jan 13 10:36:47 2024


Writing checkpoint, step 6720 at Sat Jan 13 10:51:49 2024



DD  step 9999  vol min/aver 0.952  load imb.: force  0.1%
           Step           Time
          10000       40.00000

Writing checkpoint, step 10000 at Sat Jan 13 11:06:29 2024


   Energies (kJ/mol)
  Connect Bonds          Angle    Proper Dih. Ryckaert-Bell.          LJ-
14
    0.00000e+00    3.48625e+05    1.21718e+04    7.61024e+05
2.87855e+05
     Coulomb-14        LJ (SR)   Coulomb (SR)   Coul. recip.
Potential
   -1.18856e+06    5.15431e+06   -4.37240e+07    3.52444e+05   -
3.79961e+07
    Kinetic En.   Total Energy  Conserved En.    Temperature Pressure
(bar)
    5.06965e+06   -3.29264e+07   -3.25294e+07    3.00269e+02   -
2.97175e+00
   Constr. rmsd
    9.05481e-06
```

```
Energy conservation over simulation part #1 of length 40 ps, time 0 to 40
ps
  Conserved energy drift: -4.66e-04 kJ/mol/ps per atom


      <======  ###############  ==>
      <====  A V E R A G E S  ====>
      <==  ###############  ======>

      Statistics over 10001 steps using 101 frames

   Energies (kJ/mol)
  Connect Bonds          Angle    Proper Dih. Ryckaert-Bell.          LJ-
14
    0.00000e+00    3.47762e+05    1.19200e+04    7.61140e+05
2.87373e+05
     Coulomb-14        LJ (SR)   Coulomb (SR)   Coul. recip.
Potential
   -1.18709e+06    5.15876e+06   -4.37242e+07    3.52858e+05   -
3.79915e+07
    Kinetic En.   Total Energy  Conserved En.    Temperature Pressure
(bar)
    5.06789e+06   -3.29236e+07   -3.25091e+07    3.00165e+02   -
1.58363e+01
   Constr. rmsd
    0.00000e+00

          Box-X          Box-Y          Box-Z
    3.10282e+01    3.10282e+01    2.19402e+01

   Total Virial (kJ/mol)
    1.69951e+06   -1.36984e+03   -7.54348e+02
   -1.37068e+03    1.69796e+06   -1.94080e+03
   -8.59384e+02   -1.93986e+03    1.70100e+06

   Pressure (bar)
   -1.46815e+01    1.31182e+00   -6.50089e-01
    1.31314e+00   -1.42345e+01    3.96650e+00
   -4.84961e-01    3.96502e+00   -1.85928e+01

          T-mol      T-solvent
    3.00091e+02    3.00171e+02


     M E G A - F L O P S   A C C O U N T I N G

 NB=Group-cutoff nonbonded kernels    NxN=N-by-N cluster Verlet kernels
 RF=Reaction-Field  VdW=Van der Waals  QSTab=quadratic-spline table
 W3=SPC/TIP3p  W4=TIP4p (single or pairs)
 V&F=Potential and force  V=Potential only  F=Force only

 Computing:                                M-Number         M-Flops  %
Flops
-----------------------------------------------------------------------
----
 Pair Search distance check          128185.261300     1153667.352
0.1
```

NxN Ewald Elec. + LJ [F]	7474896.739616	493343184.815	53.3
NxN Ewald Elec. + LJ [V&F]	76253.770592	8159153.453	0.9
NxN Ewald Elec. [F]	5667382.273088	345710318.658	37.4
NxN Ewald Elec. [V&F]	57815.044832	4856463.766	0.5
1,4 nonbonded interactions	6369.046841	573214.216	0.1
Calc Weights	64098.769236	2307555.692	0.2
Spread Q Bspline	1367440.410368	2734880.821	0.3
Gather F Bspline	1367440.410368	8204642.462	0.9
3D-FFT	6558947.569174	52471580.553	5.7
Solve PME	576.057600	36867.686	0.0
Reset In Box	269.187912	807.564	0.0
CG-CoM	271.324324	813.973	0.0
Angles	4258.985856	715509.624	0.1
Propers	212.081206	48566.596	0.0
RB-Dihedrals	6469.816917	1598044.778	0.2
Virial	856.809482	15422.571	0.0
Stop-CM	217.914024	2179.140	0.0
P-Coupling	856.701212	5140.207	0.0
Calc-Ekin	1713.402424	46261.865	0.0
Lincs	2132.326902	127939.614	0.0
Lincs-Mat	58633.902740	234535.611	0.0
Constraint-V	23392.092964	210528.837	0.0
Constraint-Vir	852.354322	20456.504	0.0
Settle	6376.591348	2359338.799	0.3
Virtual Site 3	91.223071	3375.254	0.0
Virtual Site 3fd	193.227552	18356.617	0.0
Virtual Site 3fad	110.344416	19420.617	0.0
Virtual Site 3out	361.968796	31491.285	0.0
Virtual Site 4fd	100.036034	11003.964	0.0

```
 Virtual Site 4fdn                        170.062298       43195.824
0.0
-----------------------------------------------------------------------
----
 Total                                                  925063918.719
100.0
-----------------------------------------------------------------------
----


    D O M A I N   D E C O M P O S I T I O N   S T A T I S T I C S

 av. #atoms communicated per step for force:  2 x 568976.0
 av. #atoms communicated per step for vsites: 3 x 5083.0
 av. #atoms communicated per step for LINCS:  3 x 70482.9


Dynamic load balancing report:
 DLB was turned on during the run due to measured imbalance.
 Average load imbalance: 1.7%.
 The balanceable part of the MD step is 63%, load imbalance is computed
from this.
 Part of the total run time spent waiting due to load imbalance: 1.1%.
 Steps where the load balancing was limited by -rdd, -rcon and/or -dds: X
0 %


     R E A L   C Y C L E   A N D   T I M E   A C C O U N T I N G

On 6 MPI ranks

 Activity:              Num   Num      Call    Wall time         Giga-
Cycles
                       Ranks Threads  Count      (s)         total sum
%
-----------------------------------------------------------------------
-------
 Domain decomp.            6    1        126      18.367        324.477
0.7
 DD comm. load             6    1        125       0.044          0.776
0.0
 DD comm. bounds           6    1        124       0.071          1.247
0.0
 Vsite constr.             6    1      10001      16.013        282.895
0.6
 Neighbor search           6    1        126      54.592        964.455
2.0
 Comm. coord.              6    1       9875      10.425        184.182
0.4
 Force                     6    1      10001    1600.731      28279.479
59.3
 Wait + Comm. F            6    1      10001       7.633        134.847
0.3
 PME mesh                  6    1      10001     777.876      13742.427
28.8
 NB X/F buffer ops.        6    1      29751      15.068        266.199
0.6
```

```
 Vsite spread                 6    1      10402      24.560         433.884
0.9
 Write traj.                  6    1          3       0.854          15.079
0.0
 Update                       6    1      10001      13.352         235.880
0.5
 Constraints                  6    1      10003     153.618        2713.915
5.7
 Comm. energies               6    1        401       0.619          10.933
0.0
 Rest                                                  4.072          71.932
0.2
-----------------------------------------------------------------------------
-------
 Total                                              2697.893       47662.605
100.0
-----------------------------------------------------------------------------
-------
 Breakdown of PME mesh activities
-----------------------------------------------------------------------------
-------
 PME redist. X/F              6    1      20002      93.400        1650.065
3.5
 PME spread                   6    1      10001     214.552        3790.404
8.0
 PME gather                   6    1      10001     212.987        3762.759
7.9
 PME 3D-FFT                   6    1      20002     199.568        3525.683
7.4
 PME 3D-FFT Comm.             6    1      20002      46.051         813.557
1.7
 PME solve Elec               6    1      10001      11.237         198.512
0.4
-----------------------------------------------------------------------------
-------

               Core t (s)   Wall t (s)        (%)
       Time:    16187.353     2697.893      600.0
                         44:57
                 (ns/day)    (hour/ns)
Performance:        1.281       18.733
Finished mdrun on rank 0 Sat Jan 13 11:06:33 2024
```

benchRIB_cpu-sev-cluster_3n

```
                :-) GROMACS - gmx mdrun, 2023.3 (-:

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                    Coordinated by the GROMACS project leaders:
                      Paul Bauer, Berk Hess, and Erik Lindahl

GROMACS:      gmx mdrun, version 2023.3
Executable:   /usr/local/gromacs/bin/gmx_mpi
Data prefix:  /usr/local/gromacs
Working dir:  /home/ubuntu
Process ID:   6506
Command line:
  gmx_mpi mdrun -v -s /mnt/shared/home/ubuntu/mpinat-gromacs/mpinat-
gromacs-standard-md-bench/benchRIB.tpr

GROMACS version:    2023.3
Precision:          mixed
Memory model:       64 bit
MPI library:        MPI
OpenMP support:     enabled (GMX_OPENMP_MAX_THREADS = 128)
GPU support:        disabled
SIMD instructions:  AVX2_256
```

```
CPU FFT library:    fftw-3.3.8-sse2-avx-avx2-avx2_128
GPU FFT library:    none
Multi-GPU FFT:      none
RDTSCP usage:       enabled
TNG support:        enabled
Hwloc support:      disabled
Tracing support:    disabled
C compiler:         /usr/bin/cc GNU 11.4.0
C compiler flags:   -fexcess-precision=fast -funroll-all-loops -mavx2 -
mfma -Wno-missing-field-initializers -O3 -DNDEBUG
C++ compiler:       /usr/bin/c++ GNU 11.4.0
C++ compiler flags: -fexcess-precision=fast -funroll-all-loops -mavx2 -
mfma -Wno-missing-field-initializers -Wno-cast-function-type-strict -
fopenmp -O3 -DNDEBUG
BLAS library:       Internal
LAPACK library:     Internal


Running on 3 nodes with total 18 cores, 18 processing units
  Cores per node:            6
  Logical processing units per node:    6
  OS CPU Limit / recommended threads to start per node:    6
Hardware detected on host cpu-sev-7 (the node of MPI rank 0):
  CPU info:
    Vendor: AMD
    Brand:  AMD EPYC-Milan Processor
    Family: 25   Model: 1   Stepping: 1
    Features: aes amd apic avx avx2 clfsh cmov cx8 cx16 f16c fma lahf
misalignsse mmx msr pcid pclmuldq pdpe1gb popcnt pse rdrnd rdtscp sha
sse2 sse3 sse4a sse4.1 sse4.2 ssse3 tdt x2apic
  Hardware topology: Basic
    Packages, cores, and logical processors:
    [indices refer to OS logical processors]
      Package  0: [   0]
      Package  1: [   1]
      Package  2: [   2]
      Package  3: [   3]
      Package  4: [   4]
      Package  5: [   5]
    CPU limit set by OS: -1   Recommended max number of threads: 6


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
M. J. Abraham, T. Murtola, R. Schulz, S. P√°ll, J. C. Smith, B. Hess, E.
Lindahl
GROMACS: High performance molecular simulations through multi-level
parallelism from laptops to supercomputers
SoftwareX 1 (2015) pp. 19-25
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. P√°ll, M. J. Abraham, C. Kutzner, B. Hess, E. Lindahl
Tackling Exascale Software Challenges in Molecular Dynamics Simulations
with
GROMACS
In S. Markidis & E. Laure (Eds.), Solving Software Challenges for
Exascale 8759 (2015) pp. 3-27
```

```
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. Pronk, S. P√°ll, R. Schulz, P. Larsson, P. Bjelkmar, R. Apostolov, M.
R.
Shirts, J. C. Smith, P. M. Kasson, D. van der Spoel, B. Hess, and E.
Lindahl
GROMACS 4.5: a high-throughput and highly parallel open source molecular
simulation toolkit
Bioinformatics 29 (2013) pp. 845-54
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
B. Hess and C. Kutzner and D. van der Spoel and E. Lindahl
GROMACS 4: Algorithms for highly efficient, load-balanced, and scalable
molecular simulation
J. Chem. Theory Comput. 4 (2008) pp. 435-447
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
D. van der Spoel, E. Lindahl, B. Hess, G. Groenhof, A. E. Mark and H. J.
C.
Berendsen
GROMACS: Fast, Flexible and Free
J. Comp. Chem. 26 (2005) pp. 1701-1719
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
E. Lindahl and B. Hess and D. van der Spoel
GROMACS 3.0: A package for molecular simulation and trajectory analysis
J. Mol. Mod. 7 (2001) pp. 306-317
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
H. J. C. Berendsen, D. van der Spoel and R. van Drunen
GROMACS: A message-passing parallel molecular dynamics implementation
Comp. Phys. Comm. 91 (1995) pp. 43-56
-------- -------- --- Thank You --- -------- --------


++++ PLEASE CITE THE DOI FOR THIS VERSION OF GROMACS ++++
https://doi.org/10.5281/zenodo.10017686
-------- -------- --- Thank You --- -------- --------


The number of OpenMP threads was set by environment variable
OMP_NUM_THREADS to 1

Input Parameters:
   integrator                     = md
   tinit                          = 0
   dt                             = 0.004
   nsteps                         = 10000
```

```
init-step                      = 0
simulation-part                = 1
mts                            = false
comm-mode                      = Linear
nstcomm                        = 100
bd-fric                        = 0
ld-seed                        = 14771
emtol                          = 1e-05
emstep                         = 0.01
niter                          = 20
fcstep                         = 0
nstcgsteep                     = 1000
nbfgscorr                      = 10
rtpi                           = 0.05
nstxout                        = 0
nstvout                        = 0
nstfout                        = 0
nstlog                         = 0
nstcalcenergy                  = 100
nstenergy                      = 500
nstxout-compressed             = 0
compressed-x-precision         = 1000
cutoff-scheme                  = Verlet
nstlist                        = 25
pbc                            = xyz
periodic-molecules             = false
verlet-buffer-tolerance        = 0.005
rlist                          = 1.041
coulombtype                    = PME
coulomb-modifier               = Potential-shift
rcoulomb-switch                = 0
rcoulomb                       = 1
epsilon-r                      = 1
epsilon-rf                     = inf
vdw-type                       = Cut-off
vdw-modifier                   = Potential-shift
rvdw-switch                    = 0
rvdw                           = 1
DispCorr                       = No
table-extension                = 1
fourierspacing                 = 0.135
fourier-nx                     = 240
fourier-ny                     = 240
fourier-nz                     = 240
pme-order                      = 4
ewald-rtol                     = 1e-06
ewald-rtol-lj                  = 1e-06
lj-pme-comb-rule               = Geometric
ewald-geometry                 = 3d
epsilon-surface                = 0
ensemble-temperature-setting   = constant
ensemble-temperature           = 300
tcoupl                         = V-rescale
nsttcouple                     = 25
nh-chain-length                = 0
print-nose-hoover-chain-variables = false
pcoupl                         = Berendsen
pcoupltype                     = Isotropic
```

```
   nstpcouple                     = 25
   tau-p                          = 1
   compressibility (3x3):
      compressibility[    0]={ 4.50000e-05,  0.00000e+00,  0.00000e+00}
      compressibility[    1]={ 0.00000e+00,  4.50000e-05,  0.00000e+00}
      compressibility[    2]={ 0.00000e+00,  0.00000e+00,  4.50000e-05}
   ref-p (3x3):
      ref-p[    0]={ 1.00000e+00,  0.00000e+00,  0.00000e+00}
      ref-p[    1]={ 0.00000e+00,  1.00000e+00,  0.00000e+00}
      ref-p[    2]={ 0.00000e+00,  0.00000e+00,  1.00000e+00}
   refcoord-scaling               = No
   posres-com (3):
      posres-com[0]= 0.00000e+00
      posres-com[1]= 0.00000e+00
      posres-com[2]= 0.00000e+00
   posres-comB (3):
      posres-comB[0]= 0.00000e+00
      posres-comB[1]= 0.00000e+00
      posres-comB[2]= 0.00000e+00
   QMMM                           = false
qm-opts:
   ngQM                           = 0
   constraint-algorithm           = Lincs
   continuation                   = false
   Shake-SOR                      = false
   shake-tol                      = 0.0001
   lincs-order                    = 6
   lincs-iter                     = 2
   lincs-warnangle                = 30
   nwall                          = 0
   wall-type                      = 9-3
   wall-r-linpot                  = -1
   wall-atomtype[0]               = -1
   wall-atomtype[1]               = -1
   wall-density[0]                = 0
   wall-density[1]                = 0
   wall-ewald-zfac                = 3
   pull                           = false
   awh                            = false
   rotation                       = false
   interactiveMD                  = false
   disre                          = No
   disre-weighting                = Equal
   disre-mixed                    = false
   dr-fc                          = 1000
   dr-tau                         = 0
   nstdisreout                    = 100
   orire-fc                       = 0
   orire-tau                      = 0
   nstorireout                    = 100
   free-energy                    = no
   cos-acceleration               = 0
   deform (3x3):
      deform[    0]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
      deform[    1]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
      deform[    2]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
   simulated-tempering            = false
   swapcoords                     = no
```

```
   userint1                       = 0
   userint2                       = 0
   userint3                       = 0
   userint4                       = 0
   userreal1                      = 0
   userreal2                      = 0
   userreal3                      = 0
   userreal4                      = 0
   applied-forces:
     electric-field:
grpopts:
   nrdf:      292326  3.76895e+06
   ref-t:         300         300
   tau-t:         0.1         0.1
annealing:          No          No
annealing-npoints:           0           0
   acc:               0           0           0
   nfreeze:           N           N           N
   energygrp-flags[  0]: 0


Changing rlist from 1.041 to 1 for non-bonded 4x4 atom kernels

Changing nstlist from 25 to 80, rlist from 1 to 1.124

Update groups can not be used for this system because an incompatible
virtual site type is used

Initializing Domain Decomposition on 18 ranks
Dynamic load balancing: auto
Minimum cell size due to atom displacement: 2.155 nm
Initial maximum distances in bonded interactions:
    two-body bonded interactions: 0.433 nm, LJ-14, atoms 176875 176884
  multi-body bonded interactions: 0.433 nm, Ryckaert-Bell., atoms 176875
176884
Minimum cell size due to bonded interactions: 0.476 nm
Maximum distance for 7 constraints, at 120 deg. angles, all-trans: 1.166
nm
Estimated maximum distance required for P-LINCS: 1.166 nm
Scaling the initial minimum size with 1/0.8 (option -dds) = 1.25
Using 0 separate PME ranks because: there are too few total ranks for
efficient splitting
Optimizing the DD grid for 18 cells with a minimum initial size of 2.694
nm
The maximum allowed number of cells is: X 9 Y 9 Z 8
Domain decomposition grid 6 x 3 x 1, separate PME ranks 0
PME domain decomposition: 6 x 3 x 1
Domain decomposition rank 0, coordinates 0 0 0

The initial number of communication pulses is: X 1 Y 1
The initial domain decomposition cell size is: X 4.25 nm Y 8.50 nm

The maximum allowed distance for atoms involved in interactions is:
                 non-bonded interactions           1.124 nm
(the following are initial values, they could change due to box
deformation)
            two-body bonded interactions  (-rdd)   1.124 nm
          multi-body bonded interactions  (-rdd)   1.124 nm
```

```
              virtual site constructions  (-rcon)  4.252 nm
  atoms separated by up to 7 constraints  (-rcon)  4.252 nm

When dynamic load balancing gets turned on, these settings will change
to:
The maximum number of communication pulses is: X 1 Y 1
The minimum size for domain decomposition cells is 2.155 nm
The requested allowed shrink of DD cells (option -dds) is: 0.80
The allowed shrink of domain decomposition cells is: X 0.51 Y 0.25
The maximum allowed distance for atoms involved in interactions is:
                 non-bonded interactions           1.124 nm
            two-body bonded interactions  (-rdd)   1.124 nm
          multi-body bonded interactions  (-rdd)   1.124 nm
              virtual site constructions  (-rcon)  2.155 nm
  atoms separated by up to 7 constraints  (-rcon)  2.155 nm
Using two step summing over 3 groups of on average 6.0 ranks


Using 18 MPI processes

Non-default thread affinity set, disabling internal thread affinity

Using 1 OpenMP thread per MPI process

System total charge: -0.000
Will do PME sum in reciprocal space for electrostatic interactions.

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
U. Essmann, L. Perera, M. L. Berkowitz, T. Darden, H. Lee and L. G.
Pedersen
A smooth particle mesh Ewald method
J. Chem. Phys. 103 (1995) pp. 8577-8592
-------- -------- --- Thank You --- -------- --------

Using a Gaussian width (1/beta) of 0.289108 nm for Ewald
Potential shift: LJ r^-12: -1.000e+00 r^-6: -1.000e+00, Ewald -1.000e-06
Initialized non-bonded Coulomb Ewald tables, spacing: 8.87e-04 size: 1129

Generated table with 1062 data points for 1-4 COUL.
Tabscale = 500 points/nm
Generated table with 1062 data points for 1-4 LJ6.
Tabscale = 500 points/nm
Generated table with 1062 data points for 1-4 LJ12.
Tabscale = 500 points/nm


Using SIMD 4x8 nonbonded short-range kernels

Using a dual 4x8 pair-list setup updated with dynamic pruning:
  outer list: updated every 80 steps, buffer 0.124 nm, rlist 1.124 nm
  inner list: updated every 30 steps, buffer 0.002 nm, rlist 1.002 nm
At tolerance 0.005 kJ/mol/ps per atom, equivalent classical 1x1 list
would be:
  outer list: updated every 80 steps, buffer 0.330 nm, rlist 1.330 nm
  inner list: updated every 30 steps, buffer 0.144 nm, rlist 1.144 nm

The non-bonded pair calculation algorithm tolerates a few missing pair
interactions close to the cut-off. This can lead to a systematic
```

```
overestimation of the pressure due to missing LJ interactions. The error
in the average pressure due to missing LJ interactions is at most 7.54
bar.
The pressure error can be controlled by setting the environment variable
GMX_VERLET_BUFFER_PRESSURE_TOLERANCE to the allowed error in units of
bar.

Using Lorentz-Berthelot Lennard-Jones combination rule
Removing pbc first time

Linking all bonded interactions to atoms
There are 98588 inter update-group virtual sites,
will perform an extra communication step for selected coordinates and
forces


Initializing Parallel LINear Constraint Solver

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
B. Hess
P-LINCS: A Parallel Linear Constraint Solver for molecular simulation
J. Chem. Theory Comput. 4 (2008) pp. 116-122
-------- -------- --- Thank You --- -------- --------

The number of constraints is 179952
There are constraints between atoms in different decomposition domains,
will communicate selected coordinates each lincs iteration
29316 constraints are involved in constraint triangles,
will apply an additional matrix expansion of order 6 for couplings
between constraints inside triangles

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. Miyamoto and P. A. Kollman
SETTLE: An Analytical Version of the SHAKE and RATTLE Algorithms for
Rigid
Water Models
J. Comp. Chem. 13 (1992) pp. 952-962
-------- -------- --- Thank You --- -------- --------


Intra-simulation communication will occur every 25 steps.

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
G. Bussi, D. Donadio and M. Parrinello
Canonical sampling through velocity rescaling
J. Chem. Phys. 126 (2007) pp. 014101
-------- -------- --- Thank You --- -------- --------

There are: 2037824 Atoms
There are: 98588 VSites
Atom distribution over 18 domains: av 118689 stddev 2667 min 115469 max
123890

Constraining the starting coordinates (step 0)

Constraining the coordinates at t0-dt (step 0)
Center of mass motion removal mode is Linear
We have the following groups for center of mass motion removal:
```

```
  0:  rest
RMS relative constraint deviation after constraining: 1.01e-05
Initial temperature: 302.747 K

Started mdrun on rank 0 Fri Jan 12 23:52:01 2024

           Step           Time
              0        0.00000

   Energies (kJ/mol)
  Connect Bonds          Angle    Proper Dih. Ryckaert-Bell.          LJ-
14
    0.00000e+00    3.47960e+05    1.20867e+04    7.60989e+05
2.87074e+05
     Coulomb-14        LJ (SR)   Coulomb (SR)   Coul. recip.
Potential
   -1.18825e+06    5.05954e+06   -4.35900e+07    3.60933e+05   -
3.79497e+07
    Kinetic En.   Total Energy  Conserved En.    Temperature Pressure
(bar)
    5.39098e+06   -3.25587e+07   -3.25484e+07    3.19301e+02   -
5.32616e+02
   Constr. rmsd
    9.94992e-06


DD  step 79 load imb.: force 29.3%

step 160 Turning on dynamic load balancing, because the performance loss
due to load imbalance is 11.0 %.
Writing checkpoint, step 4000 at Sat Jan 13 00:07:11 2024


Writing checkpoint, step 7840 at Sat Jan 13 00:22:08 2024



DD  step 9999  vol min/aver 0.740  load imb.: force 27.1%
           Step           Time
          10000       40.00000

Writing checkpoint, step 10000 at Sat Jan 13 00:30:16 2024


   Energies (kJ/mol)
  Connect Bonds          Angle    Proper Dih. Ryckaert-Bell.          LJ-
14
    0.00000e+00    3.48445e+05    1.20406e+04    7.60805e+05
2.86850e+05
     Coulomb-14        LJ (SR)   Coulomb (SR)   Coul. recip.
Potential
   -1.18602e+06    5.16137e+06   -4.37876e+07    3.52803e+05   -
3.80513e+07
    Kinetic En.   Total Energy  Conserved En.    Temperature Pressure
(bar)
    5.06608e+06   -3.29852e+07   -3.25895e+07    3.00058e+02
1.71065e+01
   Constr. rmsd
```

```
    9.37171e-06


Energy conservation over simulation part #1 of length 40 ps, time 0 to 40
ps
  Conserved energy drift: -4.81e-04 kJ/mol/ps per atom


      <======  ###############  ==>
      <====  A V E R A G E S  ====>
      <==  ###############  ======>

      Statistics over 10001 steps using 101 frames

   Energies (kJ/mol)
  Connect Bonds          Angle    Proper Dih. Ryckaert-Bell.          LJ-
14
    0.00000e+00    3.47995e+05    1.19406e+04    7.60961e+05
2.87410e+05
     Coulomb-14        LJ (SR)   Coulomb (SR)   Coul. recip.
Potential
   -1.18710e+06    5.16034e+06   -4.37865e+07    3.53180e+05   -
3.80518e+07
    Kinetic En.   Total Energy  Conserved En.    Temperature Pressure
(bar)
    5.06795e+06   -3.29839e+07   -3.25691e+07    3.00169e+02   -
1.24221e+01
   Constr. rmsd
    0.00000e+00

          Box-X          Box-Y          Box-Z
    3.10286e+01    3.10286e+01    2.19406e+01

   Total Virial (kJ/mol)
    1.69824e+06    2.53139e+02   -1.89334e+03
    2.51646e+02    1.69849e+06    3.33313e+03
   -1.88645e+03    3.33363e+03    1.69528e+06

   Pressure (bar)
   -1.28799e+01   -1.74429e+00    1.31112e+00
   -1.74193e+00   -1.49511e+01   -4.27041e+00
    1.30028e+00   -4.27120e+00   -9.43536e+00

          T-mol      T-solvent
    3.00036e+02    3.00179e+02


     M E G A - F L O P S   A C C O U N T I N G

 NB=Group-cutoff nonbonded kernels    NxN=N-by-N cluster Verlet kernels
 RF=Reaction-Field  VdW=Van der Waals  QSTab=quadratic-spline table
 W3=SPC/TIP3p  W4=TIP4p (single or pairs)
 V&F=Potential and force  V=Potential only  F=Force only

 Computing:                                M-Number         M-Flops  %
Flops
-----------------------------------------------------------------------
----
```

Pair Search distance check	128740.125026	1158661.125	0.1
NxN Ewald Elec. + LJ [F]	7581691.407120	500391632.870	53.3
NxN Ewald Elec. + LJ [V&F]	77344.082640	8275816.842	0.9
NxN Ewald Elec. [F]	5761664.572368	351461538.914	37.5
NxN Ewald Elec. [V&F]	58778.709520	4937411.600	0.5
1,4 nonbonded interactions	6369.046841	573214.216	0.1
Calc Weights	64098.769236	2307555.692	0.2
Spread Q Bspline	1367440.410368	2734880.821	0.3
Gather F Bspline	1367440.410368	8204642.462	0.9
3D-FFT	6558947.569174	52471580.553	5.6
Solve PME	1728.172800	110603.059	0.0
Reset In Box	269.187912	807.564	0.0
CG-CoM	271.324324	813.973	0.0
Angles	4258.985856	715509.624	0.1
Propers	212.081206	48566.596	0.0
RB-Dihedrals	6469.816917	1598044.778	0.2
Virial	857.026022	15426.468	0.0
Stop-CM	217.914024	2179.140	0.0
P-Coupling	856.701212	5140.207	0.0
Calc-Ekin	1713.402424	46261.865	0.0
Lincs	2296.148903	137768.934	0.0
Lincs-Mat	62996.752492	251987.010	0.0
Constraint-V	23920.186001	215281.674	0.0
Constraint-Vir	866.961270	20807.070	0.0
Settle	6443.424897	2384067.212	0.3
Virtual Site 3	91.938707	3401.732	0.0
Virtual Site 3fd	193.227552	18356.617	0.0
Virtual Site 3fad	110.344416	19420.617	0.0
Virtual Site 3out	361.968796	31491.285	0.0

```
 Virtual Site 4fd                        100.036034       11003.964
0.0
 Virtual Site 4fdn                       170.062298       43195.824
0.0
-----------------------------------------------------------------------
----
 Total                                                938197070.312
100.0
-----------------------------------------------------------------------
----


    D O M A I N   D E C O M P O S I T I O N   S T A T I S T I C S

 av. #atoms communicated per step for force:  2 x 1038367.2
 av. #atoms communicated per step for vsites: 3 x 8190.3
 av. #atoms communicated per step for LINCS:  3 x 111849.7


Dynamic load balancing report:
 DLB was turned on during the run due to measured imbalance.
 Average load imbalance: 33.2%.
 The balanceable part of the MD step is 39%, load imbalance is computed
from this.
 Part of the total run time spent waiting due to load imbalance: 12.9%.
 Steps where the load balancing was limited by -rdd, -rcon and/or -dds: X
0 % Y 0 %

NOTE: 12.9 % of the available CPU time was lost due to load imbalance
      in the domain decomposition.
      You can consider manually changing the decomposition (option -dd);
      e.g. by using fewer domains along the box dimension in which there
is
      considerable inhomogeneity in the simulated system.

      R E A L   C Y C L E   A N D   T I M E   A C C O U N T I N G

On 18 MPI ranks

 Activity:              Num   Num      Call    Wall time         Giga-
Cycles
                       Ranks Threads  Count      (s)         total sum
%
-----------------------------------------------------------------------
-------
 Domain decomp.           18    1        126      27.684       1467.234
1.2
 DD comm. load            18    1        125       0.096          5.067
0.0
 DD comm. bounds          18    1        124       0.928         49.202
0.0
 Vsite constr.            18    1      10001      17.494        927.184
0.8
 Neighbor search          18    1        126      26.800       1420.406
1.2
 Comm. coord.             18    1       9875      22.374       1185.791
1.0
```

```
 Force                  18    1      10001     820.495      43485.866
35.7
 Wait + Comm. F         18    1      10001      24.516       1299.340
1.1
 PME mesh               18    1      10001    1203.341      63776.560
52.3
 NB X/F buffer ops.     18    1      29751       9.907        525.090
0.4
 Vsite spread           18    1      10402      20.385       1080.421
0.9
 Write traj.            18    1          3       0.705         37.343
0.0
 Update                 18    1      10001       6.303        334.030
0.3
 Constraints            18    1      10003     115.185       6104.753
5.0
 Comm. energies         18    1        401       1.742         92.344
0.1
 Rest                                             2.278        120.745
0.1
-----------------------------------------------------------------------
-------
 Total                                         2300.233     121911.376
100.0
-----------------------------------------------------------------------
-------
 Breakdown of PME mesh activities
-----------------------------------------------------------------------
-------
 PME redist. X/F        18    1      20002     474.926      25170.891
20.6
 PME spread             18    1      10001     155.171       8223.998
6.7
 PME gather             18    1      10001     111.205       5893.839
4.8
 PME 3D-FFT             18    1      20002     123.268       6533.132
5.4
 PME 3D-FFT Comm.       18    1      40004     332.173      17605.032
14.4
 PME solve Elec         18    1      10001       6.398        339.087
0.3
-----------------------------------------------------------------------
-------

               Core t (s)   Wall t (s)        (%)
       Time:    41403.986     2300.233     1800.0
                         38:20
                 (ns/day)    (hour/ns)
Performance:        1.503       15.972
Finished mdrun on rank 0 Sat Jan 13 00:30:21 2024
```

benchRIB_cpu-sev-cluster_10n

```
                :-) GROMACS - gmx mdrun, 2023.3 (-:

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       Jon Vincent             Teemu Virolainen          Christian
Wennberg
       Maarten Wolf

                    Coordinated by the GROMACS project leaders:
                      Paul Bauer, Berk Hess, and Erik Lindahl

GROMACS:      gmx mdrun, version 2023.3
Executable:   /usr/local/gromacs/bin/gmx_mpi
Data prefix:  /usr/local/gromacs
Working dir:  /home/ubuntu
Process ID:   24913
Command line:
  gmx_mpi mdrun -v -s /mnt/shared/home/ubuntu/mpinat-gromacs/mpinat-
gromacs-standard-md-bench/benchRIB.tpr

GROMACS version:    2023.3
Precision:          mixed
Memory model:       64 bit
MPI library:        MPI
OpenMP support:     enabled (GMX_OPENMP_MAX_THREADS = 128)
GPU support:        disabled
SIMD instructions:  AVX2_256
```

```
CPU FFT library:    fftw-3.3.8-sse2-avx-avx2-avx2_128
GPU FFT library:    none
Multi-GPU FFT:      none
RDTSCP usage:       enabled
TNG support:        enabled
Hwloc support:      disabled
Tracing support:    disabled
C compiler:         /usr/bin/cc GNU 11.4.0
C compiler flags:   -fexcess-precision=fast -funroll-all-loops -mavx2 -
mfma -Wno-missing-field-initializers -O3 -DNDEBUG
C++ compiler:       /usr/bin/c++ GNU 11.4.0
C++ compiler flags: -fexcess-precision=fast -funroll-all-loops -mavx2 -
mfma -Wno-missing-field-initializers -Wno-cast-function-type-strict -
fopenmp -O3 -DNDEBUG
BLAS library:       Internal
LAPACK library:     Internal


Running on 10 nodes with total 60 cores, 60 processing units
  Cores per node:            6
  Logical processing units per node:    6
  OS CPU Limit / recommended threads to start per node:    6
Hardware detected on host cpu-sev-1 (the node of MPI rank 0):
  CPU info:
    Vendor: AMD
    Brand:  AMD EPYC-Milan Processor
    Family: 25   Model: 1   Stepping: 1
    Features: aes amd apic avx avx2 clfsh cmov cx8 cx16 f16c fma lahf
misalignsse mmx msr pcid pclmuldq pdpe1gb popcnt pse rdrnd rdtscp sha
sse2 sse3 sse4a sse4.1 sse4.2 ssse3 tdt x2apic
  Hardware topology: Basic
    Packages, cores, and logical processors:
    [indices refer to OS logical processors]
      Package  0: [   0]
      Package  1: [   1]
      Package  2: [   2]
      Package  3: [   3]
      Package  4: [   4]
      Package  5: [   5]
    CPU limit set by OS: -1   Recommended max number of threads: 6


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
M. J. Abraham, T. Murtola, R. Schulz, S. P√°ll, J. C. Smith, B. Hess, E.
Lindahl
GROMACS: High performance molecular simulations through multi-level
parallelism from laptops to supercomputers
SoftwareX 1 (2015) pp. 19-25
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. P√°ll, M. J. Abraham, C. Kutzner, B. Hess, E. Lindahl
Tackling Exascale Software Challenges in Molecular Dynamics Simulations
with
GROMACS
In S. Markidis & E. Laure (Eds.), Solving Software Challenges for
Exascale 8759 (2015) pp. 3-27
```

```
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. Pronk, S. P√°ll, R. Schulz, P. Larsson, P. Bjelkmar, R. Apostolov, M.
R.
Shirts, J. C. Smith, P. M. Kasson, D. van der Spoel, B. Hess, and E.
Lindahl
GROMACS 4.5: a high-throughput and highly parallel open source molecular
simulation toolkit
Bioinformatics 29 (2013) pp. 845-54
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
B. Hess and C. Kutzner and D. van der Spoel and E. Lindahl
GROMACS 4: Algorithms for highly efficient, load-balanced, and scalable
molecular simulation
J. Chem. Theory Comput. 4 (2008) pp. 435-447
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
D. van der Spoel, E. Lindahl, B. Hess, G. Groenhof, A. E. Mark and H. J.
C.
Berendsen
GROMACS: Fast, Flexible and Free
J. Comp. Chem. 26 (2005) pp. 1701-1719
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
E. Lindahl and B. Hess and D. van der Spoel
GROMACS 3.0: A package for molecular simulation and trajectory analysis
J. Mol. Mod. 7 (2001) pp. 306-317
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
H. J. C. Berendsen, D. van der Spoel and R. van Drunen
GROMACS: A message-passing parallel molecular dynamics implementation
Comp. Phys. Comm. 91 (1995) pp. 43-56
-------- -------- --- Thank You --- -------- --------


++++ PLEASE CITE THE DOI FOR THIS VERSION OF GROMACS ++++
https://doi.org/10.5281/zenodo.10017686
-------- -------- --- Thank You --- -------- --------


The number of OpenMP threads was set by environment variable
OMP_NUM_THREADS to 1

Input Parameters:
   integrator                   = md
   tinit                        = 0
   dt                           = 0.004
   nsteps                       = 10000
```

```
init-step                      = 0
simulation-part                = 1
mts                            = false
comm-mode                      = Linear
nstcomm                        = 100
bd-fric                        = 0
ld-seed                        = 14771
emtol                          = 1e-05
emstep                         = 0.01
niter                          = 20
fcstep                         = 0
nstcgsteep                     = 1000
nbfgscorr                      = 10
rtpi                           = 0.05
nstxout                        = 0
nstvout                        = 0
nstfout                        = 0
nstlog                         = 0
nstcalcenergy                  = 100
nstenergy                      = 500
nstxout-compressed             = 0
compressed-x-precision         = 1000
cutoff-scheme                  = Verlet
nstlist                        = 25
pbc                            = xyz
periodic-molecules             = false
verlet-buffer-tolerance        = 0.005
rlist                          = 1.041
coulombtype                    = PME
coulomb-modifier               = Potential-shift
rcoulomb-switch                = 0
rcoulomb                       = 1
epsilon-r                      = 1
epsilon-rf                     = inf
vdw-type                       = Cut-off
vdw-modifier                   = Potential-shift
rvdw-switch                    = 0
rvdw                           = 1
DispCorr                       = No
table-extension                = 1
fourierspacing                 = 0.135
fourier-nx                     = 240
fourier-ny                     = 240
fourier-nz                     = 240
pme-order                      = 4
ewald-rtol                     = 1e-06
ewald-rtol-lj                  = 1e-06
lj-pme-comb-rule               = Geometric
ewald-geometry                 = 3d
epsilon-surface                = 0
ensemble-temperature-setting   = constant
ensemble-temperature           = 300
tcoupl                         = V-rescale
nsttcouple                     = 25
nh-chain-length                = 0
print-nose-hoover-chain-variables = false
pcoupl                         = Berendsen
pcoupltype                     = Isotropic
```

```
   nstpcouple                     = 25
   tau-p                          = 1
   compressibility (3x3):
      compressibility[    0]={ 4.50000e-05,  0.00000e+00,  0.00000e+00}
      compressibility[    1]={ 0.00000e+00,  4.50000e-05,  0.00000e+00}
      compressibility[    2]={ 0.00000e+00,  0.00000e+00,  4.50000e-05}
   ref-p (3x3):
      ref-p[    0]={ 1.00000e+00,  0.00000e+00,  0.00000e+00}
      ref-p[    1]={ 0.00000e+00,  1.00000e+00,  0.00000e+00}
      ref-p[    2]={ 0.00000e+00,  0.00000e+00,  1.00000e+00}
   refcoord-scaling               = No
   posres-com (3):
      posres-com[0]= 0.00000e+00
      posres-com[1]= 0.00000e+00
      posres-com[2]= 0.00000e+00
   posres-comB (3):
      posres-comB[0]= 0.00000e+00
      posres-comB[1]= 0.00000e+00
      posres-comB[2]= 0.00000e+00
   QMMM                           = false
qm-opts:
   ngQM                           = 0
   constraint-algorithm           = Lincs
   continuation                   = false
   Shake-SOR                      = false
   shake-tol                      = 0.0001
   lincs-order                    = 6
   lincs-iter                     = 2
   lincs-warnangle                = 30
   nwall                          = 0
   wall-type                      = 9-3
   wall-r-linpot                  = -1
   wall-atomtype[0]               = -1
   wall-atomtype[1]               = -1
   wall-density[0]                = 0
   wall-density[1]                = 0
   wall-ewald-zfac                = 3
   pull                           = false
   awh                            = false
   rotation                       = false
   interactiveMD                  = false
   disre                          = No
   disre-weighting                = Equal
   disre-mixed                    = false
   dr-fc                          = 1000
   dr-tau                         = 0
   nstdisreout                    = 100
   orire-fc                       = 0
   orire-tau                      = 0
   nstorireout                    = 100
   free-energy                    = no
   cos-acceleration               = 0
   deform (3x3):
      deform[    0]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
      deform[    1]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
      deform[    2]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
   simulated-tempering            = false
   swapcoords                     = no
```

```
   userint1                       = 0
   userint2                       = 0
   userint3                       = 0
   userint4                       = 0
   userreal1                      = 0
   userreal2                      = 0
   userreal3                      = 0
   userreal4                      = 0
   applied-forces:
     electric-field:
grpopts:
   nrdf:      292326  3.76895e+06
   ref-t:         300         300
   tau-t:         0.1         0.1
annealing:          No          No
annealing-npoints:           0           0
   acc:               0           0           0
   nfreeze:           N           N           N
   energygrp-flags[  0]: 0


Changing rlist from 1.041 to 1 for non-bonded 4x4 atom kernels

Changing nstlist from 25 to 80, rlist from 1 to 1.124

Update groups can not be used for this system because an incompatible
virtual site type is used

Initializing Domain Decomposition on 60 ranks
Dynamic load balancing: auto
Minimum cell size due to atom displacement: 2.155 nm
Initial maximum distances in bonded interactions:
    two-body bonded interactions: 0.433 nm, LJ-14, atoms 176875 176884
  multi-body bonded interactions: 0.433 nm, Ryckaert-Bell., atoms 176875
176884
Minimum cell size due to bonded interactions: 0.476 nm
Maximum distance for 7 constraints, at 120 deg. angles, all-trans: 1.166
nm
Estimated maximum distance required for P-LINCS: 1.166 nm
Scaling the initial minimum size with 1/0.8 (option -dds) = 1.25
Guess for relative PME load: 0.22
Will use 45 particle-particle and 15 PME only ranks
This is a guess, check the performance at the end of the log file
Using 15 separate PME ranks, as guessed by mdrun
Optimizing the DD grid for 45 cells with a minimum initial size of 2.694
nm
The maximum allowed number of cells is: X 9 Y 9 Z 8
Domain decomposition grid 9 x 5 x 1, separate PME ranks 15
PME domain decomposition: 15 x 1 x 1
Interleaving PP and PME ranks
This rank does only particle-particle work.
Domain decomposition rank 0, coordinates 0 0 0

The initial number of communication pulses is: X 1 Y 1
The initial domain decomposition cell size is: X 2.83 nm Y 5.10 nm

The maximum allowed distance for atoms involved in interactions is:
                 non-bonded interactions           1.124 nm
```

```
(the following are initial values, they could change due to box
deformation)
            two-body bonded interactions  (-rdd)   1.124 nm
          multi-body bonded interactions  (-rdd)   1.124 nm
              virtual site constructions  (-rcon)  2.835 nm
  atoms separated by up to 7 constraints  (-rcon)  2.835 nm

When dynamic load balancing gets turned on, these settings will change
to:
The maximum number of communication pulses is: X 1 Y 1
The minimum size for domain decomposition cells is 2.155 nm
The requested allowed shrink of DD cells (option -dds) is: 0.80
The allowed shrink of domain decomposition cells is: X 0.76 Y 0.42
The maximum allowed distance for atoms involved in interactions is:
                 non-bonded interactions           1.124 nm
            two-body bonded interactions  (-rdd)   1.124 nm
          multi-body bonded interactions  (-rdd)   1.124 nm
              virtual site constructions  (-rcon)  2.155 nm
  atoms separated by up to 7 constraints  (-rcon)  2.155 nm
Using two step summing over 10 groups of on average 4.5 ranks


Using 60 MPI processes

Non-default thread affinity set, disabling internal thread affinity

Using 1 OpenMP thread per MPI process

System total charge: -0.000
Will do PME sum in reciprocal space for electrostatic interactions.

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
U. Essmann, L. Perera, M. L. Berkowitz, T. Darden, H. Lee and L. G.
Pedersen
A smooth particle mesh Ewald method
J. Chem. Phys. 103 (1995) pp. 8577-8592
-------- -------- --- Thank You --- -------- --------

Using a Gaussian width (1/beta) of 0.289108 nm for Ewald
Potential shift: LJ r^-12: -1.000e+00 r^-6: -1.000e+00, Ewald -1.000e-06
Initialized non-bonded Coulomb Ewald tables, spacing: 8.87e-04 size: 1129

Generated table with 1062 data points for 1-4 COUL.
Tabscale = 500 points/nm
Generated table with 1062 data points for 1-4 LJ6.
Tabscale = 500 points/nm
Generated table with 1062 data points for 1-4 LJ12.
Tabscale = 500 points/nm


Using SIMD 4x8 nonbonded short-range kernels

Using a dual 4x8 pair-list setup updated with dynamic pruning:
  outer list: updated every 80 steps, buffer 0.124 nm, rlist 1.124 nm
  inner list: updated every 30 steps, buffer 0.002 nm, rlist 1.002 nm
At tolerance 0.005 kJ/mol/ps per atom, equivalent classical 1x1 list
would be:
  outer list: updated every 80 steps, buffer 0.330 nm, rlist 1.330 nm
```

```
  inner list: updated every 30 steps, buffer 0.144 nm, rlist 1.144 nm

The non-bonded pair calculation algorithm tolerates a few missing pair
interactions close to the cut-off. This can lead to a systematic
overestimation of the pressure due to missing LJ interactions. The error
in the average pressure due to missing LJ interactions is at most 7.54
bar.
The pressure error can be controlled by setting the environment variable
GMX_VERLET_BUFFER_PRESSURE_TOLERANCE to the allowed error in units of
bar.

Using Lorentz-Berthelot Lennard-Jones combination rule
Removing pbc first time

Linking all bonded interactions to atoms
There are 98588 inter update-group virtual sites,
will perform an extra communication step for selected coordinates and
forces


Initializing Parallel LINear Constraint Solver

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
B. Hess
P-LINCS: A Parallel Linear Constraint Solver for molecular simulation
J. Chem. Theory Comput. 4 (2008) pp. 116-122
-------- -------- --- Thank You --- -------- --------

The number of constraints is 179952
There are constraints between atoms in different decomposition domains,
will communicate selected coordinates each lincs iteration
29316 constraints are involved in constraint triangles,
will apply an additional matrix expansion of order 6 for couplings
between constraints inside triangles

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. Miyamoto and P. A. Kollman
SETTLE: An Analytical Version of the SHAKE and RATTLE Algorithms for
Rigid
Water Models
J. Comp. Chem. 13 (1992) pp. 952-962
-------- -------- --- Thank You --- -------- --------


Intra-simulation communication will occur every 25 steps.

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
G. Bussi, D. Donadio and M. Parrinello
Canonical sampling through velocity rescaling
J. Chem. Phys. 126 (2007) pp. 014101
-------- -------- --- Thank You --- -------- --------

There are: 2037824 Atoms
There are: 98588 VSites
Atom distribution over 45 domains: av 47475 stddev 1177 min 45929 max
49545

Constraining the starting coordinates (step 0)
```

```
Constraining the coordinates at t0-dt (step 0)
Center of mass motion removal mode is Linear
We have the following groups for center of mass motion removal:
  0:  rest
RMS relative constraint deviation after constraining: 1.01e-05
Initial temperature: 302.751 K

Started mdrun on rank 0 Sun Jan 14 14:01:17 2024

           Step           Time
              0        0.00000

   Energies (kJ/mol)
  Connect Bonds          Angle    Proper Dih. Ryckaert-Bell.          LJ-
14
    0.00000e+00    3.47961e+05    1.20867e+04    7.60995e+05
2.87071e+05
     Coulomb-14        LJ (SR)   Coulomb (SR)   Coul. recip.
Potential
   -1.18825e+06    5.05953e+06   -4.35657e+07    3.60894e+05   -
3.79254e+07
    Kinetic En.   Total Energy  Conserved En.    Temperature Pressure
(bar)
    5.39105e+06   -3.25344e+07   -3.25241e+07    3.19305e+02   -
5.32592e+02
   Constr. rmsd
    9.94933e-06


DD  step 79 load imb.: force 34.0%  pme mesh/force 1.565
step  480: timed with pme grid 240 240 240, coulomb cutoff 1.000: 11515.7
M-cycles
step  640: timed with pme grid 216 216 216, coulomb cutoff 1.072: 11002.5
M-cycles
step  800: timed with pme grid 200 200 200, coulomb cutoff 1.157: 11854.4
M-cycles
step  960: timed with pme grid 168 168 168, coulomb cutoff 1.378: 15524.8
M-cycles
step 1120: timed with pme grid 192 192 192, coulomb cutoff 1.206: 12347.4
M-cycles
step 1280: timed with pme grid 200 200 200, coulomb cutoff 1.157: 12929.9
M-cycles
step 1440: timed with pme grid 208 208 208, coulomb cutoff 1.113: 11173.5
M-cycles
step 1600: timed with pme grid 216 216 216, coulomb cutoff 1.072: 11671.2
M-cycles
step 1760: timed with pme grid 224 224 224, coulomb cutoff 1.033: 11556.8
M-cycles
step 1920: timed with pme grid 240 240 240, coulomb cutoff 1.000: 11750.1
M-cycles
             optimal pme grid 216 216 216, coulomb cutoff 1.072

DD  step 9999 load imb.: force 33.6%  pme mesh/force 1.016
           Step           Time
          10000       40.00000

Writing checkpoint, step 10000 at Sun Jan 14 14:12:19 2024
```

```
   Energies (kJ/mol)
  Connect Bonds          Angle    Proper Dih. Ryckaert-Bell.          LJ-
14
    0.00000e+00    3.48559e+05    1.18592e+04    7.61447e+05
2.87277e+05
     Coulomb-14        LJ (SR)   Coulomb (SR)   Coul. recip.
Potential
   -1.18786e+06    5.16549e+06   -4.36813e+07    2.68475e+05   -
3.80261e+07
    Kinetic En.   Total Energy  Conserved En.    Temperature Pressure
(bar)
    5.07227e+06   -3.29538e+07   -3.25263e+07    3.00425e+02
7.86835e+00
   Constr. rmsd
    9.39030e-06


Energy conservation over simulation part #1 of length 40 ps, time 0 to 40
ps
  Conserved energy drift: -2.64e-05 kJ/mol/ps per atom


      <======  ###############  ==>
      <====  A V E R A G E S  ====>
      <==  ###############  ======>

      Statistics over 10001 steps using 101 frames

   Energies (kJ/mol)
  Connect Bonds          Angle    Proper Dih. Ryckaert-Bell.          LJ-
14
    0.00000e+00    3.47775e+05    1.19109e+04    7.61232e+05
2.87444e+05
     Coulomb-14        LJ (SR)   Coulomb (SR)   Coul. recip.
Potential
   -1.18686e+06    5.16088e+06   -4.36709e+07    2.67340e+05   -
3.80212e+07
    Kinetic En.   Total Energy  Conserved En.    Temperature Pressure
(bar)
    5.06879e+06   -3.29524e+07   -3.25223e+07    3.00218e+02   -
1.34511e+01
   Constr. rmsd
    0.00000e+00

          Box-X          Box-Y          Box-Z
    3.10283e+01    3.10283e+01    2.19403e+01

   Total Virial (kJ/mol)
    1.69813e+06   -1.27148e+03   -5.52916e+00
   -1.27304e+03    1.69649e+06    1.65007e+03
    2.78824e+00    1.65010e+03    1.70021e+06

   Pressure (bar)
   -1.20913e+01    1.08551e+00   -1.83899e+00
    1.08798e+00   -1.17002e+01   -1.65442e+00
   -1.85206e+00   -1.65446e+00   -1.65619e+01
```

```
          T-mol      T-solvent
    3.00214e+02    3.00219e+02


       P P   -   P M E   L O A D   B A L A N C I N G

 PP/PME load balancing changed the cut-off and PME settings:
           particle-particle                    PME
            rcoulomb  rlist            grid      spacing   1/beta
   initial  1.000 nm  1.002 nm     240 240 240   0.130 nm  0.289 nm
   final    1.072 nm  1.074 nm     216 216 216   0.145 nm  0.310 nm
 cost-ratio           1.23             0.73
 (note that these numbers concern only part of the total PP and PME load)


     M E G A - F L O P S   A C C O U N T I N G

 NB=Group-cutoff nonbonded kernels    NxN=N-by-N cluster Verlet kernels
 RF=Reaction-Field  VdW=Van der Waals  QSTab=quadratic-spline table
 W3=SPC/TIP3p  W4=TIP4p (single or pairs)
 V&F=Potential and force  V=Potential only  F=Force only

 Computing:                                M-Number         M-Flops  %
Flops
-----------------------------------------------------------------------
----
 Pair Search distance check          142550.107334     1282950.966
0.1
 NxN Ewald Elec. + LJ [F]           9155892.040896   604288874.699
54.7
 NxN Ewald Elec. + LJ [V&F]           93497.371472    10004218.748
0.9
 NxN Ewald Elec. [F]                6978460.610336   425686097.230
38.5
 NxN Ewald Elec. [V&F]                71263.787760     5986158.172
0.5
 1,4 nonbonded interactions            6369.046841      573214.216
0.1
 Calc Weights                         64098.769236     2307555.692
0.2
 Spread Q Bspline                   1367440.410368     2734880.821
0.2
 Gather F Bspline                   1367440.410368     8204642.462
0.7
 3D-FFT                             4712391.258148    37699130.065
3.4
 Solve PME                              466.985536       29887.074
0.0
 Reset In Box                           269.187912         807.564
0.0
 CG-CoM                                 271.324324         813.973
0.0
 Angles                                4258.985856      715509.624
0.1
 Propers                                212.081206       48566.596
0.0
```

```
 RB-Dihedrals                          6469.816917     1598044.778
0.1
 Virial                                 857.513237       15435.238
0.0
 Stop-CM                                217.914024        2179.140
0.0
 P-Coupling                             856.701212        5140.207
0.0
 Calc-Ekin                             1713.402424       46261.865
0.0
 Lincs                                 2575.674297      154540.458
0.0
 Lincs-Mat                            70441.625720      281766.503
0.0
 Constraint-V                         24813.102665      223317.924
0.0
 Constraint-Vir                         891.552929       21397.270
0.0
 Settle                                6554.744553     2425255.485
0.2
 Virtual Site 3                          93.027699        3442.025
0.0
 Virtual Site 3fd                       193.227552       18356.617
0.0
 Virtual Site 3fad                      110.344416       19420.617
0.0
 Virtual Site 3out                      361.968796       31491.285
0.0
 Virtual Site 4fd                       100.036034       11003.964
0.0
 Virtual Site 4fdn                      170.062298       43195.824
0.0
-----------------------------------------------------------------------
----
 Total                                                1104463557.104
100.0
-----------------------------------------------------------------------
----


    D O M A I N   D E C O M P O S I T I O N   S T A T I S T I C S

 av. #atoms communicated per step for force:  2 x 1636214.6
 av. #atoms communicated per step for vsites: 3 x 11755.2
 av. #atoms communicated per step for LINCS:  3 x 165950.5


Dynamic load balancing report:
 DLB was off during the run due to low measured imbalance.
 Average load imbalance: 36.9%.
 The balanceable part of the MD step is 59%, load imbalance is computed
from this.
 Part of the total run time spent waiting due to load imbalance: 21.8%.
 Average PME mesh/force load: 1.071
 Part of the total run time spent waiting due to PP/PME imbalance: 4.1 %

NOTE: 21.8 % of the available CPU time was lost due to load imbalance
      in the domain decomposition.
```

Dynamic load balancing was automatically disabled, but it might be beneficial to manually turn it on (option -dlb yes.)

You can also consider manually changing the decomposition (option -dd);

e.g. by using fewer domains along the box dimension in which there is

considerable inhomogeneity in the simulated system.

R E A L C Y C L E A N D T I M E A C C O U N T I N G

On 45 MPI ranks doing PP, and
on 15 MPI ranks doing PME

Activity:	Num Ranks	Num Threads	Call Count	Wall time (s)	Giga-Cycles total sum	%
Domain decomp.	45	1	126	16.788	2223.724	1.9
DD comm. load	45	1	23	0.006	0.775	0.0
Vsite constr.	45	1	10001	7.465	988.858	0.8
Send X to PME	45	1	10001	4.598	609.000	0.5
Neighbor search	45	1	126	10.401	1377.777	1.2
Comm. coord.	45	1	9875	26.751	3543.531	3.0
Force	45	1	10001	345.016	45701.816	38.9
Wait + Comm. F	45	1	10001	88.994	11788.415	10.0
PME mesh *	15	1	10001	513.340	22666.146	19.3
PME wait for PP *				152.129	6717.151	5.7
Wait + Recv. PME F	45	1	10001	75.339	9979.650	8.5
NB X/F buffer ops.	45	1	29751	4.349	576.120	0.5
Vsite spread	45	1	10402	23.067	3055.472	2.6
Write traj.	45	1	1	0.168	22.200	0.0
Update	45	1	10001	1.642	217.515	0.2
Constraints	45	1	10003	58.645	7768.318	6.6
Comm. energies	45	1	401	1.410	186.711	0.2
Rest				0.871	115.377	0.1

```
 Total                                                 665.509     117540.347
100.0
-----------------------------------------------------------------------------
-------
(*) Note that with separate PME ranks, the walltime column actually sums
to
    twice the total reported, but the cycle count total and % are
correct.
-----------------------------------------------------------------------------
-------
 Breakdown of PME mesh activities
-----------------------------------------------------------------------------
-------
 PME redist. X/F          15    1      20002     104.779       4626.449
3.9
 PME spread               15    1      10001     103.486       4569.339
3.9
 PME gather               15    1      10001      65.798       2905.257
2.5
 PME 3D-FFT               15    1      20002      93.049       4108.514
3.5
 PME 3D-FFT Comm.         15    1      20002     141.760       6259.328
5.3
 PME solve Elec           15    1      10001       4.376        193.226
0.2
-----------------------------------------------------------------------------
-------

               Core t (s)   Wall t (s)        (%)
       Time:    39919.275      665.509     5998.3
                 (ns/day)    (hour/ns)
Performance:        5.194        4.621
Finished mdrun on rank 0 Sun Jan 14 14:12:22 2024
```

BINDING AFFINITY STUDY BENCHMARKS

cmet_eq_cpu-cluster_1n

```
                :-) GROMACS - gmx mdrun, 2023.3 (-:

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                    Coordinated by the GROMACS project leaders:
                      Paul Bauer, Berk Hess, and Erik Lindahl

GROMACS:      gmx mdrun, version 2023.3
Executable:   /usr/local/gromacs/bin/gmx_mpi
Data prefix:  /usr/local/gromacs
Working dir:  /home/ubuntu
Process ID:   11889
Command line:
  gmx_mpi mdrun -v -s /mnt/shared/home/ubuntu/mpinat-gromacs/mpinat-
gromacs-binding-affinity-study-bench/cmet_eq.tpr

GROMACS version:    2023.3
Precision:          mixed
Memory model:       64 bit
MPI library:        MPI
OpenMP support:     enabled (GMX_OPENMP_MAX_THREADS = 128)
GPU support:        disabled
SIMD instructions:  AVX2_256
```

```
CPU FFT library:    fftw-3.3.8-sse2-avx-avx2-avx2_128
GPU FFT library:    none
Multi-GPU FFT:      none
RDTSCP usage:       enabled
TNG support:        enabled
Hwloc support:      disabled
Tracing support:    disabled
C compiler:         /usr/bin/cc GNU 11.4.0
C compiler flags:   -fexcess-precision=fast -funroll-all-loops -mavx2 -
mfma -Wno-missing-field-initializers -O3 -DNDEBUG
C++ compiler:       /usr/bin/c++ GNU 11.4.0
C++ compiler flags: -fexcess-precision=fast -funroll-all-loops -mavx2 -
mfma -Wno-missing-field-initializers -Wno-cast-function-type-strict -
fopenmp -O3 -DNDEBUG
BLAS library:       Internal
LAPACK library:     Internal


Running on 1 node with total 6 cores, 6 processing units
Hardware detected on host cpu-1 (the node of MPI rank 0):
  CPU info:
    Vendor: AMD
    Brand:  AMD EPYC-Milan Processor
    Family: 25   Model: 1   Stepping: 1
    Features: aes amd apic avx avx2 clfsh cmov cx8 cx16 f16c fma lahf
misalignsse mmx msr pcid pclmuldq pdpe1gb popcnt pse rdrnd rdtscp sha
sse2 sse3 sse4a sse4.1 sse4.2 ssse3 tdt x2apic
  Hardware topology: Basic
    Packages, cores, and logical processors:
    [indices refer to OS logical processors]
      Package  0: [   0]
      Package  1: [   1]
      Package  2: [   2]
      Package  3: [   3]
      Package  4: [   4]
      Package  5: [   5]
    CPU limit set by OS: -1   Recommended max number of threads: 6


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
M. J. Abraham, T. Murtola, R. Schulz, S. P√°ll, J. C. Smith, B. Hess, E.
Lindahl
GROMACS: High performance molecular simulations through multi-level
parallelism from laptops to supercomputers
SoftwareX 1 (2015) pp. 19-25
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. P√°ll, M. J. Abraham, C. Kutzner, B. Hess, E. Lindahl
Tackling Exascale Software Challenges in Molecular Dynamics Simulations
with
GROMACS
In S. Markidis & E. Laure (Eds.), Solving Software Challenges for
Exascale 8759 (2015) pp. 3-27
-------- -------- --- Thank You --- -------- --------
```

```
++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. Pronk, S. P√°ll, R. Schulz, P. Larsson, P. Bjelkmar, R. Apostolov, M.
R.
Shirts, J. C. Smith, P. M. Kasson, D. van der Spoel, B. Hess, and E.
Lindahl
GROMACS 4.5: a high-throughput and highly parallel open source molecular
simulation toolkit
Bioinformatics 29 (2013) pp. 845-54
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
B. Hess and C. Kutzner and D. van der Spoel and E. Lindahl
GROMACS 4: Algorithms for highly efficient, load-balanced, and scalable
molecular simulation
J. Chem. Theory Comput. 4 (2008) pp. 435-447
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
D. van der Spoel, E. Lindahl, B. Hess, G. Groenhof, A. E. Mark and H. J.
C.
Berendsen
GROMACS: Fast, Flexible and Free
J. Comp. Chem. 26 (2005) pp. 1701-1719
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
E. Lindahl and B. Hess and D. van der Spoel
GROMACS 3.0: A package for molecular simulation and trajectory analysis
J. Mol. Mod. 7 (2001) pp. 306-317
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
H. J. C. Berendsen, D. van der Spoel and R. van Drunen
GROMACS: A message-passing parallel molecular dynamics implementation
Comp. Phys. Comm. 91 (1995) pp. 43-56
-------- -------- --- Thank You --- -------- --------


++++ PLEASE CITE THE DOI FOR THIS VERSION OF GROMACS ++++
https://doi.org/10.5281/zenodo.10017686
-------- -------- --- Thank You --- -------- --------


The number of OpenMP threads was set by environment variable
OMP_NUM_THREADS to 1

Input Parameters:
   integrator                     = sd
   tinit                          = 0
   dt                             = 0.002
   nsteps                         = 3000000
   init-step                      = 0
   simulation-part                = 1
   mts                            = false
```

```
comm-mode                       = Linear
nstcomm                         = 100
bd-fric                         = 0
ld-seed                         = -1628089582
emtol                           = 100
emstep                          = 0.01
niter                           = 0
fcstep                          = 0
nstcgsteep                      = 1000
nbfgscorr                       = 10
rtpi                            = 0.05
nstxout                         = 23500
nstvout                         = 23500
nstfout                         = 0
nstlog                          = 10000
nstcalcenergy                   = 100
nstenergy                       = 23500
nstxout-compressed              = 23500
compressed-x-precision          = 1000
cutoff-scheme                   = Verlet
nstlist                         = 10
pbc                             = xyz
periodic-molecules              = false
verlet-buffer-tolerance         = 0.005
rlist                           = 1.1
coulombtype                     = PME
coulomb-modifier                = Potential-shift
rcoulomb-switch                 = 0
rcoulomb                        = 1.1
epsilon-r                       = 1
epsilon-rf                      = inf
vdw-type                        = Cut-off
vdw-modifier                    = Potential-switch
rvdw-switch                     = 1
rvdw                            = 1.1
DispCorr                        = EnerPres
table-extension                 = 1
fourierspacing                  = 0.12
fourier-nx                      = 84
fourier-ny                      = 84
fourier-nz                      = 84
pme-order                       = 4
ewald-rtol                      = 1e-05
ewald-rtol-lj                   = 0.001
lj-pme-comb-rule                = Geometric
ewald-geometry                  = 3d
epsilon-surface                 = 0
ensemble-temperature-setting    = constant
ensemble-temperature            = 298
tcoupl                          = No
nsttcouple                      = -1
nh-chain-length                 = 0
print-nose-hoover-chain-variables = false
pcoupl                          = Parrinello-Rahman
pcoupltype                      = Isotropic
nstpcouple                      = 10
tau-p                           = 5
compressibility (3x3):
```

```
      compressibility[    0]={ 4.60000e-05,  0.00000e+00,  0.00000e+00}
      compressibility[    1]={ 0.00000e+00,  4.60000e-05,  0.00000e+00}
      compressibility[    2]={ 0.00000e+00,  0.00000e+00,  4.60000e-05}
   ref-p (3x3):
      ref-p[    0]={ 1.00000e+00,  0.00000e+00,  0.00000e+00}
      ref-p[    1]={ 0.00000e+00,  1.00000e+00,  0.00000e+00}
      ref-p[    2]={ 0.00000e+00,  0.00000e+00,  1.00000e+00}
   refcoord-scaling               = COM
   posres-com (3):
      posres-com[0]= 0.00000e+00
      posres-com[1]= 0.00000e+00
      posres-com[2]= 0.00000e+00
   posres-comB (3):
      posres-comB[0]= 0.00000e+00
      posres-comB[1]= 0.00000e+00
      posres-comB[2]= 0.00000e+00
   QMMM                           = false
qm-opts:
   ngQM                           = 0
   constraint-algorithm           = Lincs
   continuation                   = true
   Shake-SOR                      = false
   shake-tol                      = 0.0001
   lincs-order                    = 4
   lincs-iter                     = 2
   lincs-warnangle                = 30
   nwall                          = 0
   wall-type                      = 9-3
   wall-r-linpot                  = -1
   wall-atomtype[0]               = -1
   wall-atomtype[1]               = -1
   wall-density[0]                = 0
   wall-density[1]                = 0
   wall-ewald-zfac                = 3
   pull                           = false
   awh                            = false
   rotation                       = false
   interactiveMD                  = false
   disre                          = No
   disre-weighting                = Equal
   disre-mixed                    = false
   dr-fc                          = 1000
   dr-tau                         = 0
   nstdisreout                    = 100
   orire-fc                       = 0
   orire-tau                      = 0
   nstorireout                    = 100
   free-energy                    = yes
   init-lambda                    = 0
   init-lambda-state              = -1
   delta-lambda                   = 0
   nstdhdl                        = 10000
   n-lambdas                      = 0
   calc-lambda-neighbors          = 1
   dhdl-print-energy              = no
   sc-alpha                       = 0.3
   sc-power                       = 1
   sc-r-power                     = 6
```

```
   sc-sigma                       = 0.25
   sc-sigma-min                   = 0.25
   sc-coul                        = true
   dh-hist-size                   = 0
   dh-hist-spacing                = 0.1
   separate-dhdl-file             = yes
   dhdl-derivatives               = yes
   sc-function                    = beutler
   sc-gapsys-scale-linpoint-lj    = 0.85
   sc-gapsys-scale-linpoint-q     = 0.3
   sc-gapsys-sigma-lj             = 0.3
   cos-acceleration               = 0
   deform (3x3):
      deform[    0]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
      deform[    1]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
      deform[    2]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
   simulated-tempering            = false
   swapcoords                     = no
   userint1                       = 0
   userint2                       = 0
   userint3                       = 0
   userint4                       = 0
   userreal1                      = 0
   userreal2                      = 0
   userreal3                      = 0
   userreal4                      = 0
   applied-forces:
     electric-field:
       x:
         E0                       = 0
         omega                    = 0
         t0                       = 0
         sigma                    = 0
       y:
         E0                       = 0
         omega                    = 0
         t0                       = 0
         sigma                    = 0
       z:
         E0                       = 0
         omega                    = 0
         t0                       = 0
         sigma                    = 0
grpopts:
   nrdf:      134649
   ref-t:         298
   tau-t:           2
annealing:          No
annealing-npoints:           0
   acc:               0           0           0
   nfreeze:           N           N           N
   energygrp-flags[  0]: 0

Changing nstlist from 10 to 80, rlist from 1.1 to 1.232

Update groups can not be used for this system because there are three or
more consecutively coupled constraints
```

```
Initializing Domain Decomposition on 6 ranks
Dynamic load balancing: auto
Minimum cell size due to atom displacement: 0.639 nm
Initial maximum distances in bonded interactions:
    two-body bonded interactions: 0.438 nm, LJ-14, atoms 4073 4080
  multi-body bonded interactions: 0.438 nm, Proper Dih., atoms 4073 4080
Minimum cell size due to bonded interactions: 0.482 nm
Maximum distance for 5 constraints, at 120 deg. angles, all-trans: 0.819
nm
Estimated maximum distance required for P-LINCS: 0.819 nm
This distance will limit the DD cell size, you can override this with -
rcon
Scaling the initial minimum size with 1/0.8 (option -dds) = 1.25
Using 0 separate PME ranks because: there are too few total ranks for
efficient splitting
Optimizing the DD grid for 6 cells with a minimum initial size of 1.024
nm
The maximum allowed number of cells is: X 7 Y 7 Z 6
Domain decomposition grid 6 x 1 x 1, separate PME ranks 0
PME domain decomposition: 6 x 1 x 1
Domain decomposition rank 0, coordinates 0 0 0

The initial number of communication pulses is: X 1
The initial domain decomposition cell size is: X 1.34 nm

The maximum allowed distance for atoms involved in interactions is:
                 non-bonded interactions           1.232 nm
(the following are initial values, they could change due to box
deformation)
            two-body bonded interactions  (-rdd)   1.232 nm
          multi-body bonded interactions  (-rdd)   1.232 nm
  atoms separated by up to 5 constraints  (-rcon)  1.338 nm

When dynamic load balancing gets turned on, these settings will change
to:
The maximum number of communication pulses is: X 2
The minimum size for domain decomposition cells is 0.910 nm
The requested allowed shrink of DD cells (option -dds) is: 0.80
The allowed shrink of domain decomposition cells is: X 0.68
The maximum allowed distance for atoms involved in interactions is:
                 non-bonded interactions           1.232 nm
            two-body bonded interactions  (-rdd)   1.232 nm
          multi-body bonded interactions  (-rdd)   0.910 nm
  atoms separated by up to 5 constraints  (-rcon)  0.910 nm

Using 6 MPI processes

Non-default thread affinity set, disabling internal thread affinity

Using 1 OpenMP thread per MPI process

System total charge, top. A: 0.000 top. B: -1.000
Will do PME sum in reciprocal space for electrostatic interactions.

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
U. Essmann, L. Perera, M. L. Berkowitz, T. Darden, H. Lee and L. G.
Pedersen
A smooth particle mesh Ewald method
```

```
J. Chem. Phys. 103 (1995) pp. 8577-8592
-------- -------- --- Thank You --- -------- --------

Using a Gaussian width (1/beta) of 0.352179 nm for Ewald
Potential shift: LJ r^-12: 0.000e+00 r^-6: 0.000e+00, Ewald -9.091e-06
Initialized non-bonded Coulomb Ewald tables, spacing: 9.79e-04 size: 2282

Generated table with 1115 data points for 1-4 COUL.
Tabscale = 500 points/nm
Generated table with 1115 data points for 1-4 LJ6.
Tabscale = 500 points/nm
Generated table with 1115 data points for 1-4 LJ12.
Tabscale = 500 points/nm
Long Range LJ corr.: <C6> 3.0958e-04


Using SIMD 4x8 nonbonded short-range kernels

Using a dual 4x8 pair-list setup updated with dynamic pruning:
  outer list: updated every 80 steps, buffer 0.132 nm, rlist 1.232 nm
  inner list: updated every 13 steps, buffer 0.003 nm, rlist 1.103 nm
At tolerance 0.005 kJ/mol/ps per atom, equivalent classical 1x1 list
would be:
  outer list: updated every 80 steps, buffer 0.270 nm, rlist 1.370 nm
  inner list: updated every 13 steps, buffer 0.052 nm, rlist 1.152 nm

The non-bonded pair calculation algorithm tolerates a few missing pair
interactions close to the cut-off. This can lead to a systematic
overestimation of the pressure due to missing LJ interactions. The error
in the average pressure due to missing LJ interactions is at most 1.25
bar.
The pressure error can be controlled by setting the environment variable
GMX_VERLET_BUFFER_PRESSURE_TOLERANCE to the allowed error in units of
bar.
There are 61 atoms and 61 charges for free energy perturbation

Linking all bonded interactions to atoms


Initializing Parallel LINear Constraint Solver

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
B. Hess
P-LINCS: A Parallel Linear Constraint Solver for molecular simulation
J. Chem. Theory Comput. 4 (2008) pp. 116-122
-------- -------- --- Thank You --- -------- --------

The number of constraints is 4701
There are constraints between atoms in different decomposition domains,
will communicate selected coordinates each lincs iteration

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. Miyamoto and P. A. Kollman
SETTLE: An Analytical Version of the SHAKE and RATTLE Algorithms for
Rigid
Water Models
J. Comp. Chem. 13 (1992) pp. 952-962
-------- -------- --- Thank You --- -------- --------
```

```
Intra-simulation communication will occur every 10 steps.
Initial vector of lambda components:[     0.0000     0.0000     0.0000
0.0000     0.0000     0.0000     0.0000 ]

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
N. Goga and A. J. Rzepiela and A. H. de Vries and S. J. Marrink and H. J.
C.
Berendsen
Efficient Algorithms for Langevin and DPD Dynamics
J. Chem. Theory Comput. 8 (2012) pp. 3637--3649
-------- -------- --- Thank You --- -------- --------

There are: 67291 Atoms
Atom distribution over 6 domains: av 11215 stddev 149 min 11078 max 11409
Center of mass motion removal mode is Linear
We have the following groups for center of mass motion removal:
  0:  rest

Started mdrun on rank 0 Fri Jan 12 23:24:57 2024

           Step           Time
              0        0.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.03471e+04    1.16572e+04    8.17096e+02    5.07276e+03
5.18934e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.21209e+05   -3.77970e+03   -1.12353e+06    4.51443e+03   -
9.21800e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.67924e+05   -7.53875e+05    2.99990e+02   -9.33422e+01
1.04721e+02
    dVremain/dl   Constr. rmsd
    7.32203e+01    3.46295e-06


DD  step 79 load imb.: force 31.1%

step 240 Turning on dynamic load balancing, because the performance loss
due to load imbalance is 13.3 %.
step 6400 Turning off dynamic load balancing, because it is degrading
performance.
Atom distribution over 6 domains: av 11215 stddev 134 min 11054 max 11382
step 8000 Turning on dynamic load balancing, because the performance loss
due to load imbalance is 8.5 %.

DD  step 9999  vol min/aver 0.773  load imb.: force 12.5%
           Step           Time
          10000       20.00000

   Energies (kJ/mol)
```

```
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.02066e+04    1.17759e+04    7.91354e+02    5.07480e+03
5.16989e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.20467e+05   -3.75734e+03   -1.12079e+06    4.73063e+03   -
9.19804e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.65512e+05   -7.54293e+05    2.95680e+02   -9.22413e+01   -
7.95764e+01
    dVremain/dl   Constr. rmsd
    1.09873e+02    3.41735e-06


DD  step 19999  vol min/aver 0.712  load imb.: force  3.9%
           Step           Time
          20000       40.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    9.97419e+03    1.18920e+04    7.52372e+02    5.14955e+03
5.18708e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.20283e+05   -3.77281e+03   -1.12151e+06    4.49136e+03   -
9.20865e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.67474e+05   -7.53391e+05    2.99186e+02   -9.30023e+01
6.12514e+01
    dVremain/dl   Constr. rmsd
    1.89722e+02    3.47746e-06


DD  step 29999  vol min/aver 0.853  load imb.: force  4.6%
           Step           Time
          30000       60.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.01678e+04    1.16215e+04    7.93203e+02    5.10045e+03
5.17514e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.20857e+05   -3.76940e+03   -1.12226e+06    4.51421e+03   -
9.21226e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.66594e+05   -7.54632e+05    2.97613e+02   -9.28343e+01
3.68348e+01
    dVremain/dl   Constr. rmsd
    2.12171e+02    3.40566e-06

Writing checkpoint, step 34000 at Fri Jan 12 23:39:57 2024
```

```
DD  step 39999  vol min/aver 0.733  load imb.: force  4.3%
           Step           Time
          40000       80.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.01545e+04    1.16572e+04    6.70985e+02    5.05400e+03
5.17533e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.19741e+05   -3.75927e+03   -1.11999e+06    4.64549e+03   -
9.20068e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.66613e+05   -7.53455e+05    2.97646e+02   -9.23361e+01   -
1.41620e+02
    dVremain/dl   Constr. rmsd
    1.13353e+02    3.50666e-06


DD  step 49999  vol min/aver 0.803  load imb.: force  0.9%
           Step           Time
          50000      100.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.02270e+04    1.17717e+04    7.46851e+02    5.03325e+03
5.16801e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.21365e+05   -3.78228e+03   -1.12424e+06    4.55364e+03   -
9.22648e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.67224e+05   -7.55424e+05    2.98739e+02   -9.34696e+01
8.02744e+00
    dVremain/dl   Constr. rmsd
    1.23261e+02    3.43612e-06


DD  step 59999  vol min/aver 0.801  load imb.: force  0.5%
           Step           Time
          60000      120.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.01037e+04    1.16710e+04    7.47495e+02    5.12394e+03
5.20332e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.20845e+05   -3.76472e+03   -1.12188e+06    4.50583e+03   -
9.20616e+05
```

```
[…]

Writing checkpoint, step 3000000 at Sat Jan 13 14:11:11 2024


   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    9.98208e+03    1.15781e+04    7.38572e+02    5.07281e+03
5.20437e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.19300e+05   -3.75477e+03   -1.11996e+06    4.55134e+03   -
9.20449e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.67042e+05   -7.53407e+05    2.98413e+02   -9.21150e+01   -
9.42448e+01
    dVremain/dl   Constr. rmsd
    1.58454e+02    3.29164e-06


      <======  ###############  ==>
      <====  A V E R A G E S  ====>
      <==  ###############  ======>

      Statistics over 3000001 steps using 30001 frames

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.00501e+04    1.16490e+04    7.25155e+02    5.11130e+03
5.21172e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.20388e+05   -3.76877e+03   -1.12199e+06    4.55221e+03   -
9.21161e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.66969e+05   -7.54192e+05    2.98283e+02   -9.28035e+01
1.52334e+00
    dVremain/dl   Constr. rmsd
    1.52174e+02    0.00000e+00

          Box-X          Box-Y          Box-Z
    9.84270e+00    9.84270e+00    6.95984e+00

   Total Virial (kJ/mol)
    5.56271e+04    3.42692e+01    8.60461e+00
    3.43489e+01    5.56883e+04    8.17092e+00
    8.43294e+00    8.06970e+00    5.55651e+04

   Pressure (bar)
    3.06858e+00    1.38022e-01    3.98567e-01
    1.34096e-01   -6.43344e-01   -1.32006e+00
    4.07024e-01   -1.31508e+00    2.14478e+00
```

M E G A - F L O P S A C C O U N T I N G

NB=Group-cutoff nonbonded kernels NxN=N-by-N cluster Verlet kernels
RF=Reaction-Field VdW=Van der Waals QSTab=quadratic-spline table
W3=SPC/TIP3p W4=TIP4p (single or pairs)
V&F=Potential and force V=Potential only F=Force only

Computing:	M-Number	M-Flops	% Flops
NB Free energy kernel	27288359.565330	27288359.565	0.2
Pair Search distance check	1416186.520336	12745678.683	0.1
NxN Ewald Elec. + LJ [F]	89258663.409440	8301055697.078	57.1
NxN Ewald Elec. + LJ [V&F]	901635.578608	114507718.483	0.8
NxN Ewald Elec. [F]	75407193.141696	4599838781.643	31.7
NxN Ewald Elec. [V&F]	761713.744560	63983954.543	0.4
1,4 nonbonded interactions	36702.012234	3303181.101	0.0
Calc Weights	605619.201873	21802291.267	0.2
Spread Q Bspline	25839752.613248	51679505.226	0.4
Gather F Bspline	25839752.613248	155038515.679	1.1
3D-FFT	136395117.465024	1091160939.720	7.5
Solve PME	42336.014112	2709504.903	0.0
Reset In Box	2523.345209	7570.036	0.0
CG-CoM	2523.479791	7570.439	0.0
Angles	25548.008516	4292065.431	0.0
Propers	39945.013315	9147408.049	0.1
Impropers	3591.001197	746928.249	0.0
Virial	20268.367561	364830.616	0.0
Update	201873.067291	6258065.086	0.0
Stop-CM	2018.797291	20187.973	0.0
Calc-Ekin	40374.734582	1090117.834	0.0
Lincs	42300.511250	2538030.675	0.0
Lincs-Mat	912651.470328	3650605.881	0.0

```
 Constraint-V                          483502.164016     4351519.476
0.0
 Constraint-Vir                         22060.148791      529443.571
0.0
 Settle                                132967.047172    49197807.454
0.3
-----------------------------------------------------------------------
----
 Total                                                14527316278.663
100.0
-----------------------------------------------------------------------
----


   D O M A I N   D E C O M P O S I T I O N   S T A T I S T I C S

 av. #atoms communicated per step for force:  2 x 61950.2
 av. #atoms communicated per step for LINCS:  3 x 6338.4


Dynamic load balancing report:
 DLB was turned on during the run due to measured imbalance.
 Average load imbalance: 4.7%.
 The balanceable part of the MD step is 61%, load imbalance is computed
from this.
 Part of the total run time spent waiting due to load imbalance: 2.9%.
 Steps where the load balancing was limited by -rdd, -rcon and/or -dds: X
0 %


     R E A L   C Y C L E   A N D   T I M E   A C C O U N T I N G

On 6 MPI ranks

 Activity:              Num   Num      Call    Wall time         Giga-
Cycles
                       Ranks Threads  Count      (s)         total sum
%
-----------------------------------------------------------------------
-------
 Domain decomp.            6    1      37500     179.299       3167.611
0.3
 DD comm. load             6    1      37483       0.376          6.636
0.0
 DD comm. bounds           6    1      37478       2.090         36.923
0.0
 Neighbor search           6    1      37501     751.667      13279.407
1.4
 Comm. coord.              6    1    2962500     179.604       3172.993
0.3
 Force                     6    1    3000001   31986.524     565093.746
60.2
 Wait + Comm. F            6    1    3000001     227.141       4012.809
0.4
 PME mesh                  6    1    3000001   16611.237     293464.408
31.2
 NB X/F buffer ops.        6    1    8925001     202.243       3572.952
0.4
```

```
 Write traj.              6    1        188       1.094         19.332
0.0
 Update                   6    1    6000002     794.822      14041.816
1.5
 Constraints              6    1    6000002    2132.669      37677.048
4.0
 Comm. energies           6    1     300001      13.278        234.570
0.0
 Rest                                            92.490       1633.984
0.2
-----------------------------------------------------------------------
-------
 Total                                        53174.533     939414.234
100.0
-----------------------------------------------------------------------
-------
 Breakdown of PME mesh activities
-----------------------------------------------------------------------
-------
 PME redist. X/F          6    1    9000003    2983.942      52716.175
5.6
 PME spread               6    1    6000002    3361.218      59381.365
6.3
 PME gather               6    1    6000002    1734.210      30637.625
3.3
 PME 3D-FFT               6    1   12000004    6438.283     113742.698
12.1
 PME 3D-FFT Comm.         6    1   12000004    1602.600      28312.523
3.0
 PME solve Elec           6    1    6000002     484.766       8564.172
0.9
-----------------------------------------------------------------------
-------

               Core t (s)   Wall t (s)        (%)
       Time:   319047.194    53174.533      600.0
                         14h46:14
                 (ns/day)    (hour/ns)
Performance:        9.749        2.462
Finished mdrun on rank 0 Sat Jan 13 14:11:11 2024
```

cmet_eq_cpu-cluster_3n

```
                :-) GROMACS - gmx mdrun, 2023.3 (-:

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    M. Eric Irrgang          Farzaneh Jalalypour           Joe Jordan
   Christoph Junghans         Prashanth Kanduri          Sebastian Keller
    Carsten Kutzner            Justin A. Lemkul          Magnus Lundborg
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                    Coordinated by the GROMACS project leaders:
                      Paul Bauer, Berk Hess, and Erik Lindahl

GROMACS:      gmx mdrun, version 2023.3
Executable:   /usr/local/gromacs/bin/gmx_mpi
Data prefix:  /usr/local/gromacs
Working dir:  /home/ubuntu
Process ID:   8684
Command line:
  gmx_mpi mdrun -v -s /mnt/shared/home/ubuntu/mpinat-gromacs/mpinat-
gromacs-binding-affinity-study-bench/cmet_eq.tpr

GROMACS version:    2023.3
Precision:          mixed
Memory model:       64 bit
MPI library:        MPI
OpenMP support:     enabled (GMX_OPENMP_MAX_THREADS = 128)
GPU support:        disabled
SIMD instructions:  AVX2_256
```

```
CPU FFT library:    fftw-3.3.8-sse2-avx-avx2-avx2_128
GPU FFT library:    none
Multi-GPU FFT:      none
RDTSCP usage:       enabled
TNG support:        enabled
Hwloc support:      disabled
Tracing support:    disabled
C compiler:         /usr/bin/cc GNU 11.4.0
C compiler flags:   -fexcess-precision=fast -funroll-all-loops -mavx2 -
mfma -Wno-missing-field-initializers -O3 -DNDEBUG
C++ compiler:       /usr/bin/c++ GNU 11.4.0
C++ compiler flags: -fexcess-precision=fast -funroll-all-loops -mavx2 -
mfma -Wno-missing-field-initializers -Wno-cast-function-type-strict -
fopenmp -O3 -DNDEBUG
BLAS library:
LAPACK library:


Running on 3 nodes with total 18 cores, 18 processing units
  Cores per node:            6
  Logical processing units per node:    6
  OS CPU Limit / recommended threads to start per node:    6
Hardware detected on host cpu-2 (the node of MPI rank 0):
  CPU info:
    Vendor: AMD
    Brand:  AMD EPYC-Milan Processor
    Family: 25   Model: 1   Stepping: 1
    Features: aes amd apic avx avx2 clfsh cmov cx8 cx16 f16c fma lahf
misalignsse mmx msr pcid pclmuldq pdpe1gb popcnt pse rdrnd rdtscp sha
sse2 sse3 sse4a sse4.1 sse4.2 ssse3 tdt x2apic
  Hardware topology: Basic
    Packages, cores, and logical processors:
    [indices refer to OS logical processors]
      Package  0: [   0]
      Package  1: [   1]
      Package  2: [   2]
      Package  3: [   3]
      Package  4: [   4]
      Package  5: [   5]
    CPU limit set by OS: -1   Recommended max number of threads: 6


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
M. J. Abraham, T. Murtola, R. Schulz, S. P√°ll, J. C. Smith, B. Hess, E.
Lindahl
GROMACS: High performance molecular simulations through multi-level
parallelism from laptops to supercomputers
SoftwareX 1 (2015) pp. 19-25
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. P√°ll, M. J. Abraham, C. Kutzner, B. Hess, E. Lindahl
Tackling Exascale Software Challenges in Molecular Dynamics Simulations
with
GROMACS
In S. Markidis & E. Laure (Eds.), Solving Software Challenges for
Exascale 8759 (2015) pp. 3-27
```

```
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. Pronk, S. P√°ll, R. Schulz, P. Larsson, P. Bjelkmar, R. Apostolov, M.
R.
Shirts, J. C. Smith, P. M. Kasson, D. van der Spoel, B. Hess, and E.
Lindahl
GROMACS 4.5: a high-throughput and highly parallel open source molecular
simulation toolkit
Bioinformatics 29 (2013) pp. 845-54
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
B. Hess and C. Kutzner and D. van der Spoel and E. Lindahl
GROMACS 4: Algorithms for highly efficient, load-balanced, and scalable
molecular simulation
J. Chem. Theory Comput. 4 (2008) pp. 435-447
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
D. van der Spoel, E. Lindahl, B. Hess, G. Groenhof, A. E. Mark and H. J.
C.
Berendsen
GROMACS: Fast, Flexible and Free
J. Comp. Chem. 26 (2005) pp. 1701-1719
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
E. Lindahl and B. Hess and D. van der Spoel
GROMACS 3.0: A package for molecular simulation and trajectory analysis
J. Mol. Mod. 7 (2001) pp. 306-317
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
H. J. C. Berendsen, D. van der Spoel and R. van Drunen
GROMACS: A message-passing parallel molecular dynamics implementation
Comp. Phys. Comm. 91 (1995) pp. 43-56
-------- -------- --- Thank You --- -------- --------


++++ PLEASE CITE THE DOI FOR THIS VERSION OF GROMACS ++++
https://doi.org/10.5281/zenodo.10017686
-------- -------- --- Thank You --- -------- --------


The number of OpenMP threads was set by environment variable
OMP_NUM_THREADS to 1

Input Parameters:
   integrator                   = sd
   tinit                        = 0
   dt                           = 0.002
   nsteps                       = 3000000
```

```
init-step                       = 0
simulation-part                 = 1
mts                             = false
comm-mode                       = Linear
nstcomm                         = 100
bd-fric                         = 0
ld-seed                         = -1628089582
emtol                           = 100
emstep                          = 0.01
niter                           = 0
fcstep                          = 0
nstcgsteep                      = 1000
nbfgscorr                       = 10
rtpi                            = 0.05
nstxout                         = 23500
nstvout                         = 23500
nstfout                         = 0
nstlog                          = 10000
nstcalcenergy                   = 100
nstenergy                       = 23500
nstxout-compressed              = 23500
compressed-x-precision          = 1000
cutoff-scheme                   = Verlet
nstlist                         = 10
pbc                             = xyz
periodic-molecules              = false
verlet-buffer-tolerance         = 0.005
rlist                           = 1.1
coulombtype                     = PME
coulomb-modifier                = Potential-shift
rcoulomb-switch                 = 0
rcoulomb                        = 1.1
epsilon-r                       = 1
epsilon-rf                      = inf
vdw-type                        = Cut-off
vdw-modifier                    = Potential-switch
rvdw-switch                     = 1
rvdw                            = 1.1
DispCorr                        = EnerPres
table-extension                 = 1
fourierspacing                  = 0.12
fourier-nx                      = 84
fourier-ny                      = 84
fourier-nz                      = 84
pme-order                       = 4
ewald-rtol                      = 1e-05
ewald-rtol-lj                   = 0.001
lj-pme-comb-rule                = Geometric
ewald-geometry                  = 3d
epsilon-surface                 = 0
ensemble-temperature-setting    = constant
ensemble-temperature            = 298
tcoupl                          = No
nsttcouple                      = -1
nh-chain-length                 = 0
print-nose-hoover-chain-variables = false
pcoupl                          = Parrinello-Rahman
pcoupltype                      = Isotropic
```

```
   nstpcouple                     = 10
   tau-p                          = 5
   compressibility (3x3):
      compressibility[    0]={ 4.60000e-05,  0.00000e+00,  0.00000e+00}
      compressibility[    1]={ 0.00000e+00,  4.60000e-05,  0.00000e+00}
      compressibility[    2]={ 0.00000e+00,  0.00000e+00,  4.60000e-05}
   ref-p (3x3):
      ref-p[    0]={ 1.00000e+00,  0.00000e+00,  0.00000e+00}
      ref-p[    1]={ 0.00000e+00,  1.00000e+00,  0.00000e+00}
      ref-p[    2]={ 0.00000e+00,  0.00000e+00,  1.00000e+00}
   refcoord-scaling               = COM
   posres-com (3):
      posres-com[0]= 0.00000e+00
      posres-com[1]= 0.00000e+00
      posres-com[2]= 0.00000e+00
   posres-comB (3):
      posres-comB[0]= 0.00000e+00
      posres-comB[1]= 0.00000e+00
      posres-comB[2]= 0.00000e+00
   QMMM                           = false
qm-opts:
   ngQM                           = 0
   constraint-algorithm           = Lincs
   continuation                   = true
   Shake-SOR                      = false
   shake-tol                      = 0.0001
   lincs-order                    = 4
   lincs-iter                     = 2
   lincs-warnangle                = 30
   nwall                          = 0
   wall-type                      = 9-3
   wall-r-linpot                  = -1
   wall-atomtype[0]               = -1
   wall-atomtype[1]               = -1
   wall-density[0]                = 0
   wall-density[1]                = 0
   wall-ewald-zfac                = 3
   pull                           = false
   awh                            = false
   rotation                       = false
   interactiveMD                  = false
   disre                          = No
   disre-weighting                = Equal
   disre-mixed                    = false
   dr-fc                          = 1000
   dr-tau                         = 0
   nstdisreout                    = 100
   orire-fc                       = 0
   orire-tau                      = 0
   nstorireout                    = 100
   free-energy                    = yes
   init-lambda                    = 0
   init-lambda-state              = -1
   delta-lambda                   = 0
   nstdhdl                        = 10000
   n-lambdas                      = 0
   calc-lambda-neighbors          = 1
   dhdl-print-energy              = no
```

```
   sc-alpha                       = 0.3
   sc-power                       = 1
   sc-r-power                     = 6
   sc-sigma                       = 0.25
   sc-sigma-min                   = 0.25
   sc-coul                        = true
   dh-hist-size                   = 0
   dh-hist-spacing                = 0.1
   separate-dhdl-file             = yes
   dhdl-derivatives               = yes
   sc-function                    = beutler
   sc-gapsys-scale-linpoint-lj    = 0.85
   sc-gapsys-scale-linpoint-q     = 0.3
   sc-gapsys-sigma-lj             = 0.3
   cos-acceleration               = 0
   deform (3x3):
      deform[    0]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
      deform[    1]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
      deform[    2]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
   simulated-tempering            = false
   swapcoords                     = no
   userint1                       = 0
   userint2                       = 0
   userint3                       = 0
   userint4                       = 0
   userreal1                      = 0
   userreal2                      = 0
   userreal3                      = 0
   userreal4                      = 0
   applied-forces:
     electric-field:
       x:
         E0                       = 0
         omega                    = 0
         t0                       = 0
         sigma                    = 0
       y:
         E0                       = 0
         omega                    = 0
         t0                       = 0
         sigma                    = 0
       z:
         E0                       = 0
         omega                    = 0
         t0                       = 0
         sigma                    = 0
grpopts:
   nrdf:      134649
   ref-t:         298
   tau-t:           2
annealing:          No
annealing-npoints:           0
   acc:               0           0           0
   nfreeze:           N           N           N
   energygrp-flags[  0]: 0

Changing nstlist from 10 to 80, rlist from 1.1 to 1.232
```

```
Update groups can not be used for this system because there are three or
more consecutively coupled constraints

Initializing Domain Decomposition on 18 ranks
Dynamic load balancing: auto
Minimum cell size due to atom displacement: 0.639 nm
Initial maximum distances in bonded interactions:
    two-body bonded interactions: 0.438 nm, LJ-14, atoms 4073 4080
  multi-body bonded interactions: 0.438 nm, Proper Dih., atoms 4073 4080
Minimum cell size due to bonded interactions: 0.482 nm
Maximum distance for 5 constraints, at 120 deg. angles, all-trans: 0.819
nm
Estimated maximum distance required for P-LINCS: 0.819 nm
This distance will limit the DD cell size, you can override this with -
rcon
Scaling the initial minimum size with 1/0.8 (option -dds) = 1.25
Using 0 separate PME ranks because: there are too few total ranks for
efficient splitting
Optimizing the DD grid for 18 cells with a minimum initial size of 1.024
nm
The maximum allowed number of cells is: X 7 Y 7 Z 6
Domain decomposition grid 6 x 3 x 1, separate PME ranks 0
PME domain decomposition: 6 x 3 x 1
Domain decomposition rank 0, coordinates 0 0 0

The initial number of communication pulses is: X 1 Y 1
The initial domain decomposition cell size is: X 1.34 nm Y 2.68 nm

The maximum allowed distance for atoms involved in interactions is:
                 non-bonded interactions           1.232 nm
(the following are initial values, they could change due to box
deformation)
            two-body bonded interactions  (-rdd)   1.232 nm
          multi-body bonded interactions  (-rdd)   1.232 nm
  atoms separated by up to 5 constraints  (-rcon)  1.338 nm

When dynamic load balancing gets turned on, these settings will change
to:
The maximum number of communication pulses is: X 2 Y 2
The minimum size for domain decomposition cells is 0.910 nm
The requested allowed shrink of DD cells (option -dds) is: 0.80
The allowed shrink of domain decomposition cells is: X 0.68 Y 0.34
The maximum allowed distance for atoms involved in interactions is:
                 non-bonded interactions           1.232 nm
            two-body bonded interactions  (-rdd)   1.232 nm
          multi-body bonded interactions  (-rdd)   0.910 nm
  atoms separated by up to 5 constraints  (-rcon)  0.910 nm
Using two step summing over 3 groups of on average 6.0 ranks


Using 18 MPI processes

Non-default thread affinity set, disabling internal thread affinity

Using 1 OpenMP thread per MPI process

System total charge, top. A: 0.000 top. B: -1.000
Will do PME sum in reciprocal space for electrostatic interactions.
```

```
++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
U. Essmann, L. Perera, M. L. Berkowitz, T. Darden, H. Lee and L. G.
Pedersen
A smooth particle mesh Ewald method
J. Chem. Phys. 103 (1995) pp. 8577-8592
-------- -------- --- Thank You --- -------- --------

Using a Gaussian width (1/beta) of 0.352179 nm for Ewald
Potential shift: LJ r^-12: 0.000e+00 r^-6: 0.000e+00, Ewald -9.091e-06
Initialized non-bonded Coulomb Ewald tables, spacing: 9.79e-04 size: 2282

Generated table with 1115 data points for 1-4 COUL.
Tabscale = 500 points/nm
Generated table with 1115 data points for 1-4 LJ6.
Tabscale = 500 points/nm
Generated table with 1115 data points for 1-4 LJ12.
Tabscale = 500 points/nm
Long Range LJ corr.: <C6> 3.0958e-04


Using SIMD 4x8 nonbonded short-range kernels

Using a dual 4x8 pair-list setup updated with dynamic pruning:
  outer list: updated every 80 steps, buffer 0.132 nm, rlist 1.232 nm
  inner list: updated every 13 steps, buffer 0.003 nm, rlist 1.103 nm
At tolerance 0.005 kJ/mol/ps per atom, equivalent classical 1x1 list
would be:
  outer list: updated every 80 steps, buffer 0.270 nm, rlist 1.370 nm
  inner list: updated every 13 steps, buffer 0.052 nm, rlist 1.152 nm

The non-bonded pair calculation algorithm tolerates a few missing pair
interactions close to the cut-off. This can lead to a systematic
overestimation of the pressure due to missing LJ interactions. The error
in the average pressure due to missing LJ interactions is at most 1.25
bar.
The pressure error can be controlled by setting the environment variable
GMX_VERLET_BUFFER_PRESSURE_TOLERANCE to the allowed error in units of
bar.
There are 61 atoms and 61 charges for free energy perturbation

Linking all bonded interactions to atoms


Initializing Parallel LINear Constraint Solver

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
B. Hess
P-LINCS: A Parallel Linear Constraint Solver for molecular simulation
J. Chem. Theory Comput. 4 (2008) pp. 116-122
-------- -------- --- Thank You --- -------- --------

The number of constraints is 4701
There are constraints between atoms in different decomposition domains,
will communicate selected coordinates each lincs iteration

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. Miyamoto and P. A. Kollman
```

```
SETTLE: An Analytical Version of the SHAKE and RATTLE Algorithms for
Rigid
Water Models
J. Comp. Chem. 13 (1992) pp. 952-962
-------- -------- --- Thank You --- -------- --------


Intra-simulation communication will occur every 10 steps.
Initial vector of lambda components:[     0.0000     0.0000     0.0000
0.0000     0.0000     0.0000     0.0000 ]

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
N. Goga and A. J. Rzepiela and A. H. de Vries and S. J. Marrink and H. J.
C.
Berendsen
Efficient Algorithms for Langevin and DPD Dynamics
J. Chem. Theory Comput. 8 (2012) pp. 3637--3649
-------- -------- --- Thank You --- -------- --------

There are: 67291 Atoms
Atom distribution over 18 domains: av 3738 stddev 80 min 3648 max 3883
Center of mass motion removal mode is Linear
We have the following groups for center of mass motion removal:
  0:  rest

Started mdrun on rank 0 Fri Jan 12 23:25:04 2024

           Step           Time
              0        0.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.03471e+04    1.16572e+04    8.17095e+02    5.07276e+03
5.18934e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.21209e+05   -3.77970e+03   -1.12353e+06    4.51451e+03   -
9.21801e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.67925e+05   -7.53876e+05    2.99990e+02   -9.33422e+01
1.04718e+02
    dVremain/dl   Constr. rmsd
    7.32098e+01    3.49022e-06


DD  step 79 load imb.: force 25.0%

step 240 Turning on dynamic load balancing, because the performance loss
due to load imbalance is 8.4 %.
step 8000 Turning off dynamic load balancing, because it is degrading
performance.
Atom distribution over 18 domains: av 3738 stddev 71 min 3674 max 3841

DD  step 9999 load imb.: force 64.3%
           Step           Time
          10000       20.00000
```

```
   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.02010e+04    1.16347e+04    7.14806e+02    5.10341e+03
5.18079e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.19887e+05   -3.77569e+03   -1.12034e+06    4.53346e+03   -
9.20235e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.66966e+05   -7.53269e+05    2.98277e+02   -9.31446e+01
2.27139e+01
    dVremain/dl   Constr. rmsd
    1.15611e+02    3.46855e-06


step 16000 Turning on dynamic load balancing, because the performance
loss due to load imbalance is 8.4 %.

DD  step 19999  vol min/aver 0.538  load imb.: force  3.8%
           Step           Time
          20000       40.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.01222e+04    1.16408e+04    6.90274e+02    5.15371e+03
5.18689e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.19006e+05   -3.77409e+03   -1.11846e+06    4.43627e+03   -
9.19318e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.66830e+05   -7.52488e+05    2.98034e+02   -9.30653e+01   -
3.98888e+01
    dVremain/dl   Constr. rmsd
    1.25969e+02    3.46677e-06


DD  step 29999  vol min/aver 0.781  load imb.: force 41.0%
           Step           Time
          30000       60.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.00584e+04    1.16875e+04    7.90742e+02    5.10638e+03
5.18258e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.21538e+05   -3.77105e+03   -1.12237e+06    4.65870e+03   -
9.20479e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
```

```
    1.68222e+05   -7.52257e+05    3.00522e+02   -9.29156e+01
5.45765e+01
    dVremain/dl   Constr. rmsd
    1.96821e+02    3.72143e-06


DD  step 39999  vol min/aver 0.465  load imb.: force 43.3%
           Step           Time
          40000       80.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.00610e+04    1.17820e+04    7.37137e+02    5.01714e+03
5.18833e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.21208e+05   -3.77753e+03   -1.12449e+06    4.59444e+03   -
9.22981e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.67176e+05   -7.55805e+05    2.98653e+02   -9.32352e+01   -
2.91461e+00
    dVremain/dl   Constr. rmsd
    1.65300e+02    3.44814e-06


DD  step 49999  vol min/aver 0.454  load imb.: force 57.9%
           Step           Time
          50000      100.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    9.93374e+03    1.17089e+04    7.13615e+02    5.05919e+03
5.17690e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.20394e+05   -3.76977e+03   -1.12226e+06    4.56301e+03   -
9.21885e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.67184e+05   -7.54702e+05    2.98667e+02   -9.28526e+01   -
1.68613e+01
    dVremain/dl   Constr. rmsd
    9.08243e+01    3.41058e-06

Writing checkpoint, step 56080 at Fri Jan 12 23:40:05 2024


DD  step 59999  vol min/aver 0.539  load imb.: force 18.0%
           Step           Time
          60000      120.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
```

```
    1.03260e+04    1.16263e+04    7.33323e+02    5.14368e+03
5.18436e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.19393e+05   -3.77488e+03   -1.12025e+06    4.61647e+03   -
9.20338e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.67390e+05   -7.52948e+05    2.99035e+02   -9.31043e+01   -
4.11863e+01
    dVremain/dl   Constr. rmsd
    1.77017e+02    3.54985e-06


DD  step 69999  vol min/aver 0.702  load imb.: force 14.2%
           Step           Time
          70000      140.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.00546e+04    1.17899e+04    7.55751e+02    5.06443e+03
5.20146e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.21338e+05   -3.76270e+03   -1.12130e+06    4.47232e+03   -
9.19570e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.66518e+05   -7.53052e+05    2.97477e+02   -9.25048e+01
4.51170e+01
    dVremain/dl   Constr. rmsd
    1.42893e+02    3.56886e-06


DD  step 79999  vol min/aver 0.610  load imb.: force  1.5%
           Step           Time
          80000      160.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    9.97882e+03    1.16320e+04    7.13555e+02    5.12380e+03
5.21487e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.20873e+05   -3.76838e+03   -1.12184e+06    4.59506e+03   -
9.20539e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.67365e+05   -7.53174e+05    2.98990e+02   -9.27840e+01
7.49017e+01
    dVremain/dl   Constr. rmsd
    1.91230e+02    3.55436e-06


DD  step 89999  vol min/aver 0.634  load imb.: force  2.7%
           Step           Time
```

```
          90000      180.00000

[…]

DD  step 2989999  vol min/aver 0.601  load imb.: force  1.7%
           Step           Time
        2990000     5980.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.00709e+04    1.16010e+04    7.50842e+02    5.17002e+03
5.15727e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.20451e+05   -3.76685e+03   -1.11960e+06    4.56116e+03   -
9.19190e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.66528e+05   -7.52661e+05    2.97495e+02   -9.27087e+01
7.98788e+01
    dVremain/dl   Constr. rmsd
    1.43497e+02    3.45570e-06


DD  step 2999999  vol min/aver 0.610  load imb.: force  1.3%
           Step           Time
        3000000     6000.00000

Writing checkpoint, step 3000000 at Sat Jan 13 09:54:13 2024


   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.01792e+04    1.16798e+04    6.46925e+02    5.18140e+03
5.15915e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.19753e+05   -3.75981e+03   -1.12157e+06    4.42603e+03   -
9.21872e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.67154e+05   -7.54719e+05    2.98613e+02   -9.23623e+01   -
5.40019e+01
    dVremain/dl   Constr. rmsd
    1.29877e+02    3.42777e-06


      <======  ###############  ==>
      <====  A V E R A G E S  ====>
      <==  ###############  ======>

      Statistics over 3000001 steps using 30001 frames

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
```

```
    1.00448e+04    1.16760e+04    7.25786e+02    5.11380e+03
5.19431e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.20277e+05   -3.76936e+03   -1.12173e+06    4.54031e+03   -
9.21175e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.66994e+05   -7.54181e+05    2.98327e+02   -9.28327e+01    3.14865e-
01
    dVremain/dl   Constr. rmsd
    1.47202e+02    0.00000e+00

          Box-X          Box-Y          Box-Z
    9.84219e+00    9.84219e+00    6.95948e+00

   Total Virial (kJ/mol)
    5.56802e+04    2.31558e+01   -1.17733e+01
    2.31366e+01    5.56941e+04   -4.73271e+01
   -1.19994e+01   -4.76071e+01    5.56046e+04

   Pressure (bar)
   -2.56229e-01    5.63197e-01    8.87378e-01
    5.64142e-01    3.72625e-01    6.18933e-01
    8.98515e-01    6.32724e-01    8.28200e-01


     M E G A - F L O P S   A C C O U N T I N G

 NB=Group-cutoff nonbonded kernels    NxN=N-by-N cluster Verlet kernels
 RF=Reaction-Field  VdW=Van der Waals  QSTab=quadratic-spline table
 W3=SPC/TIP3p  W4=TIP4p (single or pairs)
 V&F=Potential and force  V=Potential only  F=Force only

 Computing:                                M-Number         M-Flops  %
Flops
-----------------------------------------------------------------------
----
 NB Free energy kernel             27215279.634006    27215279.634
0.2
 Pair Search distance check         1479150.497748    13312354.480
0.1
 NxN Ewald Elec. + LJ [F]          93854672.032192  8728484498.994
57.3
 NxN Ewald Elec. + LJ [V&F]          948059.550080   120403562.860
0.8
 NxN Ewald Elec. [F]               79635958.611584  4857793475.307
31.9
 NxN Ewald Elec. [V&F]               804424.682336    67571673.316
0.4
 1,4 nonbonded interactions           36702.012234     3303181.101
0.0
 Calc Weights                        605619.201873    21802291.267
0.1
 Spread Q Bspline                  25839752.613248    51679505.226
0.3
 Gather F Bspline                  25839752.613248   155038515.679
1.0
```

```
 3D-FFT                          136395117.465024  1091160939.720
7.2
 Solve PME                          127008.042336     8128514.710
0.1
 Reset In Box                         2523.345209        7570.036
0.0
 CG-CoM                               2523.479791        7570.439
0.0
 Angles                              25548.008516     4292065.431
0.0
 Propers                             39945.013315     9147408.049
0.1
 Impropers                            3591.001197      746928.249
0.0
 Virial                              20430.368101      367746.626
0.0
 Update                             201873.067291     6258065.086
0.0
 Stop-CM                              2018.797291       20187.973
0.0
 Calc-Ekin                           40374.734582     1090117.834
0.0
 Lincs                               50284.108670     3017046.520
0.0
 Lincs-Mat                         1079401.207152     4317604.829
0.0
 Constraint-V                       511157.512006     4600417.608
0.0
 Constraint-Vir                      23043.739060      553049.737
0.0
 Settle                             136863.098222    50639346.342
0.3
-----------------------------------------------------------------------
----
 Total                                              15230958917.053
100.0
-----------------------------------------------------------------------
----


    D O M A I N   D E C O M P O S I T I O N   S T A T I S T I C S

 av. #atoms communicated per step for force:  2 x 123911.3
 av. #atoms communicated per step for LINCS:  3 x 10092.0


Dynamic load balancing report:
 DLB was turned on during the run due to measured imbalance.
 Average load imbalance: 11.5%.
 The balanceable part of the MD step is 33%, load imbalance is computed
from this.
 Part of the total run time spent waiting due to load imbalance: 3.7%.
 Steps where the load balancing was limited by -rdd, -rcon and/or -dds: X
0 % Y 0 %


     R E A L   C Y C L E   A N D   T I M E   A C C O U N T I N G
```

On 18 MPI ranks

Activity:	Num Ranks	Num Threads	Call Count	Wall time (s)	Giga-Cycles total sum	%
Domain decomp.	18	1	37500	142.895	7573.386	0.4
DD comm. load	18	1	37419	0.582	30.854	0.0
DD comm. bounds	18	1	37398	5.505	291.767	0.0
Neighbor search	18	1	37501	329.034	17438.725	0.9
Comm. coord.	18	1	2962500	598.616	31726.542	1.6
Force	18	1	3000001	11483.794	608639.059	30.4
Wait + Comm. F	18	1	3000001	616.275	32662.476	1.6
PME mesh	18	1	3000001	21025.943	1114371.310	55.7
NB X/F buffer ops.	18	1	8925001	124.622	6604.965	0.3
Write traj.	18	1	169	0.378	20.044	0.0
Update	18	1	6000002	310.587	16461.073	0.8
Constraints	18	1	6000002	3015.248	159807.603	8.0
Comm. energies	18	1	300001	41.984	2225.150	0.1
Rest				52.858	2801.468	0.1
Total				37748.322	2000654.423	100.0
Breakdown of PME mesh activities						
PME redist. X/F	18	1	9000003	3928.914	208231.777	10.4
PME spread	18	1	6000002	2069.749	109696.356	5.5
PME gather	18	1	6000002	1599.870	84792.845	4.2
PME 3D-FFT	18	1	12000004	2483.737	131637.630	6.6
PME 3D-FFT Comm.	18	1	24000008	10757.141	570126.575	28.5
PME solve Elec	18	1	6000002	179.369	9506.547	0.5

```
-------------------------------------------------------------------------------

               Core t (s)   Wall t (s)        (%)
       Time:   679469.783    37748.322     1800.0
                         10h29:08
                 (ns/day)    (hour/ns)
Performance:       13.733        1.748
Finished mdrun on rank 0 Sat Jan 13 09:54:13 2024
```

cmet_eq_cpu-cluster_10n

```
                :-) GROMACS - gmx mdrun, 2023.3 (-:

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Wennberg
       Maarten Wolf

                    Coordinated by the GROMACS project leaders:
                      Paul Bauer, Berk Hess, and Erik Lindahl

GROMACS:      gmx mdrun, version 2023.3
Executable:   /usr/local/gromacs/bin/gmx_mpi
Data prefix:  /usr/local/gromacs
Working dir:  /home/ubuntu
Process ID:   17672
Command line:
  gmx_mpi mdrun -v -s /mnt/shared/home/ubuntu/mpinat-gromacs/mpinat-
gromacs-binding-affinity-study-bench/cmet_eq.tpr

GROMACS version:    2023.3
Precision:          mixed
Memory model:       64 bit
MPI library:        MPI
OpenMP support:     enabled (GMX_OPENMP_MAX_THREADS = 128)
GPU support:        disabled
SIMD instructions:  AVX2_256
```

```
CPU FFT library:    fftw-3.3.8-sse2-avx-avx2-avx2_128
GPU FFT library:    none
Multi-GPU FFT:      none
RDTSCP usage:       enabled
TNG support:        enabled
Hwloc support:      disabled
Tracing support:    disabled
C compiler:         /usr/bin/cc GNU 11.4.0
C compiler flags:   -fexcess-precision=fast -funroll-all-loops -mavx2 -
mfma -Wno-missing-field-initializers -O3 -DNDEBUG
C++ compiler:       /usr/bin/c++ GNU 11.4.0
C++ compiler flags: -fexcess-precision=fast -funroll-all-loops -mavx2 -
mfma -Wno-missing-field-initializers -Wno-cast-function-type-strict -
fopenmp -O3 -DNDEBUG
BLAS library:       Internal
LAPACK library:     Internal


Running on 10 nodes with total 60 cores, 60 processing units
  Cores per node:            6
  Logical processing units per node:    6
  OS CPU Limit / recommended threads to start per node:    6
Hardware detected on host cpu-1 (the node of MPI rank 0):
  CPU info:
    Vendor: AMD
    Brand:  AMD EPYC-Milan Processor
    Family: 25   Model: 1   Stepping: 1
    Features: aes amd apic avx avx2 clfsh cmov cx8 cx16 f16c fma lahf
misalignsse mmx msr pcid pclmuldq pdpe1gb popcnt pse rdrnd rdtscp sha
sse2 sse3 sse4a sse4.1 sse4.2 ssse3 tdt x2apic
  Hardware topology: Basic
    Packages, cores, and logical processors:
    [indices refer to OS logical processors]
      Package  0: [   0]
      Package  1: [   1]
      Package  2: [   2]
      Package  3: [   3]
      Package  4: [   4]
      Package  5: [   5]
    CPU limit set by OS: -1   Recommended max number of threads: 6


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
M. J. Abraham, T. Murtola, R. Schulz, S. P√°ll, J. C. Smith, B. Hess, E.
Lindahl
GROMACS: High performance molecular simulations through multi-level
parallelism from laptops to supercomputers
SoftwareX 1 (2015) pp. 19-25
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. P√°ll, M. J. Abraham, C. Kutzner, B. Hess, E. Lindahl
Tackling Exascale Software Challenges in Molecular Dynamics Simulations
with
GROMACS
In S. Markidis & E. Laure (Eds.), Solving Software Challenges for
Exascale 8759 (2015) pp. 3-27
```

```
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. Pronk, S. P√°ll, R. Schulz, P. Larsson, P. Bjelkmar, R. Apostolov, M.
R.
Shirts, J. C. Smith, P. M. Kasson, D. van der Spoel, B. Hess, and E.
Lindahl
GROMACS 4.5: a high-throughput and highly parallel open source molecular
simulation toolkit
Bioinformatics 29 (2013) pp. 845-54
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
B. Hess and C. Kutzner and D. van der Spoel and E. Lindahl
GROMACS 4: Algorithms for highly efficient, load-balanced, and scalable
molecular simulation
J. Chem. Theory Comput. 4 (2008) pp. 435-447
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
D. van der Spoel, E. Lindahl, B. Hess, G. Groenhof, A. E. Mark and H. J.
C.
Berendsen
GROMACS: Fast, Flexible and Free
J. Comp. Chem. 26 (2005) pp. 1701-1719
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
E. Lindahl and B. Hess and D. van der Spoel
GROMACS 3.0: A package for molecular simulation and trajectory analysis
J. Mol. Mod. 7 (2001) pp. 306-317
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
H. J. C. Berendsen, D. van der Spoel and R. van Drunen
GROMACS: A message-passing parallel molecular dynamics implementation
Comp. Phys. Comm. 91 (1995) pp. 43-56
-------- -------- --- Thank You --- -------- --------


++++ PLEASE CITE THE DOI FOR THIS VERSION OF GROMACS ++++
https://doi.org/10.5281/zenodo.10017686
-------- -------- --- Thank You --- -------- --------


The number of OpenMP threads was set by environment variable
OMP_NUM_THREADS to 1

Input Parameters:
   integrator                   = sd
   tinit                        = 0
   dt                           = 0.002
   nsteps                       = 3000000
```

```
init-step                       = 0
simulation-part                 = 1
mts                             = false
comm-mode                       = Linear
nstcomm                         = 100
bd-fric                         = 0
ld-seed                         = -1628089582
emtol                           = 100
emstep                          = 0.01
niter                           = 0
fcstep                          = 0
nstcgsteep                      = 1000
nbfgscorr                       = 10
rtpi                            = 0.05
nstxout                         = 23500
nstvout                         = 23500
nstfout                         = 0
nstlog                          = 10000
nstcalcenergy                   = 100
nstenergy                       = 23500
nstxout-compressed              = 23500
compressed-x-precision          = 1000
cutoff-scheme                   = Verlet
nstlist                         = 10
pbc                             = xyz
periodic-molecules              = false
verlet-buffer-tolerance         = 0.005
rlist                           = 1.1
coulombtype                     = PME
coulomb-modifier                = Potential-shift
rcoulomb-switch                 = 0
rcoulomb                        = 1.1
epsilon-r                       = 1
epsilon-rf                      = inf
vdw-type                        = Cut-off
vdw-modifier                    = Potential-switch
rvdw-switch                     = 1
rvdw                            = 1.1
DispCorr                        = EnerPres
table-extension                 = 1
fourierspacing                  = 0.12
fourier-nx                      = 84
fourier-ny                      = 84
fourier-nz                      = 84
pme-order                       = 4
ewald-rtol                      = 1e-05
ewald-rtol-lj                   = 0.001
lj-pme-comb-rule                = Geometric
ewald-geometry                  = 3d
epsilon-surface                 = 0
ensemble-temperature-setting    = constant
ensemble-temperature            = 298
tcoupl                          = No
nsttcouple                      = -1
nh-chain-length                 = 0
print-nose-hoover-chain-variables = false
pcoupl                          = Parrinello-Rahman
pcoupltype                      = Isotropic
```

```
   nstpcouple                     = 10
   tau-p                          = 5
   compressibility (3x3):
      compressibility[    0]={ 4.60000e-05,  0.00000e+00,  0.00000e+00}
      compressibility[    1]={ 0.00000e+00,  4.60000e-05,  0.00000e+00}
      compressibility[    2]={ 0.00000e+00,  0.00000e+00,  4.60000e-05}
   ref-p (3x3):
      ref-p[    0]={ 1.00000e+00,  0.00000e+00,  0.00000e+00}
      ref-p[    1]={ 0.00000e+00,  1.00000e+00,  0.00000e+00}
      ref-p[    2]={ 0.00000e+00,  0.00000e+00,  1.00000e+00}
   refcoord-scaling               = COM
   posres-com (3):
      posres-com[0]= 0.00000e+00
      posres-com[1]= 0.00000e+00
      posres-com[2]= 0.00000e+00
   posres-comB (3):
      posres-comB[0]= 0.00000e+00
      posres-comB[1]= 0.00000e+00
      posres-comB[2]= 0.00000e+00
   QMMM                           = false
qm-opts:
   ngQM                           = 0
   constraint-algorithm           = Lincs
   continuation                   = true
   Shake-SOR                      = false
   shake-tol                      = 0.0001
   lincs-order                    = 4
   lincs-iter                     = 2
   lincs-warnangle                = 30
   nwall                          = 0
   wall-type                      = 9-3
   wall-r-linpot                  = -1
   wall-atomtype[0]               = -1
   wall-atomtype[1]               = -1
   wall-density[0]                = 0
   wall-density[1]                = 0
   wall-ewald-zfac                = 3
   pull                           = false
   awh                            = false
   rotation                       = false
   interactiveMD                  = false
   disre                          = No
   disre-weighting                = Equal
   disre-mixed                    = false
   dr-fc                          = 1000
   dr-tau                         = 0
   nstdisreout                    = 100
   orire-fc                       = 0
   orire-tau                      = 0
   nstorireout                    = 100
   free-energy                    = yes
   init-lambda                    = 0
   init-lambda-state              = -1
   delta-lambda                   = 0
   nstdhdl                        = 10000
   n-lambdas                      = 0
   calc-lambda-neighbors          = 1
   dhdl-print-energy              = no
```

```
   sc-alpha                       = 0.3
   sc-power                       = 1
   sc-r-power                     = 6
   sc-sigma                       = 0.25
   sc-sigma-min                   = 0.25
   sc-coul                        = true
   dh-hist-size                   = 0
   dh-hist-spacing                = 0.1
   separate-dhdl-file             = yes
   dhdl-derivatives               = yes
   sc-function                    = beutler
   sc-gapsys-scale-linpoint-lj    = 0.85
   sc-gapsys-scale-linpoint-q     = 0.3
   sc-gapsys-sigma-lj             = 0.3
   cos-acceleration               = 0
   deform (3x3):
      deform[    0]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
      deform[    1]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
      deform[    2]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
   simulated-tempering            = false
   swapcoords                     = no
   userint1                       = 0
   userint2                       = 0
   userint3                       = 0
   userint4                       = 0
   userreal1                      = 0
   userreal2                      = 0
   userreal3                      = 0
   userreal4                      = 0
   applied-forces:
     electric-field:
       x:
         E0                       = 0
         omega                    = 0
         t0                       = 0
         sigma                    = 0
       y:
         E0                       = 0
         omega                    = 0
         t0                       = 0
         sigma                    = 0
       z:
         E0                       = 0
         omega                    = 0
         t0                       = 0
         sigma                    = 0
grpopts:
   nrdf:      134649
   ref-t:         298
   tau-t:           2
annealing:          No
annealing-npoints:           0
   acc:               0           0           0
   nfreeze:           N           N           N
   energygrp-flags[  0]: 0

Changing nstlist from 10 to 80, rlist from 1.1 to 1.232
```

```
Update groups can not be used for this system because there are three or
more consecutively coupled constraints

Initializing Domain Decomposition on 60 ranks
Dynamic load balancing: auto
Minimum cell size due to atom displacement: 0.639 nm
Initial maximum distances in bonded interactions:
    two-body bonded interactions: 0.438 nm, LJ-14, atoms 4073 4080
  multi-body bonded interactions: 0.438 nm, Proper Dih., atoms 4073 4080
Minimum cell size due to bonded interactions: 0.482 nm
Maximum distance for 5 constraints, at 120 deg. angles, all-trans: 0.819
nm
Estimated maximum distance required for P-LINCS: 0.819 nm
This distance will limit the DD cell size, you can override this with -
rcon
Scaling the initial minimum size with 1/0.8 (option -dds) = 1.25
Guess for relative PME load: 0.29
Will use 40 particle-particle and 20 PME only ranks
This is a guess, check the performance at the end of the log file
Using 20 separate PME ranks, as guessed by mdrun
Optimizing the DD grid for 40 cells with a minimum initial size of 1.024
nm
The maximum allowed number of cells is: X 7 Y 7 Z 6
Domain decomposition grid 5 x 4 x 2, separate PME ranks 20
PME domain decomposition: 5 x 4 x 1
Interleaving PP and PME ranks
This rank does only particle-particle work.
Domain decomposition rank 0, coordinates 0 0 0

The initial number of communication pulses is: X 1 Y 1 Z 1
The initial domain decomposition cell size is: X 1.61 nm Y 2.01 nm Z 3.48
nm

The maximum allowed distance for atoms involved in interactions is:
                 non-bonded interactions           1.232 nm
(the following are initial values, they could change due to box
deformation)
            two-body bonded interactions  (-rdd)   1.232 nm
          multi-body bonded interactions  (-rdd)   1.232 nm
  atoms separated by up to 5 constraints  (-rcon)  1.606 nm

When dynamic load balancing gets turned on, these settings will change
to:
The maximum number of communication pulses is: X 1 Y 1 Z 1
The minimum size for domain decomposition cells is 1.232 nm
The requested allowed shrink of DD cells (option -dds) is: 0.80
The allowed shrink of domain decomposition cells is: X 0.77 Y 0.61 Z 0.35
The maximum allowed distance for atoms involved in interactions is:
                 non-bonded interactions           1.232 nm
            two-body bonded interactions  (-rdd)   1.232 nm
          multi-body bonded interactions  (-rdd)   1.232 nm
  atoms separated by up to 5 constraints  (-rcon)  1.232 nm
Using two step summing over 10 groups of on average 4.0 ranks


Using 60 MPI processes

Non-default thread affinity set, disabling internal thread affinity
```

```
Using 1 OpenMP thread per MPI process

System total charge, top. A: 0.000 top. B: -1.000
Will do PME sum in reciprocal space for electrostatic interactions.

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
U. Essmann, L. Perera, M. L. Berkowitz, T. Darden, H. Lee and L. G.
Pedersen
A smooth particle mesh Ewald method
J. Chem. Phys. 103 (1995) pp. 8577-8592
-------- -------- --- Thank You --- -------- --------

Using a Gaussian width (1/beta) of 0.352179 nm for Ewald
Potential shift: LJ r^-12: 0.000e+00 r^-6: 0.000e+00, Ewald -9.091e-06
Initialized non-bonded Coulomb Ewald tables, spacing: 9.79e-04 size: 2282

Generated table with 1115 data points for 1-4 COUL.
Tabscale = 500 points/nm
Generated table with 1115 data points for 1-4 LJ6.
Tabscale = 500 points/nm
Generated table with 1115 data points for 1-4 LJ12.
Tabscale = 500 points/nm
Long Range LJ corr.: <C6> 3.0958e-04


Using SIMD 4x8 nonbonded short-range kernels

Using a dual 4x8 pair-list setup updated with dynamic pruning:
  outer list: updated every 80 steps, buffer 0.132 nm, rlist 1.232 nm
  inner list: updated every 13 steps, buffer 0.003 nm, rlist 1.103 nm
At tolerance 0.005 kJ/mol/ps per atom, equivalent classical 1x1 list
would be:
  outer list: updated every 80 steps, buffer 0.270 nm, rlist 1.370 nm
  inner list: updated every 13 steps, buffer 0.052 nm, rlist 1.152 nm

The non-bonded pair calculation algorithm tolerates a few missing pair
interactions close to the cut-off. This can lead to a systematic
overestimation of the pressure due to missing LJ interactions. The error
in the average pressure due to missing LJ interactions is at most 1.25
bar.
The pressure error can be controlled by setting the environment variable
GMX_VERLET_BUFFER_PRESSURE_TOLERANCE to the allowed error in units of
bar.
There are 61 atoms and 61 charges for free energy perturbation

Linking all bonded interactions to atoms


Initializing Parallel LINear Constraint Solver

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
B. Hess
P-LINCS: A Parallel Linear Constraint Solver for molecular simulation
J. Chem. Theory Comput. 4 (2008) pp. 116-122
-------- -------- --- Thank You --- -------- --------

The number of constraints is 4701
```

```
There are constraints between atoms in different decomposition domains,
will communicate selected coordinates each lincs iteration

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. Miyamoto and P. A. Kollman
SETTLE: An Analytical Version of the SHAKE and RATTLE Algorithms for
Rigid
Water Models
J. Comp. Chem. 13 (1992) pp. 952-962
-------- -------- --- Thank You --- -------- --------


Intra-simulation communication will occur every 10 steps.
Initial vector of lambda components:[     0.0000     0.0000     0.0000
0.0000     0.0000     0.0000     0.0000 ]

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
N. Goga and A. J. Rzepiela and A. H. de Vries and S. J. Marrink and H. J.
C.
Berendsen
Efficient Algorithms for Langevin and DPD Dynamics
J. Chem. Theory Comput. 8 (2012) pp. 3637--3649
-------- -------- --- Thank You --- -------- --------

There are: 67291 Atoms
Atom distribution over 40 domains: av 1682 stddev 46 min 1621 max 1772
Center of mass motion removal mode is Linear
We have the following groups for center of mass motion removal:
  0:  rest

Started mdrun on rank 0 Sun Jan 14 18:03:05 2024

           Step           Time
              0        0.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.03471e+04    1.16572e+04    8.17095e+02    5.07276e+03
5.18933e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.21209e+05   -3.77970e+03   -1.12353e+06    4.51452e+03   -
9.21801e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.67925e+05   -7.53877e+05    2.99990e+02   -9.33422e+01
1.04726e+02
    dVremain/dl   Constr. rmsd
    7.32140e+01    3.49038e-06


DD  step 79 load imb.: force 53.9%  pme mesh/force 1.952
step  720: timed with pme grid 84 84 84, coulomb cutoff 1.100: 1089.8 M-
cycles
step  880: timed with pme grid 72 72 72, coulomb cutoff 1.252: 1315.2 M-
cycles
```

```
step 1040: timed with pme grid 80 80 80, coulomb cutoff 1.127: 1160.9 M-
cycles
step 1200: timed with pme grid 84 84 84, coulomb cutoff 1.100: 1180.4 M-
cycles
             optimal pme grid 84 84 84, coulomb cutoff 1.100

DD  step 9999 load imb.: force 48.1%  pme mesh/force 1.705
           Step           Time
          10000       20.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.01727e+04    1.17101e+04    7.41895e+02    5.10221e+03
5.19138e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.19858e+05   -3.76137e+03   -1.12037e+06    4.61936e+03   -
9.20016e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.65732e+05   -7.54283e+05    2.96074e+02   -9.24393e+01   -
9.18308e+01
    dVremain/dl   Constr. rmsd
    2.20368e+01    3.48482e-06


DD  step 19999 load imb.: force 75.2%  pme mesh/force 1.493
           Step           Time
          20000       40.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    9.92697e+03    1.17502e+04    7.49933e+02    5.19496e+03
5.19461e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.19624e+05   -3.75831e+03   -1.12151e+06    4.65719e+03   -
9.21415e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.67366e+05   -7.54049e+05    2.98992e+02   -9.22886e+01   -
7.03647e+01
    dVremain/dl   Constr. rmsd
    1.78703e+02    3.58300e-06


DD  step 29999 load imb.: force 54.4%  pme mesh/force 1.721
           Step           Time
          30000       60.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.03077e+04    1.16444e+04    7.00273e+02    5.13749e+03
5.17391e+04
```

```
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.20321e+05   -3.77794e+03   -1.12196e+06    4.56758e+03   -
9.21316e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.66570e+05   -7.54746e+05    2.97570e+02   -9.32555e+01
3.97827e+01
    dVremain/dl   Constr. rmsd
    1.06661e+02    3.60657e-06


DD  step 39999 load imb.: force 61.0%  pme mesh/force 1.579
           Step           Time
          40000       80.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    9.94073e+03    1.16704e+04    7.34059e+02    5.12605e+03
5.19438e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.21583e+05   -3.76716e+03   -1.12179e+06    4.47358e+03   -
9.20082e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.66926e+05   -7.53156e+05    2.98206e+02   -9.27239e+01
1.78899e+02
    dVremain/dl   Constr. rmsd
    1.65384e+02    3.62426e-06


DD  step 49999 load imb.: force 48.7%  pme mesh/force 1.817
           Step           Time
          50000      100.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.04724e+04    1.15445e+04    7.52346e+02    5.08040e+03
5.16231e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.21484e+05   -3.76492e+03   -1.12374e+06    4.62346e+03   -
9.21924e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.66379e+05   -7.55545e+05    2.97229e+02   -9.26137e+01   -
6.10418e+01
    dVremain/dl   Constr. rmsd
    1.04800e+02    3.58890e-06


DD  step 59999 load imb.: force 51.0%  pme mesh/force 1.729
           Step           Time
          60000      120.00000
```

```
   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.01073e+04    1.16031e+04    7.12690e+02    5.12194e+03
5.20016e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.21542e+05   -3.77574e+03   -1.12341e+06    4.55534e+03   -
9.21540e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.67680e+05   -7.53860e+05    2.99553e+02   -9.31468e+01
5.82031e+01
    dVremain/dl   Constr. rmsd
    1.28359e+02    3.44644e-06



[...]



DD  step 2999999 load imb.: force 34.4%  pme mesh/force 1.948
           Step           Time
        3000000     6000.00000

Writing checkpoint, step 3000000 at Mon Jan 15 00:05:53 2024


   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    9.86736e+03    1.17087e+04    6.76734e+02    5.07992e+03
5.22697e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.19922e+05   -3.76566e+03   -1.12259e+06    4.48341e+03   -
9.22343e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.67819e+05   -7.54523e+05    2.99802e+02   -9.26503e+01   -
7.55178e+01
    dVremain/dl   Constr. rmsd
    1.15256e+02    3.75583e-06


      <======  ###############  ==>
      <====  A V E R A G E S  ====>
      <==  ###############  ======>

      Statistics over 3000001 steps using 30001 frames

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.00524e+04    1.16505e+04    7.27051e+02    5.12332e+03
5.20993e+04
```

```
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.20327e+05   -3.76878e+03   -1.12185e+06    4.55416e+03   -
9.21085e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.66995e+05   -7.54090e+05    2.98330e+02   -9.28042e+01    9.20272e-
01
    dVremain/dl   Constr. rmsd
    1.26912e+02    0.00000e+00

          Box-X          Box-Y          Box-Z
    9.84269e+00    9.84269e+00    6.95983e+00

   Total Virial (kJ/mol)
    5.56517e+04   -1.29520e+00   -3.19727e+01
   -1.57080e+00    5.56989e+04   -4.73058e+01
   -3.21082e+01   -4.73868e+01    5.55931e+04

   Pressure (bar)
    1.38426e+00    4.07664e-01    1.67121e-01
    4.21237e-01   -4.11712e-01   -9.15071e-02
    1.73790e-01   -8.75226e-02    1.78826e+00


     M E G A - F L O P S   A C C O U N T I N G

 NB=Group-cutoff nonbonded kernels    NxN=N-by-N cluster Verlet kernels
 RF=Reaction-Field  VdW=Van der Waals  QSTab=quadratic-spline table
 W3=SPC/TIP3p  W4=TIP4p (single or pairs)
 V&F=Potential and force  V=Potential only  F=Force only

 Computing:                                M-Number         M-Flops  %
Flops
-----------------------------------------------------------------------
----
 NB Free energy kernel            27295213.389744    27295213.390
0.2
 Pair Search distance check        1511062.063992    13599558.576
0.1
 NxN Ewald Elec. + LJ [F]         93946208.351104  8736997376.653
57.1
 NxN Ewald Elec. + LJ [V&F]         948977.165952   120520100.076
0.8
 NxN Ewald Elec. [F]              80529243.547328  4912283856.387
32.1
 NxN Ewald Elec. [V&F]              813451.915264    68329960.882
0.4
 1,4 nonbonded interactions          36702.012234     3303181.101
0.0
 Calc Weights                       605619.201873    21802291.267
0.1
 Spread Q Bspline                 25839752.613248    51679505.226
0.3
 Gather F Bspline                 25839752.613248   155038515.679
1.0
 3D-FFT                          136391204.956224  1091129639.650
7.1
```

```
 Solve PME                          169340.820608    10837812.519
0.1
 Reset In Box                         2523.412500        7570.237
0.0
 CG-CoM                               2523.479791        7570.439
0.0
 Angles                              25548.008516     4292065.431
0.0
 Propers                             39945.013315     9147408.049
0.1
 Impropers                            3591.001197      746928.249
0.0
 Virial                              20727.369091      373092.644
0.0
 Update                             201873.067291     6258065.086
0.0
 Stop-CM                              2018.797291       20187.973
0.0
 Calc-Ekin                           40374.734582     1090117.834
0.0
 Lincs                               54997.867262     3299872.036
0.0
 Lincs-Mat                         1177726.220496     4710904.882
0.0
 Constraint-V                       529584.307342     4766258.766
0.0
 Constraint-Vir                      23729.393536      569505.445
0.0
 Settle                             139862.857606    51749257.314
0.3
-----------------------------------------------------------------------
----
 Total                                              15299855815.791
100.0
-----------------------------------------------------------------------
----


    D O M A I N   D E C O M P O S I T I O N   S T A T I S T I C S

 av. #atoms communicated per step for force:  2 x 174534.6
 av. #atoms communicated per step for LINCS:  3 x 12284.7


Dynamic load balancing report:
 DLB was off during the run due to low measured imbalance.
 Average load imbalance: 53.6%.
 The balanceable part of the MD step is 30%, load imbalance is computed
from this.
 Part of the total run time spent waiting due to load imbalance: 16.2%.
 Average PME mesh/force load: 1.666
 Part of the total run time spent waiting due to PP/PME imbalance: 21.4 %

NOTE: 16.2 % of the available CPU time was lost due to load imbalance
      in the domain decomposition.
      Dynamic load balancing was automatically disabled, but it might be
beneficial to manually turn it on (option -dlb yes.)
```

```
      You can also consider manually changing the decomposition (option -
dd);
      e.g. by using fewer domains along the box dimension in which there
is
      considerable inhomogeneity in the simulated system.
NOTE: 21.4 % performance was lost because the PME ranks
      had more work to do than the PP ranks.
      You might want to increase the number of PME ranks
      or increase the cut-off and the grid spacing.


      R E A L   C Y C L E   A N D   T I M E   A C C O U N T I N G

On 40 MPI ranks doing PP, and
on 20 MPI ranks doing PME

 Activity:              Num   Num      Call    Wall time         Giga-
Cycles
                       Ranks Threads  Count      (s)         total sum
%
-----------------------------------------------------------------------
-------
 Domain decomp.           40    1      37500     153.197      18043.126
0.5
 DD comm. load            40    1       7500       0.158         18.630
0.0
 Send X to PME            40    1    3000001      56.019       6597.825
0.2
 Neighbor search          40    1      37501     173.140      20392.002
0.5
 Comm. coord.             40    1    2962500     749.927      88324.375
2.3
 Force                    40    1    3000001    5588.549     658204.592
17.1
 Wait + Comm. F           40    1    3000001    2719.866     320338.645
8.3
 PME mesh *               20    1    3000001   17277.810    1017467.411
26.5
 PME wait for PP *                             4490.501     264439.669
6.9
 Wait + Recv. PME F       40    1    3000001    8123.719     956790.176
24.9
 NB X/F buffer ops.       40    1    8925001      89.384      10527.403
0.3
 Write traj.              40    1        153       0.197         23.173
0.0
 Update                   40    1    6000002     157.659      18568.648
0.5
 Constraints              40    1    6000002    3864.284     455125.174
11.8
 Comm. energies           40    1     300001      58.751       6919.540
0.2
 Rest                                           33.460       3940.837
0.1
-----------------------------------------------------------------------
-------
 Total                                         21768.311    3845721.220
100.0
```

```
-----------------------------------------------------------------------------
-------
(*) Note that with separate PME ranks, the walltime column actually sums
to
    twice the total reported, but the cycle count total and % are
correct.
-----------------------------------------------------------------------------
-------
 Breakdown of PME mesh activities
-----------------------------------------------------------------------------
-------
 PME redist. X/F          20    1    9000003    3949.148     232560.109
6.0
 PME spread               20    1    6000002    2150.430     126636.003
3.3
 PME gather               20    1    6000002    1638.899      96512.573
2.5
 PME 3D-FFT               20    1   12000004    1989.831     117178.497
3.0
 PME 3D-FFT Comm.         20    1   24000008    7381.572     434691.024
11.3
 PME solve Elec           20    1    6000002     161.771       9526.456
0.2
-----------------------------------------------------------------------------
-------

               Core t (s)   Wall t (s)        (%)
       Time:  1306098.487    21768.311     6000.0
                         6h02:48
                 (ns/day)    (hour/ns)
Performance:       23.814        1.008
Finished mdrun on rank 0 Mon Jan 15 00:05:53 2024
```

cmet_eq_cpu-sev-cluster_1n

:-) GROMACS - gmx mdrun, 2023.3 (-:

Current GROMACS contributors:

Mark Abraham, Andrey Alekseenko, Cathrine Bergh, Christian Blau, Eliane Briand, Mahesh Doijade, Stefan Fleischmann, Vytas Gapsys, Gaurav Garg, Sergey Gorelov, Gilles Gouaillardet, Alan Gray, M. Eric Irrgang, Farzaneh Jalalypour, Joe Jordan, Christoph Junghans, Prashanth Kanduri, Sebastian Keller, Carsten Kutzner, Justin A. Lemkul, Magnus Lundborg, Pascal Merz, Vedran Miletic, Dmitry Morozov, Szilard Pall, Roland Schulz, Michael Shirts, Alexey Shvetsov, Balint Soproni, David van der Spoel, Philip Turner, Carsten Uphoff, Alessandra Villa, Sebastian Wingbermuehle, Artem Zhmurov

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Coordinated by the GROMACS project leaders:
Paul Bauer, Berk Hess, and Erik Lindahl

```
GROMACS:      gmx mdrun, version 2023.3
Executable:   /usr/local/gromacs/bin/gmx_mpi
Data prefix:  /usr/local/gromacs
Working dir:  /home/ubuntu
Process ID:   8730
Command line:
  gmx_mpi mdrun -v -s /mnt/shared/home/ubuntu/mpinat-gromacs/mpinat-
gromacs-binding-affinity-study-bench/cmet_eq.tpr

GROMACS version:    2023.3
Precision:          mixed
Memory model:       64 bit
MPI library:        MPI
OpenMP support:     enabled (GMX_OPENMP_MAX_THREADS = 128)
GPU support:        disabled
SIMD instructions:  AVX2_256
```

```
CPU FFT library:    fftw-3.3.8-sse2-avx-avx2-avx2_128
GPU FFT library:    none
Multi-GPU FFT:      none
RDTSCP usage:       enabled
TNG support:        enabled
Hwloc support:      disabled
Tracing support:    disabled
C compiler:         /usr/bin/cc GNU 11.4.0
C compiler flags:   -fexcess-precision=fast -funroll-all-loops -mavx2 -
mfma -Wno-missing-field-initializers -O3 -DNDEBUG
C++ compiler:       /usr/bin/c++ GNU 11.4.0
C++ compiler flags: -fexcess-precision=fast -funroll-all-loops -mavx2 -
mfma -Wno-missing-field-initializers -Wno-cast-function-type-strict -
fopenmp -O3 -DNDEBUG
BLAS library:       Internal
LAPACK library:     Internal


Running on 1 node with total 6 cores, 6 processing units
Hardware detected on host cpu-sev-4 (the node of MPI rank 0):
  CPU info:
    Vendor: AMD
    Brand:  AMD EPYC-Milan Processor
    Family: 25   Model: 1   Stepping: 1
    Features: aes amd apic avx avx2 clfsh cmov cx8 cx16 f16c fma lahf
misalignsse mmx msr pcid pclmuldq pdpe1gb popcnt pse rdrnd rdtscp sha
sse2 sse3 sse4a sse4.1 sse4.2 ssse3 tdt x2apic
  Hardware topology: Basic
    Packages, cores, and logical processors:
    [indices refer to OS logical processors]
      Package  0: [   0]
      Package  1: [   1]
      Package  2: [   2]
      Package  3: [   3]
      Package  4: [   4]
      Package  5: [   5]
    CPU limit set by OS: -1   Recommended max number of threads: 6


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
M. J. Abraham, T. Murtola, R. Schulz, S. P√°ll, J. C. Smith, B. Hess, E.
Lindahl
GROMACS: High performance molecular simulations through multi-level
parallelism from laptops to supercomputers
SoftwareX 1 (2015) pp. 19-25
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. P√°ll, M. J. Abraham, C. Kutzner, B. Hess, E. Lindahl
Tackling Exascale Software Challenges in Molecular Dynamics Simulations
with
GROMACS
In S. Markidis & E. Laure (Eds.), Solving Software Challenges for
Exascale 8759 (2015) pp. 3-27
-------- -------- --- Thank You --- -------- --------
```

```
++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. Pronk, S. P√°ll, R. Schulz, P. Larsson, P. Bjelkmar, R. Apostolov, M.
R.
Shirts, J. C. Smith, P. M. Kasson, D. van der Spoel, B. Hess, and E.
Lindahl
GROMACS 4.5: a high-throughput and highly parallel open source molecular
simulation toolkit
Bioinformatics 29 (2013) pp. 845-54
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
B. Hess and C. Kutzner and D. van der Spoel and E. Lindahl
GROMACS 4: Algorithms for highly efficient, load-balanced, and scalable
molecular simulation
J. Chem. Theory Comput. 4 (2008) pp. 435-447
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
D. van der Spoel, E. Lindahl, B. Hess, G. Groenhof, A. E. Mark and H. J.
C.
Berendsen
GROMACS: Fast, Flexible and Free
J. Comp. Chem. 26 (2005) pp. 1701-1719
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
E. Lindahl and B. Hess and D. van der Spoel
GROMACS 3.0: A package for molecular simulation and trajectory analysis
J. Mol. Mod. 7 (2001) pp. 306-317
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
H. J. C. Berendsen, D. van der Spoel and R. van Drunen
GROMACS: A message-passing parallel molecular dynamics implementation
Comp. Phys. Comm. 91 (1995) pp. 43-56
-------- -------- --- Thank You --- -------- --------


++++ PLEASE CITE THE DOI FOR THIS VERSION OF GROMACS ++++
https://doi.org/10.5281/zenodo.10017686
-------- -------- --- Thank You --- -------- --------


The number of OpenMP threads was set by environment variable
OMP_NUM_THREADS to 1

Input Parameters:
   integrator                     = sd
   tinit                          = 0
   dt                             = 0.002
   nsteps                         = 3000000
   init-step                      = 0
   simulation-part                = 1
   mts                            = false
```

```
comm-mode                       = Linear
nstcomm                         = 100
bd-fric                         = 0
ld-seed                         = -1628089582
emtol                           = 100
emstep                          = 0.01
niter                           = 0
fcstep                          = 0
nstcgsteep                      = 1000
nbfgscorr                       = 10
rtpi                            = 0.05
nstxout                         = 23500
nstvout                         = 23500
nstfout                         = 0
nstlog                          = 10000
nstcalcenergy                   = 100
nstenergy                       = 23500
nstxout-compressed              = 23500
compressed-x-precision          = 1000
cutoff-scheme                   = Verlet
nstlist                         = 10
pbc                             = xyz
periodic-molecules              = false
verlet-buffer-tolerance         = 0.005
rlist                           = 1.1
coulombtype                     = PME
coulomb-modifier                = Potential-shift
rcoulomb-switch                 = 0
rcoulomb                        = 1.1
epsilon-r                       = 1
epsilon-rf                      = inf
vdw-type                        = Cut-off
vdw-modifier                    = Potential-switch
rvdw-switch                     = 1
rvdw                            = 1.1
DispCorr                        = EnerPres
table-extension                 = 1
fourierspacing                  = 0.12
fourier-nx                      = 84
fourier-ny                      = 84
fourier-nz                      = 84
pme-order                       = 4
ewald-rtol                      = 1e-05
ewald-rtol-lj                   = 0.001
lj-pme-comb-rule                = Geometric
ewald-geometry                  = 3d
epsilon-surface                 = 0
ensemble-temperature-setting    = constant
ensemble-temperature            = 298
tcoupl                          = No
nsttcouple                      = -1
nh-chain-length                 = 0
print-nose-hoover-chain-variables = false
pcoupl                          = Parrinello-Rahman
pcoupltype                      = Isotropic
nstpcouple                      = 10
tau-p                           = 5
compressibility (3x3):
```

```
      compressibility[    0]={ 4.60000e-05,  0.00000e+00,  0.00000e+00}
      compressibility[    1]={ 0.00000e+00,  4.60000e-05,  0.00000e+00}
      compressibility[    2]={ 0.00000e+00,  0.00000e+00,  4.60000e-05}
   ref-p (3x3):
      ref-p[    0]={ 1.00000e+00,  0.00000e+00,  0.00000e+00}
      ref-p[    1]={ 0.00000e+00,  1.00000e+00,  0.00000e+00}
      ref-p[    2]={ 0.00000e+00,  0.00000e+00,  1.00000e+00}
   refcoord-scaling               = COM
   posres-com (3):
      posres-com[0]= 0.00000e+00
      posres-com[1]= 0.00000e+00
      posres-com[2]= 0.00000e+00
   posres-comB (3):
      posres-comB[0]= 0.00000e+00
      posres-comB[1]= 0.00000e+00
      posres-comB[2]= 0.00000e+00
   QMMM                           = false
qm-opts:
   ngQM                           = 0
   constraint-algorithm           = Lincs
   continuation                   = true
   Shake-SOR                      = false
   shake-tol                      = 0.0001
   lincs-order                    = 4
   lincs-iter                     = 2
   lincs-warnangle                = 30
   nwall                          = 0
   wall-type                      = 9-3
   wall-r-linpot                  = -1
   wall-atomtype[0]               = -1
   wall-atomtype[1]               = -1
   wall-density[0]                = 0
   wall-density[1]                = 0
   wall-ewald-zfac                = 3
   pull                           = false
   awh                            = false
   rotation                       = false
   interactiveMD                  = false
   disre                          = No
   disre-weighting                = Equal
   disre-mixed                    = false
   dr-fc                          = 1000
   dr-tau                         = 0
   nstdisreout                    = 100
   orire-fc                       = 0
   orire-tau                      = 0
   nstorireout                    = 100
   free-energy                    = yes
   init-lambda                    = 0
   init-lambda-state              = -1
   delta-lambda                   = 0
   nstdhdl                        = 10000
   n-lambdas                      = 0
   calc-lambda-neighbors          = 1
   dhdl-print-energy              = no
   sc-alpha                       = 0.3
   sc-power                       = 1
   sc-r-power                     = 6
```

```
   sc-sigma                       = 0.25
   sc-sigma-min                   = 0.25
   sc-coul                        = true
   dh-hist-size                   = 0
   dh-hist-spacing                = 0.1
   separate-dhdl-file             = yes
   dhdl-derivatives               = yes
   sc-function                    = beutler
   sc-gapsys-scale-linpoint-lj    = 0.85
   sc-gapsys-scale-linpoint-q     = 0.3
   sc-gapsys-sigma-lj             = 0.3
   cos-acceleration               = 0
   deform (3x3):
      deform[    0]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
      deform[    1]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
      deform[    2]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
   simulated-tempering            = false
   swapcoords                     = no
   userint1                       = 0
   userint2                       = 0
   userint3                       = 0
   userint4                       = 0
   userreal1                      = 0
   userreal2                      = 0
   userreal3                      = 0
   userreal4                      = 0
   applied-forces:
     electric-field:
       x:
         E0                       = 0
         omega                    = 0
         t0                       = 0
         sigma                    = 0
       y:
         E0                       = 0
         omega                    = 0
         t0                       = 0
         sigma                    = 0
       z:
         E0                       = 0
         omega                    = 0
         t0                       = 0
         sigma                    = 0
grpopts:
   nrdf:      134649
   ref-t:         298
   tau-t:           2
annealing:          No
annealing-npoints:           0
   acc:               0           0           0
   nfreeze:           N           N           N
   energygrp-flags[  0]: 0

Changing nstlist from 10 to 80, rlist from 1.1 to 1.232

Update groups can not be used for this system because there are three or
more consecutively coupled constraints
```

```
Initializing Domain Decomposition on 6 ranks
Dynamic load balancing: auto
Minimum cell size due to atom displacement: 0.639 nm
Initial maximum distances in bonded interactions:
    two-body bonded interactions: 0.438 nm, LJ-14, atoms 4073 4080
  multi-body bonded interactions: 0.438 nm, Proper Dih., atoms 4073 4080
Minimum cell size due to bonded interactions: 0.482 nm
Maximum distance for 5 constraints, at 120 deg. angles, all-trans: 0.819
nm
Estimated maximum distance required for P-LINCS: 0.819 nm
This distance will limit the DD cell size, you can override this with -
rcon
Scaling the initial minimum size with 1/0.8 (option -dds) = 1.25
Using 0 separate PME ranks because: there are too few total ranks for
efficient splitting
Optimizing the DD grid for 6 cells with a minimum initial size of 1.024
nm
The maximum allowed number of cells is: X 7 Y 7 Z 6
Domain decomposition grid 6 x 1 x 1, separate PME ranks 0
PME domain decomposition: 6 x 1 x 1
Domain decomposition rank 0, coordinates 0 0 0

The initial number of communication pulses is: X 1
The initial domain decomposition cell size is: X 1.34 nm

The maximum allowed distance for atoms involved in interactions is:
                 non-bonded interactions           1.232 nm
(the following are initial values, they could change due to box
deformation)
            two-body bonded interactions  (-rdd)   1.232 nm
          multi-body bonded interactions  (-rdd)   1.232 nm
  atoms separated by up to 5 constraints  (-rcon)  1.338 nm

When dynamic load balancing gets turned on, these settings will change
to:
The maximum number of communication pulses is: X 2
The minimum size for domain decomposition cells is 0.910 nm
The requested allowed shrink of DD cells (option -dds) is: 0.80
The allowed shrink of domain decomposition cells is: X 0.68
The maximum allowed distance for atoms involved in interactions is:
                 non-bonded interactions           1.232 nm
            two-body bonded interactions  (-rdd)   1.232 nm
          multi-body bonded interactions  (-rdd)   0.910 nm
  atoms separated by up to 5 constraints  (-rcon)  0.910 nm

Using 6 MPI processes

Non-default thread affinity set, disabling internal thread affinity

Using 1 OpenMP thread per MPI process

System total charge, top. A: 0.000 top. B: -1.000
Will do PME sum in reciprocal space for electrostatic interactions.

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
U. Essmann, L. Perera, M. L. Berkowitz, T. Darden, H. Lee and L. G.
Pedersen
A smooth particle mesh Ewald method
```

```
J. Chem. Phys. 103 (1995) pp. 8577-8592
-------- -------- --- Thank You --- -------- --------

Using a Gaussian width (1/beta) of 0.352179 nm for Ewald
Potential shift: LJ r^-12: 0.000e+00 r^-6: 0.000e+00, Ewald -9.091e-06
Initialized non-bonded Coulomb Ewald tables, spacing: 9.79e-04 size: 2282

Generated table with 1115 data points for 1-4 COUL.
Tabscale = 500 points/nm
Generated table with 1115 data points for 1-4 LJ6.
Tabscale = 500 points/nm
Generated table with 1115 data points for 1-4 LJ12.
Tabscale = 500 points/nm
Long Range LJ corr.: <C6> 3.0958e-04


Using SIMD 4x8 nonbonded short-range kernels

Using a dual 4x8 pair-list setup updated with dynamic pruning:
  outer list: updated every 80 steps, buffer 0.132 nm, rlist 1.232 nm
  inner list: updated every 13 steps, buffer 0.003 nm, rlist 1.103 nm
At tolerance 0.005 kJ/mol/ps per atom, equivalent classical 1x1 list
would be:
  outer list: updated every 80 steps, buffer 0.270 nm, rlist 1.370 nm
  inner list: updated every 13 steps, buffer 0.052 nm, rlist 1.152 nm

The non-bonded pair calculation algorithm tolerates a few missing pair
interactions close to the cut-off. This can lead to a systematic
overestimation of the pressure due to missing LJ interactions. The error
in the average pressure due to missing LJ interactions is at most 1.25
bar.
The pressure error can be controlled by setting the environment variable
GMX_VERLET_BUFFER_PRESSURE_TOLERANCE to the allowed error in units of
bar.
There are 61 atoms and 61 charges for free energy perturbation

Linking all bonded interactions to atoms


Initializing Parallel LINear Constraint Solver

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
B. Hess
P-LINCS: A Parallel Linear Constraint Solver for molecular simulation
J. Chem. Theory Comput. 4 (2008) pp. 116-122
-------- -------- --- Thank You --- -------- --------

The number of constraints is 4701
There are constraints between atoms in different decomposition domains,
will communicate selected coordinates each lincs iteration

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. Miyamoto and P. A. Kollman
SETTLE: An Analytical Version of the SHAKE and RATTLE Algorithms for
Rigid
Water Models
J. Comp. Chem. 13 (1992) pp. 952-962
-------- -------- --- Thank You --- -------- --------
```

```
Intra-simulation communication will occur every 10 steps.
Initial vector of lambda components:[     0.0000     0.0000     0.0000
0.0000     0.0000     0.0000     0.0000 ]

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
N. Goga and A. J. Rzepiela and A. H. de Vries and S. J. Marrink and H. J.
C.
Berendsen
Efficient Algorithms for Langevin and DPD Dynamics
J. Chem. Theory Comput. 8 (2012) pp. 3637--3649
-------- -------- --- Thank You --- -------- --------

There are: 67291 Atoms
Atom distribution over 6 domains: av 11215 stddev 149 min 11078 max 11409
Center of mass motion removal mode is Linear
We have the following groups for center of mass motion removal:
  0:  rest

Started mdrun on rank 0 Sat Jan 13 12:39:24 2024

           Step           Time
              0        0.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.03471e+04    1.16572e+04    8.17096e+02    5.07276e+03
5.18934e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.21209e+05   -3.77970e+03   -1.12353e+06    4.51443e+03   -
9.21800e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.67924e+05   -7.53875e+05    2.99990e+02   -9.33422e+01
1.04720e+02
    dVremain/dl   Constr. rmsd
    7.32211e+01    3.46295e-06


DD  step 79 load imb.: force 19.2%

step 240 Turning on dynamic load balancing, because the performance loss
due to load imbalance is 10.9 %.

DD  step 9999  vol min/aver 0.803  load imb.: force  0.4%
           Step           Time
          10000       20.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.00150e+04    1.16358e+04    7.11841e+02    5.12583e+03
5.18132e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
```

```
    1.19005e+05   -3.76444e+03   -1.12048e+06    4.55538e+03   -
9.21383e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.66717e+05   -7.54667e+05    2.97832e+02   -9.25901e+01   -
1.22847e+02
    dVremain/dl   Constr. rmsd
    7.73340e+01    3.46697e-06


DD  step 19999  vol min/aver 0.807  load imb.: force  0.9%
          Step           Time
         20000       40.00000

   Energies (kJ/mol)
         Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.00129e+04    1.16411e+04    6.84081e+02    5.21976e+03
5.19363e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.20241e+05   -3.77721e+03   -1.12161e+06    4.52212e+03   -
9.21131e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.67564e+05   -7.53567e+05    2.99346e+02   -9.32192e+01
9.51121e+01
    dVremain/dl   Constr. rmsd
    1.05939e+02    3.46896e-06


DD  step 29999  vol min/aver 0.797  load imb.: force  0.9%
          Step           Time
         30000       60.00000

   Energies (kJ/mol)
         Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    9.95831e+03    1.16234e+04    7.57119e+02    5.07954e+03
5.17440e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.20045e+05   -3.76512e+03   -1.12039e+06    4.62069e+03   -
9.20331e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.66211e+05   -7.54120e+05    2.96930e+02   -9.26237e+01   -
2.86171e+01
    dVremain/dl   Constr. rmsd
    2.47186e+02    3.51382e-06


DD  step 39999  vol min/aver 0.796  load imb.: force  0.5%
          Step           Time
         40000       80.00000

   Energies (kJ/mol)
[...]
```

```
DD  step 2979999 load imb.: force 19.0%
           Step           Time
        2980000     5960.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.00104e+04    1.17378e+04    7.66332e+02    5.08102e+03
5.20160e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.21046e+05   -3.77814e+03   -1.12249e+06    4.59733e+03   -
9.21017e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.66904e+05   -7.54113e+05    2.98167e+02   -9.32653e+01
4.09151e+01
    dVremain/dl   Constr. rmsd
    2.87500e+02    3.31692e-06


DD  step 2989999 load imb.: force 44.3%
           Step           Time
        2990000     5980.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.00142e+04    1.17962e+04    8.04830e+02    5.11582e+03
5.18616e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.19793e+05   -3.75538e+03   -1.12063e+06    4.59564e+03   -
9.20405e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.67015e+05   -7.53390e+05    2.98366e+02   -9.21452e+01   -
1.22817e+02
    dVremain/dl   Constr. rmsd
    1.42069e+02    3.37740e-06


DD  step 2999999 load imb.: force 17.3%
           Step           Time
        3000000     6000.00000

Writing checkpoint, step 3000000 at Sun Jan 14 05:33:33 2024


   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    9.80515e+03    1.16297e+04    7.02901e+02    5.26288e+03
5.21123e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
```

```
    1.20396e+05   -3.75964e+03   -1.12158e+06    4.46765e+03   -
9.20960e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.66159e+05   -7.54801e+05    2.96836e+02   -9.23541e+01
1.19555e+02
    dVremain/dl   Constr. rmsd
    1.86993e+02    3.27206e-06


      <======  ###############  ==>
      <====  A V E R A G E S  ====>
      <==  ###############  ======>

      Statistics over 3000001 steps using 30001 frames

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.00301e+04    1.16671e+04    7.25199e+02    5.11629e+03
5.19870e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.20356e+05   -3.76884e+03   -1.12181e+06    4.55281e+03   -
9.21143e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.66968e+05   -7.54175e+05    2.98282e+02   -9.28069e+01
1.12804e+00
    dVremain/dl   Constr. rmsd
    1.41377e+02    0.00000e+00

          Box-X          Box-Y          Box-Z
    9.84264e+00    9.84264e+00    6.95980e+00

   Total Virial (kJ/mol)
    5.56355e+04    7.45454e+00    2.23143e+01
    7.58829e+00    5.56544e+04    3.09531e-01
    2.19717e+01   -2.36005e-01    5.56141e+04

   Pressure (bar)
    2.51199e+00    9.59219e-01    2.14983e-01
    9.52629e-01    1.19426e+00    9.77070e-02
    2.31863e-01    1.24580e-01   -3.22137e-01


     M E G A - F L O P S   A C C O U N T I N G

 NB=Group-cutoff nonbonded kernels    NxN=N-by-N cluster Verlet kernels
 RF=Reaction-Field  VdW=Van der Waals  QSTab=quadratic-spline table
 W3=SPC/TIP3p  W4=TIP4p (single or pairs)
 V&F=Potential and force  V=Potential only  F=Force only

 Computing:                                M-Number         M-Flops  %
Flops
-----------------------------------------------------------------------
----
```

```
 NB Free energy kernel             27234080.674542    27234080.675
0.2
 Pair Search distance check         1414741.192716    12732670.734
0.1
 NxN Ewald Elec. + LJ [F]          89322003.624848  8306946337.111
57.1
 NxN Ewald Elec. + LJ [V&F]          902277.042480   114589184.395
0.8
 NxN Ewald Elec. [F]               75567189.704016  4609598571.945
31.7
 NxN Ewald Elec. [V&F]               763327.799152    64119535.129
0.4
 1,4 nonbonded interactions           36702.012234     3303181.101
0.0
 Calc Weights                        605619.201873    21802291.267
0.1
 Spread Q Bspline                  25839752.613248    51679505.226
0.4
 Gather F Bspline                  25839752.613248   155038515.679
1.1
 3D-FFT                           136395117.465024  1091160939.720
7.5
 Solve PME                            42336.014112     2709504.903
0.0
 Reset In Box                          2523.143336        7569.430
0.0
 CG-CoM                                2523.479791        7570.439
0.0
 Angles                               25548.008516     4292065.431
0.0
 Propers                              39945.013315     9147408.049
0.1
 Impropers                             3591.001197      746928.249
0.0
 Virial                               20268.367561      364830.616
0.0
 Update                              201873.067291     6258065.086
0.0
 Stop-CM                               2018.797291       20187.973
0.0
 Calc-Ekin                            40374.734582     1090117.834
0.0
 Lincs                                40602.315488     2436138.929
0.0
 Lincs-Mat                           876002.777160     3504011.109
0.0
 Constraint-V                        480275.478004     4322479.302
0.0
 Constraint-Vir                       21983.724058      527609.377
0.0
 Settle                              133023.615676    49218737.800
0.3
-----------------------------------------------------------------------
----
 Total                                              14542858037.511
100.0
-----------------------------------------------------------------------
----
```

```
    D O M A I N   D E C O M P O S I T I O N   S T A T I S T I C S

 av. #atoms communicated per step for force:  2 x 61902.1
 av. #atoms communicated per step for LINCS:  3 x 6082.3


Dynamic load balancing report:
 DLB got disabled because it was unsuitable to use.
 Average load imbalance: 14.6%.
 The balanceable part of the MD step is 58%, load imbalance is computed
from this.
 Part of the total run time spent waiting due to load imbalance: 8.5%.

NOTE: 8.5 % of the available CPU time was lost due to load imbalance
      in the domain decomposition.
      You can consider manually changing the decomposition (option -dd);
      e.g. by using fewer domains along the box dimension in which there
is
      considerable inhomogeneity in the simulated system.

      R E A L   C Y C L E   A N D   T I M E   A C C O U N T I N G

On 6 MPI ranks

 Activity:              Num   Num      Call    Wall time         Giga-
Cycles
                       Ranks Threads  Count      (s)         total sum
%
-----------------------------------------------------------------------
-------
 Domain decomp.            6    1      37500     187.060       3304.727
0.3
 DD comm. load             6    1      11547       0.182          3.208
0.0
 DD comm. bounds           6    1       5057       0.207          3.656
0.0
 Neighbor search           6    1      37501     775.011      13691.827
1.3
 Comm. coord.              6    1    2962500     180.786       3193.883
0.3
 Force                     6    1    3000001   33687.707     595148.129
55.4
 Wait + Comm. F            6    1    3000001     213.684       3775.071
0.4
 PME mesh                  6    1    3000001   22269.500     393426.927
36.6
 NB X/F buffer ops.        6    1    8925001     209.940       3708.935
0.3
 Write traj.               6    1        196       0.623         11.012
0.0
 Update                    6    1    6000002     848.041      14982.029
1.4
 Constraints               6    1    6000002    2363.601      41756.858
3.9
 Comm. energies            6    1     300001      19.090        337.258
0.0
```

```
 Rest                                                 93.257       1647.531
0.2
-----------------------------------------------------------------------------
-------
 Total                                             60848.689    1074991.050
100.0
-----------------------------------------------------------------------------
-------
 Breakdown of PME mesh activities
-----------------------------------------------------------------------------
-------
 PME redist. X/F          6    1    9000003    8271.106     146122.533
13.6
 PME spread               6    1    6000002    3478.129      61446.807
5.7
 PME gather               6    1    6000002    1815.063      32066.047
3.0
 PME 3D-FFT               6    1   12000004    6520.734     115199.378
10.7
 PME 3D-FFT Comm.         6    1   12000004    1668.544      29477.535
2.7
 PME solve Elec           6    1    6000002     509.642       9003.663
0.8
-----------------------------------------------------------------------------
-------

               Core t (s)   Wall t (s)        (%)
       Time:   365092.133    60848.689      600.0
                         16h54:08
                 (ns/day)    (hour/ns)
Performance:        8.519        2.817
Finished mdrun on rank 0 Sun Jan 14 05:33:33 2024
```

cmet_eq_cpu-sev-cluster_3n

```
                :-) GROMACS - gmx mdrun, 2023.3 (-:

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                    Coordinated by the GROMACS project leaders:
                      Paul Bauer, Berk Hess, and Erik Lindahl

GROMACS:      gmx mdrun, version 2023.3
Executable:   /usr/local/gromacs/bin/gmx_mpi
Data prefix:  /usr/local/gromacs
Working dir:  /home/ubuntu
Process ID:   21011
Command line:
  gmx_mpi mdrun -v -s /mnt/shared/home/ubuntu/mpinat-gromacs/mpinat-
gromacs-binding-affinity-study-bench/cmet_eq.tpr

GROMACS version:    2023.3
Precision:          mixed
Memory model:       64 bit
MPI library:        MPI
OpenMP support:     enabled (GMX_OPENMP_MAX_THREADS = 128)
GPU support:        disabled
SIMD instructions:  AVX2_256
```

```
CPU FFT library:    fftw-3.3.8-sse2-avx-avx2-avx2_128
GPU FFT library:    none
Multi-GPU FFT:      none
RDTSCP usage:       enabled
TNG support:        enabled
Hwloc support:      disabled
Tracing support:    disabled
C compiler:         /usr/bin/cc GNU 11.4.0
C compiler flags:   -fexcess-precision=fast -funroll-all-loops -mavx2 -
mfma -Wno-missing-field-initializers -O3 -DNDEBUG
C++ compiler:       /usr/bin/c++ GNU 11.4.0
C++ compiler flags: -fexcess-precision=fast -funroll-all-loops -mavx2 -
mfma -Wno-missing-field-initializers -Wno-cast-function-type-strict -
fopenmp -O3 -DNDEBUG
BLAS library:       Internal
LAPACK library:     Internal


Running on 3 nodes with total 18 cores, 18 processing units
  Cores per node:            6
  Logical processing units per node:    6
  OS CPU Limit / recommended threads to start per node:    6
Hardware detected on host cpu-sev-1 (the node of MPI rank 0):
  CPU info:
    Vendor: AMD
    Brand:  AMD EPYC-Milan Processor
    Family: 25   Model: 1   Stepping: 1
    Features: aes amd apic avx avx2 clfsh cmov cx8 cx16 f16c fma lahf
misalignsse mmx msr pcid pclmuldq pdpe1gb popcnt pse rdrnd rdtscp sha
sse2 sse3 sse4a sse4.1 sse4.2 ssse3 tdt x2apic
  Hardware topology: Basic
    Packages, cores, and logical processors:
    [indices refer to OS logical processors]
      Package  0: [   0]
      Package  1: [   1]
      Package  2: [   2]
      Package  3: [   3]
      Package  4: [   4]
      Package  5: [   5]
    CPU limit set by OS: -1   Recommended max number of threads: 6


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
M. J. Abraham, T. Murtola, R. Schulz, S. P√°ll, J. C. Smith, B. Hess, E.
Lindahl
GROMACS: High performance molecular simulations through multi-level
parallelism from laptops to supercomputers
SoftwareX 1 (2015) pp. 19-25
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. P√°ll, M. J. Abraham, C. Kutzner, B. Hess, E. Lindahl
Tackling Exascale Software Challenges in Molecular Dynamics Simulations
with
GROMACS
In S. Markidis & E. Laure (Eds.), Solving Software Challenges for
Exascale 8759 (2015) pp. 3-27
```

```
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. Pronk, S. P√°ll, R. Schulz, P. Larsson, P. Bjelkmar, R. Apostolov, M.
R.
Shirts, J. C. Smith, P. M. Kasson, D. van der Spoel, B. Hess, and E.
Lindahl
GROMACS 4.5: a high-throughput and highly parallel open source molecular
simulation toolkit
Bioinformatics 29 (2013) pp. 845-54
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
B. Hess and C. Kutzner and D. van der Spoel and E. Lindahl
GROMACS 4: Algorithms for highly efficient, load-balanced, and scalable
molecular simulation
J. Chem. Theory Comput. 4 (2008) pp. 435-447
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++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
D. van der Spoel, E. Lindahl, B. Hess, G. Groenhof, A. E. Mark and H. J.
C.
Berendsen
GROMACS: Fast, Flexible and Free
J. Comp. Chem. 26 (2005) pp. 1701-1719
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
E. Lindahl and B. Hess and D. van der Spoel
GROMACS 3.0: A package for molecular simulation and trajectory analysis
J. Mol. Mod. 7 (2001) pp. 306-317
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
H. J. C. Berendsen, D. van der Spoel and R. van Drunen
GROMACS: A message-passing parallel molecular dynamics implementation
Comp. Phys. Comm. 91 (1995) pp. 43-56
-------- -------- --- Thank You --- -------- --------


++++ PLEASE CITE THE DOI FOR THIS VERSION OF GROMACS ++++
https://doi.org/10.5281/zenodo.10017686
-------- -------- --- Thank You --- -------- --------


The number of OpenMP threads was set by environment variable
OMP_NUM_THREADS to 1

Input Parameters:
   integrator                   = sd
   tinit                        = 0
   dt                           = 0.002
   nsteps                       = 3000000
```

```
init-step                      = 0
simulation-part                = 1
mts                            = false
comm-mode                      = Linear
nstcomm                        = 100
bd-fric                        = 0
ld-seed                        = -1628089582
emtol                          = 100
emstep                         = 0.01
niter                          = 0
fcstep                         = 0
nstcgsteep                     = 1000
nbfgscorr                      = 10
rtpi                           = 0.05
nstxout                        = 23500
nstvout                        = 23500
nstfout                        = 0
nstlog                         = 10000
nstcalcenergy                  = 100
nstenergy                      = 23500
nstxout-compressed             = 23500
compressed-x-precision         = 1000
cutoff-scheme                  = Verlet
nstlist                        = 10
pbc                            = xyz
periodic-molecules             = false
verlet-buffer-tolerance        = 0.005
rlist                          = 1.1
coulombtype                    = PME
coulomb-modifier               = Potential-shift
rcoulomb-switch                = 0
rcoulomb                       = 1.1
epsilon-r                      = 1
epsilon-rf                     = inf
vdw-type                       = Cut-off
vdw-modifier                   = Potential-switch
rvdw-switch                    = 1
rvdw                           = 1.1
DispCorr                       = EnerPres
table-extension                = 1
fourierspacing                 = 0.12
fourier-nx                     = 84
fourier-ny                     = 84
fourier-nz                     = 84
pme-order                      = 4
ewald-rtol                     = 1e-05
ewald-rtol-lj                  = 0.001
lj-pme-comb-rule               = Geometric
ewald-geometry                 = 3d
epsilon-surface                = 0
ensemble-temperature-setting   = constant
ensemble-temperature           = 298
tcoupl                         = No
nsttcouple                     = -1
nh-chain-length                = 0
print-nose-hoover-chain-variables = false
pcoupl                         = Parrinello-Rahman
pcoupltype                     = Isotropic
```

```
   nstpcouple                     = 10
   tau-p                          = 5
   compressibility (3x3):
      compressibility[    0]={ 4.60000e-05,  0.00000e+00,  0.00000e+00}
      compressibility[    1]={ 0.00000e+00,  4.60000e-05,  0.00000e+00}
      compressibility[    2]={ 0.00000e+00,  0.00000e+00,  4.60000e-05}
   ref-p (3x3):
      ref-p[    0]={ 1.00000e+00,  0.00000e+00,  0.00000e+00}
      ref-p[    1]={ 0.00000e+00,  1.00000e+00,  0.00000e+00}
      ref-p[    2]={ 0.00000e+00,  0.00000e+00,  1.00000e+00}
   refcoord-scaling               = COM
   posres-com (3):
      posres-com[0]= 0.00000e+00
      posres-com[1]= 0.00000e+00
      posres-com[2]= 0.00000e+00
   posres-comB (3):
      posres-comB[0]= 0.00000e+00
      posres-comB[1]= 0.00000e+00
      posres-comB[2]= 0.00000e+00
   QMMM                           = false
qm-opts:
   ngQM                           = 0
   constraint-algorithm           = Lincs
   continuation                   = true
   Shake-SOR                      = false
   shake-tol                      = 0.0001
   lincs-order                    = 4
   lincs-iter                     = 2
   lincs-warnangle                = 30
   nwall                          = 0
   wall-type                      = 9-3
   wall-r-linpot                  = -1
   wall-atomtype[0]               = -1
   wall-atomtype[1]               = -1
   wall-density[0]                = 0
   wall-density[1]                = 0
   wall-ewald-zfac                = 3
   pull                           = false
   awh                            = false
   rotation                       = false
   interactiveMD                  = false
   disre                          = No
   disre-weighting                = Equal
   disre-mixed                    = false
   dr-fc                          = 1000
   dr-tau                         = 0
   nstdisreout                    = 100
   orire-fc                       = 0
   orire-tau                      = 0
   nstorireout                    = 100
   free-energy                    = yes
   init-lambda                    = 0
   init-lambda-state              = -1
   delta-lambda                   = 0
   nstdhdl                        = 10000
   n-lambdas                      = 0
   calc-lambda-neighbors          = 1
   dhdl-print-energy              = no
```

```
   sc-alpha                       = 0.3
   sc-power                       = 1
   sc-r-power                     = 6
   sc-sigma                       = 0.25
   sc-sigma-min                   = 0.25
   sc-coul                        = true
   dh-hist-size                   = 0
   dh-hist-spacing                = 0.1
   separate-dhdl-file             = yes
   dhdl-derivatives               = yes
   sc-function                    = beutler
   sc-gapsys-scale-linpoint-lj    = 0.85
   sc-gapsys-scale-linpoint-q     = 0.3
   sc-gapsys-sigma-lj             = 0.3
   cos-acceleration               = 0
   deform (3x3):
      deform[    0]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
      deform[    1]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
      deform[    2]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
   simulated-tempering            = false
   swapcoords                     = no
   userint1                       = 0
   userint2                       = 0
   userint3                       = 0
   userint4                       = 0
   userreal1                      = 0
   userreal2                      = 0
   userreal3                      = 0
   userreal4                      = 0
   applied-forces:
     electric-field:
       x:
         E0                       = 0
         omega                    = 0
         t0                       = 0
         sigma                    = 0
       y:
         E0                       = 0
         omega                    = 0
         t0                       = 0
         sigma                    = 0
       z:
         E0                       = 0
         omega                    = 0
         t0                       = 0
         sigma                    = 0
grpopts:
   nrdf:      134649
   ref-t:         298
   tau-t:           2
annealing:          No
annealing-npoints:           0
   acc:               0           0           0
   nfreeze:           N           N           N
   energygrp-flags[  0]: 0

Changing nstlist from 10 to 80, rlist from 1.1 to 1.232
```

```
Update groups can not be used for this system because there are three or
more consecutively coupled constraints

Initializing Domain Decomposition on 18 ranks
Dynamic load balancing: auto
Minimum cell size due to atom displacement: 0.639 nm
Initial maximum distances in bonded interactions:
    two-body bonded interactions: 0.438 nm, LJ-14, atoms 4073 4080
  multi-body bonded interactions: 0.438 nm, Proper Dih., atoms 4073 4080
Minimum cell size due to bonded interactions: 0.482 nm
Maximum distance for 5 constraints, at 120 deg. angles, all-trans: 0.819
nm
Estimated maximum distance required for P-LINCS: 0.819 nm
This distance will limit the DD cell size, you can override this with -
rcon
Scaling the initial minimum size with 1/0.8 (option -dds) = 1.25
Using 0 separate PME ranks because: there are too few total ranks for
efficient splitting
Optimizing the DD grid for 18 cells with a minimum initial size of 1.024
nm
The maximum allowed number of cells is: X 7 Y 7 Z 6
Domain decomposition grid 6 x 3 x 1, separate PME ranks 0
PME domain decomposition: 6 x 3 x 1
Domain decomposition rank 0, coordinates 0 0 0

The initial number of communication pulses is: X 1 Y 1
The initial domain decomposition cell size is: X 1.34 nm Y 2.68 nm

The maximum allowed distance for atoms involved in interactions is:
                 non-bonded interactions           1.232 nm
(the following are initial values, they could change due to box
deformation)
            two-body bonded interactions  (-rdd)   1.232 nm
          multi-body bonded interactions  (-rdd)   1.232 nm
  atoms separated by up to 5 constraints  (-rcon)  1.338 nm

When dynamic load balancing gets turned on, these settings will change
to:
The maximum number of communication pulses is: X 2 Y 2
The minimum size for domain decomposition cells is 0.910 nm
The requested allowed shrink of DD cells (option -dds) is: 0.80
The allowed shrink of domain decomposition cells is: X 0.68 Y 0.34
The maximum allowed distance for atoms involved in interactions is:
                 non-bonded interactions           1.232 nm
            two-body bonded interactions  (-rdd)   1.232 nm
          multi-body bonded interactions  (-rdd)   0.910 nm
  atoms separated by up to 5 constraints  (-rcon)  0.910 nm
Using two step summing over 3 groups of on average 6.0 ranks


Using 18 MPI processes

Non-default thread affinity set, disabling internal thread affinity

Using 1 OpenMP thread per MPI process

System total charge, top. A: 0.000 top. B: -1.000
Will do PME sum in reciprocal space for electrostatic interactions.
```

```
++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
U. Essmann, L. Perera, M. L. Berkowitz, T. Darden, H. Lee and L. G.
Pedersen
A smooth particle mesh Ewald method
J. Chem. Phys. 103 (1995) pp. 8577-8592
-------- -------- --- Thank You --- -------- --------

Using a Gaussian width (1/beta) of 0.352179 nm for Ewald
Potential shift: LJ r^-12: 0.000e+00 r^-6: 0.000e+00, Ewald -9.091e-06
Initialized non-bonded Coulomb Ewald tables, spacing: 9.79e-04 size: 2282

Generated table with 1115 data points for 1-4 COUL.
Tabscale = 500 points/nm
Generated table with 1115 data points for 1-4 LJ6.
Tabscale = 500 points/nm
Generated table with 1115 data points for 1-4 LJ12.
Tabscale = 500 points/nm
Long Range LJ corr.: <C6> 3.0958e-04


Using SIMD 4x8 nonbonded short-range kernels

Using a dual 4x8 pair-list setup updated with dynamic pruning:
  outer list: updated every 80 steps, buffer 0.132 nm, rlist 1.232 nm
  inner list: updated every 13 steps, buffer 0.003 nm, rlist 1.103 nm
At tolerance 0.005 kJ/mol/ps per atom, equivalent classical 1x1 list
would be:
  outer list: updated every 80 steps, buffer 0.270 nm, rlist 1.370 nm
  inner list: updated every 13 steps, buffer 0.052 nm, rlist 1.152 nm

The non-bonded pair calculation algorithm tolerates a few missing pair
interactions close to the cut-off. This can lead to a systematic
overestimation of the pressure due to missing LJ interactions. The error
in the average pressure due to missing LJ interactions is at most 1.25
bar.
The pressure error can be controlled by setting the environment variable
GMX_VERLET_BUFFER_PRESSURE_TOLERANCE to the allowed error in units of
bar.
There are 61 atoms and 61 charges for free energy perturbation

Linking all bonded interactions to atoms


Initializing Parallel LINear Constraint Solver

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
B. Hess
P-LINCS: A Parallel Linear Constraint Solver for molecular simulation
J. Chem. Theory Comput. 4 (2008) pp. 116-122
-------- -------- --- Thank You --- -------- --------

The number of constraints is 4701
There are constraints between atoms in different decomposition domains,
will communicate selected coordinates each lincs iteration

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. Miyamoto and P. A. Kollman
```

```
SETTLE: An Analytical Version of the SHAKE and RATTLE Algorithms for
Rigid
Water Models
J. Comp. Chem. 13 (1992) pp. 952-962
-------- -------- --- Thank You --- -------- --------


Intra-simulation communication will occur every 10 steps.
Initial vector of lambda components:[     0.0000     0.0000     0.0000
0.0000     0.0000     0.0000     0.0000 ]

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
N. Goga and A. J. Rzepiela and A. H. de Vries and S. J. Marrink and H. J.
C.
Berendsen
Efficient Algorithms for Langevin and DPD Dynamics
J. Chem. Theory Comput. 8 (2012) pp. 3637--3649
-------- -------- --- Thank You --- -------- --------

There are: 67291 Atoms
Atom distribution over 18 domains: av 3738 stddev 80 min 3648 max 3883
Center of mass motion removal mode is Linear
We have the following groups for center of mass motion removal:
  0:  rest

Started mdrun on rank 0 Sat Jan 13 12:39:13 2024

           Step           Time
              0        0.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.03471e+04    1.16572e+04    8.17095e+02    5.07276e+03
5.18934e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.21209e+05   -3.77970e+03   -1.12353e+06    4.51451e+03   -
9.21801e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.67925e+05   -7.53876e+05    2.99990e+02   -9.33422e+01
1.04717e+02
    dVremain/dl   Constr. rmsd
    7.32094e+01    3.49022e-06


DD  step 79 load imb.: force 48.9%

step 240 Turning on dynamic load balancing, because the performance loss
due to load imbalance is 25.0 %.

DD  step 9999  vol min/aver 0.631  load imb.: force 11.6%
           Step           Time
          10000       20.00000

   Energies (kJ/mol)
[...]
```

```
DD  step 2979999  vol min/aver 0.480  load imb.: force  2.5%
           Step           Time
        2980000     5960.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    9.93831e+03    1.16397e+04    7.04903e+02    5.08050e+03
5.22389e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.21159e+05   -3.77522e+03   -1.12330e+06    4.63025e+03   -
9.21683e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.67355e+05   -7.54328e+05    2.98973e+02   -9.31210e+01
7.65648e+01
    dVremain/dl   Constr. rmsd
    5.93430e+01    3.38824e-06


DD  step 2989999  vol min/aver 0.473  load imb.: force 18.0%
           Step           Time
        2990000     5980.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.02338e+04    1.17305e+04    7.33066e+02    5.02029e+03
5.21852e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.19231e+05   -3.77333e+03   -1.12172e+06    4.51025e+03   -
9.21852e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.66426e+05   -7.55425e+05    2.97314e+02   -9.30282e+01   -
2.04077e+02
    dVremain/dl   Constr. rmsd
    1.08725e+02    3.45627e-06


DD  step 2999999  vol min/aver 0.473  load imb.: force  2.0%
           Step           Time
        3000000     6000.00000

Writing checkpoint, step 3000000 at Sat Jan 13 23:59:11 2024


   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    9.94768e+03    1.14698e+04    7.16617e+02    5.10908e+03
5.22220e+04
```

```
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.19050e+05   -3.77483e+03   -1.12071e+06    4.56665e+03   -
9.21406e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.68110e+05   -7.53296e+05    3.00321e+02   -9.31020e+01   -
7.83857e+01
    dVremain/dl   Constr. rmsd
    1.05897e+02    3.37282e-06


      <======  ###############  ==>
      <====  A V E R A G E S  ====>
      <==  ###############  ======>

      Statistics over 3000001 steps using 30001 frames

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.00636e+04    1.16497e+04    7.23408e+02    5.10732e+03
5.21094e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.20383e+05   -3.76847e+03   -1.12192e+06    4.55162e+03   -
9.21098e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.66976e+05   -7.54122e+05    2.98296e+02   -9.27888e+01    3.84487e-
01
    dVremain/dl   Constr. rmsd
    1.37711e+02    0.00000e+00

          Box-X          Box-Y          Box-Z
    9.84296e+00    9.84296e+00    6.96002e+00

   Total Virial (kJ/mol)
    5.56604e+04    1.00435e+01    9.32772e-01
    9.71762e+00    5.56969e+04   -1.41549e+01
    7.48227e-01   -1.41789e+01    5.55999e+04

   Pressure (bar)
    9.32960e-01    1.05543e+00    7.37149e-01
    1.07148e+00    1.41790e-02    1.83154e-01
    7.46239e-01    1.84339e-01    2.06321e-01


     M E G A - F L O P S   A C C O U N T I N G

 NB=Group-cutoff nonbonded kernels    NxN=N-by-N cluster Verlet kernels
 RF=Reaction-Field  VdW=Van der Waals  QSTab=quadratic-spline table
 W3=SPC/TIP3p  W4=TIP4p (single or pairs)
 V&F=Potential and force  V=Potential only  F=Force only

 Computing:                                M-Number         M-Flops  %
Flops
```

```
-----------------------------------------------------------------------
----
 NB Free energy kernel             27132549.054024    27132549.054
0.2
 Pair Search distance check         1477979.564242    13301816.078
0.1
 NxN Ewald Elec. + LJ [F]          93843045.270608  8727403210.167
57.3
 NxN Ewald Elec. + LJ [V&F]          947939.411568   120388305.269
0.8
 NxN Ewald Elec. [F]               79607002.984560  4856027182.058
31.9
 NxN Ewald Elec. [V&F]               804138.155952    67547605.100
0.4
 1,4 nonbonded interactions           36702.012234     3303181.101
0.0
 Calc Weights                        605619.201873    21802291.267
0.1
 Spread Q Bspline                  25839752.613248    51679505.226
0.3
 Gather F Bspline                  25839752.613248   155038515.679
1.0
 3D-FFT                           136395117.465024  1091160939.720
7.2
 Solve PME                           127008.042336     8128514.710
0.1
 Reset In Box                          2523.345209        7570.036
0.0
 CG-CoM                                2523.479791        7570.439
0.0
 Angles                               25548.008516     4292065.431
0.0
 Propers                              39945.013315     9147408.049
0.1
 Impropers                             3591.001197      746928.249
0.0
 Virial                               20430.368101      367746.626
0.0
 Update                              201873.067291     6258065.086
0.0
 Stop-CM                               2018.797291       20187.973
0.0
 Calc-Ekin                            40374.734582     1090117.834
0.0
 Lincs                                50533.671644     3032020.299
0.0
 Lincs-Mat                          1084978.950264     4339915.801
0.0
 Constraint-V                        511617.243034     4604555.187
0.0
 Constraint-Vir                       23054.247775      553301.947
0.0
 Settle                              136849.966582    50634487.635
0.3
-----------------------------------------------------------------------
----
 Total                                              15228015556.021
100.0
```

```
-------------------------------------------------------------------------
----

    D O M A I N   D E C O M P O S I T I O N   S T A T I S T I C S

 av. #atoms communicated per step for force:  2 x 125506.2
 av. #atoms communicated per step for LINCS:  3 x 10380.9


Dynamic load balancing report:
 DLB was turned on during the run due to measured imbalance.
 Average load imbalance: 14.1%.
 The balanceable part of the MD step is 33%, load imbalance is computed
from this.
 Part of the total run time spent waiting due to load imbalance: 4.7%.
 Steps where the load balancing was limited by -rdd, -rcon and/or -dds: X
0 % Y 0 %


     R E A L   C Y C L E   A N D   T I M E   A C C O U N T I N G

On 18 MPI ranks

 Activity:              Num   Num      Call    Wall time         Giga-
Cycles
                       Ranks Threads  Count      (s)         total sum
%
-------------------------------------------------------------------------
-------
 Domain decomp.           18    1      37500     159.562       8456.780
0.4
 DD comm. load            18    1      37355       0.649         34.395
0.0
 DD comm. bounds          18    1      37318       5.863        310.753
0.0
 Neighbor search          18    1      37501     350.114      18555.971
0.9
 Comm. coord.             18    1    2962500     664.201      35202.529
1.6
 Force                    18    1    3000001   12655.753     670753.002
31.0
 Wait + Comm. F           18    1    3000001     651.609      34535.159
1.6
 PME mesh                 18    1    3000001   22369.706    1185591.041
54.8
 NB X/F buffer ops.       18    1    8925001     138.975       7365.639
0.3
 Write traj.              18    1        174       0.277         14.660
0.0
 Update                   18    1    6000002     364.546      19320.908
0.9
 Constraints              18    1    6000002    3331.378     176562.517
8.2
 Comm. energies           18    1     300001      47.941       2540.882
0.1
 Rest                                             57.252       3034.352
0.1
```

```
-----------------------------------------------------------------------------
-------
 Total                                          40797.826    2162278.590
100.0
-----------------------------------------------------------------------------
-------
 Breakdown of PME mesh activities
-----------------------------------------------------------------------------
-------
 PME redist. X/F          18    1    9000003    4494.277     238196.012
11.0
 PME spread               18    1    6000002    2244.999     118984.581
5.5
 PME gather               18    1    6000002    1560.417      82701.856
3.8
 PME 3D-FFT               18    1   12000004    2701.045     143154.971
6.6
 PME 3D-FFT Comm.         18    1   24000008   11160.309     591494.709
27.4
 PME solve Elec           18    1    6000002     200.683      10636.153
0.5
-----------------------------------------------------------------------------
-------

               Core t (s)   Wall t (s)        (%)
       Time:   734360.860    40797.826     1800.0
                         11h19:57
                 (ns/day)    (hour/ns)
Performance:       12.707        1.889
Finished mdrun on rank 0 Sat Jan 13 23:59:11 2024
```

cmet_eq_cpu-sev-cluster_10n

```
                :-) GROMACS - gmx mdrun, 2023.3 (-:

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    Christoph Junghans         Prashanth Kanduri         Sebastian Keller
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       Maarten Wolf

                    Coordinated by the GROMACS project leaders:
                      Paul Bauer, Berk Hess, and Erik Lindahl

GROMACS:      gmx mdrun, version 2023.3
Executable:   /usr/local/gromacs/bin/gmx_mpi
Data prefix:  /usr/local/gromacs
Working dir:  /home/ubuntu
Process ID:   23099
Command line:
  gmx_mpi mdrun -v -s /mnt/shared/home/ubuntu/mpinat-gromacs/mpinat-
gromacs-binding-affinity-study-bench/cmet_eq.tpr

GROMACS version:    2023.3
Precision:          mixed
Memory model:       64 bit
MPI library:        MPI
OpenMP support:     enabled (GMX_OPENMP_MAX_THREADS = 128)
GPU support:        disabled
SIMD instructions:  AVX2_256
```

```
CPU FFT library:    fftw-3.3.8-sse2-avx-avx2-avx2_128
GPU FFT library:    none
Multi-GPU FFT:      none
RDTSCP usage:       enabled
TNG support:        enabled
Hwloc support:      disabled
Tracing support:    disabled
C compiler:         /usr/bin/cc GNU 11.4.0
C compiler flags:   -fexcess-precision=fast -funroll-all-loops -mavx2 -
mfma -Wno-missing-field-initializers -O3 -DNDEBUG
C++ compiler:       /usr/bin/c++ GNU 11.4.0
C++ compiler flags: -fexcess-precision=fast -funroll-all-loops -mavx2 -
mfma -Wno-missing-field-initializers -Wno-cast-function-type-strict -
fopenmp -O3 -DNDEBUG
BLAS library:       Internal
LAPACK library:     Internal


Running on 10 nodes with total 60 cores, 60 processing units
  Cores per node:            6
  Logical processing units per node:    6
  OS CPU Limit / recommended threads to start per node:    6
Hardware detected on host cpu-sev-1 (the node of MPI rank 0):
  CPU info:
    Vendor: AMD
    Brand:  AMD EPYC-Milan Processor
    Family: 25   Model: 1   Stepping: 1
    Features: aes amd apic avx avx2 clfsh cmov cx8 cx16 f16c fma lahf
misalignsse mmx msr pcid pclmuldq pdpe1gb popcnt pse rdrnd rdtscp sha
sse2 sse3 sse4a sse4.1 sse4.2 ssse3 tdt x2apic
  Hardware topology: Basic
    Packages, cores, and logical processors:
    [indices refer to OS logical processors]
      Package  0: [   0]
      Package  1: [   1]
      Package  2: [   2]
      Package  3: [   3]
      Package  4: [   4]
      Package  5: [   5]
    CPU limit set by OS: -1   Recommended max number of threads: 6


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
M. J. Abraham, T. Murtola, R. Schulz, S. P√°ll, J. C. Smith, B. Hess, E.
Lindahl
GROMACS: High performance molecular simulations through multi-level
parallelism from laptops to supercomputers
SoftwareX 1 (2015) pp. 19-25
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. P√°ll, M. J. Abraham, C. Kutzner, B. Hess, E. Lindahl
Tackling Exascale Software Challenges in Molecular Dynamics Simulations
with
GROMACS
In S. Markidis & E. Laure (Eds.), Solving Software Challenges for
Exascale 8759 (2015) pp. 3-27
```

```
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. Pronk, S. P√°ll, R. Schulz, P. Larsson, P. Bjelkmar, R. Apostolov, M.
R.
Shirts, J. C. Smith, P. M. Kasson, D. van der Spoel, B. Hess, and E.
Lindahl
GROMACS 4.5: a high-throughput and highly parallel open source molecular
simulation toolkit
Bioinformatics 29 (2013) pp. 845-54
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
B. Hess and C. Kutzner and D. van der Spoel and E. Lindahl
GROMACS 4: Algorithms for highly efficient, load-balanced, and scalable
molecular simulation
J. Chem. Theory Comput. 4 (2008) pp. 435-447
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
D. van der Spoel, E. Lindahl, B. Hess, G. Groenhof, A. E. Mark and H. J.
C.
Berendsen
GROMACS: Fast, Flexible and Free
J. Comp. Chem. 26 (2005) pp. 1701-1719
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
E. Lindahl and B. Hess and D. van der Spoel
GROMACS 3.0: A package for molecular simulation and trajectory analysis
J. Mol. Mod. 7 (2001) pp. 306-317
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
H. J. C. Berendsen, D. van der Spoel and R. van Drunen
GROMACS: A message-passing parallel molecular dynamics implementation
Comp. Phys. Comm. 91 (1995) pp. 43-56
-------- -------- --- Thank You --- -------- --------


++++ PLEASE CITE THE DOI FOR THIS VERSION OF GROMACS ++++
https://doi.org/10.5281/zenodo.10017686
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The number of OpenMP threads was set by environment variable
OMP_NUM_THREADS to 1

Input Parameters:
   integrator                   = sd
   tinit                        = 0
   dt                           = 0.002
   nsteps                       = 3000000
```

```
init-step                       = 0
simulation-part                 = 1
mts                             = false
comm-mode                       = Linear
nstcomm                         = 100
bd-fric                         = 0
ld-seed                         = -1628089582
emtol                           = 100
emstep                          = 0.01
niter                           = 0
fcstep                          = 0
nstcgsteep                      = 1000
nbfgscorr                       = 10
rtpi                            = 0.05
nstxout                         = 23500
nstvout                         = 23500
nstfout                         = 0
nstlog                          = 10000
nstcalcenergy                   = 100
nstenergy                       = 23500
nstxout-compressed              = 23500
compressed-x-precision          = 1000
cutoff-scheme                   = Verlet
nstlist                         = 10
pbc                             = xyz
periodic-molecules              = false
verlet-buffer-tolerance         = 0.005
rlist                           = 1.1
coulombtype                     = PME
coulomb-modifier                = Potential-shift
rcoulomb-switch                 = 0
rcoulomb                        = 1.1
epsilon-r                       = 1
epsilon-rf                      = inf
vdw-type                        = Cut-off
vdw-modifier                    = Potential-switch
rvdw-switch                     = 1
rvdw                            = 1.1
DispCorr                        = EnerPres
table-extension                 = 1
fourierspacing                  = 0.12
fourier-nx                      = 84
fourier-ny                      = 84
fourier-nz                      = 84
pme-order                       = 4
ewald-rtol                      = 1e-05
ewald-rtol-lj                   = 0.001
lj-pme-comb-rule                = Geometric
ewald-geometry                  = 3d
epsilon-surface                 = 0
ensemble-temperature-setting    = constant
ensemble-temperature            = 298
tcoupl                          = No
nsttcouple                      = -1
nh-chain-length                 = 0
print-nose-hoover-chain-variables = false
pcoupl                          = Parrinello-Rahman
pcoupltype                      = Isotropic
```

```
   nstpcouple                     = 10
   tau-p                          = 5
   compressibility (3x3):
      compressibility[    0]={ 4.60000e-05,  0.00000e+00,  0.00000e+00}
      compressibility[    1]={ 0.00000e+00,  4.60000e-05,  0.00000e+00}
      compressibility[    2]={ 0.00000e+00,  0.00000e+00,  4.60000e-05}
   ref-p (3x3):
      ref-p[    0]={ 1.00000e+00,  0.00000e+00,  0.00000e+00}
      ref-p[    1]={ 0.00000e+00,  1.00000e+00,  0.00000e+00}
      ref-p[    2]={ 0.00000e+00,  0.00000e+00,  1.00000e+00}
   refcoord-scaling               = COM
   posres-com (3):
      posres-com[0]= 0.00000e+00
      posres-com[1]= 0.00000e+00
      posres-com[2]= 0.00000e+00
   posres-comB (3):
      posres-comB[0]= 0.00000e+00
      posres-comB[1]= 0.00000e+00
      posres-comB[2]= 0.00000e+00
   QMMM                           = false
qm-opts:
   ngQM                           = 0
   constraint-algorithm           = Lincs
   continuation                   = true
   Shake-SOR                      = false
   shake-tol                      = 0.0001
   lincs-order                    = 4
   lincs-iter                     = 2
   lincs-warnangle                = 30
   nwall                          = 0
   wall-type                      = 9-3
   wall-r-linpot                  = -1
   wall-atomtype[0]               = -1
   wall-atomtype[1]               = -1
   wall-density[0]                = 0
   wall-density[1]                = 0
   wall-ewald-zfac                = 3
   pull                           = false
   awh                            = false
   rotation                       = false
   interactiveMD                  = false
   disre                          = No
   disre-weighting                = Equal
   disre-mixed                    = false
   dr-fc                          = 1000
   dr-tau                         = 0
   nstdisreout                    = 100
   orire-fc                       = 0
   orire-tau                      = 0
   nstorireout                    = 100
   free-energy                    = yes
   init-lambda                    = 0
   init-lambda-state              = -1
   delta-lambda                   = 0
   nstdhdl                        = 10000
   n-lambdas                      = 0
   calc-lambda-neighbors          = 1
   dhdl-print-energy              = no
```

```
   sc-alpha                       = 0.3
   sc-power                       = 1
   sc-r-power                     = 6
   sc-sigma                       = 0.25
   sc-sigma-min                   = 0.25
   sc-coul                        = true
   dh-hist-size                   = 0
   dh-hist-spacing                = 0.1
   separate-dhdl-file             = yes
   dhdl-derivatives               = yes
   sc-function                    = beutler
   sc-gapsys-scale-linpoint-lj    = 0.85
   sc-gapsys-scale-linpoint-q     = 0.3
   sc-gapsys-sigma-lj             = 0.3
   cos-acceleration               = 0
   deform (3x3):
      deform[    0]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
      deform[    1]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
      deform[    2]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
   simulated-tempering            = false
   swapcoords                     = no
   userint1                       = 0
   userint2                       = 0
   userint3                       = 0
   userint4                       = 0
   userreal1                      = 0
   userreal2                      = 0
   userreal3                      = 0
   userreal4                      = 0
   applied-forces:
     electric-field:
       x:
         E0                       = 0
         omega                    = 0
         t0                       = 0
         sigma                    = 0
       y:
         E0                       = 0
         omega                    = 0
         t0                       = 0
         sigma                    = 0
       z:
         E0                       = 0
         omega                    = 0
         t0                       = 0
         sigma                    = 0
grpopts:
   nrdf:      134649
   ref-t:         298
   tau-t:           2
annealing:          No
annealing-npoints:           0
   acc:               0           0           0
   nfreeze:           N           N           N
   energygrp-flags[  0]: 0

Changing nstlist from 10 to 80, rlist from 1.1 to 1.232
```

```
Update groups can not be used for this system because there are three or
more consecutively coupled constraints

Initializing Domain Decomposition on 60 ranks
Dynamic load balancing: auto
Minimum cell size due to atom displacement: 0.639 nm
Initial maximum distances in bonded interactions:
    two-body bonded interactions: 0.438 nm, LJ-14, atoms 4073 4080
  multi-body bonded interactions: 0.438 nm, Proper Dih., atoms 4073 4080
Minimum cell size due to bonded interactions: 0.482 nm
Maximum distance for 5 constraints, at 120 deg. angles, all-trans: 0.819
nm
Estimated maximum distance required for P-LINCS: 0.819 nm
This distance will limit the DD cell size, you can override this with -
rcon
Scaling the initial minimum size with 1/0.8 (option -dds) = 1.25
Guess for relative PME load: 0.29
Will use 40 particle-particle and 20 PME only ranks
This is a guess, check the performance at the end of the log file
Using 20 separate PME ranks, as guessed by mdrun
Optimizing the DD grid for 40 cells with a minimum initial size of 1.024
nm
The maximum allowed number of cells is: X 7 Y 7 Z 6
Domain decomposition grid 5 x 4 x 2, separate PME ranks 20
PME domain decomposition: 5 x 4 x 1
Interleaving PP and PME ranks
This rank does only particle-particle work.
Domain decomposition rank 0, coordinates 0 0 0

The initial number of communication pulses is: X 1 Y 1 Z 1
The initial domain decomposition cell size is: X 1.61 nm Y 2.01 nm Z 3.48
nm

The maximum allowed distance for atoms involved in interactions is:
                 non-bonded interactions           1.232 nm
(the following are initial values, they could change due to box
deformation)
            two-body bonded interactions  (-rdd)   1.232 nm
          multi-body bonded interactions  (-rdd)   1.232 nm
  atoms separated by up to 5 constraints  (-rcon)  1.606 nm

When dynamic load balancing gets turned on, these settings will change
to:
The maximum number of communication pulses is: X 1 Y 1 Z 1
The minimum size for domain decomposition cells is 1.232 nm
The requested allowed shrink of DD cells (option -dds) is: 0.80
The allowed shrink of domain decomposition cells is: X 0.77 Y 0.61 Z 0.35
The maximum allowed distance for atoms involved in interactions is:
                 non-bonded interactions           1.232 nm
            two-body bonded interactions  (-rdd)   1.232 nm
          multi-body bonded interactions  (-rdd)   1.232 nm
  atoms separated by up to 5 constraints  (-rcon)  1.232 nm
Using two step summing over 10 groups of on average 4.0 ranks


Using 60 MPI processes

Non-default thread affinity set, disabling internal thread affinity
```

```
Using 1 OpenMP thread per MPI process

System total charge, top. A: 0.000 top. B: -1.000
Will do PME sum in reciprocal space for electrostatic interactions.

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
U. Essmann, L. Perera, M. L. Berkowitz, T. Darden, H. Lee and L. G.
Pedersen
A smooth particle mesh Ewald method
J. Chem. Phys. 103 (1995) pp. 8577-8592
-------- -------- --- Thank You --- -------- --------

Using a Gaussian width (1/beta) of 0.352179 nm for Ewald
Potential shift: LJ r^-12: 0.000e+00 r^-6: 0.000e+00, Ewald -9.091e-06
Initialized non-bonded Coulomb Ewald tables, spacing: 9.79e-04 size: 2282

Generated table with 1115 data points for 1-4 COUL.
Tabscale = 500 points/nm
Generated table with 1115 data points for 1-4 LJ6.
Tabscale = 500 points/nm
Generated table with 1115 data points for 1-4 LJ12.
Tabscale = 500 points/nm
Long Range LJ corr.: <C6> 3.0958e-04


Using SIMD 4x8 nonbonded short-range kernels

Using a dual 4x8 pair-list setup updated with dynamic pruning:
  outer list: updated every 80 steps, buffer 0.132 nm, rlist 1.232 nm
  inner list: updated every 13 steps, buffer 0.003 nm, rlist 1.103 nm
At tolerance 0.005 kJ/mol/ps per atom, equivalent classical 1x1 list
would be:
  outer list: updated every 80 steps, buffer 0.270 nm, rlist 1.370 nm
  inner list: updated every 13 steps, buffer 0.052 nm, rlist 1.152 nm

The non-bonded pair calculation algorithm tolerates a few missing pair
interactions close to the cut-off. This can lead to a systematic
overestimation of the pressure due to missing LJ interactions. The error
in the average pressure due to missing LJ interactions is at most 1.25
bar.
The pressure error can be controlled by setting the environment variable
GMX_VERLET_BUFFER_PRESSURE_TOLERANCE to the allowed error in units of
bar.
There are 61 atoms and 61 charges for free energy perturbation

Linking all bonded interactions to atoms


Initializing Parallel LINear Constraint Solver

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
B. Hess
P-LINCS: A Parallel Linear Constraint Solver for molecular simulation
J. Chem. Theory Comput. 4 (2008) pp. 116-122
-------- -------- --- Thank You --- -------- --------

The number of constraints is 4701
```

```
There are constraints between atoms in different decomposition domains,
will communicate selected coordinates each lincs iteration

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. Miyamoto and P. A. Kollman
SETTLE: An Analytical Version of the SHAKE and RATTLE Algorithms for
Rigid
Water Models
J. Comp. Chem. 13 (1992) pp. 952-962
-------- -------- --- Thank You --- -------- --------


Intra-simulation communication will occur every 10 steps.
Initial vector of lambda components:[     0.0000     0.0000     0.0000
0.0000     0.0000     0.0000     0.0000 ]

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
N. Goga and A. J. Rzepiela and A. H. de Vries and S. J. Marrink and H. J.
C.
Berendsen
Efficient Algorithms for Langevin and DPD Dynamics
J. Chem. Theory Comput. 8 (2012) pp. 3637--3649
-------- -------- --- Thank You --- -------- --------

There are: 67291 Atoms
Atom distribution over 40 domains: av 1682 stddev 46 min 1621 max 1772
Center of mass motion removal mode is Linear
We have the following groups for center of mass motion removal:
  0:  rest

Started mdrun on rank 0 Sun Jan 14 05:33:44 2024

           Step           Time
              0        0.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.03471e+04    1.16572e+04    8.17095e+02    5.07276e+03
5.18933e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.21209e+05   -3.77970e+03   -1.12353e+06    4.51452e+03   -
9.21801e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.67925e+05   -7.53877e+05    2.99990e+02   -9.33422e+01
1.04729e+02
    dVremain/dl   Constr. rmsd
    7.32135e+01    3.49038e-06


DD  step 79 load imb.: force 96.0%  pme mesh/force 1.853
step  560: timed with pme grid 84 84 84, coulomb cutoff 1.100: 1272.7 M-
cycles
step  720: timed with pme grid 72 72 72, coulomb cutoff 1.252: 1113.7 M-
cycles
```

```
step  880: timed with pme grid 64 64 64, coulomb cutoff 1.408: 1260.5 M-
cycles
step 1040: timed with pme grid 72 72 72, coulomb cutoff 1.252: 1082.6 M-
cycles
step 1200: timed with pme grid 80 80 80, coulomb cutoff 1.127: 1102.6 M-
cycles
step 1360: timed with pme grid 72 72 72, coulomb cutoff 1.252: 1232.2 M-
cycles
step 1520: timed with pme grid 80 80 80, coulomb cutoff 1.127: 1096.7 M-
cycles
              optimal pme grid 72 72 72, coulomb cutoff 1.252

DD  step 9999 load imb.: force 50.6%  pme mesh/force 1.272
           Step           Time
          10000       20.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.00955e+04    1.16174e+04    6.93379e+02    5.07993e+03
5.15630e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.20565e+05   -3.76331e+03   -1.11957e+06    2.86977e+03   -
9.20845e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.66944e+05   -7.53902e+05    2.98238e+02   -9.25345e+01   -
2.84468e+01
    dVremain/dl   Constr. rmsd
    1.13981e+02    3.50748e-06


DD  step 19999 load imb.: force 71.4%  pme mesh/force 1.064
           Step           Time
          20000       40.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    9.95589e+03    1.16972e+04    6.79389e+02    5.07811e+03
5.16134e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.19297e+05   -3.76968e+03   -1.11734e+06    2.96438e+03   -
9.19820e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.66705e+05   -7.53115e+05    2.97812e+02   -9.28481e+01   -
6.53924e+01
    dVremain/dl   Constr. rmsd
    1.92183e+02    3.44489e-06


DD  step 29999 load imb.: force 66.9%  pme mesh/force 1.065
           Step           Time
          30000       60.00000
```

```
   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    9.89727e+03    1.16349e+04    7.50352e+02    5.11659e+03
5.17321e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.18205e+05   -3.76631e+03   -1.11750e+06    2.96683e+03   -
9.20968e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.67489e+05   -7.53479e+05    2.99213e+02   -9.26824e+01   -
1.49395e+02
    dVremain/dl   Constr. rmsd
    1.43396e+02    3.50826e-06


DD  step 39999 load imb.: force 55.2%  pme mesh/force 1.223
           Step           Time
          40000       80.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.00909e+04    1.17076e+04    7.29114e+02    5.07208e+03
5.18558e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.19617e+05   -3.76895e+03   -1.11845e+06    2.96725e+03   -
9.20175e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.65472e+05   -7.54704e+05    2.95608e+02   -9.28122e+01   -
2.19450e+01
    dVremain/dl   Constr. rmsd
    1.45020e+02    3.44374e-06


DD  step 49999 load imb.: force 75.0%  pme mesh/force 1.104
           Step           Time
          50000      100.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.00872e+04    1.15343e+04    7.33005e+02    5.03478e+03
5.19624e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.20901e+05   -3.77085e+03   -1.12063e+06    2.98718e+03   -
9.21160e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.67236e+05   -7.53923e+05    2.98761e+02   -9.29059e+01
7.27376e+01
    dVremain/dl   Constr. rmsd
    2.28303e+02    3.54792e-06
```

```
DD  step 59999 load imb.: force 61.1%  pme mesh/force 1.135
           Step           Time
          60000      120.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.00775e+04    1.15899e+04    7.49812e+02    5.03202e+03
5.15223e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.22443e+05   -3.77826e+03   -1.12344e+06    2.97600e+03   -
9.22825e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.66363e+05   -7.56462e+05    2.97200e+02   -9.32710e+01
8.46019e+01
    dVremain/dl   Constr. rmsd
    1.48262e+02    3.48798e-06


DD  step 69999 load imb.: force 64.4%  pme mesh/force 1.130
           Step           Time
          70000      140.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    9.82911e+03    1.16468e+04    7.23746e+02    5.06293e+03
5.17987e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.20052e+05   -3.77680e+03   -1.11977e+06    2.96580e+03   -
9.21468e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.66528e+05   -7.54939e+05    2.97496e+02   -9.31993e+01   -
8.34895e+01
    dVremain/dl   Constr. rmsd
    1.91611e+02    3.46565e-06


DD  step 79999 load imb.: force 52.7%  pme mesh/force 1.086
           Step           Time
          80000      160.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.01666e+04    1.16666e+04    7.17069e+02    5.16111e+03
5.19615e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.20240e+05   -3.76090e+03   -1.11947e+06    2.90298e+03   -
9.20412e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
```

```
    1.65623e+05   -7.54789e+05    2.95879e+02   -9.24162e+01   -
2.18173e+01
    dVremain/dl   Constr. rmsd
    2.23762e+02    3.42073e-06


DD  step 89999 load imb.: force 47.3%  pme mesh/force 1.235
           Step           Time
          90000      180.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.02469e+04    1.16181e+04    7.05407e+02    5.06620e+03
5.17472e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.19410e+05   -3.76559e+03   -1.12040e+06    2.89797e+03   -
9.22478e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.66640e+05   -7.55838e+05    2.97695e+02   -9.26470e+01   -
2.03348e+02
    dVremain/dl   Constr. rmsd
    1.54210e+02    3.51303e-06


DD  step 99999 load imb.: force 46.5%  pme mesh/force 1.301
           Step           Time
         100000      200.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.03425e+04    1.17853e+04    7.30054e+02    5.03094e+03
5.17245e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.20091e+05   -3.76039e+03   -1.11963e+06    2.97713e+03   -
9.20708e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.66120e+05   -7.54588e+05    2.96767e+02   -9.23908e+01   -
1.98461e+02
    dVremain/dl   Constr. rmsd
    1.40325e+02    3.55986e-06
[...]

    1.66542e+05   -7.53876e+05    2.97521e+02   -9.27776e+01   -
1.10817e+02
    dVremain/dl   Constr. rmsd
    1.60507e+02    3.26983e-06


DD  load balancing is limited by minimum cell size in dimension X Y
DD  step 2979999  vol min/aver 0.431! load imb.: force 28.8%  pme
mesh/force 1.308
           Step           Time
```

```
        2980000     5960.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    9.92435e+03    1.16344e+04    7.73686e+02    5.08618e+03
5.21595e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.20946e+05   -3.77706e+03   -1.12122e+06    2.94840e+03   -
9.21522e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.67392e+05   -7.54129e+05    2.99039e+02   -9.32122e+01
4.28988e+01
    dVremain/dl   Constr. rmsd
    7.21903e+01    3.27908e-06

Writing checkpoint, step 2988320 at Sun Jan 14 11:48:44 2024



DD  load balancing is limited by minimum cell size in dimension Y
DD  step 2989999  vol min/aver 0.370! load imb.: force 16.3%  pme
mesh/force 1.534
           Step           Time
        2990000     5980.00000

   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.00134e+04    1.17068e+04    7.48604e+02    5.21980e+03
5.23396e+04
        LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.20248e+05   -3.77902e+03   -1.12029e+06    2.87345e+03   -
9.20915e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.67875e+05   -7.53040e+05    2.99901e+02   -9.33087e+01
9.75005e+01
    dVremain/dl   Constr. rmsd
    1.38993e+02    3.30095e-06


DD  step 2999999  vol min/aver 0.564  load imb.: force 17.7%  pme
mesh/force 1.429
           Step           Time
        3000000     6000.00000

Writing checkpoint, step 3000000 at Sun Jan 14 11:50:11 2024


   Energies (kJ/mol)
          Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.00548e+04    1.16047e+04    7.28459e+02    5.12188e+03
5.21427e+04
```

```
       LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.20496e+05   -3.78357e+03   -1.12070e+06    2.99760e+03   -
9.21333e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.65826e+05   -7.55507e+05    2.96242e+02   -9.35336e+01
1.02348e+02
    dVremain/dl   Constr. rmsd
    1.97984e+02    3.22734e-06


      <======  ###############  ==>
      <====  A V E R A G E S  ====>
      <==  ###############  ======>

      Statistics over 3000001 steps using 30001 frames

   Energies (kJ/mol)
         Angle    Proper Dih. Per. Imp. Dih.          LJ-14     Coulomb-
14
    1.00386e+04    1.16745e+04    7.23417e+02    5.11614e+03
5.20492e+04
       LJ (SR)  Disper. corr.   Coulomb (SR)   Coul. recip.
Potential
    1.20293e+05   -3.76884e+03   -1.12019e+06    2.94159e+03   -
9.21119e+05
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure
(bar)
    1.66981e+05   -7.54138e+05    2.98304e+02   -9.28071e+01    7.80075e-
01
    dVremain/dl   Constr. rmsd
    1.37948e+02    0.00000e+00

          Box-X          Box-Y          Box-Z
    9.84264e+00    9.84264e+00    6.95980e+00

   Total Virial (kJ/mol)
    5.56955e+04    3.01411e+01   -1.00749e+01
    3.00032e+01    5.56511e+04   -1.05169e+01
   -1.00974e+01   -1.05751e+01    5.55911e+04

   Pressure (bar)
   -5.57080e-02   -6.94588e-02   -4.81087e-01
   -6.26675e-02    1.10018e+00   -6.01558e-01
   -4.79977e-01   -5.98687e-01    1.29576e+00


       P P   -   P M E   L O A D   B A L A N C I N G

 PP/PME load balancing changed the cut-off and PME settings:
           particle-particle                    PME
            rcoulomb  rlist            grid      spacing   1/beta
   initial  1.100 nm  1.103 nm      84  84  84   0.117 nm  0.352 nm
   final    1.252 nm  1.255 nm      72  72  72   0.137 nm  0.401 nm
 cost-ratio           1.47             0.63
 (note that these numbers concern only part of the total PP and PME load)
```

M E G A - F L O P S A C C O U N T I N G

NB=Group-cutoff nonbonded kernels NxN=N-by-N cluster Verlet kernels
RF=Reaction-Field VdW=Van der Waals QSTab=quadratic-spline table
W3=SPC/TIP3p W4=TIP4p (single or pairs)
V&F=Potential and force V=Potential only F=Force only

Computing:	M-Number	M-Flops	% Flops
NB Free energy kernel	38060290.567074	38060290.567	0.2
Pair Search distance check	1842835.791974	16585522.128	0.1
NxN Ewald Elec. + LJ [F]	125877982.918080	11706652411.381	59.8
NxN Ewald Elec. + LJ [V&F]	1271526.777840	161483900.786	0.8
NxN Ewald Elec. [F]	107956844.327328	6585367503.967	33.6
NxN Ewald Elec. [V&F]	1090495.706352	91601639.334	0.5
1,4 nonbonded interactions	36702.012234	3303181.101	0.0
Calc Weights	605619.201873	21802291.267	0.1
Spread Q Bspline	25839752.613248	51679505.226	0.3
Gather F Bspline	25839752.613248	155038515.679	0.8
3D-FFT	82917029.021184	663336232.169	3.4
Solve PME	124426.148352	7963273.495	0.0
Reset In Box	2523.345209	7570.036	0.0
CG-CoM	2523.479791	7570.439	0.0
Angles	25548.008516	4292065.431	0.0
Propers	39945.013315	9147408.049	0.0
Impropers	3591.001197	746928.249	0.0
Virial	20727.369091	373092.644	0.0
Update	201873.067291	6258065.086	0.0
Stop-CM	2018.797291	20187.973	0.0
Calc-Ekin	40374.734582	1090117.834	0.0
Lincs	58023.183682	3481391.021	0.0
Lincs-Mat	1240745.165640	4962980.663	0.0

```
 Constraint-V                           535313.312870     4817819.816
0.0
 Constraint-Vir                          23864.578058      572749.873
0.0
 Settle                                 139755.648502    51709589.946
0.3
-----------------------------------------------------------------------
----
 Total                                                 19590361804.160
100.0
-----------------------------------------------------------------------
----


    D O M A I N   D E C O M P O S I T I O N   S T A T I S T I C S

 av. #atoms communicated per step for force:  2 x 223144.5
 av. #atoms communicated per step for LINCS:  3 x 14014.9


Dynamic load balancing report:
 DLB was turned on during the run due to measured imbalance.
 Average load imbalance: 23.9%.
 The balanceable part of the MD step is 41%, load imbalance is computed
from this.
 Part of the total run time spent waiting due to load imbalance: 9.8%.
 Steps where the load balancing was limited by -rdd, -rcon and/or -dds: X
0 % Y 0 % Z 0 %
 Average PME mesh/force load: 1.429
 Part of the total run time spent waiting due to PP/PME imbalance: 15.5 %

NOTE: 9.8 % of the available CPU time was lost due to load imbalance
      in the domain decomposition.
      You can consider manually changing the decomposition (option -dd);
      e.g. by using fewer domains along the box dimension in which there
is
      considerable inhomogeneity in the simulated system.
NOTE: 15.5 % performance was lost because the PME ranks
      had more work to do than the PP ranks.
      You might want to increase the number of PME ranks
      or increase the cut-off and the grid spacing.


      R E A L   C Y C L E   A N D   T I M E   A C C O U N T I N G

On 40 MPI ranks doing PP, and
on 20 MPI ranks doing PME

 Activity:              Num   Num      Call    Wall time         Giga-
Cycles
                       Ranks Threads  Count      (s)         total sum
%
-----------------------------------------------------------------------
-------
 Domain decomp.           40    1      37500     203.380      23953.595
0.6
 DD comm. load            40    1      35340       0.946        111.395
0.0
```

```
 DD comm. bounds          40    1      34801      11.051       1301.597
0.0
 Send X to PME            40    1    3000001      68.355       8050.698
0.2
 Neighbor search          40    1      37501     215.338      25361.923
0.6
 Comm. coord.             40    1    2962500     995.706     117271.589
2.9
 Force                    40    1    3000001    8022.118     944823.390
23.7
 Wait + Comm. F           40    1    3000001    2502.549     294743.440
7.4
 PME mesh *               20    1    3000001   17151.087    1010004.375
25.3
 PME wait for PP *                             5436.468     320146.279
8.0
 Wait + Recv. PME F       40    1    3000001    5577.093     656854.926
16.5
 NB X/F buffer ops.       40    1    8925001     105.753      12455.313
0.3
 Write traj.              40    1        154       0.183         21.531
0.0
 Update                   40    1    6000002     170.165      20041.570
0.5
 Constraints              40    1    6000002    4603.093     542139.890
13.6
 Comm. energies           40    1     300001      69.363       8169.353
0.2
 Rest                                           42.461       5000.924
0.1
-----------------------------------------------------------------------
-------
 Total                                       22587.554    3990451.700
100.0
-----------------------------------------------------------------------
-------
(*) Note that with separate PME ranks, the walltime column actually sums
to
    twice the total reported, but the cycle count total and % are
correct.
-----------------------------------------------------------------------
-------
 Breakdown of PME mesh activities
-----------------------------------------------------------------------
-------
 PME redist. X/F          20    1    9000003    4170.753     245610.009
6.2
 PME spread               20    1    6000002    2445.563     144015.926
3.6
 PME gather               20    1    6000002    1644.090      96818.237
2.4
 PME 3D-FFT               20    1   12000004    1092.392      64329.461
1.6
 PME 3D-FFT Comm.         20    1   24000008    7676.157     452038.541
11.3
 PME solve Elec           20    1    6000002     114.150       6722.117
0.2
```

```
-------------------------------------------------------------------------------

               Core t (s)   Wall t (s)        (%)
       Time:  1355252.592    22587.554     6000.0
                         6h16:27
                 (ns/day)    (hour/ns)
Performance:       22.951        1.046
Finished mdrun on rank 0 Sun Jan 14 11:50:11 2024
```

OTHER FREE ENERGY BENCHMARKS

benchBFC_cpu-cluster_1n

```
                :-) GROMACS - gmx mdrun, 2023.3 (-:

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                    Coordinated by the GROMACS project leaders:
                      Paul Bauer, Berk Hess, and Erik Lindahl

GROMACS:      gmx mdrun, version 2023.3
Executable:   /usr/local/gromacs/bin/gmx_mpi
Data prefix:  /usr/local/gromacs
Working dir:  /home/ubuntu
Process ID:   3893
Command line:
  gmx_mpi mdrun -v -s /mnt/shared/home/ubuntu/mpinat-gromacs/mpinat-
gromacs-free-energy-bench/benchBFC.tpr

GROMACS version:    2023.3
Precision:          mixed
Memory model:       64 bit
MPI library:        MPI
OpenMP support:     enabled (GMX_OPENMP_MAX_THREADS = 128)
GPU support:        disabled
SIMD instructions:  AVX2_256
```

```
CPU FFT library:    fftw-3.3.8-sse2-avx-avx2-avx2_128
GPU FFT library:    none
Multi-GPU FFT:      none
RDTSCP usage:       enabled
TNG support:        enabled
Hwloc support:      disabled
Tracing support:    disabled
C compiler:         /usr/bin/cc GNU 11.4.0
C compiler flags:   -fexcess-precision=fast -funroll-all-loops -mavx2 -
mfma -Wno-missing-field-initializers -O3 -DNDEBUG
C++ compiler:       /usr/bin/c++ GNU 11.4.0
C++ compiler flags: -fexcess-precision=fast -funroll-all-loops -mavx2 -
mfma -Wno-missing-field-initializers -Wno-cast-function-type-strict -
fopenmp -O3 -DNDEBUG
BLAS library:
LAPACK library:


Running on 1 node with total 6 cores, 6 processing units
Hardware detected on host cpu-9 (the node of MPI rank 0):
  CPU info:
    Vendor: AMD
    Brand:  AMD EPYC-Milan Processor
    Family: 25   Model: 1   Stepping: 1
    Features: aes amd apic avx avx2 clfsh cmov cx8 cx16 f16c fma lahf
misalignsse mmx msr pcid pclmuldq pdpe1gb popcnt pse rdrnd rdtscp sha
sse2 sse3 sse4a sse4.1 sse4.2 ssse3 tdt x2apic
  Hardware topology: Basic
    Packages, cores, and logical processors:
    [indices refer to OS logical processors]
      Package  0: [   0]
      Package  1: [   1]
      Package  2: [   2]
      Package  3: [   3]
      Package  4: [   4]
      Package  5: [   5]
    CPU limit set by OS: -1   Recommended max number of threads: 6


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
M. J. Abraham, T. Murtola, R. Schulz, S. P√°ll, J. C. Smith, B. Hess, E.
Lindahl
GROMACS: High performance molecular simulations through multi-level
parallelism from laptops to supercomputers
SoftwareX 1 (2015) pp. 19-25
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. P√°ll, M. J. Abraham, C. Kutzner, B. Hess, E. Lindahl
Tackling Exascale Software Challenges in Molecular Dynamics Simulations
with
GROMACS
In S. Markidis & E. Laure (Eds.), Solving Software Challenges for
Exascale 8759 (2015) pp. 3-27
-------- -------- --- Thank You --- -------- --------
```

```
++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. Pronk, S. P√°ll, R. Schulz, P. Larsson, P. Bjelkmar, R. Apostolov, M.
R.
Shirts, J. C. Smith, P. M. Kasson, D. van der Spoel, B. Hess, and E.
Lindahl
GROMACS 4.5: a high-throughput and highly parallel open source molecular
simulation toolkit
Bioinformatics 29 (2013) pp. 845-54
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
B. Hess and C. Kutzner and D. van der Spoel and E. Lindahl
GROMACS 4: Algorithms for highly efficient, load-balanced, and scalable
molecular simulation
J. Chem. Theory Comput. 4 (2008) pp. 435-447
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
D. van der Spoel, E. Lindahl, B. Hess, G. Groenhof, A. E. Mark and H. J.
C.
Berendsen
GROMACS: Fast, Flexible and Free
J. Comp. Chem. 26 (2005) pp. 1701-1719
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
E. Lindahl and B. Hess and D. van der Spoel
GROMACS 3.0: A package for molecular simulation and trajectory analysis
J. Mol. Mod. 7 (2001) pp. 306-317
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
H. J. C. Berendsen, D. van der Spoel and R. van Drunen
GROMACS: A message-passing parallel molecular dynamics implementation
Comp. Phys. Comm. 91 (1995) pp. 43-56
-------- -------- --- Thank You --- -------- --------


++++ PLEASE CITE THE DOI FOR THIS VERSION OF GROMACS ++++
https://doi.org/10.5281/zenodo.10017686
-------- -------- --- Thank You --- -------- --------


The number of OpenMP threads was set by environment variable
OMP_NUM_THREADS to 1

Input Parameters:
   integrator                     = sd
   tinit                          = 0
   dt                             = 0.002
   nsteps                         = 10000
   init-step                      = 0
   simulation-part                = 1
   mts                            = false
```

```
comm-mode                      = Linear
nstcomm                        = 100
bd-fric                        = 0
ld-seed                        = -1287569705
emtol                          = 10
emstep                         = 0.01
niter                          = 20
fcstep                         = 0
nstcgsteep                     = 1000
nbfgscorr                      = 10
rtpi                           = 0.05
nstxout                        = 0
nstvout                        = 0
nstfout                        = 0
nstlog                         = 0
nstcalcenergy                  = 100
nstenergy                      = 0
nstxout-compressed             = 0
compressed-x-precision         = 1000
cutoff-scheme                  = Verlet
nstlist                        = 10
pbc                            = xyz
periodic-molecules             = false
verlet-buffer-tolerance        = 0.005
rlist                          = 1.2
coulombtype                    = PME
coulomb-modifier               = Potential-shift
rcoulomb-switch                = 0
rcoulomb                       = 1.2
epsilon-r                      = 1
epsilon-rf                     = inf
vdw-type                       = Cut-off
vdw-modifier                   = Potential-shift
rvdw-switch                    = 0
rvdw                           = 1.2
DispCorr                       = EnerPres
table-extension                = 1
fourierspacing                 = 0.1
fourier-nx                     = 96
fourier-ny                     = 96
fourier-nz                     = 96
pme-order                      = 4
ewald-rtol                     = 1e-05
ewald-rtol-lj                  = 0.001
lj-pme-comb-rule               = Geometric
ewald-geometry                 = 3d
epsilon-surface                = 0
ensemble-temperature-setting   = constant
ensemble-temperature           = 298.15
tcoupl                         = No
nsttcouple                     = -1
nh-chain-length                = 0
print-nose-hoover-chain-variables = false
pcoupl                         = Parrinello-Rahman
pcoupltype                     = Isotropic
nstpcouple                     = 10
tau-p                          = 2
compressibility (3x3):
```

```
      compressibility[    0]={ 4.50000e-05,  0.00000e+00,  0.00000e+00}
      compressibility[    1]={ 0.00000e+00,  4.50000e-05,  0.00000e+00}
      compressibility[    2]={ 0.00000e+00,  0.00000e+00,  4.50000e-05}
   ref-p (3x3):
      ref-p[    0]={ 1.00000e+00,  0.00000e+00,  0.00000e+00}
      ref-p[    1]={ 0.00000e+00,  1.00000e+00,  0.00000e+00}
      ref-p[    2]={ 0.00000e+00,  0.00000e+00,  1.00000e+00}
   refcoord-scaling               = No
   posres-com (3):
      posres-com[0]= 0.00000e+00
      posres-com[1]= 0.00000e+00
      posres-com[2]= 0.00000e+00
   posres-comB (3):
      posres-comB[0]= 0.00000e+00
      posres-comB[1]= 0.00000e+00
      posres-comB[2]= 0.00000e+00
   QMMM                           = false
qm-opts:
   ngQM                           = 0
   constraint-algorithm           = Lincs
   continuation                   = false
   Shake-SOR                      = false
   shake-tol                      = 0.0001
   lincs-order                    = 4
   lincs-iter                     = 1
   lincs-warnangle                = 30
   nwall                          = 0
   wall-type                      = 9-3
   wall-r-linpot                  = -1
   wall-atomtype[0]               = -1
   wall-atomtype[1]               = -1
   wall-density[0]                = 0
   wall-density[1]                = 0
   wall-ewald-zfac                = 3
   pull                           = false
   awh                            = false
   rotation                       = false
   interactiveMD                  = false
   disre                          = No
   disre-weighting                = Conservative
   disre-mixed                    = false
   dr-fc                          = 1000
   dr-tau                         = 0
   nstdisreout                    = 100
   orire-fc                       = 0
   orire-tau                      = 0
   nstorireout                    = 100
   free-energy                    = yes
   init-lambda                    = -1
   init-lambda-state              = 10
   delta-lambda                   = 0
   nstdhdl                        = 100
   n-lambdas                      = 20
   separate-dvdl:
       fep-lambdas =   FALSE
      mass-lambdas =   FALSE
      coul-lambdas =   TRUE
       vdw-lambdas =   TRUE
```

```
    bonded-lambdas =   FALSE
 restraint-lambdas =   FALSE
temperature-lambdas =   FALSE
all-lambdas:
       fep-lambdas =            0           0           0           0
0           0           0           0           0           0           0
0           0           0           0           0           0           0
0           0
      mass-lambdas =            0           0           0           0
0           0           0           0           0           0           0
0           0           0           0           0           0           0
0           0
      coul-lambdas =            0        0.25         0.5        0.75
1           1           1           1           1           1           1
1           1           1           1           1           1           1
1           1
       vdw-lambdas =            0           0           0           0
0        0.05         0.1         0.2         0.3         0.4         0.5
0.6        0.65         0.7        0.75         0.8        0.85
0.9        0.95           1
    bonded-lambdas =            0           0           0           0
0           0           0           0           0           0           0
0           0           0           0           0           0           0
0           0
 restraint-lambdas =            0           0           0           0
0           0           0           0           0           0           0
0           0           0           0           0           0           0
0           0
temperature-lambdas =            0           0           0           0
0           0           0           0           0           0           0
0           0           0           0           0           0           0
0           0
   calc-lambda-neighbors         = -1
   dhdl-print-energy             = no
   sc-alpha                      = 0.5
   sc-power                      = 1
   sc-r-power                    = 6
   sc-sigma                      = 0.3
   sc-sigma-min                  = 0.3
   sc-coul                       = true
   dh-hist-size                  = 0
   dh-hist-spacing               = 0.1
   separate-dhdl-file            = yes
   dhdl-derivatives              = yes
   sc-function                   = beutler
   sc-gapsys-scale-linpoint-lj   = 0.85
   sc-gapsys-scale-linpoint-q    = 0.3
   sc-gapsys-sigma-lj            = 0.3
   cos-acceleration              = 0
   deform (3x3):
      deform[    0]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
      deform[    1]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
      deform[    2]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
   simulated-tempering           = false
   swapcoords                    = no
   userint1                      = 0
   userint2                      = 0
   userint3                      = 0
```

```
   userint4                       = 0
   userreal1                      = 0
   userreal2                      = 0
   userreal3                      = 0
   userreal4                      = 0
   applied-forces:
     electric-field:
grpopts:
   nrdf:       89026
   ref-t:      298.15
   tau-t:           1
annealing:          No
annealing-npoints:           0
   acc:                0           0           0
   nfreeze:            N           N           N
   energygrp-flags[  0]: 0

Changing nstlist from 10 to 80, rlist from 1.2 to 1.322

Update groups can not be used for this system because atoms that are
(in)directly constrained together are interdispersed with other atoms

Initializing Domain Decomposition on 6 ranks
Dynamic load balancing: auto
Minimum cell size due to atom displacement: 0.632 nm
Initial maximum distances in bonded interactions:
    two-body bonded interactions: 1.223 nm, LJC Pairs NB, atoms 2065 2079
  multi-body bonded interactions: 0.698 nm, Improper Dih., atoms 2034
1556
Minimum cell size due to bonded interactions: 0.768 nm
Maximum distance for 5 constraints, at 120 deg. angles, all-trans: 0.219
nm
Estimated maximum distance required for P-LINCS: 0.219 nm
Scaling the initial minimum size with 1/0.8 (option -dds) = 1.25
Using 0 separate PME ranks because: there are too few total ranks for
efficient splitting
Optimizing the DD grid for 6 cells with a minimum initial size of 0.960
nm
The maximum allowed number of cells is: X 7 Y 7 Z 6
Domain decomposition grid 6 x 1 x 1, separate PME ranks 0
PME domain decomposition: 6 x 1 x 1
Domain decomposition rank 0, coordinates 0 0 0

The initial number of communication pulses is: X 2
The initial domain decomposition cell size is: X 1.16 nm

The maximum allowed distance for atoms involved in interactions is:
                 non-bonded interactions           1.322 nm
(the following are initial values, they could change due to box
deformation)
            two-body bonded interactions  (-rdd)   1.322 nm
          multi-body bonded interactions  (-rdd)   1.163 nm
  atoms separated by up to 5 constraints  (-rcon)  1.163 nm

When dynamic load balancing gets turned on, these settings will change
to:
The maximum number of communication pulses is: X 2
The minimum size for domain decomposition cells is 0.931 nm
```

```
The requested allowed shrink of DD cells (option -dds) is: 0.80
The allowed shrink of domain decomposition cells is: X 0.80
The maximum allowed distance for atoms involved in interactions is:
                 non-bonded interactions           1.322 nm
            two-body bonded interactions  (-rdd)   1.322 nm
          multi-body bonded interactions  (-rdd)   0.931 nm
  atoms separated by up to 5 constraints  (-rcon)  0.931 nm

Using 6 MPI processes

Non-default thread affinity set, disabling internal thread affinity

Using 1 OpenMP thread per MPI process

System total charge, top. A: -0.000 top. B: 0.000
Will do PME sum in reciprocal space for electrostatic interactions.

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
U. Essmann, L. Perera, M. L. Berkowitz, T. Darden, H. Lee and L. G.
Pedersen
A smooth particle mesh Ewald method
J. Chem. Phys. 103 (1995) pp. 8577-8592
-------- -------- --- Thank You --- -------- --------

Using a Gaussian width (1/beta) of 0.384195 nm for Ewald
Potential shift: LJ r^-12: -1.122e-01 r^-6: -3.349e-01, Ewald -8.333e-06
Initialized non-bonded Coulomb Ewald tables, spacing: 1.02e-03 size: 2273

Generated table with 1161 data points for 1-4 COUL.
Tabscale = 500 points/nm
Generated table with 1161 data points for 1-4 LJ6.
Tabscale = 500 points/nm
Generated table with 1161 data points for 1-4 LJ12.
Tabscale = 500 points/nm
Long Range LJ corr.: <C6> 3.0077e-04


Using SIMD 4x8 nonbonded short-range kernels

Using a dual 4x8 pair-list setup updated with dynamic pruning:
  outer list: updated every 80 steps, buffer 0.122 nm, rlist 1.322 nm
  inner list: updated every 13 steps, buffer 0.003 nm, rlist 1.203 nm
At tolerance 0.005 kJ/mol/ps per atom, equivalent classical 1x1 list
would be:
  outer list: updated every 80 steps, buffer 0.266 nm, rlist 1.466 nm
  inner list: updated every 13 steps, buffer 0.052 nm, rlist 1.252 nm

The non-bonded pair calculation algorithm tolerates a few missing pair
interactions close to the cut-off. This can lead to a systematic
overestimation of the pressure due to missing LJ interactions. The error
in the average pressure due to missing LJ interactions is at most 0.26
bar.
The pressure error can be controlled by setting the environment variable
GMX_VERLET_BUFFER_PRESSURE_TOLERANCE to the allowed error in units of
bar.

Using Lorentz-Berthelot Lennard-Jones combination rule
There are 48 atoms and 48 charges for free energy perturbation
```

```
Removing pbc first time

Linking all bonded interactions to atoms


Initializing Parallel LINear Constraint Solver

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
B. Hess
P-LINCS: A Parallel Linear Constraint Solver for molecular simulation
J. Chem. Theory Comput. 4 (2008) pp. 116-122
-------- -------- --- Thank You --- -------- --------

The number of constraints is 1037
There are constraints between atoms in different decomposition domains,
will communicate selected coordinates each lincs iteration

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. Miyamoto and P. A. Kollman
SETTLE: An Analytical Version of the SHAKE and RATTLE Algorithms for
Rigid
Water Models
J. Comp. Chem. 13 (1992) pp. 952-962
-------- -------- --- Thank You --- -------- --------


Intra-simulation communication will occur every 10 steps.
Initial vector of lambda components:[     0.0000     0.0000     1.0000
0.5000     0.0000     0.0000     0.0000 ]

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
N. Goga and A. J. Rzepiela and A. H. de Vries and S. J. Marrink and H. J.
C.
Berendsen
Efficient Algorithms for Langevin and DPD Dynamics
J. Chem. Theory Comput. 8 (2012) pp. 3637--3649
-------- -------- --- Thank You --- -------- --------

There are: 43952 Atoms
Atom distribution over 6 domains: av 7325 stddev 93 min 7261 max 7447

Constraining the starting coordinates (step 0)

Constraining the coordinates at t0-dt (step 0)
Center of mass motion removal mode is Linear
We have the following groups for center of mass motion removal:
  0:  rest
RMS relative constraint deviation after constraining: 2.99e-06
Initial temperature: 297.767 K

Started mdrun on rank 0 Fri Jan 12 00:05:25 2024

           Step           Time
              0        0.00000

   Energies (kJ/mol)
           Bond  Harmonic Pot.          Angle    Proper Dih.  Improper
Dih.
```

```
    1.74496e+03    0.00000e+00    4.45123e+03    5.17096e+03
0.00000e+00
 Per. Imp. Dih.          LJ-14     Coulomb-14        LJ (SR)  Disper.
corr.
    2.79362e+02    2.02835e+03    1.20238e+04    8.34149e+04   -
3.18065e+03
   Coulomb (SR)   Coul. recip.      Potential    Kinetic En.   Total
Energy
   -7.21755e+05    2.18051e+03   -6.13641e+05    1.10125e+05   -
5.03516e+05
    Temperature Pres. DC (bar) Pressure (bar)      dVcoul/dl
dVvdw/dl
    2.97553e+02   -1.19688e+02   -8.81475e+01    2.54752e+01
2.47544e+02
   Constr. rmsd
    3.01294e-06


DD  step 79 load imb.: force 22.5%

step 160 Turning on dynamic load balancing, because the performance loss
due to load imbalance is 12.1 %.

DD  load balancing is limited by minimum cell size in dimension X
DD  step 9999  vol min/aver 0.801! load imb.: force 35.9%
          Step           Time
         10000       20.00000

Writing checkpoint, step 10000 at Fri Jan 12 00:08:59 2024


   Energies (kJ/mol)
          Bond  Harmonic Pot.          Angle    Proper Dih.  Improper
Dih.
    1.52916e+03    0.00000e+00    4.32794e+03    5.16629e+03
0.00000e+00
 Per. Imp. Dih.          LJ-14     Coulomb-14        LJ (SR)  Disper.
corr.
    3.06232e+02    2.05002e+03    1.22443e+04    8.40895e+04   -
3.19181e+03
   Coulomb (SR)   Coul. recip.      Potential    Kinetic En.   Total
Energy
   -7.23563e+05    2.12148e+03   -6.14920e+05    1.10648e+05   -
5.04272e+05
    Temperature Pres. DC (bar) Pressure (bar)      dVcoul/dl
dVvdw/dl
    2.98968e+02   -1.20529e+02    1.11560e+02    2.38251e+01
5.86457e+01
   Constr. rmsd
    3.36803e-06


      <======  ###############  ==>
      <====  A V E R A G E S  ====>
      <==  ###############  ======>

      Statistics over 10001 steps using 101 frames
```

```
   Energies (kJ/mol)
           Bond  Harmonic Pot.          Angle    Proper Dih.  Improper
Dih.
    1.63207e+03    0.00000e+00    4.41683e+03    5.12516e+03
0.00000e+00
 Per. Imp. Dih.          LJ-14     Coulomb-14        LJ (SR)  Disper.
corr.
    2.75378e+02    2.01304e+03    1.20595e+04    8.40503e+04   -
3.18279e+03
   Coulomb (SR)   Coul. recip.      Potential    Kinetic En.   Total
Energy
   -7.23102e+05    2.15379e+03   -6.14559e+05    1.10305e+05   -
5.04254e+05
    Temperature Pres. DC (bar) Pressure (bar)      dVcoul/dl
dVvdw/dl
    2.98039e+02   -1.19850e+02    1.07909e+01    2.60116e+01
1.08904e+02
   Constr. rmsd
    0.00000e+00

          Box-X          Box-Y          Box-Z
    8.54568e+00    8.54568e+00    6.04272e+00

   Total Virial (kJ/mol)
    3.67523e+04    4.57322e+01   -4.45912e+01
    4.56065e+01    3.67182e+04    2.02157e+02
   -4.36197e+01    2.03140e+02    3.64087e+04

   Pressure (bar)
    2.24598e+00   -2.08189e+00    2.64827e+00
   -2.07238e+00    7.18807e+00   -1.65456e+01
    2.57517e+00   -1.66196e+01    2.29388e+01


     M E G A - F L O P S   A C C O U N T I N G

 NB=Group-cutoff nonbonded kernels    NxN=N-by-N cluster Verlet kernels
 RF=Reaction-Field  VdW=Van der Waals  QSTab=quadratic-spline table
 W3=SPC/TIP3p  W4=TIP4p (single or pairs)
 V&F=Potential and force  V=Potential only  F=Force only

 Computing:                                M-Number         M-Flops  %
Flops
-----------------------------------------------------------------------
----
 NB Free energy kernel                104262.762624      104262.763
0.3
 Pair Search distance check             3381.345928       30432.113
0.1
 NxN Ewald Elec. + LJ [F]             228457.569408    15078199.581
44.1
 NxN Ewald Elec. + LJ [V&F]             2331.073632      249424.879
0.7
 NxN Ewald Elec. [F]                  201956.022048    12319317.345
36.0
 NxN Ewald Elec. [V&F]                  2060.553120      173086.462
0.5
```

```
 1,4 nonbonded interactions              63.186318        5686.769
0.0
 Calc Weights                          1318.691856       47472.907
0.1
 Spread Q Bspline                     56264.185856      112528.372
0.3
 Gather F Bspline                     56264.185856      337585.115
1.0
 3D-FFT                              699184.311440     5593474.492
16.3
 Solve PME                             184.338432       11797.660
0.0
 Reset In Box                            5.537952          16.614
0.0
 CG-CoM                                  5.581904          16.746
0.0
 Bonds                                  10.603181         625.588
0.0
 Angles                                 37.838025        6356.788
0.0
 Propers                                57.785778       13232.943
0.0
 Impropers                               4.236786         881.251
0.0
 Virial                                 44.266222         796.792
0.0
 Update                                439.563952       13626.483
0.0
 Stop-CM                                 4.483104          44.831
0.0
 Calc-Ekin                              87.991904        2375.781
0.0
 Lincs                                  22.368324        1342.099
0.0
 Lincs-Mat                             124.674960         498.700
0.0
 Constraint-V                          942.048528        8478.437
0.0
 Constraint-Vir                         46.023183        1104.556
0.0
 Settle                                299.119626      110674.262
0.3
-----------------------------------------------------------------------
----
 Total                                                34223340.327
100.0
-----------------------------------------------------------------------
----


   D O M A I N   D E C O M P O S I T I O N   S T A T I S T I C S

 av. #atoms communicated per step for force:  2 x 49956.1
 av. #atoms communicated per step for LINCS:  2 x 3194.0


Dynamic load balancing report:
 DLB was turned on during the run due to measured imbalance.
```

```
 Average load imbalance: 13.7%.
 The balanceable part of the MD step is 47%, load imbalance is computed
from this.
 Part of the total run time spent waiting due to load imbalance: 6.5%.
 Steps where the load balancing was limited by -rdd, -rcon and/or -dds: X
0 %

NOTE: 6.5 % of the available CPU time was lost due to load imbalance
      in the domain decomposition.
      You can consider manually changing the decomposition (option -dd);
      e.g. by using fewer domains along the box dimension in which there
is
      considerable inhomogeneity in the simulated system.

      R E A L   C Y C L E   A N D   T I M E   A C C O U N T I N G

On 6 MPI ranks

 Activity:              Num   Num      Call    Wall time         Giga-
Cycles
                       Ranks Threads  Count      (s)         total sum
%
-----------------------------------------------------------------------
-------
 Domain decomp.            6    1        126       0.631         11.155
0.3
 DD comm. load             6    1        125       0.004          0.069
0.0
 DD comm. bounds           6    1        124       0.012          0.218
0.0
 Neighbor search           6    1        126       2.667         47.113
1.2
 Comm. coord.              6    1       9875       1.121         19.802
0.5
 Force                     6    1      10001      99.514       1758.080
46.5
 Wait + Comm. F            6    1      10001       1.062         18.764
0.5
 PME mesh                  6    1      10001      99.621       1759.961
46.5
 NB X/F buffer ops.        6    1      29751       0.905         15.988
0.4
 Write traj.               6    1          1       0.023          0.399
0.0
 Update                    6    1      20002       3.561         62.912
1.7
 Constraints               6    1      20004       4.251         75.102
2.0
 Comm. energies            6    1       1001       0.128          2.253
0.1
 Rest                                               0.509          8.986
0.2
-----------------------------------------------------------------------
-------
 Total                                            214.008       3780.801
100.0
-----------------------------------------------------------------------
-------
```

```
 Breakdown of PME mesh activities
------------------------------------------------------------------------
-------
 PME redist. X/F           6    1      30003      24.492        432.689
11.4
 PME spread                6    1      20002      15.483        273.541
7.2
 PME gather                6    1      20002       8.790        155.285
4.1
 PME 3D-FFT                6    1      40004      35.959        635.278
16.8
 PME 3D-FFT Comm.          6    1      40004      11.118        196.414
5.2
 PME solve Elec            6    1      20002       3.724         65.791
1.7
------------------------------------------------------------------------
-------

               Core t (s)   Wall t (s)        (%)
       Time:     1284.048      214.008      600.0
                 (ns/day)    (hour/ns)
Performance:        8.075        2.972
Finished mdrun on rank 0 Fri Jan 12 00:08:59 2024
```

benchBFC_cpu-cluster_3n

```
                    :-) GROMACS - gmx mdrun, 2023.3 (-:

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Wennberg
       Maarten Wolf

                    Coordinated by the GROMACS project leaders:
                      Paul Bauer, Berk Hess, and Erik Lindahl

GROMACS:      gmx mdrun, version 2023.3
Executable:   /usr/local/gromacs/bin/gmx_mpi
Data prefix:  /usr/local/gromacs
Working dir:  /home/ubuntu
Process ID:   9126
Command line:
  gmx_mpi mdrun -v -s /mnt/shared/home/ubuntu/mpinat-gromacs/mpinat-
gromacs-free-energy-bench/benchBFC.tpr

GROMACS version:    2023.3
Precision:          mixed
Memory model:       64 bit
MPI library:        MPI
OpenMP support:     enabled (GMX_OPENMP_MAX_THREADS = 128)
GPU support:        disabled
SIMD instructions:  AVX2_256
```

```
CPU FFT library:    fftw-3.3.8-sse2-avx-avx2-avx2_128
GPU FFT library:    none
Multi-GPU FFT:      none
RDTSCP usage:       enabled
TNG support:        enabled
Hwloc support:      disabled
Tracing support:    disabled
C compiler:         /usr/bin/cc GNU 11.4.0
C compiler flags:   -fexcess-precision=fast -funroll-all-loops -mavx2 -
mfma -Wno-missing-field-initializers -O3 -DNDEBUG
C++ compiler:       /usr/bin/c++ GNU 11.4.0
C++ compiler flags: -fexcess-precision=fast -funroll-all-loops -mavx2 -
mfma -Wno-missing-field-initializers -Wno-cast-function-type-strict -
fopenmp -O3 -DNDEBUG
BLAS library:       Internal
LAPACK library:     Internal


Running on 3 nodes with total 18 cores, 18 processing units
  Cores per node:            6
  Logical processing units per node:    6
  OS CPU Limit / recommended threads to start per node:    6
Hardware detected on host cpu-1 (the node of MPI rank 0):
  CPU info:
    Vendor: AMD
    Brand:  AMD EPYC-Milan Processor
    Family: 25   Model: 1   Stepping: 1
    Features: aes amd apic avx avx2 clfsh cmov cx8 cx16 f16c fma lahf
misalignsse mmx msr pcid pclmuldq pdpe1gb popcnt pse rdrnd rdtscp sha
sse2 sse3 sse4a sse4.1 sse4.2 ssse3 tdt x2apic
  Hardware topology: Basic
    Packages, cores, and logical processors:
    [indices refer to OS logical processors]
      Package  0: [   0]
      Package  1: [   1]
      Package  2: [   2]
      Package  3: [   3]
      Package  4: [   4]
      Package  5: [   5]
    CPU limit set by OS: -1   Recommended max number of threads: 6


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
M. J. Abraham, T. Murtola, R. Schulz, S. P√°ll, J. C. Smith, B. Hess, E.
Lindahl
GROMACS: High performance molecular simulations through multi-level
parallelism from laptops to supercomputers
SoftwareX 1 (2015) pp. 19-25
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. P√°ll, M. J. Abraham, C. Kutzner, B. Hess, E. Lindahl
Tackling Exascale Software Challenges in Molecular Dynamics Simulations
with
GROMACS
In S. Markidis & E. Laure (Eds.), Solving Software Challenges for
Exascale 8759 (2015) pp. 3-27
```

```
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. Pronk, S. P√°ll, R. Schulz, P. Larsson, P. Bjelkmar, R. Apostolov, M.
R.
Shirts, J. C. Smith, P. M. Kasson, D. van der Spoel, B. Hess, and E.
Lindahl
GROMACS 4.5: a high-throughput and highly parallel open source molecular
simulation toolkit
Bioinformatics 29 (2013) pp. 845-54
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
B. Hess and C. Kutzner and D. van der Spoel and E. Lindahl
GROMACS 4: Algorithms for highly efficient, load-balanced, and scalable
molecular simulation
J. Chem. Theory Comput. 4 (2008) pp. 435-447
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
D. van der Spoel, E. Lindahl, B. Hess, G. Groenhof, A. E. Mark and H. J.
C.
Berendsen
GROMACS: Fast, Flexible and Free
J. Comp. Chem. 26 (2005) pp. 1701-1719
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
E. Lindahl and B. Hess and D. van der Spoel
GROMACS 3.0: A package for molecular simulation and trajectory analysis
J. Mol. Mod. 7 (2001) pp. 306-317
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
H. J. C. Berendsen, D. van der Spoel and R. van Drunen
GROMACS: A message-passing parallel molecular dynamics implementation
Comp. Phys. Comm. 91 (1995) pp. 43-56
-------- -------- --- Thank You --- -------- --------


++++ PLEASE CITE THE DOI FOR THIS VERSION OF GROMACS ++++
https://doi.org/10.5281/zenodo.10017686
-------- -------- --- Thank You --- -------- --------


The number of OpenMP threads was set by environment variable
OMP_NUM_THREADS to 1

Input Parameters:
   integrator                   = sd
   tinit                        = 0
   dt                           = 0.002
   nsteps                       = 10000
```

```
init-step                      = 0
simulation-part                = 1
mts                            = false
comm-mode                      = Linear
nstcomm                        = 100
bd-fric                        = 0
ld-seed                        = -1287569705
emtol                          = 10
emstep                         = 0.01
niter                          = 20
fcstep                         = 0
nstcgsteep                     = 1000
nbfgscorr                      = 10
rtpi                           = 0.05
nstxout                        = 0
nstvout                        = 0
nstfout                        = 0
nstlog                         = 0
nstcalcenergy                  = 100
nstenergy                      = 0
nstxout-compressed             = 0
compressed-x-precision         = 1000
cutoff-scheme                  = Verlet
nstlist                        = 10
pbc                            = xyz
periodic-molecules             = false
verlet-buffer-tolerance        = 0.005
rlist                          = 1.2
coulombtype                    = PME
coulomb-modifier               = Potential-shift
rcoulomb-switch                = 0
rcoulomb                       = 1.2
epsilon-r                      = 1
epsilon-rf                     = inf
vdw-type                       = Cut-off
vdw-modifier                   = Potential-shift
rvdw-switch                    = 0
rvdw                           = 1.2
DispCorr                       = EnerPres
table-extension                = 1
fourierspacing                 = 0.1
fourier-nx                     = 96
fourier-ny                     = 96
fourier-nz                     = 96
pme-order                      = 4
ewald-rtol                     = 1e-05
ewald-rtol-lj                  = 0.001
lj-pme-comb-rule               = Geometric
ewald-geometry                 = 3d
epsilon-surface                = 0
ensemble-temperature-setting   = constant
ensemble-temperature           = 298.15
tcoupl                         = No
nsttcouple                     = -1
nh-chain-length                = 0
print-nose-hoover-chain-variables = false
pcoupl                         = Parrinello-Rahman
pcoupltype                     = Isotropic
```

```
   nstpcouple                     = 10
   tau-p                          = 2
   compressibility (3x3):
      compressibility[    0]={ 4.50000e-05,  0.00000e+00,  0.00000e+00}
      compressibility[    1]={ 0.00000e+00,  4.50000e-05,  0.00000e+00}
      compressibility[    2]={ 0.00000e+00,  0.00000e+00,  4.50000e-05}
   ref-p (3x3):
      ref-p[    0]={ 1.00000e+00,  0.00000e+00,  0.00000e+00}
      ref-p[    1]={ 0.00000e+00,  1.00000e+00,  0.00000e+00}
      ref-p[    2]={ 0.00000e+00,  0.00000e+00,  1.00000e+00}
   refcoord-scaling               = No
   posres-com (3):
      posres-com[0]= 0.00000e+00
      posres-com[1]= 0.00000e+00
      posres-com[2]= 0.00000e+00
   posres-comB (3):
      posres-comB[0]= 0.00000e+00
      posres-comB[1]= 0.00000e+00
      posres-comB[2]= 0.00000e+00
   QMMM                           = false
qm-opts:
   ngQM                           = 0
   constraint-algorithm           = Lincs
   continuation                   = false
   Shake-SOR                      = false
   shake-tol                      = 0.0001
   lincs-order                    = 4
   lincs-iter                     = 1
   lincs-warnangle                = 30
   nwall                          = 0
   wall-type                      = 9-3
   wall-r-linpot                  = -1
   wall-atomtype[0]               = -1
   wall-atomtype[1]               = -1
   wall-density[0]                = 0
   wall-density[1]                = 0
   wall-ewald-zfac                = 3
   pull                           = false
   awh                            = false
   rotation                       = false
   interactiveMD                  = false
   disre                          = No
   disre-weighting                = Conservative
   disre-mixed                    = false
   dr-fc                          = 1000
   dr-tau                         = 0
   nstdisreout                    = 100
   orire-fc                       = 0
   orire-tau                      = 0
   nstorireout                    = 100
   free-energy                    = yes
   init-lambda                    = -1
   init-lambda-state              = 10
   delta-lambda                   = 0
   nstdhdl                        = 100
   n-lambdas                      = 20
   separate-dvdl:
       fep-lambdas =   FALSE
```

```
      mass-lambdas =   FALSE
      coul-lambdas =   TRUE
       vdw-lambdas =   TRUE
    bonded-lambdas =   FALSE
 restraint-lambdas =   FALSE
temperature-lambdas =   FALSE
all-lambdas:
       fep-lambdas =            0           0           0           0
0           0           0           0           0           0           0
0           0           0           0           0           0           0
0           0
      mass-lambdas =            0           0           0           0
0           0           0           0           0           0           0
0           0           0           0           0           0           0
0           0
      coul-lambdas =            0        0.25         0.5        0.75
1           1           1           1           1           1           1
1           1           1           1           1           1           1
1           1
       vdw-lambdas =            0           0           0           0
0        0.05         0.1         0.2         0.3         0.4         0.5
0.6        0.65         0.7        0.75         0.8        0.85
0.9        0.95           1
    bonded-lambdas =            0           0           0           0
0           0           0           0           0           0           0
0           0           0           0           0           0           0
0           0
 restraint-lambdas =            0           0           0           0
0           0           0           0           0           0           0
0           0           0           0           0           0           0
0           0
temperature-lambdas =            0           0           0           0
0           0           0           0           0           0           0
0           0           0           0           0           0           0
0           0
   calc-lambda-neighbors         = -1
   dhdl-print-energy             = no
   sc-alpha                      = 0.5
   sc-power                      = 1
   sc-r-power                    = 6
   sc-sigma                      = 0.3
   sc-sigma-min                  = 0.3
   sc-coul                       = true
   dh-hist-size                  = 0
   dh-hist-spacing               = 0.1
   separate-dhdl-file            = yes
   dhdl-derivatives              = yes
   sc-function                   = beutler
   sc-gapsys-scale-linpoint-lj   = 0.85
   sc-gapsys-scale-linpoint-q    = 0.3
   sc-gapsys-sigma-lj            = 0.3
   cos-acceleration              = 0
   deform (3x3):
      deform[    0]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
      deform[    1]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
      deform[    2]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
   simulated-tempering           = false
   swapcoords                    = no
```

```
   userint1                       = 0
   userint2                       = 0
   userint3                       = 0
   userint4                       = 0
   userreal1                      = 0
   userreal2                      = 0
   userreal3                      = 0
   userreal4                      = 0
   applied-forces:
     electric-field:
grpopts:
   nrdf:       89026
   ref-t:      298.15
   tau-t:           1
annealing:          No
annealing-npoints:           0
   acc:                0           0           0
   nfreeze:            N           N           N
   energygrp-flags[  0]: 0

Changing nstlist from 10 to 80, rlist from 1.2 to 1.322

Update groups can not be used for this system because atoms that are
(in)directly constrained together are interdispersed with other atoms

Initializing Domain Decomposition on 18 ranks
Dynamic load balancing: auto
Minimum cell size due to atom displacement: 0.632 nm
Initial maximum distances in bonded interactions:
    two-body bonded interactions: 1.223 nm, LJC Pairs NB, atoms 2065 2079
  multi-body bonded interactions: 0.698 nm, Improper Dih., atoms 2034
1556
Minimum cell size due to bonded interactions: 0.768 nm
Maximum distance for 5 constraints, at 120 deg. angles, all-trans: 0.219
nm
Estimated maximum distance required for P-LINCS: 0.219 nm
Scaling the initial minimum size with 1/0.8 (option -dds) = 1.25
Using 0 separate PME ranks because: there are too few total ranks for
efficient splitting
Optimizing the DD grid for 18 cells with a minimum initial size of 0.960
nm
The maximum allowed number of cells is: X 7 Y 7 Z 6
Domain decomposition grid 6 x 3 x 1, separate PME ranks 0
PME domain decomposition: 6 x 3 x 1
Domain decomposition rank 0, coordinates 0 0 0

The initial number of communication pulses is: X 2 Y 1
The initial domain decomposition cell size is: X 1.16 nm Y 2.33 nm

The maximum allowed distance for atoms involved in interactions is:
                 non-bonded interactions           1.322 nm
(the following are initial values, they could change due to box
deformation)
            two-body bonded interactions  (-rdd)   1.322 nm
          multi-body bonded interactions  (-rdd)   1.163 nm
  atoms separated by up to 5 constraints  (-rcon)  1.163 nm
```

```
When dynamic load balancing gets turned on, these settings will change
to:
The maximum number of communication pulses is: X 2 Y 2
The minimum size for domain decomposition cells is 0.931 nm
The requested allowed shrink of DD cells (option -dds) is: 0.80
The allowed shrink of domain decomposition cells is: X 0.80 Y 0.40
The maximum allowed distance for atoms involved in interactions is:
                 non-bonded interactions           1.322 nm
            two-body bonded interactions  (-rdd)   1.322 nm
          multi-body bonded interactions  (-rdd)   0.931 nm
  atoms separated by up to 5 constraints  (-rcon)  0.931 nm
Using two step summing over 3 groups of on average 6.0 ranks


Using 18 MPI processes

Non-default thread affinity set, disabling internal thread affinity

Using 1 OpenMP thread per MPI process

System total charge, top. A: -0.000 top. B: 0.000
Will do PME sum in reciprocal space for electrostatic interactions.

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
U. Essmann, L. Perera, M. L. Berkowitz, T. Darden, H. Lee and L. G.
Pedersen
A smooth particle mesh Ewald method
J. Chem. Phys. 103 (1995) pp. 8577-8592
-------- -------- --- Thank You --- -------- --------

Using a Gaussian width (1/beta) of 0.384195 nm for Ewald
Potential shift: LJ r^-12: -1.122e-01 r^-6: -3.349e-01, Ewald -8.333e-06
Initialized non-bonded Coulomb Ewald tables, spacing: 1.02e-03 size: 2273

Generated table with 1161 data points for 1-4 COUL.
Tabscale = 500 points/nm
Generated table with 1161 data points for 1-4 LJ6.
Tabscale = 500 points/nm
Generated table with 1161 data points for 1-4 LJ12.
Tabscale = 500 points/nm
Long Range LJ corr.: <C6> 3.0077e-04


Using SIMD 4x8 nonbonded short-range kernels

Using a dual 4x8 pair-list setup updated with dynamic pruning:
  outer list: updated every 80 steps, buffer 0.122 nm, rlist 1.322 nm
  inner list: updated every 13 steps, buffer 0.003 nm, rlist 1.203 nm
At tolerance 0.005 kJ/mol/ps per atom, equivalent classical 1x1 list
would be:
  outer list: updated every 80 steps, buffer 0.266 nm, rlist 1.466 nm
  inner list: updated every 13 steps, buffer 0.052 nm, rlist 1.252 nm

The non-bonded pair calculation algorithm tolerates a few missing pair
interactions close to the cut-off. This can lead to a systematic
overestimation of the pressure due to missing LJ interactions. The error
in the average pressure due to missing LJ interactions is at most 0.26
bar.
```

```
The pressure error can be controlled by setting the environment variable
GMX_VERLET_BUFFER_PRESSURE_TOLERANCE to the allowed error in units of
bar.

Using Lorentz-Berthelot Lennard-Jones combination rule
There are 48 atoms and 48 charges for free energy perturbation
Removing pbc first time

Linking all bonded interactions to atoms


Initializing Parallel LINear Constraint Solver

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
B. Hess
P-LINCS: A Parallel Linear Constraint Solver for molecular simulation
J. Chem. Theory Comput. 4 (2008) pp. 116-122
-------- -------- --- Thank You --- -------- --------

The number of constraints is 1037
There are constraints between atoms in different decomposition domains,
will communicate selected coordinates each lincs iteration

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. Miyamoto and P. A. Kollman
SETTLE: An Analytical Version of the SHAKE and RATTLE Algorithms for
Rigid
Water Models
J. Comp. Chem. 13 (1992) pp. 952-962
-------- -------- --- Thank You --- -------- --------


Intra-simulation communication will occur every 10 steps.
Initial vector of lambda components:[     0.0000     0.0000     1.0000
0.5000     0.0000     0.0000     0.0000 ]

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
N. Goga and A. J. Rzepiela and A. H. de Vries and S. J. Marrink and H. J.
C.
Berendsen
Efficient Algorithms for Langevin and DPD Dynamics
J. Chem. Theory Comput. 8 (2012) pp. 3637--3649
-------- -------- --- Thank You --- -------- --------

There are: 43952 Atoms
Atom distribution over 18 domains: av 2441 stddev 77 min 2387 max 2574

Constraining the starting coordinates (step 0)

Constraining the coordinates at t0-dt (step 0)
Center of mass motion removal mode is Linear
We have the following groups for center of mass motion removal:
  0:  rest
RMS relative constraint deviation after constraining: 2.99e-06
Initial temperature: 297.767 K

Started mdrun on rank 0 Fri Jan 12 10:03:05 2024
```

```
           Step           Time
              0        0.00000

   Energies (kJ/mol)
           Bond  Harmonic Pot.          Angle    Proper Dih.  Improper
Dih.
    1.74496e+03    0.00000e+00    4.45123e+03    5.17097e+03
0.00000e+00
 Per. Imp. Dih.          LJ-14     Coulomb-14        LJ (SR)  Disper.
corr.
    2.79362e+02    2.02835e+03    1.20238e+04    8.34149e+04   -
3.18065e+03
   Coulomb (SR)   Coul. recip.      Potential    Kinetic En.   Total
Energy
   -7.21758e+05    2.18054e+03   -6.13645e+05    1.10125e+05   -
5.03520e+05
    Temperature Pres. DC (bar) Pressure (bar)      dVcoul/dl
dVvdw/dl
    2.97553e+02   -1.19688e+02   -8.81538e+01    2.54722e+01
2.47544e+02
   Constr. rmsd
    3.01589e-06


DD  step 79 load imb.: force 40.4%

step 160 Turning on dynamic load balancing, because the performance loss
due to load imbalance is 10.2 %.
step 4800 Turning off dynamic load balancing, because it is degrading
performance.
Atom distribution over 18 domains: av 2441 stddev 74 min 2376 max 2555
step 8000 Turning on dynamic load balancing, because the performance loss
due to load imbalance is 4.2 %.
step 9600 Turning off dynamic load balancing, because it is degrading
performance.
Atom distribution over 18 domains: av 2441 stddev 73 min 2357 max 2524

DD  step 9999 load imb.: force 39.1%
           Step           Time
          10000       20.00000

Writing checkpoint, step 10000 at Fri Jan 12 10:04:52 2024


   Energies (kJ/mol)
           Bond  Harmonic Pot.          Angle    Proper Dih.  Improper
Dih.
    1.53408e+03    0.00000e+00    4.42931e+03    5.13098e+03
0.00000e+00
 Per. Imp. Dih.          LJ-14     Coulomb-14        LJ (SR)  Disper.
corr.
    2.81527e+02    2.02570e+03    1.20477e+04    8.48897e+04   -
3.18289e+03
   Coulomb (SR)   Coul. recip.      Potential    Kinetic En.   Total
Energy
   -7.23420e+05    2.15516e+03   -6.14109e+05    1.10440e+05   -
5.03669e+05
```

```
    Temperature Pres. DC (bar) Pressure (bar)      dVcoul/dl
dVvdw/dl
    2.98404e+02   -1.19857e+02    1.53210e+02    5.16672e+01
6.69937e+01
   Constr. rmsd
    3.11705e-06


      <======  ###############  ==>
      <====  A V E R A G E S  ====>
      <==  ###############  ======>

      Statistics over 10001 steps using 101 frames

   Energies (kJ/mol)
          Bond  Harmonic Pot.          Angle    Proper Dih.  Improper
Dih.
    1.63246e+03    0.00000e+00    4.42483e+03    5.14537e+03
0.00000e+00
 Per. Imp. Dih.          LJ-14     Coulomb-14        LJ (SR)  Disper.
corr.
    2.77493e+02    2.01536e+03    1.20492e+04    8.42717e+04   -
3.18167e+03
   Coulomb (SR)   Coul. recip.      Potential    Kinetic En.   Total
Energy
   -7.23829e+05    2.15606e+03   -6.15038e+05    1.10173e+05   -
5.04865e+05
    Temperature Pres. DC (bar) Pressure (bar)      dVcoul/dl
dVvdw/dl
    2.97682e+02   -1.19765e+02    1.73827e+00    2.43952e+01
1.04594e+02
   Constr. rmsd
    0.00000e+00

          Box-X          Box-Y          Box-Z
    8.54667e+00    8.54667e+00    6.04342e+00

   Total Virial (kJ/mol)
    3.68256e+04   -1.09825e+02    2.82388e+01
   -1.10602e+02    3.67130e+04   -7.23328e+01
    2.70633e+01   -7.31024e+01    3.65681e+04

   Pressure (bar)
   -6.25507e+00    6.49034e+00   -5.70145e+00
    6.54878e+00    4.86362e+00    3.18912e+00
   -5.61304e+00    3.24702e+00    6.60628e+00


     M E G A - F L O P S   A C C O U N T I N G

 NB=Group-cutoff nonbonded kernels    NxN=N-by-N cluster Verlet kernels
 RF=Reaction-Field  VdW=Van der Waals  QSTab=quadratic-spline table
 W3=SPC/TIP3p  W4=TIP4p (single or pairs)
 V&F=Potential and force  V=Potential only  F=Force only

 Computing:                                M-Number         M-Flops  %
Flops
```

```
-----------------------------------------------------------------------
----
 NB Free energy kernel               103794.439308      103794.439
0.3
 Pair Search distance check            3624.940764       32624.467
0.1
 NxN Ewald Elec. + LJ [F]            241171.922576    15917346.890
44.3
 NxN Ewald Elec. + LJ [V&F]            2460.740128      263299.194
0.7
 NxN Ewald Elec. [F]                 215002.604848    13115158.896
36.5
 NxN Ewald Elec. [V&F]                 2193.583584      184261.021
0.5
 1,4 nonbonded interactions              63.186318        5686.769
0.0
 Calc Weights                          1318.691856       47472.907
0.1
 Spread Q Bspline                     56264.185856      112528.372
0.3
 Gather F Bspline                     56264.185856      337585.115
0.9
 3D-FFT                              699184.311440     5593474.492
15.6
 Solve PME                             553.015296       35392.979
0.1
 Reset In Box                            5.450048          16.350
0.0
 CG-CoM                                  5.581904          16.746
0.0
 Bonds                                  10.603181         625.588
0.0
 Angles                                 37.838025        6356.788
0.0
 Propers                                57.785778       13232.943
0.0
 Impropers                               4.236786         881.251
0.0
 Virial                                 44.806762         806.522
0.0
 Update                                439.563952       13626.483
0.0
 Stop-CM                                 4.483104          44.831
0.0
 Calc-Ekin                              87.991904        2375.781
0.0
 Lincs                                  22.792978        1367.579
0.0
 Lincs-Mat                             126.199512         504.798
0.0
 Constraint-V                          972.795931        8755.163
0.0
 Constraint-Vir                         47.540661        1140.976
0.0
 Settle                                309.086186      114361.889
0.3
-----------------------------------------------------------------------
----
```

```
 Total                                                 35912739.227
100.0
-------------------------------------------------------------------------
----


   D O M A I N   D E C O M P O S I T I O N   S T A T I S T I C S

 av. #atoms communicated per step for force:  2 x 104546.3
 av. #atoms communicated per step for LINCS:  2 x 4862.9


Dynamic load balancing report:
 DLB was off during the run due to low measured imbalance.
 Average load imbalance: 19.1%.
 The balanceable part of the MD step is 22%, load imbalance is computed
from this.
 Part of the total run time spent waiting due to load imbalance: 4.2%.


     R E A L   C Y C L E   A N D   T I M E   A C C O U N T I N G

On 18 MPI ranks

 Activity:              Num   Num      Call    Wall time         Giga-
Cycles
                       Ranks Threads  Count      (s)         total sum
%
-------------------------------------------------------------------------
-------
 Domain decomp.           18    1        126       0.377         19.986
0.4
 DD comm. load            18    1         89       0.001          0.051
0.0
 DD comm. bounds          18    1         78       0.010          0.522
0.0
 Neighbor search          18    1        126       0.821         43.489
0.8
 Comm. coord.             18    1       9875       2.107        111.665
2.0
 Force                    18    1      10001      20.667       1095.357
19.4
 Wait + Comm. F           18    1      10001       2.040        108.124
1.9
 PME mesh                 18    1      10001      75.619       4007.755
71.0
 NB X/F buffer ops.       18    1      29751       0.307         16.247
0.3
 Write traj.              18    1          1       0.006          0.302
0.0
 Update                   18    1      20002       0.635         33.640
0.6
 Constraints              18    1      20004       3.623        192.034
3.4
 Comm. energies           18    1       1001       0.147          7.776
0.1
 Rest                                               0.131          6.943
0.1
```

```
-----------------------------------------------------------------------------
-------
 Total                                                106.490       5643.892
100.0
-----------------------------------------------------------------------------
-------
 Breakdown of PME mesh activities
-----------------------------------------------------------------------------
-------
 PME redist. X/F          18    1      30003      13.927        738.110
13.1
 PME spread               18    1      20002       6.073        321.871
5.7
 PME gather               18    1      20002       4.739        251.162
4.5
 PME 3D-FFT               18    1      40004       8.195        434.353
7.7
 PME 3D-FFT Comm.         18    1      80008      41.825       2216.708
39.3
 PME solve Elec           18    1      20002       0.839         44.452
0.8
-----------------------------------------------------------------------------
-------

               Core t (s)   Wall t (s)        (%)
       Time:     1916.798      106.490     1800.0
                 (ns/day)    (hour/ns)
Performance:       16.228        1.479
Finished mdrun on rank 0 Fri Jan 12 10:04:52 2024
```

benchBFC_cpu-cluster_10n

```
                :-) GROMACS - gmx mdrun, 2023.3 (-:

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                    Coordinated by the GROMACS project leaders:
                      Paul Bauer, Berk Hess, and Erik Lindahl

GROMACS:      gmx mdrun, version 2023.3
Executable:   /usr/local/gromacs/bin/gmx_mpi
Data prefix:  /usr/local/gromacs
Working dir:  /home/ubuntu
Process ID:   8799
Command line:
  gmx_mpi mdrun -v -s /mnt/shared/home/ubuntu/mpinat-gromacs/mpinat-
gromacs-free-energy-bench/benchBFC.tpr

GROMACS version:    2023.3
Precision:          mixed
Memory model:       64 bit
MPI library:        MPI
OpenMP support:     enabled (GMX_OPENMP_MAX_THREADS = 128)
GPU support:        disabled
SIMD instructions:  AVX2_256
```

```
CPU FFT library:    fftw-3.3.8-sse2-avx-avx2-avx2_128
GPU FFT library:    none
Multi-GPU FFT:      none
RDTSCP usage:       enabled
TNG support:        enabled
Hwloc support:      disabled
Tracing support:    disabled
C compiler:         /usr/bin/cc GNU 11.4.0
C compiler flags:   -fexcess-precision=fast -funroll-all-loops -mavx2 -
mfma -Wno-missing-field-initializers -O3 -DNDEBUG
C++ compiler:       /usr/bin/c++ GNU 11.4.0
C++ compiler flags: -fexcess-precision=fast -funroll-all-loops -mavx2 -
mfma -Wno-missing-field-initializers -Wno-cast-function-type-strict -
fopenmp -O3 -DNDEBUG
BLAS library:       Internal
LAPACK library:     Internal


Running on 10 nodes with total 60 cores, 60 processing units
  Cores per node:            6
  Logical processing units per node:    6
  OS CPU Limit / recommended threads to start per node:    6
Hardware detected on host cpu-1 (the node of MPI rank 0):
  CPU info:
    Vendor: AMD
    Brand:  AMD EPYC-Milan Processor
    Family: 25   Model: 1   Stepping: 1
    Features: aes amd apic avx avx2 clfsh cmov cx8 cx16 f16c fma lahf
misalignsse mmx msr pcid pclmuldq pdpe1gb popcnt pse rdrnd rdtscp sha
sse2 sse3 sse4a sse4.1 sse4.2 ssse3 tdt x2apic
  Hardware topology: Basic
    Packages, cores, and logical processors:
    [indices refer to OS logical processors]
      Package  0: [   0]
      Package  1: [   1]
      Package  2: [   2]
      Package  3: [   3]
      Package  4: [   4]
      Package  5: [   5]
    CPU limit set by OS: -1   Recommended max number of threads: 6


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
M. J. Abraham, T. Murtola, R. Schulz, S. P√°ll, J. C. Smith, B. Hess, E.
Lindahl
GROMACS: High performance molecular simulations through multi-level
parallelism from laptops to supercomputers
SoftwareX 1 (2015) pp. 19-25
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. P√°ll, M. J. Abraham, C. Kutzner, B. Hess, E. Lindahl
Tackling Exascale Software Challenges in Molecular Dynamics Simulations
with
GROMACS
In S. Markidis & E. Laure (Eds.), Solving Software Challenges for
Exascale 8759 (2015) pp. 3-27
```

```
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. Pronk, S. P√°ll, R. Schulz, P. Larsson, P. Bjelkmar, R. Apostolov, M.
R.
Shirts, J. C. Smith, P. M. Kasson, D. van der Spoel, B. Hess, and E.
Lindahl
GROMACS 4.5: a high-throughput and highly parallel open source molecular
simulation toolkit
Bioinformatics 29 (2013) pp. 845-54
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
B. Hess and C. Kutzner and D. van der Spoel and E. Lindahl
GROMACS 4: Algorithms for highly efficient, load-balanced, and scalable
molecular simulation
J. Chem. Theory Comput. 4 (2008) pp. 435-447
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
D. van der Spoel, E. Lindahl, B. Hess, G. Groenhof, A. E. Mark and H. J.
C.
Berendsen
GROMACS: Fast, Flexible and Free
J. Comp. Chem. 26 (2005) pp. 1701-1719
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
E. Lindahl and B. Hess and D. van der Spoel
GROMACS 3.0: A package for molecular simulation and trajectory analysis
J. Mol. Mod. 7 (2001) pp. 306-317
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
H. J. C. Berendsen, D. van der Spoel and R. van Drunen
GROMACS: A message-passing parallel molecular dynamics implementation
Comp. Phys. Comm. 91 (1995) pp. 43-56
-------- -------- --- Thank You --- -------- --------


++++ PLEASE CITE THE DOI FOR THIS VERSION OF GROMACS ++++
https://doi.org/10.5281/zenodo.10017686
-------- -------- --- Thank You --- -------- --------


The number of OpenMP threads was set by environment variable
OMP_NUM_THREADS to 1

Input Parameters:
   integrator                   = sd
   tinit                        = 0
   dt                           = 0.002
   nsteps                       = 10000
```

```
init-step                       = 0
simulation-part                 = 1
mts                             = false
comm-mode                       = Linear
nstcomm                         = 100
bd-fric                         = 0
ld-seed                         = -1287569705
emtol                           = 10
emstep                          = 0.01
niter                           = 20
fcstep                          = 0
nstcgsteep                      = 1000
nbfgscorr                       = 10
rtpi                            = 0.05
nstxout                         = 0
nstvout                         = 0
nstfout                         = 0
nstlog                          = 0
nstcalcenergy                   = 100
nstenergy                       = 0
nstxout-compressed              = 0
compressed-x-precision          = 1000
cutoff-scheme                   = Verlet
nstlist                         = 10
pbc                             = xyz
periodic-molecules              = false
verlet-buffer-tolerance         = 0.005
rlist                           = 1.2
coulombtype                     = PME
coulomb-modifier                = Potential-shift
rcoulomb-switch                 = 0
rcoulomb                        = 1.2
epsilon-r                       = 1
epsilon-rf                      = inf
vdw-type                        = Cut-off
vdw-modifier                    = Potential-shift
rvdw-switch                     = 0
rvdw                            = 1.2
DispCorr                        = EnerPres
table-extension                 = 1
fourierspacing                  = 0.1
fourier-nx                      = 96
fourier-ny                      = 96
fourier-nz                      = 96
pme-order                       = 4
ewald-rtol                      = 1e-05
ewald-rtol-lj                   = 0.001
lj-pme-comb-rule                = Geometric
ewald-geometry                  = 3d
epsilon-surface                 = 0
ensemble-temperature-setting    = constant
ensemble-temperature            = 298.15
tcoupl                          = No
nsttcouple                      = -1
nh-chain-length                 = 0
print-nose-hoover-chain-variables = false
pcoupl                          = Parrinello-Rahman
pcoupltype                      = Isotropic
```

```
   nstpcouple                     = 10
   tau-p                          = 2
   compressibility (3x3):
      compressibility[    0]={ 4.50000e-05,  0.00000e+00,  0.00000e+00}
      compressibility[    1]={ 0.00000e+00,  4.50000e-05,  0.00000e+00}
      compressibility[    2]={ 0.00000e+00,  0.00000e+00,  4.50000e-05}
   ref-p (3x3):
      ref-p[    0]={ 1.00000e+00,  0.00000e+00,  0.00000e+00}
      ref-p[    1]={ 0.00000e+00,  1.00000e+00,  0.00000e+00}
      ref-p[    2]={ 0.00000e+00,  0.00000e+00,  1.00000e+00}
   refcoord-scaling               = No
   posres-com (3):
      posres-com[0]= 0.00000e+00
      posres-com[1]= 0.00000e+00
      posres-com[2]= 0.00000e+00
   posres-comB (3):
      posres-comB[0]= 0.00000e+00
      posres-comB[1]= 0.00000e+00
      posres-comB[2]= 0.00000e+00
   QMMM                           = false
qm-opts:
   ngQM                           = 0
   constraint-algorithm           = Lincs
   continuation                   = false
   Shake-SOR                      = false
   shake-tol                      = 0.0001
   lincs-order                    = 4
   lincs-iter                     = 1
   lincs-warnangle                = 30
   nwall                          = 0
   wall-type                      = 9-3
   wall-r-linpot                  = -1
   wall-atomtype[0]               = -1
   wall-atomtype[1]               = -1
   wall-density[0]                = 0
   wall-density[1]                = 0
   wall-ewald-zfac                = 3
   pull                           = false
   awh                            = false
   rotation                       = false
   interactiveMD                  = false
   disre                          = No
   disre-weighting                = Conservative
   disre-mixed                    = false
   dr-fc                          = 1000
   dr-tau                         = 0
   nstdisreout                    = 100
   orire-fc                       = 0
   orire-tau                      = 0
   nstorireout                    = 100
   free-energy                    = yes
   init-lambda                    = -1
   init-lambda-state              = 10
   delta-lambda                   = 0
   nstdhdl                        = 100
   n-lambdas                      = 20
   separate-dvdl:
       fep-lambdas =   FALSE
```

```
      mass-lambdas =   FALSE
      coul-lambdas =   TRUE
       vdw-lambdas =   TRUE
    bonded-lambdas =   FALSE
 restraint-lambdas =   FALSE
temperature-lambdas =   FALSE
all-lambdas:
       fep-lambdas =            0           0           0           0
0           0           0           0           0           0           0
0           0           0           0           0           0           0
0           0
      mass-lambdas =            0           0           0           0
0           0           0           0           0           0           0
0           0           0           0           0           0           0
0           0
      coul-lambdas =            0        0.25         0.5        0.75
1           1           1           1           1           1           1
1           1           1           1           1           1           1
1           1
       vdw-lambdas =            0           0           0           0
0        0.05         0.1         0.2         0.3         0.4         0.5
0.6        0.65         0.7        0.75         0.8        0.85
0.9        0.95           1
    bonded-lambdas =            0           0           0           0
0           0           0           0           0           0           0
0           0           0           0           0           0           0
0           0
 restraint-lambdas =            0           0           0           0
0           0           0           0           0           0           0
0           0           0           0           0           0           0
0           0
temperature-lambdas =            0           0           0           0
0           0           0           0           0           0           0
0           0           0           0           0           0           0
0           0
   calc-lambda-neighbors         = -1
   dhdl-print-energy             = no
   sc-alpha                      = 0.5
   sc-power                      = 1
   sc-r-power                    = 6
   sc-sigma                      = 0.3
   sc-sigma-min                  = 0.3
   sc-coul                       = true
   dh-hist-size                  = 0
   dh-hist-spacing               = 0.1
   separate-dhdl-file            = yes
   dhdl-derivatives              = yes
   sc-function                   = beutler
   sc-gapsys-scale-linpoint-lj   = 0.85
   sc-gapsys-scale-linpoint-q    = 0.3
   sc-gapsys-sigma-lj            = 0.3
   cos-acceleration              = 0
   deform (3x3):
      deform[    0]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
      deform[    1]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
      deform[    2]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
   simulated-tempering           = false
   swapcoords                    = no
```

```
   userint1                       = 0
   userint2                       = 0
   userint3                       = 0
   userint4                       = 0
   userreal1                      = 0
   userreal2                      = 0
   userreal3                      = 0
   userreal4                      = 0
   applied-forces:
     electric-field:
grpopts:
   nrdf:       89026
   ref-t:      298.15
   tau-t:           1
annealing:          No
annealing-npoints:           0
   acc:               0           0           0
   nfreeze:           N           N           N
   energygrp-flags[  0]: 0

Changing nstlist from 10 to 80, rlist from 1.2 to 1.322

Update groups can not be used for this system because atoms that are
(in)directly constrained together are interdispersed with other atoms

Initializing Domain Decomposition on 60 ranks
Dynamic load balancing: auto
Minimum cell size due to atom displacement: 0.632 nm
Initial maximum distances in bonded interactions:
    two-body bonded interactions: 1.223 nm, LJC Pairs NB, atoms 2065 2079
  multi-body bonded interactions: 0.698 nm, Improper Dih., atoms 2034
1556
Minimum cell size due to bonded interactions: 0.768 nm
Maximum distance for 5 constraints, at 120 deg. angles, all-trans: 0.219
nm
Estimated maximum distance required for P-LINCS: 0.219 nm
Scaling the initial minimum size with 1/0.8 (option -dds) = 1.25
Guess for relative PME load: 0.38
Will use 36 particle-particle and 24 PME only ranks
This is a guess, check the performance at the end of the log file
Using 24 separate PME ranks, as guessed by mdrun
Optimizing the DD grid for 36 cells with a minimum initial size of 0.960
nm
The maximum allowed number of cells is: X 7 Y 7 Z 6
Domain decomposition grid 3 x 4 x 3, separate PME ranks 24
PME domain decomposition: 3 x 8 x 1
Interleaving PP and PME ranks
This rank does only particle-particle work.
Domain decomposition rank 0, coordinates 0 0 0

The initial number of communication pulses is: X 1 Y 1 Z 1
The initial domain decomposition cell size is: X 2.33 nm Y 1.74 nm Z 2.01
nm

The maximum allowed distance for atoms involved in interactions is:
                 non-bonded interactions           1.322 nm
(the following are initial values, they could change due to box
deformation)
```

```
           two-body bonded interactions  (-rdd)   1.322 nm
         multi-body bonded interactions  (-rdd)   1.322 nm
  atoms separated by up to 5 constraints  (-rcon)  1.745 nm

When dynamic load balancing gets turned on, these settings will change
to:
The maximum number of communication pulses is: X 1 Y 1 Z 1
The minimum size for domain decomposition cells is 1.322 nm
The requested allowed shrink of DD cells (option -dds) is: 0.80
The allowed shrink of domain decomposition cells is: X 0.57 Y 0.76 Z 0.66
The maximum allowed distance for atoms involved in interactions is:
                 non-bonded interactions           1.322 nm
           two-body bonded interactions  (-rdd)   1.322 nm
         multi-body bonded interactions  (-rdd)   1.322 nm
  atoms separated by up to 5 constraints  (-rcon)  1.322 nm
Using two step summing over 10 groups of on average 3.6 ranks


Using 60 MPI processes

Non-default thread affinity set, disabling internal thread affinity

Using 1 OpenMP thread per MPI process

System total charge, top. A: -0.000 top. B: 0.000
Will do PME sum in reciprocal space for electrostatic interactions.

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
U. Essmann, L. Perera, M. L. Berkowitz, T. Darden, H. Lee and L. G.
Pedersen
A smooth particle mesh Ewald method
J. Chem. Phys. 103 (1995) pp. 8577-8592
-------- -------- --- Thank You --- -------- --------

Using a Gaussian width (1/beta) of 0.384195 nm for Ewald
Potential shift: LJ r^-12: -1.122e-01 r^-6: -3.349e-01, Ewald -8.333e-06
Initialized non-bonded Coulomb Ewald tables, spacing: 1.02e-03 size: 2273

Generated table with 1161 data points for 1-4 COUL.
Tabscale = 500 points/nm
Generated table with 1161 data points for 1-4 LJ6.
Tabscale = 500 points/nm
Generated table with 1161 data points for 1-4 LJ12.
Tabscale = 500 points/nm
Long Range LJ corr.: <C6> 3.0077e-04


Using SIMD 4x8 nonbonded short-range kernels

Using a dual 4x8 pair-list setup updated with dynamic pruning:
  outer list: updated every 80 steps, buffer 0.122 nm, rlist 1.322 nm
  inner list: updated every 13 steps, buffer 0.003 nm, rlist 1.203 nm
At tolerance 0.005 kJ/mol/ps per atom, equivalent classical 1x1 list
would be:
  outer list: updated every 80 steps, buffer 0.266 nm, rlist 1.466 nm
  inner list: updated every 13 steps, buffer 0.052 nm, rlist 1.252 nm
```

```
The non-bonded pair calculation algorithm tolerates a few missing pair
interactions close to the cut-off. This can lead to a systematic
overestimation of the pressure due to missing LJ interactions. The error
in the average pressure due to missing LJ interactions is at most 0.26
bar.
The pressure error can be controlled by setting the environment variable
GMX_VERLET_BUFFER_PRESSURE_TOLERANCE to the allowed error in units of
bar.

Using Lorentz-Berthelot Lennard-Jones combination rule
There are 48 atoms and 48 charges for free energy perturbation
Removing pbc first time

Linking all bonded interactions to atoms


Initializing Parallel LINear Constraint Solver

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
B. Hess
P-LINCS: A Parallel Linear Constraint Solver for molecular simulation
J. Chem. Theory Comput. 4 (2008) pp. 116-122
-------- -------- --- Thank You --- -------- --------

The number of constraints is 1037
There are constraints between atoms in different decomposition domains,
will communicate selected coordinates each lincs iteration

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. Miyamoto and P. A. Kollman
SETTLE: An Analytical Version of the SHAKE and RATTLE Algorithms for
Rigid
Water Models
J. Comp. Chem. 13 (1992) pp. 952-962
-------- -------- --- Thank You --- -------- --------


Intra-simulation communication will occur every 10 steps.
Initial vector of lambda components:[     0.0000     0.0000     1.0000
0.5000     0.0000     0.0000     0.0000 ]

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
N. Goga and A. J. Rzepiela and A. H. de Vries and S. J. Marrink and H. J.
C.
Berendsen
Efficient Algorithms for Langevin and DPD Dynamics
J. Chem. Theory Comput. 8 (2012) pp. 3637--3649
-------- -------- --- Thank You --- -------- --------

There are: 43952 Atoms
Atom distribution over 36 domains: av 1220 stddev 52 min 1185 max 1310

Constraining the starting coordinates (step 0)

Constraining the coordinates at t0-dt (step 0)
Center of mass motion removal mode is Linear
We have the following groups for center of mass motion removal:
  0:  rest
```

```
RMS relative constraint deviation after constraining: 2.97e-06
Initial temperature: 297.767 K

Started mdrun on rank 0 Fri Jan 12 09:30:05 2024

           Step           Time
              0        0.00000

   Energies (kJ/mol)
           Bond  Harmonic Pot.          Angle    Proper Dih.  Improper
Dih.
    1.74496e+03    0.00000e+00    4.45122e+03    5.17096e+03
0.00000e+00
 Per. Imp. Dih.          LJ-14     Coulomb-14        LJ (SR)  Disper.
corr.
    2.79362e+02    2.02835e+03    1.20239e+04    8.34149e+04   -
3.18065e+03
   Coulomb (SR)   Coul. recip.      Potential    Kinetic En.   Total
Energy
   -7.21773e+05    2.18054e+03   -6.13660e+05    1.10125e+05   -
5.03535e+05
    Temperature Pres. DC (bar) Pressure (bar)      dVcoul/dl
dVvdw/dl
    2.97553e+02   -1.19688e+02   -8.81549e+01    2.54638e+01
2.47544e+02
   Constr. rmsd
    3.01526e-06


DD  step 79 load imb.: force 79.6%  pme mesh/force 2.432
step  640: timed with pme grid 96 96 96, coulomb cutoff 1.200: 1872.6 M-
cycles
step  800: timed with pme grid 80 80 80, coulomb cutoff 1.282: 2076.4 M-
cycles
step  960: timed with pme grid 72 72 72, coulomb cutoff 1.425: 1662.3 M-
cycles
step 1120: timed with pme grid 64 64 64, coulomb cutoff 1.603: 1039.5 M-
cycles
step 1120: the domain decomposition limits the PME load balancing to a
coulomb cut-off of 1.603
step 1280: timed with pme grid 64 64 64, coulomb cutoff 1.603: 1411.7 M-
cycles
             optimal pme grid 64 64 64, coulomb cutoff 1.603

DD  step 9999 load imb.: force 55.6%  pme mesh/force 1.225
           Step           Time
          10000       20.00000

Writing checkpoint, step 10000 at Fri Jan 12 09:31:32 2024


   Energies (kJ/mol)
           Bond  Harmonic Pot.          Angle    Proper Dih.  Improper
Dih.
    1.53368e+03    0.00000e+00    4.40259e+03    5.10209e+03
0.00000e+00
 Per. Imp. Dih.          LJ-14     Coulomb-14        LJ (SR)  Disper.
corr.
```

```
    2.41460e+02    2.03033e+03    1.19017e+04    8.37755e+04   -
3.17924e+03
   Coulomb (SR)   Coul. recip.      Potential    Kinetic En.   Total
Energy
   -7.20440e+05    8.45330e+02   -6.13786e+05    1.10933e+05   -
5.02853e+05
    Temperature Pres. DC (bar) Pressure (bar)      dVcoul/dl
dVvdw/dl
    2.99738e+02   -1.19582e+02    1.01001e+02    3.14836e+01   -
8.61920e+00
   Constr. rmsd
    3.32001e-06


      <======  ###############  ==>
      <====  A V E R A G E S  ====>
      <==  ###############  ======>

      Statistics over 10001 steps using 101 frames

   Energies (kJ/mol)
          Bond  Harmonic Pot.          Angle    Proper Dih.  Improper
Dih.
    1.62926e+03    0.00000e+00    4.42349e+03    5.14648e+03
0.00000e+00
 Per. Imp. Dih.          LJ-14     Coulomb-14        LJ (SR)  Disper.
corr.
    2.80637e+02    2.01998e+03    1.20176e+04    8.38276e+04   -
3.18085e+03
   Coulomb (SR)   Coul. recip.      Potential    Kinetic En.   Total
Energy
   -7.21381e+05    9.58329e+02   -6.14259e+05    1.10524e+05   -
5.03735e+05
    Temperature Pres. DC (bar) Pressure (bar)      dVcoul/dl
dVvdw/dl
    2.98630e+02   -1.19703e+02   -2.59812e+00    2.04624e+01
1.21399e+02
   Constr. rmsd
    0.00000e+00

          Box-X          Box-Y          Box-Z
    8.54741e+00    8.54741e+00    6.04394e+00

   Total Virial (kJ/mol)
    3.69762e+04   -7.91773e+01    1.94534e+02
   -7.98641e+01    3.68371e+04   -3.14901e+01
    1.94600e+02   -3.10624e+01    3.68170e+04

   Pressure (bar)
   -9.41428e+00    3.81931e+00   -1.56148e+01
    3.87099e+00    3.38478e+00    1.97721e+00
   -1.56198e+01    1.94502e+00   -1.76486e+00


       P P   -   P M E   L O A D   B A L A N C I N G

 NOTE: The PP/PME load balancing was limited by the domain decomposition,
       you might not have reached a good load balance.
```

```
       Try different mdrun -dd settings or lower the -dds value.

 PP/PME load balancing changed the cut-off and PME settings:
           particle-particle                    PME
            rcoulomb  rlist            grid      spacing   1/beta
   initial  1.200 nm  1.203 nm      96  96  96   0.089 nm  0.384 nm
   final    1.603 nm  1.606 nm      64  64  64   0.134 nm  0.513 nm
 cost-ratio           2.38             0.30
 (note that these numbers concern only part of the total PP and PME load)

NOTE: PME load balancing increased the non-bonded workload by more than
50%.
      For better performance, use (more) PME ranks (mdrun -npme),
      or if you are beyond the scaling limit, use fewer total ranks (or
nodes).

     M E G A - F L O P S   A C C O U N T I N G

 NB=Group-cutoff nonbonded kernels    NxN=N-by-N cluster Verlet kernels
 RF=Reaction-Field  VdW=Van der Waals  QSTab=quadratic-spline table
 W3=SPC/TIP3p  W4=TIP4p (single or pairs)
 V&F=Potential and force  V=Potential only  F=Force only

 Computing:                                M-Number         M-Flops  %
Flops
-----------------------------------------------------------------------
----
 NB Free energy kernel              212165.695032      212165.695
0.4
 Pair Search distance check           5855.013098       52695.118
0.1
 NxN Ewald Elec. + LJ [F]           458389.846192    30253729.849
51.4
 NxN Ewald Elec. + LJ [V&F]           4671.291488      499828.189
0.8
 NxN Ewald Elec. [F]                408959.943312    24946556.542
42.4
 NxN Ewald Elec. [V&F]                4167.476512      350068.027
0.6
 1,4 nonbonded interactions             63.186318        5686.769
0.0
 Calc Weights                         1318.691856       47472.907
0.1
 Spread Q Bspline                    56264.185856      112528.372
0.2
 Gather F Bspline                    56264.185856      337585.115
0.6
 3D-FFT                             226022.781568     1808182.253
3.1
 Solve PME                            716.537856       45858.423
0.1
 Reset In Box                           5.537952          16.614
0.0
 CG-CoM                                 5.581904          16.746
0.0
 Bonds                                 10.603181         625.588
0.0
```

```
 Angles                                   37.838025        6356.788
0.0
 Propers                                  57.785778       13232.943
0.0
 Impropers                                 4.236786         881.251
0.0
 Virial                                   45.617572         821.116
0.0
 Update                                  439.563952       13626.483
0.0
 Stop-CM                                   4.483104          44.831
0.0
 Calc-Ekin                                87.991904        2375.781
0.0
 Lincs                                    23.909890        1434.593
0.0
 Lincs-Mat                               136.214520         544.858
0.0
 Constraint-V                            988.551022        8896.959
0.0
 Constraint-Vir                           48.273048        1158.553
0.0
 Settle                                  313.593556      116029.616
0.2
-----------------------------------------------------------------------
----
 Total                                                 58838419.978
100.0
-----------------------------------------------------------------------
----


    D O M A I N   D E C O M P O S I T I O N   S T A T I S T I C S

 av. #atoms communicated per step for force:  2 x 193089.7
 av. #atoms communicated per step for LINCS:  2 x 5615.8


Dynamic load balancing report:
 DLB was off during the run due to low measured imbalance.
 Average load imbalance: 84.8%.
 The balanceable part of the MD step is 38%, load imbalance is computed
from this.
 Part of the total run time spent waiting due to load imbalance: 32.1%.
 Average PME mesh/force load: 1.190
 Part of the total run time spent waiting due to PP/PME imbalance: 8.1 %

NOTE: 32.1 % of the available CPU time was lost due to load imbalance
      in the domain decomposition.
      Dynamic load balancing was automatically disabled, but it might be
beneficial to manually turn it on (option -dlb yes.)
      You can also consider manually changing the decomposition (option -
dd);
      e.g. by using fewer domains along the box dimension in which there
is
      considerable inhomogeneity in the simulated system.
NOTE: 8.1 % performance was lost because the PME ranks
      had more work to do than the PP ranks.
```

```
      You might want to increase the number of PME ranks
      or increase the cut-off and the grid spacing.


      R E A L   C Y C L E   A N D   T I M E   A C C O U N T I N G

On 36 MPI ranks doing PP, and
on 24 MPI ranks doing PME

 Activity:              Num   Num      Call    Wall time         Giga-
Cycles
                       Ranks Threads  Count      (s)         total sum
%
-----------------------------------------------------------------------
-------
 Domain decomp.           36    1        126       2.648        280.631
1.8
 DD comm. load            36    1         25       0.001          0.103
0.0
 Send X to PME            36    1      10001       0.175         18.510
0.1
 Neighbor search          36    1        126       0.713         75.592
0.5
 Comm. coord.             36    1       9875       4.722        500.444
3.3
 Force                    36    1      10001      24.715       2619.622
17.2
 Wait + Comm. F           36    1      10001      20.315       2153.202
14.1
 PME mesh *               24    1      10001      67.836       4793.386
31.5
 PME wait for PP *                             18.394       1299.718
8.5
 Wait + Recv. PME F       36    1      10001      21.843       2315.188
15.2
 NB X/F buffer ops.       36    1      29751       0.318         33.736
0.2
 Write traj.              36    1          1       0.019          1.967
0.0
 Update                   36    1      20002       0.431         45.641
0.3
 Constraints              36    1      20004      10.236       1084.978
7.1
 Comm. energies           36    1       1001       0.243         25.767
0.2
-----------------------------------------------------------------------
-------
 Total                                           86.232      15233.117
100.0
-----------------------------------------------------------------------
-------
(*) Note that with separate PME ranks, the walltime column actually sums
to
    twice the total reported, but the cycle count total and % are
correct.
-----------------------------------------------------------------------
-------
 Breakdown of PME mesh activities
```

```
-----------------------------------------------------------------------------
-------
 PME redist. X/F          24    1      30003      22.053       1558.279
10.2
 PME spread               24    1      20002       6.558        463.377
3.0
 PME gather               24    1      20002       5.545        391.809
2.6
 PME 3D-FFT               24    1      40004       2.644        186.856
1.2
 PME 3D-FFT Comm.         24    1      80008      30.730       2171.439
14.3
 PME solve Elec           24    1      20002       0.283         19.967
0.1
-----------------------------------------------------------------------------
-------

               Core t (s)   Wall t (s)        (%)
       Time:     5173.522       86.232     5999.5
                 (ns/day)    (hour/ns)
Performance:       20.041        1.198
Finished mdrun on rank 0 Fri Jan 12 09:31:32 2024
```

benchBFC_cpu-sev-cluster_1n

```
                :-) GROMACS - gmx mdrun, 2023.3 (-:

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                    Coordinated by the GROMACS project leaders:
                      Paul Bauer, Berk Hess, and Erik Lindahl

GROMACS:      gmx mdrun, version 2023.3
Executable:   /usr/local/gromacs/bin/gmx_mpi
Data prefix:  /usr/local/gromacs
Working dir:  /home/ubuntu
Process ID:   6834
Command line:
  gmx_mpi mdrun -v -s /mnt/shared/home/ubuntu/mpinat-gromacs/mpinat-
gromacs-free-energy-bench/benchBFC.tpr

GROMACS version:    2023.3
Precision:          mixed
Memory model:       64 bit
MPI library:        MPI
OpenMP support:     enabled (GMX_OPENMP_MAX_THREADS = 128)
GPU support:        disabled
SIMD instructions:  AVX2_256
```

```
CPU FFT library:    fftw-3.3.8-sse2-avx-avx2-avx2_128
GPU FFT library:    none
Multi-GPU FFT:      none
RDTSCP usage:       enabled
TNG support:        enabled
Hwloc support:      disabled
Tracing support:    disabled
C compiler:         /usr/bin/cc GNU 11.4.0
C compiler flags:   -fexcess-precision=fast -funroll-all-loops -mavx2 -
mfma -Wno-missing-field-initializers -O3 -DNDEBUG
C++ compiler:       /usr/bin/c++ GNU 11.4.0
C++ compiler flags: -fexcess-precision=fast -funroll-all-loops -mavx2 -
mfma -Wno-missing-field-initializers -Wno-cast-function-type-strict -
fopenmp -O3 -DNDEBUG
BLAS library:       Internal
LAPACK library:     Internal


Running on 1 node with total 6 cores, 6 processing units
Hardware detected on host cpu-sev-5 (the node of MPI rank 0):
  CPU info:
    Vendor: AMD
    Brand:  AMD EPYC-Milan Processor
    Family: 25   Model: 1   Stepping: 1
    Features: aes amd apic avx avx2 clfsh cmov cx8 cx16 f16c fma lahf
misalignsse mmx msr pcid pclmuldq pdpe1gb popcnt pse rdrnd rdtscp sha
sse2 sse3 sse4a sse4.1 sse4.2 ssse3 tdt x2apic
  Hardware topology: Basic
    Packages, cores, and logical processors:
    [indices refer to OS logical processors]
      Package  0: [   0]
      Package  1: [   1]
      Package  2: [   2]
      Package  3: [   3]
      Package  4: [   4]
      Package  5: [   5]
    CPU limit set by OS: -1   Recommended max number of threads: 6


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
M. J. Abraham, T. Murtola, R. Schulz, S. P√°ll, J. C. Smith, B. Hess, E.
Lindahl
GROMACS: High performance molecular simulations through multi-level
parallelism from laptops to supercomputers
SoftwareX 1 (2015) pp. 19-25
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. P√°ll, M. J. Abraham, C. Kutzner, B. Hess, E. Lindahl
Tackling Exascale Software Challenges in Molecular Dynamics Simulations
with
GROMACS
In S. Markidis & E. Laure (Eds.), Solving Software Challenges for
Exascale 8759 (2015) pp. 3-27
-------- -------- --- Thank You --- -------- --------
```

```
++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. Pronk, S. P√°ll, R. Schulz, P. Larsson, P. Bjelkmar, R. Apostolov, M.
R.
Shirts, J. C. Smith, P. M. Kasson, D. van der Spoel, B. Hess, and E.
Lindahl
GROMACS 4.5: a high-throughput and highly parallel open source molecular
simulation toolkit
Bioinformatics 29 (2013) pp. 845-54
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
B. Hess and C. Kutzner and D. van der Spoel and E. Lindahl
GROMACS 4: Algorithms for highly efficient, load-balanced, and scalable
molecular simulation
J. Chem. Theory Comput. 4 (2008) pp. 435-447
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
D. van der Spoel, E. Lindahl, B. Hess, G. Groenhof, A. E. Mark and H. J.
C.
Berendsen
GROMACS: Fast, Flexible and Free
J. Comp. Chem. 26 (2005) pp. 1701-1719
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
E. Lindahl and B. Hess and D. van der Spoel
GROMACS 3.0: A package for molecular simulation and trajectory analysis
J. Mol. Mod. 7 (2001) pp. 306-317
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
H. J. C. Berendsen, D. van der Spoel and R. van Drunen
GROMACS: A message-passing parallel molecular dynamics implementation
Comp. Phys. Comm. 91 (1995) pp. 43-56
-------- -------- --- Thank You --- -------- --------


++++ PLEASE CITE THE DOI FOR THIS VERSION OF GROMACS ++++
https://doi.org/10.5281/zenodo.10017686
-------- -------- --- Thank You --- -------- --------


The number of OpenMP threads was set by environment variable
OMP_NUM_THREADS to 1

Input Parameters:
   integrator                     = sd
   tinit                          = 0
   dt                             = 0.002
   nsteps                         = 10000
   init-step                      = 0
   simulation-part                = 1
   mts                            = false
```

```
comm-mode                      = Linear
nstcomm                        = 100
bd-fric                        = 0
ld-seed                        = -1287569705
emtol                          = 10
emstep                         = 0.01
niter                          = 20
fcstep                         = 0
nstcgsteep                     = 1000
nbfgscorr                      = 10
rtpi                           = 0.05
nstxout                        = 0
nstvout                        = 0
nstfout                        = 0
nstlog                         = 0
nstcalcenergy                  = 100
nstenergy                      = 0
nstxout-compressed             = 0
compressed-x-precision         = 1000
cutoff-scheme                  = Verlet
nstlist                        = 10
pbc                            = xyz
periodic-molecules             = false
verlet-buffer-tolerance        = 0.005
rlist                          = 1.2
coulombtype                    = PME
coulomb-modifier               = Potential-shift
rcoulomb-switch                = 0
rcoulomb                       = 1.2
epsilon-r                      = 1
epsilon-rf                     = inf
vdw-type                       = Cut-off
vdw-modifier                   = Potential-shift
rvdw-switch                    = 0
rvdw                           = 1.2
DispCorr                       = EnerPres
table-extension                = 1
fourierspacing                 = 0.1
fourier-nx                     = 96
fourier-ny                     = 96
fourier-nz                     = 96
pme-order                      = 4
ewald-rtol                     = 1e-05
ewald-rtol-lj                  = 0.001
lj-pme-comb-rule               = Geometric
ewald-geometry                 = 3d
epsilon-surface                = 0
ensemble-temperature-setting   = constant
ensemble-temperature           = 298.15
tcoupl                         = No
nsttcouple                     = -1
nh-chain-length                = 0
print-nose-hoover-chain-variables = false
pcoupl                         = Parrinello-Rahman
pcoupltype                     = Isotropic
nstpcouple                     = 10
tau-p                          = 2
compressibility (3x3):
```

```
      compressibility[    0]={ 4.50000e-05,  0.00000e+00,  0.00000e+00}
      compressibility[    1]={ 0.00000e+00,  4.50000e-05,  0.00000e+00}
      compressibility[    2]={ 0.00000e+00,  0.00000e+00,  4.50000e-05}
   ref-p (3x3):
      ref-p[    0]={ 1.00000e+00,  0.00000e+00,  0.00000e+00}
      ref-p[    1]={ 0.00000e+00,  1.00000e+00,  0.00000e+00}
      ref-p[    2]={ 0.00000e+00,  0.00000e+00,  1.00000e+00}
   refcoord-scaling               = No
   posres-com (3):
      posres-com[0]= 0.00000e+00
      posres-com[1]= 0.00000e+00
      posres-com[2]= 0.00000e+00
   posres-comB (3):
      posres-comB[0]= 0.00000e+00
      posres-comB[1]= 0.00000e+00
      posres-comB[2]= 0.00000e+00
   QMMM                           = false
qm-opts:
   ngQM                           = 0
   constraint-algorithm           = Lincs
   continuation                   = false
   Shake-SOR                      = false
   shake-tol                      = 0.0001
   lincs-order                    = 4
   lincs-iter                     = 1
   lincs-warnangle                = 30
   nwall                          = 0
   wall-type                      = 9-3
   wall-r-linpot                  = -1
   wall-atomtype[0]               = -1
   wall-atomtype[1]               = -1
   wall-density[0]                = 0
   wall-density[1]                = 0
   wall-ewald-zfac                = 3
   pull                           = false
   awh                            = false
   rotation                       = false
   interactiveMD                  = false
   disre                          = No
   disre-weighting                = Conservative
   disre-mixed                    = false
   dr-fc                          = 1000
   dr-tau                         = 0
   nstdisreout                    = 100
   orire-fc                       = 0
   orire-tau                      = 0
   nstorireout                    = 100
   free-energy                    = yes
   init-lambda                    = -1
   init-lambda-state              = 10
   delta-lambda                   = 0
   nstdhdl                        = 100
   n-lambdas                      = 20
   separate-dvdl:
       fep-lambdas =   FALSE
      mass-lambdas =   FALSE
      coul-lambdas =   TRUE
       vdw-lambdas =   TRUE
```

```
    bonded-lambdas =   FALSE
 restraint-lambdas =   FALSE
temperature-lambdas =   FALSE
all-lambdas:
       fep-lambdas =            0           0           0           0
0           0           0           0           0           0           0
0           0           0           0           0           0           0
0           0
      mass-lambdas =            0           0           0           0
0           0           0           0           0           0           0
0           0           0           0           0           0           0
0           0
      coul-lambdas =            0        0.25         0.5        0.75
1           1           1           1           1           1           1
1           1           1           1           1           1           1
1           1
       vdw-lambdas =            0           0           0           0
0        0.05         0.1         0.2         0.3         0.4         0.5
0.6        0.65         0.7        0.75         0.8        0.85
0.9        0.95           1
    bonded-lambdas =            0           0           0           0
0           0           0           0           0           0           0
0           0           0           0           0           0           0
0           0
 restraint-lambdas =            0           0           0           0
0           0           0           0           0           0           0
0           0           0           0           0           0           0
0           0
temperature-lambdas =           0           0           0           0
0           0           0           0           0           0           0
0           0           0           0           0           0           0
0           0
   calc-lambda-neighbors         = -1
   dhdl-print-energy             = no
   sc-alpha                      = 0.5
   sc-power                      = 1
   sc-r-power                    = 6
   sc-sigma                      = 0.3
   sc-sigma-min                  = 0.3
   sc-coul                       = true
   dh-hist-size                  = 0
   dh-hist-spacing               = 0.1
   separate-dhdl-file            = yes
   dhdl-derivatives              = yes
   sc-function                   = beutler
   sc-gapsys-scale-linpoint-lj   = 0.85
   sc-gapsys-scale-linpoint-q    = 0.3
   sc-gapsys-sigma-lj            = 0.3
   cos-acceleration              = 0
   deform (3x3):
      deform[    0]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
      deform[    1]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
      deform[    2]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
   simulated-tempering           = false
   swapcoords                    = no
   userint1                      = 0
   userint2                      = 0
   userint3                      = 0
```

```
   userint4                       = 0
   userreal1                      = 0
   userreal2                      = 0
   userreal3                      = 0
   userreal4                      = 0
   applied-forces:
     electric-field:
grpopts:
   nrdf:       89026
   ref-t:      298.15
   tau-t:           1
annealing:          No
annealing-npoints:           0
   acc:               0           0           0
   nfreeze:           N           N           N
   energygrp-flags[  0]: 0

Changing nstlist from 10 to 80, rlist from 1.2 to 1.322

Update groups can not be used for this system because atoms that are
(in)directly constrained together are interdispersed with other atoms

Initializing Domain Decomposition on 6 ranks
Dynamic load balancing: auto
Minimum cell size due to atom displacement: 0.632 nm
Initial maximum distances in bonded interactions:
    two-body bonded interactions: 1.223 nm, LJC Pairs NB, atoms 2065 2079
  multi-body bonded interactions: 0.698 nm, Improper Dih., atoms 2034
1556
Minimum cell size due to bonded interactions: 0.768 nm
Maximum distance for 5 constraints, at 120 deg. angles, all-trans: 0.219
nm
Estimated maximum distance required for P-LINCS: 0.219 nm
Scaling the initial minimum size with 1/0.8 (option -dds) = 1.25
Using 0 separate PME ranks because: there are too few total ranks for
efficient splitting
Optimizing the DD grid for 6 cells with a minimum initial size of 0.960
nm
The maximum allowed number of cells is: X 7 Y 7 Z 6
Domain decomposition grid 6 x 1 x 1, separate PME ranks 0
PME domain decomposition: 6 x 1 x 1
Domain decomposition rank 0, coordinates 0 0 0

The initial number of communication pulses is: X 2
The initial domain decomposition cell size is: X 1.16 nm

The maximum allowed distance for atoms involved in interactions is:
                 non-bonded interactions           1.322 nm
(the following are initial values, they could change due to box
deformation)
            two-body bonded interactions  (-rdd)   1.322 nm
          multi-body bonded interactions  (-rdd)   1.163 nm
  atoms separated by up to 5 constraints  (-rcon)  1.163 nm

When dynamic load balancing gets turned on, these settings will change
to:
The maximum number of communication pulses is: X 2
The minimum size for domain decomposition cells is 0.931 nm
```

```
The requested allowed shrink of DD cells (option -dds) is: 0.80
The allowed shrink of domain decomposition cells is: X 0.80
The maximum allowed distance for atoms involved in interactions is:
                 non-bonded interactions           1.322 nm
            two-body bonded interactions  (-rdd)   1.322 nm
          multi-body bonded interactions  (-rdd)   0.931 nm
  atoms separated by up to 5 constraints  (-rcon)  0.931 nm

Using 6 MPI processes

Non-default thread affinity set, disabling internal thread affinity

Using 1 OpenMP thread per MPI process

System total charge, top. A: -0.000 top. B: 0.000
Will do PME sum in reciprocal space for electrostatic interactions.

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
U. Essmann, L. Perera, M. L. Berkowitz, T. Darden, H. Lee and L. G.
Pedersen
A smooth particle mesh Ewald method
J. Chem. Phys. 103 (1995) pp. 8577-8592
-------- -------- --- Thank You --- -------- --------

Using a Gaussian width (1/beta) of 0.384195 nm for Ewald
Potential shift: LJ r^-12: -1.122e-01 r^-6: -3.349e-01, Ewald -8.333e-06
Initialized non-bonded Coulomb Ewald tables, spacing: 1.02e-03 size: 2273

Generated table with 1161 data points for 1-4 COUL.
Tabscale = 500 points/nm
Generated table with 1161 data points for 1-4 LJ6.
Tabscale = 500 points/nm
Generated table with 1161 data points for 1-4 LJ12.
Tabscale = 500 points/nm
Long Range LJ corr.: <C6> 3.0077e-04


Using SIMD 4x8 nonbonded short-range kernels

Using a dual 4x8 pair-list setup updated with dynamic pruning:
  outer list: updated every 80 steps, buffer 0.122 nm, rlist 1.322 nm
  inner list: updated every 13 steps, buffer 0.003 nm, rlist 1.203 nm
At tolerance 0.005 kJ/mol/ps per atom, equivalent classical 1x1 list
would be:
  outer list: updated every 80 steps, buffer 0.266 nm, rlist 1.466 nm
  inner list: updated every 13 steps, buffer 0.052 nm, rlist 1.252 nm

The non-bonded pair calculation algorithm tolerates a few missing pair
interactions close to the cut-off. This can lead to a systematic
overestimation of the pressure due to missing LJ interactions. The error
in the average pressure due to missing LJ interactions is at most 0.26
bar.
The pressure error can be controlled by setting the environment variable
GMX_VERLET_BUFFER_PRESSURE_TOLERANCE to the allowed error in units of
bar.

Using Lorentz-Berthelot Lennard-Jones combination rule
There are 48 atoms and 48 charges for free energy perturbation
```

```
Removing pbc first time

Linking all bonded interactions to atoms


Initializing Parallel LINear Constraint Solver

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
B. Hess
P-LINCS: A Parallel Linear Constraint Solver for molecular simulation
J. Chem. Theory Comput. 4 (2008) pp. 116-122
-------- -------- --- Thank You --- -------- --------

The number of constraints is 1037
There are constraints between atoms in different decomposition domains,
will communicate selected coordinates each lincs iteration

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. Miyamoto and P. A. Kollman
SETTLE: An Analytical Version of the SHAKE and RATTLE Algorithms for
Rigid
Water Models
J. Comp. Chem. 13 (1992) pp. 952-962
-------- -------- --- Thank You --- -------- --------


Intra-simulation communication will occur every 10 steps.
Initial vector of lambda components:[     0.0000     0.0000     1.0000
0.5000     0.0000     0.0000     0.0000 ]

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
N. Goga and A. J. Rzepiela and A. H. de Vries and S. J. Marrink and H. J.
C.
Berendsen
Efficient Algorithms for Langevin and DPD Dynamics
J. Chem. Theory Comput. 8 (2012) pp. 3637--3649
-------- -------- --- Thank You --- -------- --------

There are: 43952 Atoms
Atom distribution over 6 domains: av 7325 stddev 93 min 7261 max 7447

Constraining the starting coordinates (step 0)

Constraining the coordinates at t0-dt (step 0)
Center of mass motion removal mode is Linear
We have the following groups for center of mass motion removal:
  0:  rest
RMS relative constraint deviation after constraining: 2.99e-06
Initial temperature: 297.767 K

Started mdrun on rank 0 Fri Jan 12 23:50:05 2024

           Step           Time
              0        0.00000

   Energies (kJ/mol)
           Bond  Harmonic Pot.          Angle    Proper Dih.  Improper
Dih.
```

```
    1.74496e+03    0.00000e+00    4.45123e+03    5.17096e+03
0.00000e+00
 Per. Imp. Dih.          LJ-14     Coulomb-14        LJ (SR)  Disper.
corr.
    2.79362e+02    2.02835e+03    1.20238e+04    8.34149e+04   -
3.18065e+03
   Coulomb (SR)   Coul. recip.      Potential    Kinetic En.   Total
Energy
   -7.21755e+05    2.18051e+03   -6.13641e+05    1.10125e+05   -
5.03516e+05
    Temperature Pres. DC (bar) Pressure (bar)      dVcoul/dl
dVvdw/dl
    2.97553e+02   -1.19688e+02   -8.81484e+01    2.54752e+01
2.47544e+02
   Constr. rmsd
    3.01294e-06


DD  step 79 load imb.: force 15.7%

step 160 Turning on dynamic load balancing, because the performance loss
due to load imbalance is 7.8 %.
step 3200 Turning off dynamic load balancing, because it is degrading
performance.
Atom distribution over 6 domains: av 7325 stddev 99 min 7233 max 7443
step 8000 Turning on dynamic load balancing, because the performance loss
due to load imbalance is 5.7 %.

DD  load balancing is limited by minimum cell size in dimension X
DD  step 9999  vol min/aver 0.800! load imb.: force 12.3%
          Step           Time
         10000       20.00000

Writing checkpoint, step 10000 at Fri Jan 12 23:52:36 2024


   Energies (kJ/mol)
         Bond  Harmonic Pot.          Angle    Proper Dih.  Improper
Dih.
    1.54527e+03    0.00000e+00    4.26371e+03    5.12226e+03
0.00000e+00
 Per. Imp. Dih.          LJ-14     Coulomb-14        LJ (SR)  Disper.
corr.
    2.75412e+02    2.06052e+03    1.21763e+04    8.26960e+04   -
3.16862e+03
   Coulomb (SR)   Coul. recip.      Potential    Kinetic En.   Total
Energy
   -7.21024e+05    2.14597e+03   -6.13908e+05    1.10366e+05   -
5.03542e+05
    Temperature Pres. DC (bar) Pressure (bar)      dVcoul/dl
dVvdw/dl
    2.98204e+02   -1.18785e+02   -1.18796e+02    1.94211e+01
8.95465e+01
   Constr. rmsd
    3.23522e-06


      <======  ###############  ==>
```

```
      <====  A V E R A G E S  ====>
      <==  ###############  ======>

      Statistics over 10001 steps using 101 frames

   Energies (kJ/mol)
           Bond  Harmonic Pot.          Angle    Proper Dih.  Improper
Dih.
    1.63069e+03    0.00000e+00    4.39620e+03    5.14440e+03
0.00000e+00
 Per. Imp. Dih.          LJ-14     Coulomb-14        LJ (SR)  Disper.
corr.
    2.79706e+02    2.02288e+03    1.20460e+04    8.40467e+04   -
3.17937e+03
   Coulomb (SR)   Coul. recip.      Potential    Kinetic En.   Total
Energy
   -7.23014e+05    2.17069e+03   -6.14456e+05    1.10428e+05   -
5.04029e+05
    Temperature Pres. DC (bar) Pressure (bar)      dVcoul/dl
dVvdw/dl
    2.98372e+02   -1.19593e+02    6.20562e+00    2.01828e+01
1.34022e+02
   Constr. rmsd
    0.00000e+00

          Box-X          Box-Y          Box-Z
    8.54874e+00    8.54874e+00    6.04488e+00

   Total Virial (kJ/mol)
    3.67689e+04    2.04143e+02    2.74675e+01
    2.04436e+02    3.68350e+04   -1.20322e+02
    2.77769e+01   -1.20365e+02    3.65816e+04

   Pressure (bar)
    3.84561e+00   -1.42209e+01   -3.80354e+00
   -1.42429e+01   -8.08124e-01    1.01385e+01
   -3.82681e+00    1.01417e+01    1.55794e+01


      M E G A - F L O P S   A C C O U N T I N G

 NB=Group-cutoff nonbonded kernels    NxN=N-by-N cluster Verlet kernels
 RF=Reaction-Field  VdW=Van der Waals  QSTab=quadratic-spline table
 W3=SPC/TIP3p  W4=TIP4p (single or pairs)
 V&F=Potential and force  V=Potential only  F=Force only

 Computing:                                M-Number         M-Flops  %
Flops
-----------------------------------------------------------------------
----
 NB Free energy kernel                104715.345420      104715.345
0.3
 Pair Search distance check             3403.693148       30633.238
0.1
 NxN Ewald Elec. + LJ [F]             228949.063760    15110638.208
44.1
 NxN Ewald Elec. + LJ [V&F]             2335.672240      249916.930
0.7
```

```
 NxN Ewald Elec. [F]                202447.503856    12349297.735
36.0
 NxN Ewald Elec. [V&F]                2065.291312      173484.470
0.5
 1,4 nonbonded interactions             63.186318        5686.769
0.0
 Calc Weights                         1318.691856       47472.907
0.1
 Spread Q Bspline                    56264.185856      112528.372
0.3
 Gather F Bspline                    56264.185856      337585.115
1.0
 3D-FFT                             699184.311440     5593474.492
16.3
 Solve PME                             184.338432       11797.660
0.0
 Reset In Box                            5.494000          16.482
0.0
 CG-CoM                                  5.581904          16.746
0.0
 Bonds                                  10.603181         625.588
0.0
 Angles                                 37.838025        6356.788
0.0
 Propers                                57.785778       13232.943
0.0
 Impropers                               4.236786         881.251
0.0
 Virial                                 44.266222         796.792
0.0
 Update                                439.563952       13626.483
0.0
 Stop-CM                                 4.483104          44.831
0.0
 Calc-Ekin                              87.991904        2375.781
0.0
 Lincs                                  22.195932        1331.756
0.0
 Lincs-Mat                             123.140472         492.562
0.0
 Constraint-V                          941.643030        8474.787
0.0
 Constraint-Vir                         46.011606        1104.279
0.0
 Settle                                299.099388      110666.774
0.3
-----------------------------------------------------------------------
----
 Total                                                 34287275.083
100.0
-----------------------------------------------------------------------
----


   D O M A I N   D E C O M P O S I T I O N   S T A T I S T I C S

 av. #atoms communicated per step for force:  2 x 49955.1
 av. #atoms communicated per step for LINCS:  2 x 3179.3
```

```
Dynamic load balancing report:
 DLB was turned on during the run due to measured imbalance.
 Average load imbalance: 12.0%.
 The balanceable part of the MD step is 47%, load imbalance is computed
from this.
 Part of the total run time spent waiting due to load imbalance: 5.6%.
 Steps where the load balancing was limited by -rdd, -rcon and/or -dds: X
0 %

NOTE: 5.6 % of the available CPU time was lost due to load imbalance
      in the domain decomposition.
      You can consider manually changing the decomposition (option -dd);
      e.g. by using fewer domains along the box dimension in which there
is
      considerable inhomogeneity in the simulated system.

      R E A L   C Y C L E   A N D   T I M E   A C C O U N T I N G

On 6 MPI ranks

 Activity:              Num   Num      Call    Wall time         Giga-
Cycles
                       Ranks Threads  Count      (s)         total sum
%
-----------------------------------------------------------------------
-------
 Domain decomp.            6    1        126       0.489          8.639
0.3
 DD comm. load             6    1         77       0.003          0.044
0.0
 DD comm. bounds           6    1         64       0.004          0.064
0.0
 Neighbor search           6    1        126       2.102         37.138
1.4
 Comm. coord.              6    1       9875       0.822         14.531
0.5
 Force                     6    1      10001      68.024       1201.753
44.8
 Wait + Comm. F            6    1      10001       0.875         15.453
0.6
 PME mesh                  6    1      10001      72.925       1288.339
48.1
 NB X/F buffer ops.        6    1      29751       0.601         10.613
0.4
 Write traj.               6    1          1       0.018          0.320
0.0
 Update                    6    1      20002       2.226         39.320
1.5
 Constraints               6    1      20004       3.270         57.778
2.2
 Comm. energies            6    1       1001       0.086          1.525
0.1
 Rest                                               0.312          5.520
0.2
-----------------------------------------------------------------------
-------
```

```
 Total                                                 151.757       2681.037
100.0
-----------------------------------------------------------------------------
-------
 Breakdown of PME mesh activities
-----------------------------------------------------------------------------
-------
 PME redist. X/F          6    1      30003      16.499        291.479
10.9
 PME spread               6    1      20002      11.217        198.159
7.4
 PME gather               6    1      20002       6.895        121.816
4.5
 PME 3D-FFT               6    1      40004      26.554        469.122
17.5
 PME 3D-FFT Comm.         6    1      40004       8.977        158.590
5.9
 PME solve Elec           6    1      20002       2.753         48.632
1.8
-----------------------------------------------------------------------------
-------

               Core t (s)   Wall t (s)        (%)
       Time:      910.543      151.757      600.0
                 (ns/day)    (hour/ns)
Performance:       11.388        2.108
Finished mdrun on rank 0 Fri Jan 12 23:52:36 2024
```

benchBFC_cpu-sev-cluster_3n

```
                :-) GROMACS - gmx mdrun, 2023.3 (-:

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                    Coordinated by the GROMACS project leaders:
                      Paul Bauer, Berk Hess, and Erik Lindahl

GROMACS:      gmx mdrun, version 2023.3
Executable:   /usr/local/gromacs/bin/gmx_mpi
Data prefix:  /usr/local/gromacs
Working dir:  /home/ubuntu
Process ID:   5972
Command line:
  gmx_mpi mdrun -v -s /mnt/shared/home/ubuntu/mpinat-gromacs/mpinat-
gromacs-free-energy-bench/benchBFC.tpr

GROMACS version:    2023.3
Precision:          mixed
Memory model:       64 bit
MPI library:        MPI
OpenMP support:     enabled (GMX_OPENMP_MAX_THREADS = 128)
GPU support:        disabled
SIMD instructions:  AVX2_256
```

```
CPU FFT library:    fftw-3.3.8-sse2-avx-avx2-avx2_128
GPU FFT library:    none
Multi-GPU FFT:      none
RDTSCP usage:       enabled
TNG support:        enabled
Hwloc support:      disabled
Tracing support:    disabled
C compiler:         /usr/bin/cc GNU 11.4.0
C compiler flags:   -fexcess-precision=fast -funroll-all-loops -mavx2 -
mfma -Wno-missing-field-initializers -O3 -DNDEBUG
C++ compiler:       /usr/bin/c++ GNU 11.4.0
C++ compiler flags: -fexcess-precision=fast -funroll-all-loops -mavx2 -
mfma -Wno-missing-field-initializers -Wno-cast-function-type-strict -
fopenmp -O3 -DNDEBUG
BLAS library:       Internal
LAPACK library:     Internal


Running on 3 nodes with total 18 cores, 18 processing units
  Cores per node:            6
  Logical processing units per node:    6
  OS CPU Limit / recommended threads to start per node:    6
Hardware detected on host cpu-sev-1 (the node of MPI rank 0):
  CPU info:
    Vendor: AMD
    Brand:  AMD EPYC-Milan Processor
    Family: 25   Model: 1   Stepping: 1
    Features: aes amd apic avx avx2 clfsh cmov cx8 cx16 f16c fma lahf
misalignsse mmx msr pcid pclmuldq pdpe1gb popcnt pse rdrnd rdtscp sha
sse2 sse3 sse4a sse4.1 sse4.2 ssse3 tdt x2apic
  Hardware topology: Basic
    Packages, cores, and logical processors:
    [indices refer to OS logical processors]
      Package  0: [   0]
      Package  1: [   1]
      Package  2: [   2]
      Package  3: [   3]
      Package  4: [   4]
      Package  5: [   5]
    CPU limit set by OS: -1   Recommended max number of threads: 6


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
M. J. Abraham, T. Murtola, R. Schulz, S. P√°ll, J. C. Smith, B. Hess, E.
Lindahl
GROMACS: High performance molecular simulations through multi-level
parallelism from laptops to supercomputers
SoftwareX 1 (2015) pp. 19-25
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. P√°ll, M. J. Abraham, C. Kutzner, B. Hess, E. Lindahl
Tackling Exascale Software Challenges in Molecular Dynamics Simulations
with
GROMACS
In S. Markidis & E. Laure (Eds.), Solving Software Challenges for
Exascale 8759 (2015) pp. 3-27
```

```
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. Pronk, S. P√°ll, R. Schulz, P. Larsson, P. Bjelkmar, R. Apostolov, M.
R.
Shirts, J. C. Smith, P. M. Kasson, D. van der Spoel, B. Hess, and E.
Lindahl
GROMACS 4.5: a high-throughput and highly parallel open source molecular
simulation toolkit
Bioinformatics 29 (2013) pp. 845-54
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
B. Hess and C. Kutzner and D. van der Spoel and E. Lindahl
GROMACS 4: Algorithms for highly efficient, load-balanced, and scalable
molecular simulation
J. Chem. Theory Comput. 4 (2008) pp. 435-447
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
D. van der Spoel, E. Lindahl, B. Hess, G. Groenhof, A. E. Mark and H. J.
C.
Berendsen
GROMACS: Fast, Flexible and Free
J. Comp. Chem. 26 (2005) pp. 1701-1719
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
E. Lindahl and B. Hess and D. van der Spoel
GROMACS 3.0: A package for molecular simulation and trajectory analysis
J. Mol. Mod. 7 (2001) pp. 306-317
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
H. J. C. Berendsen, D. van der Spoel and R. van Drunen
GROMACS: A message-passing parallel molecular dynamics implementation
Comp. Phys. Comm. 91 (1995) pp. 43-56
-------- -------- --- Thank You --- -------- --------


++++ PLEASE CITE THE DOI FOR THIS VERSION OF GROMACS ++++
https://doi.org/10.5281/zenodo.10017686
-------- -------- --- Thank You --- -------- --------


The number of OpenMP threads was set by environment variable
OMP_NUM_THREADS to 1

Input Parameters:
   integrator                   = sd
   tinit                        = 0
   dt                           = 0.002
   nsteps                       = 10000
```

```
init-step                      = 0
simulation-part                = 1
mts                            = false
comm-mode                      = Linear
nstcomm                        = 100
bd-fric                        = 0
ld-seed                        = -1287569705
emtol                          = 10
emstep                         = 0.01
niter                          = 20
fcstep                         = 0
nstcgsteep                     = 1000
nbfgscorr                      = 10
rtpi                           = 0.05
nstxout                        = 0
nstvout                        = 0
nstfout                        = 0
nstlog                         = 0
nstcalcenergy                  = 100
nstenergy                      = 0
nstxout-compressed             = 0
compressed-x-precision         = 1000
cutoff-scheme                  = Verlet
nstlist                        = 10
pbc                            = xyz
periodic-molecules             = false
verlet-buffer-tolerance        = 0.005
rlist                          = 1.2
coulombtype                    = PME
coulomb-modifier               = Potential-shift
rcoulomb-switch                = 0
rcoulomb                       = 1.2
epsilon-r                      = 1
epsilon-rf                     = inf
vdw-type                       = Cut-off
vdw-modifier                   = Potential-shift
rvdw-switch                    = 0
rvdw                           = 1.2
DispCorr                       = EnerPres
table-extension                = 1
fourierspacing                 = 0.1
fourier-nx                     = 96
fourier-ny                     = 96
fourier-nz                     = 96
pme-order                      = 4
ewald-rtol                     = 1e-05
ewald-rtol-lj                  = 0.001
lj-pme-comb-rule               = Geometric
ewald-geometry                 = 3d
epsilon-surface                = 0
ensemble-temperature-setting   = constant
ensemble-temperature           = 298.15
tcoupl                         = No
nsttcouple                     = -1
nh-chain-length                = 0
print-nose-hoover-chain-variables = false
pcoupl                         = Parrinello-Rahman
pcoupltype                     = Isotropic
```

```
   nstpcouple                     = 10
   tau-p                          = 2
   compressibility (3x3):
      compressibility[    0]={ 4.50000e-05,  0.00000e+00,  0.00000e+00}
      compressibility[    1]={ 0.00000e+00,  4.50000e-05,  0.00000e+00}
      compressibility[    2]={ 0.00000e+00,  0.00000e+00,  4.50000e-05}
   ref-p (3x3):
      ref-p[    0]={ 1.00000e+00,  0.00000e+00,  0.00000e+00}
      ref-p[    1]={ 0.00000e+00,  1.00000e+00,  0.00000e+00}
      ref-p[    2]={ 0.00000e+00,  0.00000e+00,  1.00000e+00}
   refcoord-scaling               = No
   posres-com (3):
      posres-com[0]= 0.00000e+00
      posres-com[1]= 0.00000e+00
      posres-com[2]= 0.00000e+00
   posres-comB (3):
      posres-comB[0]= 0.00000e+00
      posres-comB[1]= 0.00000e+00
      posres-comB[2]= 0.00000e+00
   QMMM                           = false
qm-opts:
   ngQM                           = 0
   constraint-algorithm           = Lincs
   continuation                   = false
   Shake-SOR                      = false
   shake-tol                      = 0.0001
   lincs-order                    = 4
   lincs-iter                     = 1
   lincs-warnangle                = 30
   nwall                          = 0
   wall-type                      = 9-3
   wall-r-linpot                  = -1
   wall-atomtype[0]               = -1
   wall-atomtype[1]               = -1
   wall-density[0]                = 0
   wall-density[1]                = 0
   wall-ewald-zfac                = 3
   pull                           = false
   awh                            = false
   rotation                       = false
   interactiveMD                  = false
   disre                          = No
   disre-weighting                = Conservative
   disre-mixed                    = false
   dr-fc                          = 1000
   dr-tau                         = 0
   nstdisreout                    = 100
   orire-fc                       = 0
   orire-tau                      = 0
   nstorireout                    = 100
   free-energy                    = yes
   init-lambda                    = -1
   init-lambda-state              = 10
   delta-lambda                   = 0
   nstdhdl                        = 100
   n-lambdas                      = 20
   separate-dvdl:
       fep-lambdas =   FALSE
```

```
      mass-lambdas =   FALSE
      coul-lambdas =   TRUE
       vdw-lambdas =   TRUE
    bonded-lambdas =   FALSE
 restraint-lambdas =   FALSE
temperature-lambdas =   FALSE
all-lambdas:
       fep-lambdas =            0           0           0           0
0           0           0           0           0           0           0
0           0           0           0           0           0           0
0           0
      mass-lambdas =            0           0           0           0
0           0           0           0           0           0           0
0           0           0           0           0           0           0
0           0
      coul-lambdas =            0        0.25         0.5        0.75
1           1           1           1           1           1           1
1           1           1           1           1           1           1
1           1
       vdw-lambdas =            0           0           0           0
0        0.05         0.1         0.2         0.3         0.4         0.5
0.6        0.65         0.7        0.75         0.8        0.85
0.9        0.95           1
    bonded-lambdas =            0           0           0           0
0           0           0           0           0           0           0
0           0           0           0           0           0           0
0           0
 restraint-lambdas =            0           0           0           0
0           0           0           0           0           0           0
0           0           0           0           0           0           0
0           0
temperature-lambdas =            0           0           0           0
0           0           0           0           0           0           0
0           0           0           0           0           0           0
0           0
   calc-lambda-neighbors         = -1
   dhdl-print-energy             = no
   sc-alpha                      = 0.5
   sc-power                      = 1
   sc-r-power                    = 6
   sc-sigma                      = 0.3
   sc-sigma-min                  = 0.3
   sc-coul                       = true
   dh-hist-size                  = 0
   dh-hist-spacing               = 0.1
   separate-dhdl-file            = yes
   dhdl-derivatives              = yes
   sc-function                   = beutler
   sc-gapsys-scale-linpoint-lj   = 0.85
   sc-gapsys-scale-linpoint-q    = 0.3
   sc-gapsys-sigma-lj            = 0.3
   cos-acceleration              = 0
   deform (3x3):
      deform[    0]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
      deform[    1]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
      deform[    2]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
   simulated-tempering           = false
   swapcoords                    = no
```

```
   userint1                       = 0
   userint2                       = 0
   userint3                       = 0
   userint4                       = 0
   userreal1                      = 0
   userreal2                      = 0
   userreal3                      = 0
   userreal4                      = 0
   applied-forces:
     electric-field:
grpopts:
   nrdf:       89026
   ref-t:      298.15
   tau-t:           1
annealing:          No
annealing-npoints:           0
   acc:                0           0           0
   nfreeze:            N           N           N
   energygrp-flags[  0]: 0

Changing nstlist from 10 to 80, rlist from 1.2 to 1.322

Update groups can not be used for this system because atoms that are
(in)directly constrained together are interdispersed with other atoms

Initializing Domain Decomposition on 18 ranks
Dynamic load balancing: auto
Minimum cell size due to atom displacement: 0.632 nm
Initial maximum distances in bonded interactions:
    two-body bonded interactions: 1.223 nm, LJC Pairs NB, atoms 2065 2079
  multi-body bonded interactions: 0.698 nm, Improper Dih., atoms 2034
1556
Minimum cell size due to bonded interactions: 0.768 nm
Maximum distance for 5 constraints, at 120 deg. angles, all-trans: 0.219
nm
Estimated maximum distance required for P-LINCS: 0.219 nm
Scaling the initial minimum size with 1/0.8 (option -dds) = 1.25
Using 0 separate PME ranks because: there are too few total ranks for
efficient splitting
Optimizing the DD grid for 18 cells with a minimum initial size of 0.960
nm
The maximum allowed number of cells is: X 7 Y 7 Z 6
Domain decomposition grid 6 x 3 x 1, separate PME ranks 0
PME domain decomposition: 6 x 3 x 1
Domain decomposition rank 0, coordinates 0 0 0

The initial number of communication pulses is: X 2 Y 1
The initial domain decomposition cell size is: X 1.16 nm Y 2.33 nm

The maximum allowed distance for atoms involved in interactions is:
                 non-bonded interactions           1.322 nm
(the following are initial values, they could change due to box
deformation)
            two-body bonded interactions  (-rdd)   1.322 nm
          multi-body bonded interactions  (-rdd)   1.163 nm
  atoms separated by up to 5 constraints  (-rcon)  1.163 nm
```

```
When dynamic load balancing gets turned on, these settings will change
to:
The maximum number of communication pulses is: X 2 Y 2
The minimum size for domain decomposition cells is 0.931 nm
The requested allowed shrink of DD cells (option -dds) is: 0.80
The allowed shrink of domain decomposition cells is: X 0.80 Y 0.40
The maximum allowed distance for atoms involved in interactions is:
                 non-bonded interactions           1.322 nm
            two-body bonded interactions  (-rdd)   1.322 nm
          multi-body bonded interactions  (-rdd)   0.931 nm
  atoms separated by up to 5 constraints  (-rcon)  0.931 nm
Using two step summing over 3 groups of on average 6.0 ranks


Using 18 MPI processes

Non-default thread affinity set, disabling internal thread affinity

Using 1 OpenMP thread per MPI process

System total charge, top. A: -0.000 top. B: 0.000
Will do PME sum in reciprocal space for electrostatic interactions.

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
U. Essmann, L. Perera, M. L. Berkowitz, T. Darden, H. Lee and L. G.
Pedersen
A smooth particle mesh Ewald method
J. Chem. Phys. 103 (1995) pp. 8577-8592
-------- -------- --- Thank You --- -------- --------

Using a Gaussian width (1/beta) of 0.384195 nm for Ewald
Potential shift: LJ r^-12: -1.122e-01 r^-6: -3.349e-01, Ewald -8.333e-06
Initialized non-bonded Coulomb Ewald tables, spacing: 1.02e-03 size: 2273

Generated table with 1161 data points for 1-4 COUL.
Tabscale = 500 points/nm
Generated table with 1161 data points for 1-4 LJ6.
Tabscale = 500 points/nm
Generated table with 1161 data points for 1-4 LJ12.
Tabscale = 500 points/nm
Long Range LJ corr.: <C6> 3.0077e-04


Using SIMD 4x8 nonbonded short-range kernels

Using a dual 4x8 pair-list setup updated with dynamic pruning:
  outer list: updated every 80 steps, buffer 0.122 nm, rlist 1.322 nm
  inner list: updated every 13 steps, buffer 0.003 nm, rlist 1.203 nm
At tolerance 0.005 kJ/mol/ps per atom, equivalent classical 1x1 list
would be:
  outer list: updated every 80 steps, buffer 0.266 nm, rlist 1.466 nm
  inner list: updated every 13 steps, buffer 0.052 nm, rlist 1.252 nm

The non-bonded pair calculation algorithm tolerates a few missing pair
interactions close to the cut-off. This can lead to a systematic
overestimation of the pressure due to missing LJ interactions. The error
in the average pressure due to missing LJ interactions is at most 0.26
bar.
```

```
The pressure error can be controlled by setting the environment variable
GMX_VERLET_BUFFER_PRESSURE_TOLERANCE to the allowed error in units of
bar.

Using Lorentz-Berthelot Lennard-Jones combination rule
There are 48 atoms and 48 charges for free energy perturbation
Removing pbc first time

Linking all bonded interactions to atoms


Initializing Parallel LINear Constraint Solver

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
B. Hess
P-LINCS: A Parallel Linear Constraint Solver for molecular simulation
J. Chem. Theory Comput. 4 (2008) pp. 116-122
-------- -------- --- Thank You --- -------- --------

The number of constraints is 1037
There are constraints between atoms in different decomposition domains,
will communicate selected coordinates each lincs iteration

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. Miyamoto and P. A. Kollman
SETTLE: An Analytical Version of the SHAKE and RATTLE Algorithms for
Rigid
Water Models
J. Comp. Chem. 13 (1992) pp. 952-962
-------- -------- --- Thank You --- -------- --------


Intra-simulation communication will occur every 10 steps.
Initial vector of lambda components:[     0.0000     0.0000     1.0000
0.5000     0.0000     0.0000     0.0000 ]

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
N. Goga and A. J. Rzepiela and A. H. de Vries and S. J. Marrink and H. J.
C.
Berendsen
Efficient Algorithms for Langevin and DPD Dynamics
J. Chem. Theory Comput. 8 (2012) pp. 3637--3649
-------- -------- --- Thank You --- -------- --------

There are: 43952 Atoms
Atom distribution over 18 domains: av 2441 stddev 77 min 2387 max 2574

Constraining the starting coordinates (step 0)

Constraining the coordinates at t0-dt (step 0)
Center of mass motion removal mode is Linear
We have the following groups for center of mass motion removal:
  0:  rest
RMS relative constraint deviation after constraining: 2.99e-06
Initial temperature: 297.767 K

Started mdrun on rank 0 Fri Jan 12 10:02:38 2024
```

```
           Step           Time
              0        0.00000

   Energies (kJ/mol)
           Bond  Harmonic Pot.          Angle    Proper Dih.  Improper
Dih.
    1.74496e+03    0.00000e+00    4.45123e+03    5.17097e+03
0.00000e+00
 Per. Imp. Dih.          LJ-14     Coulomb-14        LJ (SR)  Disper.
corr.
    2.79362e+02    2.02835e+03    1.20238e+04    8.34149e+04   -
3.18065e+03
   Coulomb (SR)   Coul. recip.      Potential    Kinetic En.   Total
Energy
   -7.21758e+05    2.18054e+03   -6.13645e+05    1.10125e+05   -
5.03520e+05
    Temperature Pres. DC (bar) Pressure (bar)      dVcoul/dl
dVvdw/dl
    2.97553e+02   -1.19688e+02   -8.81522e+01    2.54720e+01
2.47544e+02
   Constr. rmsd
    3.01589e-06


DD  step 79 load imb.: force 143.7%

step 160 Turning on dynamic load balancing, because the performance loss
due to load imbalance is 16.7 %.

DD  step 9999  vol min/aver 0.522  load imb.: force  3.1%
           Step           Time
          10000       20.00000

Writing checkpoint, step 10000 at Fri Jan 12 10:04:25 2024


   Energies (kJ/mol)
           Bond  Harmonic Pot.          Angle    Proper Dih.  Improper
Dih.
    1.47853e+03    0.00000e+00    4.40461e+03    5.08336e+03
0.00000e+00
 Per. Imp. Dih.          LJ-14     Coulomb-14        LJ (SR)  Disper.
corr.
    3.08101e+02    2.06333e+03    1.20067e+04    8.42194e+04   -
3.18022e+03
   Coulomb (SR)   Coul. recip.      Potential    Kinetic En.   Total
Energy
   -7.23452e+05    2.18702e+03   -6.14881e+05    1.10762e+05   -
5.04119e+05
    Temperature Pres. DC (bar) Pressure (bar)      dVcoul/dl
dVvdw/dl
    2.99274e+02   -1.19656e+02    8.97367e+01    2.69519e+01
2.45593e+01
   Constr. rmsd
    3.46279e-06


      <======  ###############  ==>
```

```
      <====  A V E R A G E S  ====>
      <==  ###############  ======>

      Statistics over 10001 steps using 101 frames

   Energies (kJ/mol)
           Bond  Harmonic Pot.          Angle    Proper Dih.  Improper
Dih.
    1.62094e+03    0.00000e+00    4.41686e+03    5.15081e+03
0.00000e+00
 Per. Imp. Dih.          LJ-14     Coulomb-14        LJ (SR)  Disper.
corr.
    2.76755e+02    2.01756e+03    1.20572e+04    8.41430e+04   -
3.17948e+03
   Coulomb (SR)   Coul. recip.      Potential    Kinetic En.   Total
Energy
   -7.22913e+05    2.16182e+03   -6.14247e+05    1.10347e+05   -
5.03900e+05
    Temperature Pres. DC (bar) Pressure (bar)      dVcoul/dl
dVvdw/dl
    2.98154e+02   -1.19601e+02    1.51780e+01    2.92071e+01
1.13965e+02
   Constr. rmsd
    0.00000e+00

          Box-X          Box-Y          Box-Z
    8.54863e+00    8.54863e+00    6.04480e+00

   Total Virial (kJ/mol)
    3.66544e+04   -1.71336e+02    1.57566e+02
   -1.70217e+02    3.68031e+04    1.78182e+02
    1.57955e+02    1.78328e+02    3.62885e+04

   Pressure (bar)
    1.18971e+01    1.42690e+01   -1.53771e+01
    1.41848e+01    5.31692e-01   -1.48640e+01
   -1.54064e+01   -1.48749e+01    3.31053e+01


     M E G A - F L O P S   A C C O U N T I N G

 NB=Group-cutoff nonbonded kernels    NxN=N-by-N cluster Verlet kernels
 RF=Reaction-Field  VdW=Van der Waals  QSTab=quadratic-spline table
 W3=SPC/TIP3p  W4=TIP4p (single or pairs)
 V&F=Potential and force  V=Potential only  F=Force only

 Computing:                                M-Number         M-Flops  %
Flops
-----------------------------------------------------------------------
----
 NB Free energy kernel                104166.584946      104166.585
0.3
 Pair Search distance check             3626.600436       32639.404
0.1
 NxN Ewald Elec. + LJ [F]             241053.471008    15909529.087
44.3
 NxN Ewald Elec. + LJ [V&F]             2459.396464      263155.422
0.7
```

```
 NxN Ewald Elec. [F]                214974.217184    13113427.248
36.5
 NxN Ewald Elec. [V&F]                2193.318320      184238.739
0.5
 1,4 nonbonded interactions             63.186318        5686.769
0.0
 Calc Weights                         1318.691856       47472.907
0.1
 Spread Q Bspline                    56264.185856      112528.372
0.3
 Gather F Bspline                    56264.185856      337585.115
0.9
 3D-FFT                             699184.311440     5593474.492
15.6
 Solve PME                             553.015296       35392.979
0.1
 Reset In Box                            5.537952          16.614
0.0
 CG-CoM                                  5.581904          16.746
0.0
 Bonds                                  10.603181         625.588
0.0
 Angles                                 37.838025        6356.788
0.0
 Propers                                57.785778       13232.943
0.0
 Impropers                               4.236786         881.251
0.0
 Virial                                 44.806762         806.522
0.0
 Update                                439.563952       13626.483
0.0
 Stop-CM                                 4.483104          44.831
0.0
 Calc-Ekin                              87.991904        2375.781
0.0
 Lincs                                  22.945998        1376.760
0.0
 Lincs-Mat                             127.747224         510.989
0.0
 Constraint-V                          973.560431        8762.044
0.0
 Constraint-Vir                         47.571073        1141.706
0.0
 Settle                                309.239006      114418.432
0.3
-----------------------------------------------------------------------
----
 Total                                                 35903490.594
100.0
-----------------------------------------------------------------------
----


   D O M A I N   D E C O M P O S I T I O N   S T A T I S T I C S

 av. #atoms communicated per step for force:  2 x 105092.0
 av. #atoms communicated per step for LINCS:  2 x 4960.0
```

```
Dynamic load balancing report:
 DLB was turned on during the run due to measured imbalance.
 Average load imbalance: 13.4%.
 The balanceable part of the MD step is 22%, load imbalance is computed
from this.
 Part of the total run time spent waiting due to load imbalance: 2.9%.
 Steps where the load balancing was limited by -rdd, -rcon and/or -dds: X
0 % Y 0 %


     R E A L   C Y C L E   A N D   T I M E   A C C O U N T I N G

On 18 MPI ranks

 Activity:              Num   Num      Call    Wall time         Giga-
Cycles
                       Ranks Threads  Count      (s)         total sum
%
-----------------------------------------------------------------------
-------
 Domain decomp.           18    1        126       0.396         20.965
0.4
 DD comm. load            18    1        125       0.002          0.082
0.0
 DD comm. bounds          18    1        124       0.016          0.824
0.0
 Neighbor search          18    1        126       0.824         43.690
0.8
 Comm. coord.             18    1       9875       2.328        123.391
2.2
 Force                    18    1      10001      20.718       1098.058
19.3
 Wait + Comm. F           18    1      10001       2.309        122.361
2.1
 PME mesh                 18    1      10001      75.945       4025.040
70.6
 NB X/F buffer ops.       18    1      29751       0.307         16.291
0.3
 Write traj.              18    1          1       0.004          0.228
0.0
 Update                   18    1      20002       0.661         35.044
0.6
 Constraints              18    1      20004       3.767        199.654
3.5
 Comm. energies           18    1       1001       0.151          8.022
0.1
 Rest                                               0.134          7.119
0.1
-----------------------------------------------------------------------
-------
 Total                                            107.563       5700.769
100.0
-----------------------------------------------------------------------
-------
 Breakdown of PME mesh activities
```

```
-----------------------------------------------------------------------------
-------
 PME redist. X/F          18    1      30003      10.754        569.945
10.0
 PME spread               18    1      20002       6.347        336.366
5.9
 PME gather               18    1      20002       4.785        253.604
4.4
 PME 3D-FFT               18    1      40004       8.651        458.496
8.0
 PME 3D-FFT Comm.         18    1      80008      44.510       2358.991
41.4
 PME solve Elec           18    1      20002       0.878         46.553
0.8
-----------------------------------------------------------------------------
-------

               Core t (s)   Wall t (s)        (%)
       Time:     1936.119      107.563     1800.0
                 (ns/day)    (hour/ns)
Performance:       16.067        1.494
Finished mdrun on rank 0 Fri Jan 12 10:04:25 2024
```

benchBFC_cpu-sev-cluster_10n

```
                :-) GROMACS - gmx mdrun, 2023.3 (-:

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       Jon Vincent             Teemu Virolainen          Christian
Wennberg
       Maarten Wolf

                    Coordinated by the GROMACS project leaders:
                      Paul Bauer, Berk Hess, and Erik Lindahl

GROMACS:      gmx mdrun, version 2023.3
Executable:   /usr/local/gromacs/bin/gmx_mpi
Data prefix:  /usr/local/gromacs
Working dir:  /home/ubuntu
Process ID:   4854
Command line:
  gmx_mpi mdrun -v -s /mnt/shared/home/ubuntu/mpinat-gromacs/mpinat-
gromacs-free-energy-bench/benchBFC.tpr

GROMACS version:    2023.3
Precision:          mixed
Memory model:       64 bit
MPI library:        MPI
OpenMP support:     enabled (GMX_OPENMP_MAX_THREADS = 128)
GPU support:        disabled
SIMD instructions:  AVX2_256
```

```
CPU FFT library:    fftw-3.3.8-sse2-avx-avx2-avx2_128
GPU FFT library:    none
Multi-GPU FFT:      none
RDTSCP usage:       enabled
TNG support:        enabled
Hwloc support:      disabled
Tracing support:    disabled
C compiler:         /usr/bin/cc GNU 11.4.0
C compiler flags:   -fexcess-precision=fast -funroll-all-loops -mavx2 -
mfma -Wno-missing-field-initializers -O3 -DNDEBUG
C++ compiler:       /usr/bin/c++ GNU 11.4.0
C++ compiler flags: -fexcess-precision=fast -funroll-all-loops -mavx2 -
mfma -Wno-missing-field-initializers -Wno-cast-function-type-strict -
fopenmp -O3 -DNDEBUG
BLAS library:       Internal
LAPACK library:     Internal


Running on 10 nodes with total 60 cores, 60 processing units
  Cores per node:            6
  Logical processing units per node:    6
  OS CPU Limit / recommended threads to start per node:    6
Hardware detected on host cpu-sev-1 (the node of MPI rank 0):
  CPU info:
    Vendor: AMD
    Brand:  AMD EPYC-Milan Processor
    Family: 25   Model: 1   Stepping: 1
    Features: aes amd apic avx avx2 clfsh cmov cx8 cx16 f16c fma lahf
misalignsse mmx msr pcid pclmuldq pdpe1gb popcnt pse rdrnd rdtscp sha
sse2 sse3 sse4a sse4.1 sse4.2 ssse3 tdt x2apic
  Hardware topology: Basic
    Packages, cores, and logical processors:
    [indices refer to OS logical processors]
      Package  0: [   0]
      Package  1: [   1]
      Package  2: [   2]
      Package  3: [   3]
      Package  4: [   4]
      Package  5: [   5]
    CPU limit set by OS: -1   Recommended max number of threads: 6


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
M. J. Abraham, T. Murtola, R. Schulz, S. P√°ll, J. C. Smith, B. Hess, E.
Lindahl
GROMACS: High performance molecular simulations through multi-level
parallelism from laptops to supercomputers
SoftwareX 1 (2015) pp. 19-25
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. P√°ll, M. J. Abraham, C. Kutzner, B. Hess, E. Lindahl
Tackling Exascale Software Challenges in Molecular Dynamics Simulations
with
GROMACS
In S. Markidis & E. Laure (Eds.), Solving Software Challenges for
Exascale 8759 (2015) pp. 3-27
```

```
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. Pronk, S. P√°ll, R. Schulz, P. Larsson, P. Bjelkmar, R. Apostolov, M.
R.
Shirts, J. C. Smith, P. M. Kasson, D. van der Spoel, B. Hess, and E.
Lindahl
GROMACS 4.5: a high-throughput and highly parallel open source molecular
simulation toolkit
Bioinformatics 29 (2013) pp. 845-54
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
B. Hess and C. Kutzner and D. van der Spoel and E. Lindahl
GROMACS 4: Algorithms for highly efficient, load-balanced, and scalable
molecular simulation
J. Chem. Theory Comput. 4 (2008) pp. 435-447
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
D. van der Spoel, E. Lindahl, B. Hess, G. Groenhof, A. E. Mark and H. J.
C.
Berendsen
GROMACS: Fast, Flexible and Free
J. Comp. Chem. 26 (2005) pp. 1701-1719
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
E. Lindahl and B. Hess and D. van der Spoel
GROMACS 3.0: A package for molecular simulation and trajectory analysis
J. Mol. Mod. 7 (2001) pp. 306-317
-------- -------- --- Thank You --- -------- --------


++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
H. J. C. Berendsen, D. van der Spoel and R. van Drunen
GROMACS: A message-passing parallel molecular dynamics implementation
Comp. Phys. Comm. 91 (1995) pp. 43-56
-------- -------- --- Thank You --- -------- --------


++++ PLEASE CITE THE DOI FOR THIS VERSION OF GROMACS ++++
https://doi.org/10.5281/zenodo.10017686
-------- -------- --- Thank You --- -------- --------


The number of OpenMP threads was set by environment variable
OMP_NUM_THREADS to 1

Input Parameters:
   integrator                   = sd
   tinit                        = 0
   dt                           = 0.002
   nsteps                       = 10000
```

```
init-step                       = 0
simulation-part                 = 1
mts                             = false
comm-mode                       = Linear
nstcomm                         = 100
bd-fric                         = 0
ld-seed                         = -1287569705
emtol                           = 10
emstep                          = 0.01
niter                           = 20
fcstep                          = 0
nstcgsteep                      = 1000
nbfgscorr                       = 10
rtpi                            = 0.05
nstxout                         = 0
nstvout                         = 0
nstfout                         = 0
nstlog                          = 0
nstcalcenergy                   = 100
nstenergy                       = 0
nstxout-compressed              = 0
compressed-x-precision          = 1000
cutoff-scheme                   = Verlet
nstlist                         = 10
pbc                             = xyz
periodic-molecules              = false
verlet-buffer-tolerance         = 0.005
rlist                           = 1.2
coulombtype                     = PME
coulomb-modifier                = Potential-shift
rcoulomb-switch                 = 0
rcoulomb                        = 1.2
epsilon-r                       = 1
epsilon-rf                      = inf
vdw-type                        = Cut-off
vdw-modifier                    = Potential-shift
rvdw-switch                     = 0
rvdw                            = 1.2
DispCorr                        = EnerPres
table-extension                 = 1
fourierspacing                  = 0.1
fourier-nx                      = 96
fourier-ny                      = 96
fourier-nz                      = 96
pme-order                       = 4
ewald-rtol                      = 1e-05
ewald-rtol-lj                   = 0.001
lj-pme-comb-rule                = Geometric
ewald-geometry                  = 3d
epsilon-surface                 = 0
ensemble-temperature-setting    = constant
ensemble-temperature            = 298.15
tcoupl                          = No
nsttcouple                      = -1
nh-chain-length                 = 0
print-nose-hoover-chain-variables = false
pcoupl                          = Parrinello-Rahman
pcoupltype                      = Isotropic
```

```
   nstpcouple                     = 10
   tau-p                          = 2
   compressibility (3x3):
      compressibility[    0]={ 4.50000e-05,  0.00000e+00,  0.00000e+00}
      compressibility[    1]={ 0.00000e+00,  4.50000e-05,  0.00000e+00}
      compressibility[    2]={ 0.00000e+00,  0.00000e+00,  4.50000e-05}
   ref-p (3x3):
      ref-p[    0]={ 1.00000e+00,  0.00000e+00,  0.00000e+00}
      ref-p[    1]={ 0.00000e+00,  1.00000e+00,  0.00000e+00}
      ref-p[    2]={ 0.00000e+00,  0.00000e+00,  1.00000e+00}
   refcoord-scaling               = No
   posres-com (3):
      posres-com[0]= 0.00000e+00
      posres-com[1]= 0.00000e+00
      posres-com[2]= 0.00000e+00
   posres-comB (3):
      posres-comB[0]= 0.00000e+00
      posres-comB[1]= 0.00000e+00
      posres-comB[2]= 0.00000e+00
   QMMM                           = false
qm-opts:
   ngQM                           = 0
   constraint-algorithm           = Lincs
   continuation                   = false
   Shake-SOR                      = false
   shake-tol                      = 0.0001
   lincs-order                    = 4
   lincs-iter                     = 1
   lincs-warnangle                = 30
   nwall                          = 0
   wall-type                      = 9-3
   wall-r-linpot                  = -1
   wall-atomtype[0]               = -1
   wall-atomtype[1]               = -1
   wall-density[0]                = 0
   wall-density[1]                = 0
   wall-ewald-zfac                = 3
   pull                           = false
   awh                            = false
   rotation                       = false
   interactiveMD                  = false
   disre                          = No
   disre-weighting                = Conservative
   disre-mixed                    = false
   dr-fc                          = 1000
   dr-tau                         = 0
   nstdisreout                    = 100
   orire-fc                       = 0
   orire-tau                      = 0
   nstorireout                    = 100
   free-energy                    = yes
   init-lambda                    = -1
   init-lambda-state              = 10
   delta-lambda                   = 0
   nstdhdl                        = 100
   n-lambdas                      = 20
   separate-dvdl:
       fep-lambdas =   FALSE
```

```
      mass-lambdas =   FALSE
      coul-lambdas =   TRUE
       vdw-lambdas =   TRUE
    bonded-lambdas =   FALSE
 restraint-lambdas =   FALSE
temperature-lambdas =   FALSE
all-lambdas:
       fep-lambdas =            0           0           0           0
0           0           0           0           0           0           0
0           0           0           0           0           0           0
0           0
      mass-lambdas =            0           0           0           0
0           0           0           0           0           0           0
0           0           0           0           0           0           0
0           0
      coul-lambdas =            0        0.25         0.5        0.75
1           1           1           1           1           1           1
1           1           1           1           1           1           1
1           1
       vdw-lambdas =            0           0           0           0
0        0.05         0.1         0.2         0.3         0.4         0.5
0.6        0.65         0.7        0.75         0.8        0.85
0.9        0.95           1
    bonded-lambdas =            0           0           0           0
0           0           0           0           0           0           0
0           0           0           0           0           0           0
0           0
 restraint-lambdas =            0           0           0           0
0           0           0           0           0           0           0
0           0           0           0           0           0           0
0           0
temperature-lambdas =            0           0           0           0
0           0           0           0           0           0           0
0           0           0           0           0           0           0
0           0
   calc-lambda-neighbors         = -1
   dhdl-print-energy             = no
   sc-alpha                      = 0.5
   sc-power                      = 1
   sc-r-power                    = 6
   sc-sigma                      = 0.3
   sc-sigma-min                  = 0.3
   sc-coul                       = true
   dh-hist-size                  = 0
   dh-hist-spacing               = 0.1
   separate-dhdl-file            = yes
   dhdl-derivatives              = yes
   sc-function                   = beutler
   sc-gapsys-scale-linpoint-lj   = 0.85
   sc-gapsys-scale-linpoint-q    = 0.3
   sc-gapsys-sigma-lj            = 0.3
   cos-acceleration              = 0
   deform (3x3):
      deform[    0]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
      deform[    1]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
      deform[    2]={ 0.00000e+00,  0.00000e+00,  0.00000e+00}
   simulated-tempering           = false
   swapcoords                    = no
```

```
   userint1                       = 0
   userint2                       = 0
   userint3                       = 0
   userint4                       = 0
   userreal1                      = 0
   userreal2                      = 0
   userreal3                      = 0
   userreal4                      = 0
   applied-forces:
     electric-field:
grpopts:
   nrdf:       89026
   ref-t:      298.15
   tau-t:           1
annealing:          No
annealing-npoints:           0
   acc:               0           0           0
   nfreeze:           N           N           N
   energygrp-flags[  0]: 0

Changing nstlist from 10 to 80, rlist from 1.2 to 1.322

Update groups can not be used for this system because atoms that are
(in)directly constrained together are interdispersed with other atoms

Initializing Domain Decomposition on 60 ranks
Dynamic load balancing: auto
Minimum cell size due to atom displacement: 0.632 nm
Initial maximum distances in bonded interactions:
    two-body bonded interactions: 1.223 nm, LJC Pairs NB, atoms 2065 2079
  multi-body bonded interactions: 0.698 nm, Improper Dih., atoms 2034
1556
Minimum cell size due to bonded interactions: 0.768 nm
Maximum distance for 5 constraints, at 120 deg. angles, all-trans: 0.219
nm
Estimated maximum distance required for P-LINCS: 0.219 nm
Scaling the initial minimum size with 1/0.8 (option -dds) = 1.25
Guess for relative PME load: 0.38
Will use 36 particle-particle and 24 PME only ranks
This is a guess, check the performance at the end of the log file
Using 24 separate PME ranks, as guessed by mdrun
Optimizing the DD grid for 36 cells with a minimum initial size of 0.960
nm
The maximum allowed number of cells is: X 7 Y 7 Z 6
Domain decomposition grid 3 x 4 x 3, separate PME ranks 24
PME domain decomposition: 3 x 8 x 1
Interleaving PP and PME ranks
This rank does only particle-particle work.
Domain decomposition rank 0, coordinates 0 0 0

The initial number of communication pulses is: X 1 Y 1 Z 1
The initial domain decomposition cell size is: X 2.33 nm Y 1.74 nm Z 2.01
nm

The maximum allowed distance for atoms involved in interactions is:
                 non-bonded interactions           1.322 nm
(the following are initial values, they could change due to box
deformation)
```

```
           two-body bonded interactions  (-rdd)   1.322 nm
         multi-body bonded interactions  (-rdd)   1.322 nm
  atoms separated by up to 5 constraints  (-rcon)  1.745 nm

When dynamic load balancing gets turned on, these settings will change
to:
The maximum number of communication pulses is: X 1 Y 1 Z 1
The minimum size for domain decomposition cells is 1.322 nm
The requested allowed shrink of DD cells (option -dds) is: 0.80
The allowed shrink of domain decomposition cells is: X 0.57 Y 0.76 Z 0.66
The maximum allowed distance for atoms involved in interactions is:
                 non-bonded interactions           1.322 nm
           two-body bonded interactions  (-rdd)   1.322 nm
         multi-body bonded interactions  (-rdd)   1.322 nm
  atoms separated by up to 5 constraints  (-rcon)  1.322 nm
Using two step summing over 10 groups of on average 3.6 ranks


Using 60 MPI processes

Non-default thread affinity set, disabling internal thread affinity

Using 1 OpenMP thread per MPI process

System total charge, top. A: -0.000 top. B: 0.000
Will do PME sum in reciprocal space for electrostatic interactions.

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
U. Essmann, L. Perera, M. L. Berkowitz, T. Darden, H. Lee and L. G.
Pedersen
A smooth particle mesh Ewald method
J. Chem. Phys. 103 (1995) pp. 8577-8592
-------- -------- --- Thank You --- -------- --------

Using a Gaussian width (1/beta) of 0.384195 nm for Ewald
Potential shift: LJ r^-12: -1.122e-01 r^-6: -3.349e-01, Ewald -8.333e-06
Initialized non-bonded Coulomb Ewald tables, spacing: 1.02e-03 size: 2273

Generated table with 1161 data points for 1-4 COUL.
Tabscale = 500 points/nm
Generated table with 1161 data points for 1-4 LJ6.
Tabscale = 500 points/nm
Generated table with 1161 data points for 1-4 LJ12.
Tabscale = 500 points/nm
Long Range LJ corr.: <C6> 3.0077e-04


Using SIMD 4x8 nonbonded short-range kernels

Using a dual 4x8 pair-list setup updated with dynamic pruning:
  outer list: updated every 80 steps, buffer 0.122 nm, rlist 1.322 nm
  inner list: updated every 13 steps, buffer 0.003 nm, rlist 1.203 nm
At tolerance 0.005 kJ/mol/ps per atom, equivalent classical 1x1 list
would be:
  outer list: updated every 80 steps, buffer 0.266 nm, rlist 1.466 nm
  inner list: updated every 13 steps, buffer 0.052 nm, rlist 1.252 nm
```

```
The non-bonded pair calculation algorithm tolerates a few missing pair
interactions close to the cut-off. This can lead to a systematic
overestimation of the pressure due to missing LJ interactions. The error
in the average pressure due to missing LJ interactions is at most 0.26
bar.
The pressure error can be controlled by setting the environment variable
GMX_VERLET_BUFFER_PRESSURE_TOLERANCE to the allowed error in units of
bar.

Using Lorentz-Berthelot Lennard-Jones combination rule
There are 48 atoms and 48 charges for free energy perturbation
Removing pbc first time

Linking all bonded interactions to atoms


Initializing Parallel LINear Constraint Solver

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
B. Hess
P-LINCS: A Parallel Linear Constraint Solver for molecular simulation
J. Chem. Theory Comput. 4 (2008) pp. 116-122
-------- -------- --- Thank You --- -------- --------

The number of constraints is 1037
There are constraints between atoms in different decomposition domains,
will communicate selected coordinates each lincs iteration

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
S. Miyamoto and P. A. Kollman
SETTLE: An Analytical Version of the SHAKE and RATTLE Algorithms for
Rigid
Water Models
J. Comp. Chem. 13 (1992) pp. 952-962
-------- -------- --- Thank You --- -------- --------


Intra-simulation communication will occur every 10 steps.
Initial vector of lambda components:[     0.0000     0.0000     1.0000
0.5000     0.0000     0.0000     0.0000 ]

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
N. Goga and A. J. Rzepiela and A. H. de Vries and S. J. Marrink and H. J.
C.
Berendsen
Efficient Algorithms for Langevin and DPD Dynamics
J. Chem. Theory Comput. 8 (2012) pp. 3637--3649
-------- -------- --- Thank You --- -------- --------

There are: 43952 Atoms
Atom distribution over 36 domains: av 1220 stddev 52 min 1185 max 1310

Constraining the starting coordinates (step 0)

Constraining the coordinates at t0-dt (step 0)
Center of mass motion removal mode is Linear
We have the following groups for center of mass motion removal:
  0:  rest
```

```
RMS relative constraint deviation after constraining: 2.97e-06
Initial temperature: 297.767 K

Started mdrun on rank 0 Fri Jan 12 09:32:10 2024

           Step           Time
              0        0.00000

   Energies (kJ/mol)
          Bond  Harmonic Pot.          Angle    Proper Dih.  Improper
Dih.
    1.74496e+03    0.00000e+00    4.45122e+03    5.17096e+03
0.00000e+00
 Per. Imp. Dih.          LJ-14     Coulomb-14        LJ (SR)  Disper.
corr.
    2.79362e+02    2.02835e+03    1.20239e+04    8.34149e+04   -
3.18065e+03
   Coulomb (SR)   Coul. recip.      Potential    Kinetic En.   Total
Energy
   -7.21773e+05    2.18054e+03   -6.13660e+05    1.10125e+05   -
5.03535e+05
    Temperature Pres. DC (bar) Pressure (bar)      dVcoul/dl
dVvdw/dl
    2.97553e+02   -1.19688e+02   -8.81549e+01    2.54637e+01
2.47544e+02
   Constr. rmsd
    3.01526e-06


DD  step 79 load imb.: force 112.4%  pme mesh/force 2.510
step  480: timed with pme grid 96 96 96, coulomb cutoff 1.200: 1440.5 M-
cycles
step  640: timed with pme grid 80 80 80, coulomb cutoff 1.282: 1300.8 M-
cycles
step  800: timed with pme grid 72 72 72, coulomb cutoff 1.425: 1021.7 M-
cycles
step  960: timed with pme grid 64 64 64, coulomb cutoff 1.603: 1087.2 M-
cycles
step  960: the domain decomposition limits the PME load balancing to a
coulomb cut-off of 1.603
step 1120: timed with pme grid 64 64 64, coulomb cutoff 1.603: 1045.2 M-
cycles
step 1280: timed with pme grid 72 72 72, coulomb cutoff 1.425: 1052.4 M-
cycles
step 1440: timed with pme grid 64 64 64, coulomb cutoff 1.603: 1066.1 M-
cycles
step 1600: timed with pme grid 72 72 72, coulomb cutoff 1.425: 1072.1 M-
cycles
             optimal pme grid 72 72 72, coulomb cutoff 1.425

DD  step 9999 load imb.: force 62.1%  pme mesh/force 1.632
           Step           Time
          10000       20.00000

Writing checkpoint, step 10000 at Fri Jan 12 09:33:37 2024


   Energies (kJ/mol)
```

```
          Bond  Harmonic Pot.          Angle    Proper Dih.  Improper
Dih.
    1.54699e+03    0.00000e+00    4.36210e+03    5.20778e+03
0.00000e+00
 Per. Imp. Dih.          LJ-14     Coulomb-14        LJ (SR)  Disper.
corr.
    2.59741e+02    2.01494e+03    1.19912e+04    8.35744e+04   -
3.17236e+03
   Coulomb (SR)   Coul. recip.      Potential    Kinetic En.   Total
Energy
   -7.20910e+05    1.21119e+03   -6.13914e+05    1.10055e+05   -
5.03859e+05
    Temperature Pres. DC (bar) Pressure (bar)      dVcoul/dl
dVvdw/dl
    2.97363e+02   -1.19066e+02   -6.62119e+01    2.34155e+01
1.31210e+02
   Constr. rmsd
    3.47489e-06


      <======  ###############  ==>
      <====  A V E R A G E S  ====>
      <==  ###############  ======>

      Statistics over 10001 steps using 101 frames

   Energies (kJ/mol)
          Bond  Harmonic Pot.          Angle    Proper Dih.  Improper
Dih.
    1.65181e+03    0.00000e+00    4.44934e+03    5.15649e+03
0.00000e+00
 Per. Imp. Dih.          LJ-14     Coulomb-14        LJ (SR)  Disper.
corr.
    2.83069e+02    2.01439e+03    1.20149e+04    8.40583e+04   -
3.17893e+03
   Coulomb (SR)   Coul. recip.      Potential    Kinetic En.   Total
Energy
   -7.21815e+05    1.27604e+03   -6.14090e+05    1.10481e+05   -
5.03609e+05
    Temperature Pres. DC (bar) Pressure (bar)      dVcoul/dl
dVvdw/dl
    2.98515e+02   -1.19559e+02    3.83085e+00    2.22134e+01
1.14222e+02
   Constr. rmsd
    0.00000e+00

          Box-X          Box-Y          Box-Z
    8.54913e+00    8.54913e+00    6.04516e+00

   Total Virial (kJ/mol)
    3.66370e+04   -2.61344e+01    8.56668e+01
   -2.81910e+01    3.69396e+04    4.03206e+01
    8.51894e+01    4.12893e+01    3.67575e+04

   Pressure (bar)
    1.89225e+01    5.40537e+00   -1.04522e+01
    5.56007e+00   -6.03280e+00   -2.60347e+00
   -1.04163e+01   -2.67628e+00   -1.39716e+00
```

P P - P M E L O A D B A L A N C I N G

PP/PME load balancing changed the cut-off and PME settings:

	particle-particle					PME	
	rcoulomb	rlist	grid			spacing	1/beta
initial	1.200 nm	1.203 nm	96	96	96	0.089 nm	0.384 nm
final	1.425 nm	1.428 nm	72	72	72	0.119 nm	0.456 nm
cost-ratio		1.67		0.42			

(note that these numbers concern only part of the total PP and PME load)

NOTE: PME load balancing increased the non-bonded workload by more than 50%.
For better performance, use (more) PME ranks (mdrun -npme),
or if you are beyond the scaling limit, use fewer total ranks (or nodes).

M E G A - F L O P S A C C O U N T I N G

NB=Group-cutoff nonbonded kernels NxN=N-by-N cluster Verlet kernels
RF=Reaction-Field VdW=Van der Waals QSTab=quadratic-spline table
W3=SPC/TIP3p W4=TIP4p (single or pairs)
V&F=Potential and force V=Potential only F=Force only

Computing:	M-Number	M-Flops	% Flops
NB Free energy kernel	162353.961762	162353.962	0.3
Pair Search distance check	4935.319330	44417.874	0.1
NxN Ewald Elec. + LJ [F]	358806.472960	23681227.215	50.3
NxN Ewald Elec. + LJ [V&F]	3669.229424	392607.548	0.8
NxN Ewald Elec. [F]	319459.735808	19487043.884	41.4
NxN Ewald Elec. [V&F]	3267.183408	274443.406	0.6
1,4 nonbonded interactions	63.186318	5686.769	0.0
Calc Weights	1318.691856	47472.907	0.1
Spread Q Bspline	56264.185856	112528.372	0.2
Gather F Bspline	56264.185856	337585.115	0.7
3D-FFT	294257.833344	2354062.667	5.0
Solve PME	855.245824	54735.733	0.1
Reset In Box	5.537952	16.614	0.0
CG-CoM	5.581904	16.746	0.0

```
 Bonds                                    10.603181         625.588
0.0
 Angles                                   37.838025        6356.788
0.0
 Propers                                  57.785778       13232.943
0.0
 Impropers                                 4.236786         881.251
0.0
 Virial                                   45.617572         821.116
0.0
 Update                                  439.563952       13626.483
0.0
 Stop-CM                                   4.483104          44.831
0.0
 Calc-Ekin                                87.991904        2375.781
0.0
 Lincs                                    23.789556        1427.373
0.0
 Lincs-Mat                               135.333168         541.333
0.0
 Constraint-V                            988.691594        8898.224
0.0
 Constraint-Vir                           48.286141        1158.867
0.0
 Settle                                  313.720636      116076.635
0.2
-----------------------------------------------------------------------
----
 Total                                                 47120266.026
100.0
-----------------------------------------------------------------------
----


    D O M A I N   D E C O M P O S I T I O N   S T A T I S T I C S

 av. #atoms communicated per step for force:  2 x 169325.1
 av. #atoms communicated per step for LINCS:  2 x 5629.6


Dynamic load balancing report:
 DLB was off during the run due to low measured imbalance.
 Average load imbalance: 78.5%.
 The balanceable part of the MD step is 28%, load imbalance is computed
from this.
 Part of the total run time spent waiting due to load imbalance: 21.8%.
 Average PME mesh/force load: 1.643
 Part of the total run time spent waiting due to PP/PME imbalance: 21.0 %

NOTE: 21.8 % of the available CPU time was lost due to load imbalance
      in the domain decomposition.
      Dynamic load balancing was automatically disabled, but it might be
beneficial to manually turn it on (option -dlb yes.)
      You can also consider manually changing the decomposition (option -
dd);
      e.g. by using fewer domains along the box dimension in which there
is
      considerable inhomogeneity in the simulated system.
```

```
NOTE: 21.0 % performance was lost because the PME ranks
      had more work to do than the PP ranks.
      You might want to increase the number of PME ranks
      or increase the cut-off and the grid spacing.


     R E A L   C Y C L E   A N D   T I M E   A C C O U N T I N G

On 36 MPI ranks doing PP, and
on 24 MPI ranks doing PME

 Activity:              Num   Num      Call    Wall time         Giga-
Cycles
                       Ranks Threads  Count      (s)         total sum
%
-----------------------------------------------------------------------
-------
 Domain decomp.          36    1        126       2.835        300.414
2.0
 DD comm. load           36    1         23       0.001          0.128
0.0
 Send X to PME           36    1      10001       0.192         20.400
0.1
 Neighbor search         36    1        126       0.670         70.985
0.5
 Comm. coord.            36    1       9875       4.459        472.607
3.1
 Force                   36    1      10001      20.022       2122.081
13.8
 Wait + Comm. F          36    1      10001      17.678       1873.651
12.2
 PME mesh *              24    1      10001      72.305       5108.827
33.2
 PME wait for PP *                            14.705       1038.980
6.8
 Wait + Recv. PME F      36    1      10001      31.683       3357.912
21.8
 NB X/F buffer ops.      36    1      29751       0.301         31.908
0.2
 Write traj.             36    1          1       0.013          1.340
0.0
 Update                  36    1      20002       0.462         49.014
0.3
 Constraints             36    1      20004       8.616        913.137
5.9
 Comm. energies          36    1       1001       0.268         28.355
0.2
-----------------------------------------------------------------------
-------
 Total                                           87.012      15369.874
100.0
-----------------------------------------------------------------------
-------
(*) Note that with separate PME ranks, the walltime column actually sums
to
    twice the total reported, but the cycle count total and % are
correct.
```

```
-----------------------------------------------------------------------------
-------
 Breakdown of PME mesh activities
-----------------------------------------------------------------------------
-------
 PME redist. X/F          24    1      30003      22.150       1565.052
10.2
 PME spread               24    1      20002       6.767        478.168
3.1
 PME gather               24    1      20002       6.141        433.889
2.8
 PME 3D-FFT               24    1      40004       3.122        220.569
1.4
 PME 3D-FFT Comm.         24    1      80008      33.759       2385.303
15.5
 PME solve Elec           24    1      20002       0.340         24.056
0.2
-----------------------------------------------------------------------------
-------

               Core t (s)   Wall t (s)        (%)
       Time:     5219.928       87.012     5999.1
                 (ns/day)    (hour/ns)
Performance:       19.861        1.208
Finished mdrun on rank 0 Fri Jan 12 09:33:37 2024
```

"Hereby, I assure that the attached work has been created autonomously and without any support. The quotations have been done properly and I do not have used any sources beyond the scope of my bibliography."

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