

PRACE RESEARCH INFRASTRUCTURE OFFER FOR POLISH R&D COMMUNITY

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Abstract: The mission of the PRACE Research Infrastructure is to enable high impact scientific discovery and engineering research and development across all disciplines to enhance European competitiveness for the benefit of society. The paper presents the current state of the computational infrastructure, which is unique on the European level and procedures helping with the seamless access to the European HPC infrastructure: supercomputers, applications, storage. Several Polish computational grants have been called in the paper in order to present examples of the Polish domestic scientific engagement.

Keywords: PRACE-RI, Tier-1, Tier-0, Petaflop HPC, European Research Area, DECI, SHAPE

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1. Introduction

The PRACE Research Infrastructure (PRACE-RI) has been established over the past ten years to provide a pan-European world-class High Performance Computing (HPC) infrastructure to support the advanced modeling and simulation needs of European researchers from across the scientific and industrial domains.

From the user perspective, the overall goal of the PRACE-RI is to fulfill the scientific user requirements regarding their computing efficiency which cannot be achieved at the domestic HPC sites [1].

The Partnership for Advanced Computing in Europe (PRACE) has the overall objective to prepare for the creation of a persistent pan-European HPC service, consisting of 4–6 Tier-0 centers, similar to the US HPC infrastructure. PRACE is the top-Tier-0 and Tier-1 level of the European HPC ecosystem pyramid. PRACE-RI is not only computer hardware, but also user scientific support, tutorials, HPC programming schools and workshops, application benchmark repositories, legal co-operation with the existing Centers of Excellence and more.

The PRACE Research Infrastructure is managed as a single European entity. The current operation of Tier-0 production systems is the responsibility of several European HPC centers that have the expertise, competency, and the required infrastructure to provide a comprehensive service to meet the challenging demands of user groups from academia and industry. A well-defined procurement and renewal process permits to update the infrastructure to remain in a leadership position since technology and product offerings evolve very rapidly.

Since April 2010 the PRACE-RI has been established as a legal entity in Belgium – the PRACE AISBL (“Association Internationale Sans But Lucratif” under Belgian law). The work of the legal entity, which brings together 27 countries from across the European Union and associated countries, is being supported by a series of collaborative projects, part-funded by the European Commission. Poland is the founding member of the PRACE-AISBL. This paper presents the offer and benefits gained from the PRACE-RI for scientific applications. It also presents several user use cases being completed with scientific and computational success.

2. PRACE Calls

PRACE provides HPC resources to researchers and scientists from academia and industry through Preparatory Access (code scaling and optimization), through Project Access (large-scale, computationally intensive projects) and DECI (for smaller scale but still computationally intensive projects). SMEs are invited to make use of the tailored SHAPE programme, which will help them overcome barriers to the adoption of HPC in their business model. In this chapter we present an overview of the Project Access, DECI and SHAPE computational calls.

2.1. PRACE Project Access

PRACE encourages researchers from across Europe to apply for access to its world class resources for research with potential high European and international

impact. PRACE resources are available through three forms of access: Multi-year Access, Project Access and Preparatory Access [2]. Multi-year Access is available to major European projects or infrastructures that can benefit from PRACE resources and for which Project Access is not appropriate. Project Access is intended for individual researchers and research groups including multi-national research groups and has a one year duration. Calls for Proposals for Project Access are issued twice yearly in Spring and Autumn. Preparatory Access is intended for the resource use required to prepare proposals for Project Access. That include scalability tests of software to be used in Project Access computations and optimization and development codes to run smoothly on big Tier-0 systems. The upcoming Call for Proposals for 19th PRACE Project Access (Tier-0) is foreseen to open in March 2019.

Table 1. The list of Tier-0 system available for Call 19th

System	Architecture	Site (Country)	Core Hours (node hours) [Million]	Minimum request [Million]
Joliot Curie – SKL	BULL Sequana X1000	GENCI@CEA (FR)	142 (3)	15 core hours
Joliot Curie – KNL	BULL Sequana X1000	GENCI@CEA (FR)	101 (1.5)	15 core hours
JUWELS	BULL Sequana X1000	GCS@JSC (DE)	70 (1.5)	35 core hours
Marconi-Broadwell	Lenovo System	CINECA (IT)	36 (1)	15 core hours
Marconi-KNL	Lenovo System	CINECA (IT)	610 (9)	30 core hours
MareNostrum	Lenovo System	BSC (ES)	240 (5)	30 core hours
Piz Daint	Cray XC50 System	ETH Zurich / CSCS (CH)	510 (7.5)	68 core hours Use of GPUs
SuperMUC-NG*	Lenovo ThinkSystem	GCS@LRZ (DE)	125 (2.2)	35 core hours

The PRACE Project Access Calls for Proposals are intended for large-scale projects of excellent scientific merit and for which a significant European added-value and major impact at international level is anticipated. Proposals for receiving PRACE resources are subject to the PRACE peer review process [2], which consists of a technical review and a scientific review. Technical reviewers are selected based on the experience with PRACE systems, environment and software and preferably an application area. Scientific reviewers are selected based on their expertise in at least one scientific aspect of the proposal. Scientific reviewers may be selected from among reviewers proposed by applicants, but for a given proposal only one reviewer may be selected from the applicants' list of suggested reviewers. Each proposal is reviewed by experts selected by the PRACE AISBL peer review staff seeking to assure as good coverage as possible of the scientific aspects of the proposal. Scientific reviewers work independently from each other and their assessments are submitted to the PRACE AISBL peer review staff.

2.2. DECI Calls

Distributed European Computing Initiative (DECI) provides cross-national access to European Tier-1 resources (national systems). Access rights are awarded for a period of one year. Resources are available on systems from the various vendors such as: SGI, MEGWARE, Bull Bullx, Intel, CRAY, IBM, HP. Some of them available HPC systems are equipped with an accelerator: Intel/PHI and Nvidia GPGPUs. Those Tier-1 systems have computational power as big as 2.5 PFLOPS (in 2018). Applicants do not need to specify a particular machine or architecture, but if they do, their preferences are taken into account [3].

DECI enables European researchers to obtain access to the most powerful national (Tier-1) computing resources in Europe regardless of their country of origin or employment and to enhance the impact of European science and technology at the highest level. Proposals must deal with complex, demanding, innovative simulations that would not be possible without Tier-1 access. In addition to offering access to computing resources, applications-enabling and porting, assistance from experts at the leading European HPC centers is offered (on request and depending on availability) to enable projects to be run on the most appropriate Tier-1 platforms in PRACE.

Proposals from academia and industry are eligible, as long as the project leader is undertaking non-proprietary research in a European Union country or a PRACE Association member country. Project leaders will typically be employed in research organizations (academic or industrial). Individual HPC centers may have further restrictions on who is eligible to use the machines, *e.g.* due to US export regulations.

2.3. SHAPE

SHAPE (SME HPC Adoption Programme in Europe) invites applications from European SMEs with an interesting idea that would benefit from High Performance Computing for increasing their competitiveness.

SHAPE aims to work with selected SMEs to introduce HPC-based tools and techniques into their business, operational, or production environment. The selected solutions should bring a potential tangible Return on Investment to the SME's business.

The SHAPE process is as follows: the SME applies to the programme via an online or downloadable form – at this stage assistance is available from PRACE, if required, but also the form includes guidelines on the expected content. Applications are then reviewed and rated, based principally on the strength of the business case and technical feasibility of the proposed work. The successful SMEs can then receive machine time on a PRACE system, and – most importantly – effort from a PRACE expert to work alongside the SME in evaluating and/or developing the HPC-based solution. In return the SME provides in-kind effort, publicity of their participation in SHAPE, and a public white paper on the work achieved in the project at its conclusion.

PRACE experts will work with the selected SMEs in order to develop their solutions, providing the participating SMEs with knowledge that will allow them to make an informed decision on the selected HPC solution. Consideration will be given to independent service providers to become involved with the implementation at a later stage.

Since its inception in 2013, SHAPE has enabled over 40 SMEs located throughout Europe, working in many fields (including computational fluids dynamics, steel casting, medicine, genomics, environment and renewable energies, artificial intelligence), to demonstrate the tangible benefits of using HPC for improving their competitiveness. Via participation in SHAPE, jobs have been created, costs reduced, contracts won and new and innovative services have been offered. For more information about SHAPE, see [4].

3. PRACE User Support

PRACE, as an initiative, offers the HPC user community a wide range of support services. In addition to regular calls giving access to HPC resources PRACE organizes a set of smaller calls called Preparatory Access. In parallel, the PRACE Projects, with EU and national funding, offer specific support to user groups, communities or more formalized Centres of Excellence, in a form of Work Package “Application Enabling and Support”. The objective of these actions is to allow users to solve their scientific cases and challenges, and above all, solve them faster or in a more efficient way.

3.1. Preparatory Access

The PRACE Preparatory Access focuses on short-term access to a relatively small amount of computing resources and HPC experts’ time in order to optimize, scale and test codes on PRACE Tier-0 systems before applying to PRACE Project Access calls for Tier-0 Access. It means that no production runs are allowed, it is all about testing and improving codes. There are four schemes defined for Preparatory Access with differences in the peer-review process, the amount of resources granted and the allocation time.

The basic assumption for the peer-review is to keep it a light-weight procedure, it means that only administrative check and technical assessment of the submitted project is performed. The scientific value of the proposal is not checked.

Access to these calls is open to researchers from both public and private institutions. The eligibility criteria restrict the principal investigator or the headquarters of the company to be based in Europe. Access will be free of charge, but the user needs to fulfill the terms of access. This means providing a final report with the project results to PRACE, with the use of the PRACE template, and acknowledge the role of the HPC center(s) and PRACE in all publications which include results from PRACE allocations.

Type A

In this scheme the user gets access to a Tier-0 system and is supposed to perform test runs of his/her code and produce scalability plots on the system. Then, the results may be used as a reference for the scalability of the code, necessary to apply for PRACE calls for Tier-0 Project Access. The maximum duration of Type A projects is 2 months. Usually all Tier-0 systems are available in this scheme. The maximum time allocation varies between systems and changes in time, but should be at a level of 20 000–100 000 core hours per project. The Call for Proposals for this scheme is a continuously open call. The maximum time-to-resources-access (start-date) is two weeks after the date of submission.

There is no PRACE expert support available by default in this scheme, so the user is supposed to compile and run the code on his/her own. There is only a regular Tier-0 system support service provided by the Tier-0 site. However, Polish scientists can agree before submission and count on the support of experts from one of the four Polish HPC Centers engaged in PRACE. This action is possible thanks to additional national funding.

It might be worth submitting a Type A proposal even for well known and widely tested codes. The user's scientific case may be new or specific enough and use a different combination of code functionalities and linked libraries than tested so far on a given architecture. Thus, the case may significantly affect the scalability results.

Type B

In this scheme the user gets access to a Tier-0 system and is supposed to undertake code development and optimization. Applicants will need to describe the proposed work plan in detail, including the human resources and expertise available in the team to implement the project. The maximum duration of Type B projects is 6 months. Usually all Tier-0 systems are available in this scheme. The maximum time allocation varies between systems, but should be at a level of 50 000–250 000 core hours per project. The Call for Proposals for this scheme is continuously open. The maximum time-to-resources-access (start-date) is two weeks after the date of submission.

There is no PRACE expert support available by default, however, like in the Type A scheme, Polish scientists can agree before submission and count on the support of experts from one of the four Polish HPC Centers engaged in PRACE.

Type C

In this scheme, the user gets access to a Tier-0 system and requests the support of PRACE experts to provide the necessary adaptations (development and optimization) to the user's codes. The maximum support that can be requested is the equivalent of 6 person-months of effort. In addition, Polish projects can count on the support of experts from one of the four Polish HPC Centers engaged in PRACE. The maximum duration of Type C projects is 6 months. Not all Tier-0 systems are available in this scheme, the availability needs to be checked

on the PRACE website before submission. The maximum time allocation varies between the systems, but typically it should be at a level of 50 000–250 000 core hours per project. Applications for a Type C scheme are evaluated and granted on a quarterly basis, with cut-offs for evaluations to be set at 11:00 AM CEST/CET of the first working day of March, June, September and December. The winning proposals will have a maximum time-to-resources-access (start date) of two months after the relevant cut-off date.

Type D

In this scheme the user gets access to a Tier-1 and Tier-0 system and to the support of PRACE experts. The first stage of the project is to perform the code adaption and optimization process on a Tier-1 system. The second stage is to perform scalability test on a Tier-0 system in a form of a Type A project. The work is supported by PRACE experts. The maximum support that can be requested is the equivalent of 6 person-months of effort. In addition, like in other preparatory access types, Polish projects can count on the support of experts from one of the four Polish HPC Centers engaged in PRACE. The maximum duration of Type D projects is 12 months. Not all Tier-1 systems are available in this scheme. Currently, the following PRACE members provide the systems: CaSToRC representing Cyprus, CINECA representing Italy, CSC representing Finland, EPCC representing the United Kingdom, GRNET representing Greece, IT4I representing the Czech Republic, KTH-PDC representing Sweden, SURFsara representing the Netherlands and WCSS representing Poland. The exact availability needs to be checked on the PRACE website before submission. At the second stage one of the Tier-0 systems available in the Type A access scheme can be granted. The maximum time allocation varies between systems, but it should be at a level of 50 000–250 000 core hours per project.

Applications for a Type D scheme are evaluated and granted with the same quarterly schedule as Type C. Cut-offs for evaluations are set at 11:00 AM CEST/CET of the first working day of March, June, September and December. The winning proposals will have an approximate time-to-resources-access (start date) up to two months after the relevant cut-off date.

3.2. Application Enabling and Support

In parallel to Preparatory Access Calls, the PRACE Projects offer specific support to user groups and communities. These activities are grouped in a Work Package “Application Enabling and Support”. A set of long-term actions is taken to establish more permanent cooperation with users, to better know their scientific challenges and needs regarding the HPC research infrastructure.

The last PRACE-5IP project is focused on establishing a sustainable link to Centers of Excellence funded by the European Commission. The gap between the scientific case (a scientific question) and the complexity of the infrastructure (how to run *in silico* simulation) is being reduced. A set of 9 mini-projects of PRACE experts and scientists from CoEs has been established in order to solve

certain issues. The work looks further ahead to future PRACE Exascale systems, investigating new tools and techniques by applying them to important applications codes.

Topics of Mini-Projects on Novel Algorithms (Key Exascale Elements, PRACE site, Collaborators):

- Scalability, reducing synchronization overheads – PRACE: Bilkent; Collaborators: NLAFFET;
- Optimization, performance, big data – PRACE: IT4I; Collaborators: ExCAPE and PoP;
- System usability and programmability, scalability, energy efficiency, application portability – PRACE: HPC2N, BSC; Collaborators: DEEP-EST and EoCoE;

Topics of Mini-Projects on Novel Programming Models (Key Exascale Elements, PRACE site, Collaborators):

- Scalability, development of performance models – PRACE: NTNU; Collaborator: INTERTWinE;
- Scalability, development of performance models, dealing with architectural bottlenecks – PRACE: NTNU; Collaborator: INTERTWinE;
- Resilience, big data, novel algorithms – PRACE: CCSAS; Collaborator: INTERTWinE;

Topics of Mini-Projects on Novel Coding and I/O Techniques (Key Exascale Elements, PRACE site, Collaborators):

- Optimization, load balancing/task scheduling – PRACE: WCSS; Collaborator: E-CAM;
- Scalability, I/O and Storage – PRACE: CaSToRC; Collaborator: EoCoE;

Topic of Mini-Project on Energy Efficiency (Key Exascale Elements, PRACE site, Collaborators):

- Performance, energy usage – PRACE: ICHEC; Collaborators: READEX and EoCoE.

4. PRACE services

PRACE participates in various initiatives aimed at presenting HPC methods to a wide range of potential customers and stimulate their interest in these methods. The customers might come from distinct areas of interests: students, SMEs – all who can benefit from the HPC resources not only those provided within PRACE.

One group includes events and activities conducted periodically, like real and virtual meetings [5].

The second group includes all publications, training materials and tutorials.

Most of PRACE activities are collected on single hub for the PRACE training events [6].

4.1. PRACE Training Centers

PRACE operates ten PRACE Training Centers (PTCs) and they have established a state-of-the-art curriculum for training in HPC and scientific computing. PTCs carry out and coordinate training and education activities that enable both European academic researchers and the European industry to utilize the computational infrastructure available through PRACE and provide top-class education and training opportunities for computational scientists in Europe.

With approximately 100 training events each year, the ten PRACE Training Centers (PTCs) are based at the PRACE Training Center and cover basic and advanced needs across Europe.

The PRACE training centers are located at:

IT4I – National Supercomputing Center VSB Technical University of Ostrava (Czech Republic)

CSC – IT Center for Science Ltd. (Finland)

Maison de la Simulation (France)

Gauss Centre for Supercomputing (Germany)

GRNET – Greek Research and Technology Network (Greece)

ICHEC – Irish Centre for High-End Computing (Ireland)

Consorzio Interuniversitario, CINECA (Italy)

Barcelona Supercomputing Center (Spain)

SURFsara (The Netherlands)

EPCC at the University of Edinburgh (UK)

4.2. PRACE Schools

Seasonal schools

Offering top-quality face-to-face training events organized all around Europe.

The topics range from generic intermediate to advanced, covering programming techniques and more specialized topics.

Seasonal schools complement the PTC training program with three such events, usually held throughout the year. One is usually held in autumn, one in winter and one in spring. Each of these are held in a non-PTC country and at different geographical locations. Their curriculum is also different and usually varies from that of the TC events.

Summer School

The main goal of the Summer of HPC school is: to inspire the next generation of software engineers, system administrators, and general HPC users.

Summer of HPC is a programme that offers undergraduate and junior postgraduate university students the opportunity to spend two months of summer at a HPC center in a PRACE partner country. Students will undertake a project based on the outcomes of PRACE technical work or other work using the PRACE resources.

The programme aims to ensure a positive experience for all students and to encourage them in their path to become the next generation of HPC users. The programme aims to produce videos and visualizations to use in outreach activities. The programme also aims to generate interest in HPC and PRACE through social media.

Students over the age of 18 who are registered in an academic institution in European Union Member States or Associated Countries and PRACE member countries are eligible to apply. The desired applicants are late stage undergraduates or early stage postgraduates, with some coding experience and an interest in HPC. Advantages are a visual flair and/or interest in blogging or social media. Application instructions for the newest Summer School Call are available on the website [7].

All participants will be reimbursed for travel expenses (subject to a cap). Accommodation will be provided for participants. A daily allowance for living expenses is payable to participants. There is no salary associated with this programme.

There were 23 participants in the 2018 programme edition.

4.3. PRACEdays

PRACEdays is one of Europe's most important conferences on HPC in science and industry. Held annually in spring, PRACEdays conference programs are traditionally packed with high-level international keynote speakers and a broad range of many parallel sessions dealing with different HPC topics in science and industry.

The PRACE Scientific and Industrial Conference – PRACEdays was formed in 2014 through the merging of the PRACE Industrial Seminar and the PRACE Scientific Conference, formerly held at ISC. More information about the Industrial Seminars is available on the PRACE Website. Information on past PRACE Scientific Conferences held at ISC can be found there as well.

PRACEdays 2018 was held at ULFME – University of Ljubljana, Ljubljana, Slovenia on 29–31 May.

4.4. Massive Open Online Courses

PRACE has developed two Massive Open Online Courses (MOOCs) and these are hosted on the Future Learn Platform. As at the end of 2018 these are:

- **Supercomputing** This free online course will introduce the participant to what supercomputers are, how they are used, how their full computational potential can be exploited to empower scientific breakthroughs;
- **Managing Big Data with R and Hadoop** This free online course will introduce the participant to various high performance computing (HPC) facilities for big data analysis such as the R programming language and Hadoop, and how these tools can be used in the most efficient manner;

- **Defensive Programming and Debugging** A course to find information how to write a clean and robust code and to explore techniques to minimize the number of bugs during development.

All MOOCs are free and periodically re-run – opening for new enrollments at different times of the year. In addition, PRACE will also create new MOOCs.

Each PRACE’s MOOC attracts hundreds of participants from around the world.

4.5. Other services

CodeVault

PRACE experts have prepared and showed various examples and model solutions of common HPC programming tasks to be used in training and as building blocks of real-world applications.

The repository of Open Source code samples is placed on Github on the website: <https://gitlab.com/PRACE-4IP/CodeVault> with anonymous read access.

Best Practice Guides

Topics for the best practice guides include: optimal porting of applications (*e.g.* a choice of numerical libraries and compiler options); architecture-specific optimization and petascaling techniques; optimal system environment (*e.g.*, tunable system parameters, job placement and optimized system libraries); debuggers, performance analysis tools and a programming environment.

White Papers

A list of public whitepapers produced by the various tasks of PRACE projects. All PRACE White Papers are also available on OpenAire:

- Resource management and monitoring
- Evaluations on Intel MIC
- Benchmarking
- Libraries
- Parallel programming interfaces
- Application scalability
- Industrial Application Support
- Prototyping
- Visualization
- Meshing
- Publications
- PRACE Digest – Annual Summer

5. Polish Projects – Success Stories

The Polish scientific community is using the PRACE services and infrastructure whether through projects submitted to PRACE Calls for Tier-0 and Tier-1

Access, or through cooperation with PRACE experts within Preparatory Access or PRACE projects support services. Examples of projects carried out recently are presented below.

5.1. *High-precision nonadiabatic rotational states of hydrogen molecule*

Experimental spectroscopy continuously increases its capability for supplying highly accurate energy levels of atoms and molecules. In the particular case of the hydrogen molecule which has been a ubiquitous benchmark system since the very beginning of quantum chemistry, contemporary measurements have reached the accuracy of 10^{-5} cm^{-1} (relative 10^{-9}) for selected energy transitions. The complexity of the Schroedinger equation prevents its exact solution in a general multiparticle case and enforces approximations to be made. The most common approximation applied in solving the molecular time-independent Schroedinger equation is separation of electronic and nuclear variables (often referred to as the adiabatic or Born-Oppenheimer approximation). The main scientific objective of this project is to develop a variational method, based on four-body exponential wave functions, without introducing separation of the variables. Such an approach accounts for complete finite mass (nonadiabatic) effects. The first working scheme of such a method is already undergoing intensive tests in our laboratory. These tests allow us to anticipate that it will be possible to determine the eigenvalues of the four-body Schroedinger equation with the relative accuracy of 10^{-12} , which means improvement in accuracy by 2–3 orders of magnitude over the best currently available results. Reaching this unprecedented accuracy is a measurable effect of this scientific project. It is our goal to extend these capabilities to all bound rovibrational states of both homo- and heteronuclear isotopomers of the hydrogen molecule and create an ultimate database of their nonrelativistic dissociation energies. Obtaining this level of accuracy is possible when large expansions of the wave function are employed. This, in turn, involves large dense matrices for representing the Hamiltonian of the system. The main numerical effort of this project was to solve the general symmetric eigenvalue problem for such matrices.

The most time consuming part of an application is the matrix decomposition of quad-double float precision real elements. Basing on the chosen benchmarks, the LDL algorithm implemented in Elemental library scales very well on quad-double float precision real data.

The main goal of optimizing the application is to distribute it across many nodes to break the physical memory limits on a single node. The Elemental library (<http://libelemental.org>) – which is “open-source, openly-developed, software for distributed-memory dense and sparse-direct linear algebra and optimization which supports a wide range of functionality not available elsewhere” was the first option for the consideration. The most important achievement of optimized application based on the Elemental library was to allow the use of larger matrices, up to $22\,3380 \times 22\,3380$, *i. e.* almost 6 times more elements than original application could handle on the 256 GB node. The application performance also improved.

Comparing to the original application, the calculation time on 16-nodes was shortened by almost 12 times. It is worth mentioning that in the meantime the authors of the application optimized the original code using the Plasma library, which resulted in acceleration by about 7 times. Compared with the Plasma library, the memory distributed approach is about 1.7 times faster on 16-nodes compared with the Plasma based version run on a single node.

Project type: Preparatory Access Type-D;

Principal Investigator: Prof. Jacek Komasa, Adam Mickiewicz University, Poznan, Poland.

5.2. Abeta4: Computational study of tetramers of amyloid-beta peptides

The project aims at providing structural models of A oligomers, with and without Cu ions bound to the A peptides. The PI is focused on the type of binding put in evidence in vitro (the so-called component observed by the PI via electron spin resonance at physiological pH), already addressed in previous publications. This binding involves N and O of Asp 1, N1 of His 6 and N2 of His 13, the last one belonging to the same monomer of Asp 1 and His 6 or to a different monomer. The first topology is indicated as Cu-buried (a single Cu ion buried into a monomer), while the second topology is indicated as Cu-bridging, being a single Cu ion involved in a bridge of covalent bonds between two A monomers.

Contrary to the project proposal, the PI decided to start with structures of monomers and dimers already simulated by us, instead of starting from disrupting fibrillar seeds.

A number of 128 configurations of tetramers with composition [A]4, [Cu-A]4 and [Cu-A]2[A]2 were built starting from the most likely configurations of [A]2, [Cu-A]2 and [Cu-A][A] dimers, respectively. The PI also built [Cu-A]2 dimers with the Cu-bridging topology that had not been simulated yet. These dimers were compared to Cu-buried dimers of the same composition, built as in the case of tetramers.

We applied a multiple-walker metadynamics approach, using the altruistic method to combine into a unique statistical ensemble trajectories originating from different initial configurations. With this approach we built a unique bias potential based on the same collective variable, shared by all trajectories. We used the number of salt-bridges formed in the assembly, since this parameter was found to be able to discriminate between different molecular topologies in our previous work. The bias was not cancelled because histogram reweighting and free energy measurements in metadynamics require huge statistics. The biased trajectories, with and without Cu, are compared when the same bias is applied. This (and other related methods) is a promising strategy for high performance parallel calculation in the field of molecular statistics, when the object of study are such chemical perturbations (like Cu binding to the same peptide).

The accessibility of well managed high-performance computational infrastructures is a requirement to develop and apply models of the size suitable to address biological problems. In this project the PI applied a multiple-walker strategy, still at an approximate level, that is well suited for atomistic models in the size of 100 k-atoms in a simulation cell with sides of about 10 nm. The intrinsic disorder of proteins involved in the disease requires statistical models, where multiple configurations representing the same system are simulated in parallel, within the same statistical ensemble. Within this simulation frame, we can model the effects of chemical perturbations, like the Cu binding, on the protein assembly.

To apply this type of modeling, the assistance of HPC staff was essential for the two tasks: i) obtaining the best performance on a single compute node (mostly a compiling task, where the knowledge of the simulation software and hardware is required); ii) setting and managing efficient software for batch queue systems, equipped with modern job-arrays. Both these tasks were perfectly performed on the Eagle cluster in Poznan (PL).

Even if the original project was designed to perform on GPU nodes, the same achievements were possible using many-integrated core architectures.

Project type: DECI Tier-1 access;

Principal Investigator: Prof. Mai Suan Li, Polish Academy of Sciences, Institute of Physics, Warsaw, Poland.

5.3. Using GPU accelerators for parallel simulations in material physics

In this work a problem of electron–electron interaction systems was solved by diagonalizing a many-body Hamiltonian matrix in a basis of configurations of electrons distributed among possible single particle energy levels – a configuration interaction method [8]. A configuration interaction method is a universal method for quantum-mechanical many-body problems. It can be used in quantum chemistry, solid state physics [9–11], to quantum dots [12] and other nanostructures [13] in order to determine their electronic, magnetic and optical properties. In this particular project, we apply this method to find the many-body ground state of a system of a finite number of electrons occupying a topologically non-trivial energy band, which can lead to the appearance of a topological order (*i.e.* Fractional Chern insulators) [9–11]. To solve the problem of electron–electron interaction system the Modified Lanczos Method for the Two Particle Creation Annihilation Problem (MLM42PCAP) was implemented. The prepared GPU implementation improved the performance and scalability of solving the considered problem. During the technical work most promising routines of the Fortran [14] and OpenMP [15] code were identified and ported to the GPU accelerators using CUDA [16]. In many places OpenMP was also used to utilize processors and the final step was creating hybrid MPI+CUDA implementation.

The Tier-1 Polish infrastructure was used for testing. Initial versions for the use with OpenMP and GPU were developed and tested with the Nova system

(3 fat nodes with four sixteen core AMD Opteron 6274 processors with 256 GB of memory and two NVIDIA Tesla M2075 each), and at BEM cluster (with 720 computing nodes with 24-core Intel Xeon E5-2670 v3 2.3 GHz each, Haswell and 192 nodes with 28-cores Intel Xeon E5-2697 v3 2.6 GHz, Haswell each), both located at the Wrocław Centre for Networking and Supercomputing (WCSS). Final tests of the hybrid implementation were conducted at the Prometheus supercomputer at AGH Cyfronet Supercomputing Centre (Intel Xeon E5-2680 v3 processors with 24 cores each and clock at 2.5 GHz working under the Linux CentOS 7 operating system, 128 GB system memory and two Nvidia Tesla K40 XL).

The implementation work started from basic code improvements such as: the porting code from Fortran77 to Fortran90, code reorganization and refactoring. Some effort was also put in improving the implementation for the generation of configurations of electrons distributed among possible single particle energy levels. The next step was a compilation of the application using gfortran from the GNU compiler suite (v4.9.2) and a performance bottleneck analysis. The application was analyzed with the gprof (v2.20) tool. The medium size problem was taken as an example for performance tests. The interesting parts of the code were identified and implemented in several versions with the use of CUDA and MPI.

The project demonstrated the potential of using GPU accelerators for improving performance and scalability in material physics simulations. The prepared GPU implementation provides a significant increase in performance (speedup) in comparison with a parallel OpenMP base implementation. Further improvements were possible due to the nature of the problem by enabling code execution on multiple GPUs, as it was possible to perform independent computations for each subspace of the space of configurations. The multi GPU approach provided x10 speedup of computations with the use of two GPUs. The next step was to split the calculations between independent computing nodes with GPUs. The data was distributed within a set of MPI nodes which had 2 GPUs each. The hybrid MPI+CUDA approach results in a significant increase in performance – x40 speedup for execution with 16 MPI nodes. In conclusion, the proposed solution results in shortening the computation time and gives the possibility to simulate larger electron-electron interaction systems in future exascale HPC systems with GPUs.

Project type: Users community support services within PRACE-4IP and PRACE 2.0;

Principal Investigator: Paweł Potasz, Ph.D., Department of Theoretical Physics, Wrocław University of Science and Technology, Wrocław, Poland;

PRACE experts: Mariusz Uchroński Ph.D., Agnieszka Szymańska-Kwiecień, Mariusz Hruszowiec, Wrocław Centre of Networking and Supercomputing, Wrocław, Poland.

5.4. Task scheduling library for optimizing time-scale molecular dynamics simulations

This mini-project is conducted within the PRACE-5IP WP7.3 activity by WCSS and E-CAM Centre of Excellence [17] experts and is focused on the implementation of a new library in the Python programming language, taking advantage of its flexibility in optimizing the task scheduling.

The project targets some of the key workload requirements of E-CAM on the path to achieve the exascale. The E-CAM community has stated that it is the time scales and not the system sizes that are a common factor limiting the computing scale of their HTC applications (with non-independent instances). There is a large number of use cases within the E-CAM CoE target community where the same molecular dynamics application can be run many thousand times with varying inputs. The goal of the mini-project is to allow the scientific community to leverage the large-scale resources to efficiently manage this form of high-throughput computing. The goal is addressed by preparing a library for optimizing molecular dynamics simulations in terms of task scheduling for a particular use case of the OpenPathSampling (OPS) application. From the user perspective it is important to remove the requirement of interfacing with a resource manager system to manage the workload (and by that allowing the manager to work "in real-time" with the available resources). This is achieved by using the `Dask.jobqueue` library.

As computational resources become more powerful, path sampling has the promise to provide insight into rare events in larger systems, and into events with even longer timescales, for example:

- Drug/protein binding and unbinding (timescales of minutes) which is essential for predicting the efficacy of drugs;
- Association processes of proteins (large systems), which is at the core of communication in biochemical path-ways;
- Self assembly processes for complex systems (many intermediates), which can be important for the design of new materials.

In the particular use case for the mini-project described here, E-CAM is interested in the challenge of bridging timescales. Timesteps must be used on the order of a femto-second to study molecular dynamics with atomistic detail. Many problems in biological chemistry, materials science, and other fields involve events that only spontaneously occur after a millisecond or longer (for example, biomolecular conformational changes, or nucleation processes).

The Python scheduling library using the `Dask.jobqueue` library was implemented during the technical work. The JURECA Tier-0 system was used for development and experiment runs.

Two types of predefined clusters are provided:

- `ShortBatchCluster` – a custom cluster with the default parameters for the JURECA *batch* partition;

- ShortDevelCluster – the same configuration as ShortBatchCluster but on the *devel* partition.

The cluster represents some amount of computation resources (*i.e.* nodes in the HPC system). Computations within a Cluster are controlled with decorators `@task` (gets client from a cluster controller and submits a wrapped function to a given cluster) and `@on_cluster` (gets or creates clusters from a cluster controller).

Preliminary experiments were performed for a different number of nodes on JURECA. Two OpenPathSampling engines were tested: Toy Engine and OpenMM Engine. In general, for a small number of tasks, an increasing number of nodes results in increasing the speedup value. When the number of tasks is bigger the speedup value is decreasing (significantly for the OpenMM engine).

Finally, the outcome of this project will allow the E-CAM user community to leverage extreme-scale resources in a transparent way, with the use of algorithms that are optimized for addressing large times for rare event sampling.

Project type: PRACE-5IP WP7 T7.3 Mini-project;

CoE Collaborators: Alan O’Cais, E-CAM, Jülich Supercomputing Centre, Germany; David Swenson, E-CAM, Universiteit van Amsterdam, the Netherlands;

PRACE experts: Mariusz Uchroński, Ph.D., Adam Włodarczyk, Wrocław Centre for Networking and Supercomputing, Wrocław, Poland.

6. PRACE Roadmap

PRACE will continue to support the development of the European HPC ecosystem in accordance with ESFRI. It is being materialized in upcoming PRACE-6IP (Implementation Phase) by continuing the support for the world-class European PRACE HPC infrastructure. This includes its further expansion for both academia and industry, while providing state-of-the-art services that can be accessed by users regardless of their location. A unique catalogue of services is provided by PRACE 2 and complemented by services provided by the PRACE-6IP project.

Seven Tier-0 systems (JOLIOT-CURIE@GENCI, MARCONI@CINECA, Hazel Hen@HLRS, JUWELS@JSC, MareNostrum@BSC, Piz Daint@CSCS, and SuperMUC-NG@LRZ) will be offered by the five hosting member countries in 2019. The roadmap of PRACE Tier-0 systems foresees a total performance of more than 100 Pflop/s in late 2019. A key component for effective usage of the PRACE Tier-0 infrastructure is the ability for applications to use large parts of a Tier-0 system in an efficient way.

PRACE will extend its collaboration with the Centers of Excellence (CoEs) in HPC and establish a strong working relationship with the CoEs and other national and EU funded activities. It offers training and on demand events for other European initiatives, such as CoEs, HPC-Europa, EUDAT, ESFRI RIs, and ETP4HPC and possibly other research infrastructures in Europe.

As in the past, PRACE’s access to resources and corresponding support of users is solely based on scientific excellence or innovation potential. Outreach to industry and SMEs has been significantly addressed in the previous PRACE

Implementation Projects by calls for enabling support to SMEs (SHAPE). This will be continued and enhanced in the proposed project under the guidance of the PRACE Industrial Advisory Committee.

Most of the PRACE-RI members are also providers of national HPC services. PRACE-6IP will further build on these national activities to strengthen and extend the European HPC ecosystem. DECI Tier-1 calls will be integrated in PRACE-6IP.

PRACE-6IP will continue to coordinate the established HPC training activities on European level including the development of curricula of the PRACE Training Centers based on the input from engaged scientific and industrial communities, the CoEs and ETP4HPC. Along with MOOCs (Massively Open Online Courses), PRACE Seasonal Schools and PRACE on-demand events, they address the training requirements of academic users, industrial users and CoE participants. The new PRACE outreach to industry and the current outreach to university campaigns will focus on attracting more users from academia and industry.

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