PRACE 2.0 for Austria

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Abstract

PRACE (Partnership for Advanced Computing in Europe) is the premium European infrastructure, research, and training network for large-scale high performance computing. Among 25 European countries, also Austria has been from 2010–2015 member of PRACE and profited from access to its research infrastructure, scientific projects, and training and education events. In 2016–2020, PRACE will enter its next phase "PRACE 2.0". We describe the background of PRACE and its initial phase, the benefits of Austria's further participation in PRACE 2.0, and the contributions that are correspondingly required. By describing a number of projects from various Austrian scientific institutions, we demonstrate how the Austrian scientific landscape will profit from this participation.

Contents

1 PRACE Background

PRACE (Partnership for Advanced Computing in Europe) is an international non-profit association (aisbl) with seat in Brussels. It has 25 member countries whose representative organizations create a pan-European supercomputing infrastructure, providing access to computing and data management resources and services for large-scale scientific and engineering applications at the highest performance level [5].

History The members and founders of PRACE have been working together for more than a decade now. Building on EU funded initiatives since 2004 (HPCEUR, HET) and on the first Scientific Case for HPC in Europe, they started the PRACE Preparatory Phase in 2008, which resulted in the founding of PRACE aisbl in April 2010. The four "hosting members" (France, Germany, Italy, and Spain, see below) secured funding for the initial period from 2010 to 2015, while the PRACE Project partners continued to develop the brand and services of PRACE through three FP7-funded Implementation Phase projects. PRACE started with 21 members and grew to 25 by end 2012; several more governments are showing interest. The activities of PRACE are documented in annual reports [10].

Research Infrastructure Researchers and scientists (from both academia and industry) affiliated with PRACE member countries may for the purpose of basic research and development access six leading-edge high performance computing systems via regular calls and a peer-reviewed selection process [4]. These systems are provided and operated by four PRACE "hosting members" (the Barcelona Supercomputing Center BSC representing Spain, the Academic Consortium CINECA representing Italy, the Gauss Supercomputing Center GCS representing Germany, and the Grand Equipement National de Calcul Intensif GENCI representing France) [6]. In pace with the needs of the scientific communities and technical developments, systems deployed by PRACE are continuously updated and upgraded to be at the apex of HPC technology. Additionally, PRACE supports via various implementation projects and regular training activities users and user communities in porting, scaling and optimizing their applications to fully exploit the capabilities of the PRACE systems.

Funding PRACE receives funding from three sources:

- The PRACE HPC systems are funded and operated by the four hosting countries France, Germany, Italy and Spain. Their commitment for the establishment and operation of PRACE systems adds up to €400 million over a five year period (2010—2015).
- All 25 members of PRACE pay an annual fee; some of them provide national HPC resources as additional in-kind contributions.
- The European Commission supports the PRACE Implementation Projects for a total of €67 million under grant agreements RI-261557 (PRACE-1IP, 2010–2012), RI-283493 (PRACE-2IP, 2011–2013) and RI-312763 (PRACE-3IP, 2012–2014). These grants are complemented by a consortium budget of €43 million.

Austria and PRACE Austria is represented in PRACE by the Johannes Kepler University (JKU) Linz; the PRACE membership is currently jointly funded by the budgets of JKU Linz and the University of Innsbruck. Concretely Austria is represented in the PRACE Council (the body that decides on all matters of the association which is composed of one representative from each member) by Wolfgang Schreiner (RISC Institute, JKU Linz) and Michael Krieger (RISC Software); members of the Scientific Steering Committee (responsible for advice and guidance on all matters of a scientific and technical nature) are Christoph Dellago (University of Vienna) and Christian Lang (University of Graz). Information about PRACE relevant to Austrian researchers is available on a central Web page and mailing list [3].

2 PRACE Participation

Countries profit from the participation in PRACE

- by access to its research infrastructure,
- by cooperation in its implementation projects,
- by participation in its education and training activities,

and thus, all in all, by being linked to the *principal pan-European network for high-end computing activities*. These benefits are elaborated below in more detail.

PRACE Research Infrastructure PRACE systems are available to scientists and researchers from PRACE member countries through three forms of access:

- *Preparatory Access* is intended for resource use required to prepare proposals for Project Access. Applications for Preparatory Access are accepted at any time, with a cut-off date every three months.
- *Project Access* is intended for individual researchers and research groups including multi-national research groups and has one-year duration.
- *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.

Multi-year and Project Access are subject to the PRACE peer review process. Leading scientists evaluate the proposals submitted in response to the bi-annual calls [4].

PRACE Implementation Projects In three EU-sponsored implementation projects (PRACE-1IP, PRACE-2IP, and PRACE3-IP) partners have been collaborating to develop a long-term, high-quality infrastructure for European (Tier-0) systems, managing the coordination between the shared portion of the national (Tier-1) HPC resources, and also strengthening the established relationships with industrial users. In particular, the following four activities are central in the current PRACE3-IP [9]:

- *Pre-Commercial Procurement:* Pilot exercise for a joint procurement and joint ownership of innovative HPC prototypes, focusing on high-energy efficiency.
- *Deployment of HPC services for European industry:* Proposes a broad set of services suitable for use by industry, including access to HPC resources, knowledge transfer through application support, training and expertise.
- *Application scaling and support to address major socio-economic challenges:* Tackles major socio-economic challenges and the use of simulation and modeling to deal with them.
- *Training and outreach for growth:* Establishes a broad training and outreach activities specifically designed to engage more user communities, including industry, in the use of HPC systems.

This goal is approached via various networking activities (including dissemination and training), service activities (e.g., supporting applications on Tier-0 and Tier-1 systems), and joint research activities (including development of software prototypes).

PRACE Training and Education PRACE undergoes an extensive education and training effort for effective use of HPC systems by six PRACE Advanced Training Centres (PATC), quarterly seasonal schools, and regular workshops and scientific and industrial seminars throughout Europe. Seasonal Schools target broad HPC audiences, whereas workshops are focused on particular technologies, tools or disciplines or research areas [8].

In 2014, PRACE will organize its first Scientific and Industrial Conference, the first edition of the "PRACE Days", under the motto "HPC for Innovation —- when Science meets Industry". The conference combines the previously separate PRACE Scientific Conferences and PRACE Industrial Seminars and will bring together experts from academia and industry who will present their advancements in HPC-supported science and engineering [7].

Austrian Participation Since 2011, Austrian researchers have been granted access to the PRACE research infrastructure in the frame of the following projects (joint collaborations with multiple international partners):

- MHD turbulence in the Interstellar Medium: Linking Star Formation and Galaxy Dynamics (Austrian collaborators from University of Vienna),
- Modeling gravitational wave signals from black hole binaries (Austrian collaborators from University of Vienna),
- CAMEL — CArdiac MechanoELectrophysiology (Austrian collaborators from Medical University of Graz).

The rewards granted to these projects amounted to approximately *32.5 million core hours* (which would keep a 1024 core machine busy for 3.5 years) on various of the PRACE high-performance systems.

Various institutions of JKU Linz (ICA, RISC Institute and Software) have participated since 2010 in the three PRACE implementation projects.

- In the former project PRACE-1IP and PRACE-2IP, ICA investigated topics in advanced computer systems design, including parallel systems and acceleration technologies, from hardware to software. The goal was the principled development of system architectures and components that push the boundaries of high performance compute fabrics and simplify their use and programming environment.
- In the current project PRACE-3IP, RISC is engaged in work packages WP 3 (dissemination and outreach), WP 4 (training), WP 7 (application enabling and support). For instance, within WP 7 researchers of RISC have coordinated the project "Multidiscipline Simulations for Aircraft Design" on the coupling of computational fluid dynamics (CFD) code and computational structural mechanics (CSM) code for high-performance simulation systems.

As for training and dissemination activities, the PRACE 2014 Spring School on "Software Engineering for Supercomputers in Research and Industry" was organized in Hagenberg, Austria, from April 15-17 with an international audience of 40 trainees (with 7 of the 12 speakers/trainers and approx. 50% of the trainees from Austria) [2]; similarly Austrian participants have participated at various foreign seasonal schools and training events.

3 PRACE 2.0

PRACE is currently planning the next phase *PRACE 2.0* (2016–2020) of its operation (with PRACE 1.0 representing the initial phase 2010–2015). Part of the preparation of this phase is the elaboration of a proposal for the EU Horizon 2020 call for "e-Infrastructures" (budget: € 82 million) for which the PRACE partner will make a bid in September 2014 [1].

As a major change to the "business model", in PRACE 2.0 the costs for the development of the infrastructure (which was in PRACE 1.0 essentially covered by the four hosting members) will be shared between the hosting members and the general partners. The currently discussed PRACE 2.0 model (status: May 6, 2014) is based on the following principles:

1. An annual fee of € 60 000 of every member will contribute to the general PRACE operation (in addition to European projects in the frame of Horizon 2020).
2. There will be three categories of members:
   a) full members that host Tier 0 systems for PRACE,
   b) full members that do not host such systems, and
   c) associate members

   (see below for the definition of a Tier 0 system).

   Associate members will not contribute to the investment of PRACE 2.0 systems and have no voting rights in the PRACE council. However, they can participate in PRACE 2.0

projects and they will be invited to apply for the use of PRACE 2.0 systems, but with a limit of 1% usage for each of them.

3. The PRACE 2.0 infrastructure will consist of a certain number of "Tier 0 systems" which are broadly defined as

   > *high performance supercomputers that are much more powerful than national machines and could not be afforded by individual countries alone.*

   The general criteria of such a machine are

   - at least 10 PFLOPS performance,
   - about € 50 million hardware investment.

   The total cost of ownership (TCO) over a five year period is estimated to be twice the hardware investment (i.e., it is evenly split between investment and operational costs).

4. Full members contribute to the TCO based on a index that averages the corresponding nation's GDP and the past usage of that system in comparison to all other members. For full members that host PRACE systems, this index is weighted with a factor of 3; for the other full members the weight factor is 1.

   The sum of the weighted indices of full members is currently estimated at 206.4; Austria is assigned an index of about 1.1 which would mean a contribution of about 0.53% to the TCO of the PRACE 2.0 systems.

5. Current estimations for realistic investments run from two to four Tier-0 systems yielding a TCO of about € 200–400 million over a five year period; thus according to above criteria as a full member Austria's total contribution would be € 1–2 million. Austria's yearly contribution to the TCO would be € 200–400 thousand for a period of five years.

Since the discussion among PRACE members is still ongoing, above figures are only preliminary estimations but give a range within which the final figures will most probably reside. In a nutshell, we have the following result:

> **The total cost of Austria's participation in PRACE 2.0 as a full member that does not host a Tier 0 system is in the range of**
>
> **€ 260 000–460 000**
>
> **per year for a period of five years (2016–2020).**
>
> **For this investment, Austria gets access to 2–4 Tier-0 (European level) HPC systems with a total performance of at least 10 PFLOPS each; the amount of access is limited by scientific excellence (as measured in the success in the corresponding project calls) only. Furthermore, Austria is by this investment linked to the premium European research and education network for large scale high performance computing with corresponding profits for its scientific and industrial institutions.**

In comparison, the fastest HPC system in Austria, the soon to be installed VSC-3 at the Vienna Scientific Cluster [11], has a performance of about 0.584 PFLOPS; this Tier-1 system thus achieves less than 6% performance of a single of the planned PRACE 2.0 Tier-0 systems. Access to such European Tier-0 systems (in addition to that of national Tier-1 systems) is for many activities indispensable:

1. Project grants in PRACE 1.0 were typically in the region of about 10–100 million core hours; similar figures can be expected for PRACE 2.0. A typical 50 million core hours grant would occupy the biggest Austrian machine (the VSC-3 with 28 096 cores) busy for 74 days, which makes the execution of such jobs on a Tier-1 system unrealistic.

2. The number of processor cores in a Tier-0 system is an order of magnitude larger than that of a Tier-1 system (the Munich SuperMuc system currently employed in PRACE has more than 155 000 cores). With Tier-0 therefore scalability experiments can be performed in a range that is not possible with Tier-1 systems.

3. The PRACE 2.0 infrastructure provides access to multiple systems with different architectures and performance characteristics. Past experience shows that not all applications perform well on every system; thus access to different systems allows to run a much wider range of applications in an efficient way.

4. The economy of scale of running a Tier-0 system provides several advantages: apart from reducing the general overhead of operation, it allows to bundle a comparatively much larger amount of human expertise with respect to the efficient utilization of a system which can be shared with its users.

As documented in the appendices, there are many Austrian high quality research projects that will profit tremendously from a participation in PRACE 2.0. Taking into account the status of Austria as a research-oriented industrial country and comparing it with other European countries of the same status (Germany has 18,63% GDP among PRACE members and used 20.81% of the PRACE resources in the past), also researchers from Austria (2,14% GDP) will be able to profit from access to a corresponding share of this modern European research infrastructure as well as from being linked to the premium European research and education network in large-scale high performance computing.

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Potential PRACE 2.0 Projects

A Your Project Title

Proposer

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Topic

A general overview on the contents of your project including citations.

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Previous Work

What you previously did in this topic; what computational resources you used (in PRACE 1.0, in Austria, and elsewhere).

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Planned PRACE Activites and Infrastructure Access

Why you want to participate in PRACE, what you plan to do in your project, what computational resources you need and to which extent for this access to the PRACE infrastructure is needed (be as concrete as possible).

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