



“Advancements in PetaFlop Computing” Report on DEISA PRACE Symposium 2010

Wolfgang Gentzsch

For the second time, the two large European supercomputing projects DEISA (the Distributed European Infrastructure for Supercomputing Applications) and PRACE (the Partnership for Advanced Computing in Europe) jointly organised their annual science conference, the DEISA PRACE Symposium in Barcelona, May 10 – 12, 2010, and hosted by the Barcelona Supercomputing Center (BSC). The Symposium attracted over 130 participants from 23 countries from Europe, America and Asia. Scientific users, HPC technology experts and vendors, government representatives and industry partners.

The Symposium took place at the famous *Casa Milà*, better known as *La Pedrera* (Catalan for ‘The Quarry’). The beautiful building was designed by the Catalan architect Antoni Gaudí and is located in the heart of Barcelona.

The symposium was structured into five main areas: World-Wide Perspectives, DEISA PRACE Updates, Challenges in Computational Science, Technology for the Future, Collaboration between DEISA, PRACE, and TeraGrid, and selected results from the DEISA Extreme Computing Initiative (DECI).

World-Wide Perspectives

Prominent keynote speakers from all over the world started with the global perspectives of High Performance Computing (HPC) in the Petascale era of supercomputers for grand-challenge scientific research. Speakers on the first day included **Montserrat Torné** from the Ministry of Science (Spain); **Kostas Glinos** from the European Commission; **José Muñoz** from the NSF Office of Cyberinfrastructure (USA); **Akira Ukawa** from the University of Tsukuba (Japan); **Thomas Zacharia** from the Oak Ridge National Laboratory (USA); and **Catherine Rivière** from GENCI (France). In the following, we sketch a few of their key messages, and we recommend to visit the DEISA website for their detailed presentations.



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Montserrat Torné, Director General for International Cooperation and Institutional Relations of the Ministry of Science in Spain, presented conclusions of the European conference on research infrastructures (ECRI2010) and their influence on HPC. Main findings were that research infrastructures (RIs) are essential to develop the European Research Area (ERA) and address grand challenges under the EU 2020 strategy. A European policy has been developed in the field of RI in recent years, and the work of ESFRI has been crucial in this context. Finally, to be well prepared for the future, a closer partnership between the Member States and European Commission is needed with ESFRI providing an important bridge function.

Kostas Glinos, Head of Unit GÉANT & e-Infrastructures, at DG INFSO of the European Commission, was highlighting HPC from a European Perspective, aiming at staying competitive in science. In 2009 the Competitiveness Council stated that Member States and the Commission should pool investments under PRACE, in order to strengthen the position of European industry and academia in the use, development and manufacturing of advanced computing products, services and technologies. Europe is on its way to build a competitive HPC ecosystem, consisting of Tier-0 (PRACE1) resources, Tier-1 (DEISA and PRACE2) infrastructure, including the HP-SEE and Link-SCREAM2 projects, and the Tier-2 grid layer with EGI and numerous other grid projects.

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This e-Infrastructure ecosystem will provide the platforms for data and computation-intensive collaborative science. Glinos concluded that HPC now becomes part of EU policy, with DEISA and PRACE delivering tangible results. However, the impact of “tier 0” HPC beyond science needs further substantiation, and a comprehensive EU strategy for HPC still has to be developed.

José Muñoz, Acting Director of the Office of Cyberinfrastructure at the US National Science Foundation looked at high-performance computing and the cyberinfrastructure ecosystem. He demonstrated with many recent simulation results how science is radically revolutionized by Cyberinfrastructures. But at the same time, we are facing five grand challenges on our way to exascale: new computing technologies such as multicore, programming models, and paradigms (clouds, grids, etc.); data, provenance, and visualization; software; multi-disciplinary computational science; and education (how do we develop a workforce to provide leadership, expertise, and support?). Then he discussed the different components of a cyberinfrastructure ecosystem: organizations, scientific instruments, data, networking, computational resources, software, and expertise, and he highlighted specific projects in each of these areas in the US on the way to exascale computing, like Blue Waters, Gordon, and FutureGrid, forming the end-to-end integrated cyberinfrastructure that will further drive science innovation.

Akira Ukawa, Vice President of the University of Tsukuba in Japan presented an update on the NGS next-generation 10-petaflops supercomputer project and the future of high-end computing in Japan. The government’s 4th Science and Technology Basic Plan 2011-2015 consists of exaflops class HPC technology, including new chip device, software, and hardware. Goals are to develop a 10 pflops-class system and grand challenge applications in nano science and life science, to federate the 10 pflops-class and other supercomputers installations throughout Japan, and to build a research center in computational science around the 10 pflops-class system.

Thomas Zacharia, Deputy Director at the US Department of Energy’s Oak Ridge National Laboratory, described the world’s bold move from terascale to exascale computing - the latter expected to become a reality in about 2018 – 2020. One of his main findings was that already today with real petaflops

performance we now have access to length scales, time scales, and numbers of particles that can transform science! And he presented a few impressive results from turbulence, nuclear energy, bio fuels, nano science, energy storage, and fusion energy, which demonstrate scientific progress at petascale, and that exascale computing has the potential to further stimulate innovation.

Catherine Rivière, from the French HPC organization for ‘Grand Equipment National de Calcul Intensif’(GENCI), closed the day with her presentation on the European Exascale Software Initiative, EESI, which is coordinating the European contribution to the International Exascale Software Project (IESP). Both projects are based on the general awareness of the steep ascent from terascale to petascale to exascale. The two projects IESP and EESI are aiming at “improving the world’s simulation and modelling capability by improving the coordination and development of the HPC software environment.” The main goal of EESI is “to build a European vision and roadmap to address the challenge of performing scientific computing on the new generation of computers which will provide multi-Petaflop performances in 2010 and Exaflop performances in 2020.”

DEISA and PRACE Updates

The second day began with two project updates for PRACE and DEISA. **Thomas Eickermann** from the Research Center in Jülich summarized the main achievements of the PRACE preparatory phase: among others, 400 Mio € funding have been secured for the next 5 years from France, Germany, Italy, and Spain. Also, the decisions about additional 200 Mio € from The Netherlands and UK are expected soon. The architectures for the Tier-0 systems were identified (the first one an IBM Blue Gene/P in Gauss@Jülich). The 2-year PRACE Implementation Phase Project will start in July this year with 20 European partners and with a budget of 28.5 Mio € (20 Mio € EC funding). An overview on seamless services and ecosystem integration concluded his talk.

Hermann Lederer from the Garching Computing Centre of the Max Planck Society gave an update on the DEISA Extreme Computing Initiative (DECI), with now its sixth DECI call in 2010 for (multi-national) proposals for complex, demanding, innovative science simulations. Over the last five years, the number of proposals increased from 51 with 30 mio



cpu-hours, to 122 proposals with 570 mio cpu-hours requested, with over 180 research institutes and universities involved from 25 European countries. The demand for cpu-hours increased at a much faster rate than the supply. Recently, more and more virtual communities are supported, in the areas of life sciences, climate research, space science, and fusion energy research.

Challenges in Computational Science

In the next session, under the umbrella of ‘Challenges in Computational Science’, the symposium featured speakers from different science communities which are supported by DEISA and are planning to use the PRACE petaflop systems. The science fields covered in these talks were astrophysics, materials science, earth sciences, fusion for energy, and life sciences.

Wolfgang Hillebrandt from the MPI for Astrophysics in Garching presented an amazing set of videos showing very large scale supercomputer simulations about supernovae, core-collapse supernovae and gravitational waves, thermonuclear supernovae, and supernova cosmology. It was impressive to see that several important discoveries over the last 15 years were directly related to very challenging simulations on very different time and length scales. **Thomas Schulthess** from ETH Zurich and the CSCS in Manno reported on ‘Ab Initio calculations of free energies in nanoscale sys-

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tems’. **José Maria Baldasano** from the Earth Sciences Department of the Barcelona Supercomputer Center presented computation and data in an Earth system modelling framework. **Laurent Villard** from the EPFL in Lausanne talked about HPC simulations of magnetic fusion plasmas. And **Ivo Gut** from the Centro Nacional de Analisis Genomico in Spain discussed informatic issues of Genomics.

Technologies for the Future

The last session of that day was dedicated to “Technologies for the Future”, starting with programming models and tools, presented by **Jesus Labarta** from Barcelona Supercomputing Center. **Ana Bela Dias** from NCF National Computing Facilities Foundation explained the early access to PRACE systems, starting with a Call for Proposals in May this year, for run time allocated on the JUGENE IBM BlueGene/P at FZJ in Jülich. Finally, in this session, **Herbert Huber** from Leibniz Computer Center LRZ provided an outlook to emerging and future technologies.

The third day started with a presentation featuring the close collaboration between DEISA and the US TeraGrid project. **Shantenu Jha** from the Louisiana State University reported on ‘accurate and precise patient-specific treatment using large-scale free energy calculations’ addressed through a joint project with Peter Coveney, University College London, DEISA and TeraGrid.

In the following nine computational science grand-challenge projects from all over Europe were presented, with six of them from the DEISA Extreme Computing Initiative,: **Richard Kenway** on ‘Solving the mysteries of Quarks’; **Stephan Stellmach** on ‘Turbulent transport in buoyancy-driven geophysical flows’; **Roel Verstappen** on ‘Regularizing isotropic turbulence’; **Marco Bernasconi** on ‘Ab-initio study of GeSbTe phase change alloys’; **Stefan Gottloeber** on ‘The small-scale structure of the Universe’; **Philip Eric Hoggan** on a ‘Slater type orbital project for Quantum monte carlo large molecule simulations’; **Patrick Joeckel** on ‘Coupling the chemistry in Earth system models on multiple scales’; **Vassilis Theofilis** on ‘Global instability analysis of turbulent separated flows’; and last but not least, **Sandor Katz** on ‘Lattice QCD thermodynamics with improved dynamical fermions’.

Looking back, in summary, this year’s symposium was covering a vast spectrum from valuable presentations, intensive networking, great food and drinks, all mixed together nicely by a perfect host, the Barcelona Supercomputer Center BSC. Thank You !

The presentations from the symposium are available on the DEISA and PRACE web sites at: www.deisa.eu/news_press/symposium/barcelona2010 and www.prace-project.eu/documents

New DEISA publication: DEISA Digest 2010

The new DEISA Digest 2010 was published on 10th of May 2010. DEISA Digest 2010 presents articles about the key results of the research projects carried out using the DEISA research infrastructure during the recent years. It includes 15 popular science articles. The DEISA Digest 2010 is available online as a pdf at:

www.deisa.eu/news_press/DEISA_DIGEST2010.pdf

Or if you prefer reading a printed version, order your free copy from heli.autere@csc.fi

