NEWSletter

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New insights into using "the process that powers the stars" with PRACE resources

Minna Keinonen

Turbulence simulations, carried out in the framework of the PRACE Research Infrastructure, have provided new insights into the fundamental processes of turbulent transport. This research is contributing to the understanding and optimisation of magnetic confinement in fusion devices.

Ultimately, the goal is to be able to make predictions for ITER, an international flagship fusion experiment being built in Southern France.

"The research conducted in our team is part of a world-wide effort to understand and predict turbulent transport in magnetically confined fusion plasmas. Our work is contributing to a better grasp of the underlying processes and helping to establish predictive and control capabilities," tells Professor **Frank Jenko** at the Max Planck Institute for Plasma Physics (IPP) in Garching, Germany.

Professor Jenko headed the team from several European research institutes, including the IPP, the Ecole Polytechnique Fédérale in Lausanne in Switzerland and the University of Oxford in England.

CO2 free energy

Nuclear fusion is a promising carbon-free option to meet the increasing global demand for electricity in the future. A world-wide consortium including the European Union is currently constructing the flagship fusion facility ITER, one of the most challenging scientific projects ever undertaken. Construction of the facility began in 2007 and the first plasma is expected in 2019.

"We hope that ITER will, in a few years, help us to demonstrate the physical feasibility of power plants based on fusion which is the process that powers the stars. Given the predicted rise in energy demands over the next few decades, the world will need safe, carbon-free power plants. The fusion of magnetically confined hydrogen plasma at a temperature of 100 million degrees offers a very interesting way of meeting these challenges."

In order for ITER to achieve its main goal – the creation of a self-sustaining or "burning" plasma – the unavoidable heat losses induced by turbulent flows have to be kept in check.

Turbulence to be unravelled

Understanding turbulent flows and their behaviour is a challenging task.

"Turbulence has often been called one of the most important unsolved problems of classical physics," states Professor Jenko.

Many famous physicists have attempted to tackle turbulence using analytical tools but with only limited success. Today, modern supercomputers offer a different approach to investigating these phenomena.

"We can make progress in this area by state-of-the-art simulations on some of the world's most powerful supercomputers. Simulations are especially useful for studying turbulence in hot plasmas, which must be described by means of five-dimensional kinetic models."

A single simulation aiming to be as physically comprehensive as possible could take several months or even a year, if run on medium-size computers. With PRACE offering the most powerful hardware available today in Europe, investigation of turbulence becomes feasible in a reasonable time.

"We have performed plasma turbulence ab initio simulations with the sophisticated plasma turbulence GENE code on the JUGENE

gene.rzg.mpg.de GENE

Snapshot from an ab initio simulation of the ITER-like fusion device ASDEX Upgrade with the sophisticated plasma turbulence code GENE.

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supercomputer, which is one of the Tier-0 systems of the pan-European PRACE Research Infrastructure. It lets us investigate important physical effects at a level that had not been possible before. These simulations are closely linked to the ITER experiment."

Correlation between turbulent transport and size of device

"For the first time, physically comprehensive turbulence simulations of the fusion experiment device ASDEX Upgrade in Garching could be performed over time scales that are comparable to the duration of an actual discharge. ASDEX Upgrade is conceptually very similar to the ITER facility, although smaller by a factor of four in its linear dimensions," Professor Jenko points out.

A further set of simulations helped to develop a better understanding of how turbulent transport depends on the size of the device.

"This is a crucial question because transport sets the energy confinement time, which is a key factor when determining the expected performance of the fusion device."

Ongoing work

"Following up on these successful simulation campaigns and building on the ongoing improvements in the employed software and hardware, the time seems right to finally tackle a long-standing enigma of plasma turbulence research. This is the formation of so-called transport barriers – radially extended regions in which the turbulent transport is suppressed by about an order of magnitude. This effect greatly improves plasma confinement and is therefore highly desirable. However, it currently still lacks a satisfying theoretical explanation, which is necessary for reliable predictions to ITER."

Professor Frank Jenko, Max Planck Institute for Plasma Physics.

And the winning paper is… the PRACE Award 2011

The PRACE Scientific Steering Committee (SSC) selected the winner of the PRACE Award in 2011. The award was presented at ISC'11 (International Supercomputing Conference) in Hamburg.

This year's PRACE Award goes to the paper titled "*Astrophysical Particle Simulations with Large Custom GPU Clusters on Three Continents*" signed by a group of authors: **R. Spurzem, P. Berczik, T. Hamada, K. Nitadori, G. Marcus, A. Kugel, R. Manner, I. Berentzen, J. Fiestas, R. Banerjee** and **R. Klessen**.

All papers that were submitted to ISC'11 Research Paper Sessions were reviewed by the PRACE Scientific Steering Committee.

"This paper is an excellent example of what can be achieved through international and interdisciplinary collaboration to exploit new HPC technologies", says Prof. **Richard Kenway**, Chairman of the PRACE Scientific Steering Committee.

"Astrophysicists and computer scientists in Germany and China demonstrate nearly linear strong scaling on up to 170 GPUs at a third of peak performance for large-scale simulations of dense star clusters using machines in Europe, China and the USA. The work points the way to exploit exascale technologies for problems at the forefront of science", Kenway continues.

The PRACE award was presented to **Peter Berczick** and **Guillermo Marcus** at ISC'11. The winner will receive sponsorship for participation in a training event or a conference relevant to petascale computing.

Presentations from ISC'11 BoF:
www.prace-ri.eu/ISC-11-E-infrastructure-for

More images from ISC'11:
www.prace-ri.eu/ISC-11-19-23-June-Hamburg-Germany

The PRACE Award 2011 was presented at ISC'11 to Peter Berczick and Guillermo Marcus by Prof. Richard Kenway (right), the Chairman of the PRACE Scientific Steering Committee. © ISC

PRACE offers optimisation service for researchers

PRACE provides researchers an unique opportunity to improve the parallel performance of application codes with the help of experts from PRACE centres. As an outcome of optimisation project, researchers should be ready for large scale production usage of PRACE resources.

Proposals in the PRACE Regular calls have to show good parallel scaling of the application code. Currently scalability requirement is at least 8192 CPU cores in the JUGENE system, and at least 2048 CPU cores in the CURIE and HERMIT systems.

Some applications codes are capable of required parallel scaling as such, but for many software packages further optimisations are needed in order to reach the scalability requirements. As the optimisations can be non-trivial for the users of the application code, PRACE provides support for optimisation and petascaling.

PRACE experts provide help

Depending on the application code, the PRACE experts can provide help for example in the following tasks:

•Understanding the scalability bottlenecks through extensive profiling of the application code

•Improving the present communication schemes

•Implementing additional parallelisation strategies, for example a hybrid thread/MPI parallelisation

•Improving the I/O for example through the use of parallel I/O

Continuous call for proposals

The PRACE optimisation service is available through the **PRACE Preparatory Access** call. Currently, there are three types of preparatory access (A, B, and C), and the optimisation support is provided for **type C** projects. Proposals for type C preparatory access can be submitted continuously, and the proposals are evaluated every two-three months.

Successful type C preparatory access projects receive access to relevant Tier-0 system(s) for 6 months, together with CPU time for test and development. Each project gets assigned a contact person from PRACE who will be responsible for the PRACE optimisation work. Additional PRACE staff may be involved in the actual optimisation.

The maximum amount of PRACE support for type C preparatory access projects is 6 person months. PRACE staff will work in close collaboration with the applicant in all stages of the project. In the end of the project, applicant has to write a report in collaboration with the involved PRACE experts.

A successful type C preparatory access proposal has the following features:

•A good potential for Tier-0 scalability. Thus, existing scalability data should be provided for high enough number of processor cores. As an example, it is not very likely that scalability can be improved from 32 to 2048 CPU cores in a short project, however, improvement from 512 to 4096 CPU cores is much more feasible.

•A detailed work plan. In the optimum case, applicant has already good information about the scalability bottlenecks of the application code, even though that is not strictly required.

•The performed optimisations should benefit a larger user base. Thus, open-source application codes are preferred over commercial codes.

Remarkable benefits

The writing of preparatory access proposal is relatively light-weight process, while the benefits of successful project can be quite remarkable.

As an example, mesh subdivision of computational mechanics code Alya was parallelised in PRACE preparatory access project. The optimisation project achieved good parallel scalability, and the previous bottleneck for large scale calculations was thus removed.

The next evaluation cut-off dates for preparatory access proposals are **1 December 2011**, **1 March 2012**, and **1 June 2012**. We would like to encourage all researchers interested in better utilisation of PRACE resources to submit a type C preparatory access proposal.

More information about PRACE calls:
www.prace-ri.eu/hpc-access

Hungary joins PRACE

PRACE got a new member country as Hungary joined the PRACE Research Infrastructure on 8 June 2011.

The overall number of partners in the PRACE Research Infrastructure has increased to 21 countries. The Memorandum of Understanding was signed on 8 June 2011 Paris.

"PRACE welcomes Hungary as its 21st member. This is another major step in involving the new European Union member states in this important endeavour. It demonstrates both the attractiveness of PRACE and its commitment to provide service to and cooperate with all Europeans. We are looking forward to cooperate with our new colleagues in Hungary which shall foster our HPC-competence in Europe", said Prof. Dr. **Achim Bachem**, Chairman of the PRACE Council.

The following countries collaborate in PRACE: Germany (project coordinator), Austria, Bulgaria, Cyprus, Czech Republic, Finland, France, Greece, Hungary, Ireland, Italy, The Netherlands, Norway, Poland, Portugal, Serbia, Spain, Sweden, Switzerland, Turkey and UK.

HPC programming at the PRACE Summer School

Anni Jakobsson

PRACE Summer School was arranged at CSC, Finland on 29 August – 1 September 2011.

The school was hosted by CSC – IT Center for Science Ltd. and co-organised together by CSC and SNIC/PDC-Center for High Performance Computing at KTH.

"We had 38 students from Europe and the USA. In addition, there were 10 lecturers and 6 organisers", tells CSC's Head of education, outreach and training **Pekka Manninen**.

In this four-day event the participants learned advanced parallel programming skills, which are necessary for taking the most out of the largest (Tier-0) supercomputers the PRACE Research Infrastructure is offering for European scientists and engineers.

The speaker list included **William Gropp** (University of Illinois Urbana-Champaign), one of the key authors of MPI (Message Passing Interface) programming paradigm, who talked about advanced features of the MPI; and **Rolf Rabenseifner** (HLRS), one of the most renown researchers of hybrid parallel programming models. The largest supercomputers in Scandinavia, i.e. the brand new Cray XE6 system at PDC/KTH and CSC's Cray XT4/XT5 system Louhi were in disposal of the participants.

Reconstructing 3D images

One of the students of the school was **Taha Sabri Koltukluoglu** from Technical University of Munich. He is a diploma student in Computer Science, currently working on his diploma thesis in the laboratory of Machine Vision and Perception Group of the Robotics Laboratory. He got familiar with PRACE at the International Supercomputing Conference 2011 (ISC'11) in Hamburg.

"Afterwards I was interested in reading more about PRACE at the internet, where I stumbled into the PRACE Summer School", he tells.

He is conducting research in the field of Computer Vision, especially 3D reconstruction and image registration.

"The work is about creating 3D images from monocular image sequences with moving light source. The work does not depend on any features to be segmented from the images, but only on the intensity values, including the alignment of participating images from the sequence – thus intensity-based image registration, to define the three-dimensional modal of the region of interest."

This type of reconstruction can be applied e.g. in medical endoscopy. Creating such images needs massively parallel architectures such as GPUs or GPU clusters.

Aiming to use GPUs

Mr. Koltukluoglu found the PRACE Summer School very useful.

"I learned a lot of fine issues. From the parallel programming point of view, I actually apply GPUs only to accelerate the scientific calculations of my diploma thesis. In the PRACE Summer School, I had the chance to practice on other parallel programming paradigms such as Message Passing Interface and OpenMP, and I learned more about hybrid programming. I was allowed to run the exercises on both CPU and GPU clusters. I have always been interested in these issues, but never had the time nor hardware to start practicing. I will continue that, and now I am especially more interested in hybrid MPI/CUDA solutions."

He is considering applying for the PRACE RI resources in the future.

"I would definitely like to go for GPU clusters. 3D reconstruction consists in most cases of dense mathematical inverse problems – especially iterative reconstruction approaches are computationally challenging. The potential of such approaches to be divided in sub parallelisable processes make them a top candidate for GPU clusters. Therefore I would consider the use of PRACE services in the future."

During the intensive four-day school he didn't have a lot of time to see Helsinki, but he liked it.

Taha Sabri Koltukluoglu was one of the students at the PRACE Summer School 2011. © PRACE

"Helsinki is a great historical city. At this point I want to thank to PRACE organisers for providing us with a very special sightseeing on Suomenlinna Fortress Island with historical background. I was fascinated."

The next PRACE seasonal school will be arranged in France in October 2011.

Training videos from the school will later be available at:
www.prace-ri.eu/training

38 students from Europe and USA took part to the PRACE Summer School 2011. © PRACE

Training jointly with HP-SEE and LinkSCEEM-2

The HPC Summer Training, jointly organized by PRACE, HP-SEE and LinkSCEEM-2, was held on 13 – 15 June at the training Center of the Hellenic Telecommunications Organization (OTE Academy) in Athens, Greece.

It gathered 55 researchers from 15 countries working in the wide variety of scientific disciplines including for instance: computational physics, life sciences, computational chemistry, engineering, computer science, earth sciences.

Main goals of the training were to enhance the knowledge of current HPC users, engage new user communities in the use of HPC infrastructure.

During the three days of training participants learned about methods and tools that are necessary for developing highly efficient HPC application and optimal usage of the available computing resources.

The main subjects that were covered in the training sessions were advanced modules in MPI, OpenMP, Hybrid Programming, CUDA Programming, Profiling Optimization and Benchmarking. Every module was accompanied with the hands-on sessions where participants had the chance to try out the HPC resources provided by IPB and IICT-BAS trough a series of examples and exercises.

The training was complemented with the Introduction to IBM Blue Gene and WS-PGRADE/gUSE, and it was preceded by the LinkSCEEM-2 session where the project, its user support system, sites, users and activities were presented.

Training material is available at: http://indico.ipb.ac.rs/conferenceDisplay.py?confId=163

A group photo taken at the PRACE / HP-SEE / LinkSCEEM2 HPC Summer Training in Athens, Greece. © GRNET

Featured project: EUDAT

EUDAT is a new European initiative including 25 partners: national data centers, technology providers, research communities, and funding agencies from 13 countries who will work together to deliver a Collaborative Data Infrastructure (CDI) with the capacity and capability for meeting future researchers' needs in a sustainable way. EUDAT is coordinated by CSC - IT Center for Science, Finland, and co-funded by the EC FP7 programme starting in October 2011.

EUDAT

www.eudat.eu

Europe's science and research communities from a wide range of scientific fields are faced with increasingly large amounts of valuable data that stem from new sources such as powerful new sensors and scientific instruments used in analyses, experiments and observations as well as growing volumes of data from simulations and from the digitization of library resources. This accelerated proliferation of data is a fantastic opportunity for science but also creates new challenges related to data management, integration and interoperability, access and preservation.

Multi-disciplinary collaboration and data sharing

These challenges can only be tackled through a systematic and focused approach, encouraging collaboration between the various stakeholders and covering the entire life cycle of data objects. EUDAT will contribute to develop a Collaborative Data Infrastructure by building a generic infrastructure layer on which research communities and existing infrastructures can rely for some of their basic data service requirements – some of which are common to multiple disciplines and can be deployed for use by diverse communities.

EUDAT will offer a trusted domain for long term data preservation accompanied with related services to store, identify, authenticate and mine these data, and facilitate progress towards a cross-disciplinary and open data-intensive science by providing a unique opportunity for multi-disciplinary collaboration and data sharing.

Featured events

Supercomputing 2011
November 12 –18, Seattle, WA, USA

PRACE project members will welcome SC'11 visitors to the PRACE booth (#5001) in Seattle, WA, on November 14–17.

Thursday, **November 17** at **12:15pm–1:15pm** PRACE organizes a BoF session entitled "**PRACE – The European HPC Infrastructure**". We will present some of our outstanding research results achieved with PRACE resources and give information on the PRACE's Tier-0 and Tier-1 services. This will be an excellent opportunity to learn how to apply for resources and application support. PRACE representatives will be on hand to chat about everything PRACE and answer any questions you may have.

PRACE also organizes a treasure hunt at the SC'11 PRACE booth. Don't miss the change to win a great prize!

Read more at: www.prace-ri.eu

EESI Final International Conference
10 – 11 October 2011, Barcelona, Spain

The main goals of EESI (European Exascale Software Initiative) are to build a European vision and roadmap to address the international outstanding challenge of performing scientific computing on the new generation of computers which will provide hundreds of Petaflop performances in 2015 and Exaflop performances in 2020.

The main objective of the EESI Final International Conference is presenting the project results to the stakeholders, scientists and policy makers containing presentations and discussions with all experts participating to the WG activities. Beyond the EESI vision and roadmap, the presentation will include societal impact of using Exascale computing, cost for using exascale computing, and cost for the society not using Exascale computing.

More information at: http://www.eesi-project.eu/pages/menu/news-events/final-conference.php

PRACE-1IP all-hands and 2IP kick-off meeting

The PRACE 1IP All Hands & 2IP Kick-Off Meeting was held in Barcelona on 14 – 16 September 2011 with nearly 200 attendees from all PRACE member countries. The meeting was organised by the local host Barcelona Supercomputing Center.

This three-day event consisted of two parts: the first and a half day, the attendees participated in the all-hands meetings of the first implementation phase and the second part consisted of the kick-off meeting of the second implementation phase. This activity allowed aligning everybody with the main ideas of PRACE. During the parallel sessions of all different work packages, the partners discussed working tasks and planned the next steps of the projects. On Friday the agenda also included the innovative "interpillar meetings" of the second implementation phase. These meetings allow the combination of different sets of work packages in order to indentify synergies amongst them and facilitate their collaboration.

Nearly 200 attendees took part to the PRACE-1IP all-hands and 2IP kick-off meeting held in Barcelona on 14-16 September. © BSC

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