

Press release
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PRACE granted over 4.3 Million Core Hours to PRACE Prototype Systems

Six projects, two from France and one from Norway, Denmark, UK, and the Netherlands, have been granted access to the PRACE (Partnership for Advanced Computing in Europe) prototype systems. These projects will spend a total of 4 311 272 core hours on the PRACE prototypes. So far, PRACE has granted a total of over 8.7 million core hours on the PRACE prototypes.

The purpose of this granting access is to enable future Tier-0 users to assess the prototypes and to prepare their applications for the Petaflop infrastructure. The evaluation process has focused on technical feasibility and the expected benefits of the tests both for PRACE and the prototype users.

Cryptanalytic Performance Evaluation

Tanja Lange's (Eindhoven University of Technology, the Netherlands) research group is evaluating the performance of various cryptanalytic computations on five of the six PRACE prototype platforms. Today's e-commerce relies critically on the various cryptographic mechanisms such as SHA-1 and RSA-1024. Understanding the security of these mechanisms requires analyzing and optimizing a wide variety of cryptanalytic algorithms. The most convincing way to resolve uncertainty and disputes regarding the performance of these algorithms is to actually try the algorithms on an increasingly difficult series of cryptanalytic challenges. This can help to sort out some major issues such as the ongoing debate about whether the internet needs to switch from RSA-1024 to higher-security standards, to reduce possible criminal attacks.

Lange leads the implementation lab in the FP7-funded ECRYPT II Network of Excellence in Cryptology, and in particular leads the ECRYPT Benchmarking of Cryptographic Systems project (<http://bench.cr.yp.to>), which has collected 580 implementations of 164 different cryptographic functions into a single unified benchmarking framework; this framework provides a convenient starting point for this project to start immediately collecting useful performance data. Subsequent plans include microarchitectural "superoptimization" (trying many machine-language sequences to identify the fastest) and experimenting with higher-level cryptanalytic algorithms.

This project will use 100 000 core hours on the following PRACE prototypes: FZJ IBM BlueGene/P (Germany), CSC-CSCS CrayXT5 (Finland-Switzerland), CEA-FZJ Intel Xeon Nehalem (France-Germany), NCF/SARA IBM Power 6 (The Netherlands) and BSC IBM Cell (Spain).

Solar Atmospheric Modelling

Mats Carlsson's (University of Oslo, Norway) research group tests a 3D radiation magnetohydrodynamic code for solar atmospheric modeling. The Sun offers a unique opportunity to test and improve the physical description of the mechanisms occurring in stars in general, the methods and approximations involved in the construction of numerical stellar models as well as their computer implementation. The project aims at testing the scalability of the code to a very large number

of cores, and explore various architectures with the goal of enabling even more realistic simulations of the solar outer atmosphere on future Petascale systems.

The project was allocated 10000 core hours on the FZJ IBM BlueGene/P (Germany) and 8640 core hours on the CSC-CSCS Cray XT5 (Finland-Switzerland).

Ab Initio Calculation of Complex Doping of a Photovoltaic Material

Fabien Bruneval's (CEA, France) research group is studying how to improve the scalability of codes implementing the GW approximation. The calculation of the doping of materials requires numerical schemes that produce realistic band gaps for semiconductors and insulators. All the common approximations of Density Functional Theory (DFT) badly fail with this central property. The so-called GW approximation that goes beyond the usual DFT is a predictive method to calculate band gaps. Unfortunately, the GW approximation is extremely cumbersome and scales very badly with the system size, but fortunately can be efficiently parallelized. The ABINIT code provides a highly parallel implementation of the GW approximation. The group tests the scalability and the feasibility of large scale GW calculations for a doped photovoltaic material.

Bruneval's research group will use 786 432 core hours on the CEA-FZJ Intel Xeon Nehalem (France-Germany).

Porting MESO-NH to PRACE Prototype

Escobar Munoz's (Université Paul Sabatier Toulouse, France) research group tests and optimizes the scalability of Méso-NH code, which is a non-hydrostatic mesoscale atmospheric model. The preliminary goal of the test is to extend the scalability and optimization of the code beyond 100 000 cores on the BlueGene architecture and to make initial tests of the code in the new architecture of the Cray XT5.

The group will use one million core hours on the FZJ IBM BlueGene/P prototype (Germany) and 100 000 core hours on the CSC-CSCS CrayXT5 prototype (Finland-Switzerland).

Incompact3d: High Performance Computing for Turbulence

Sylvain Laizet's (Imperial College London, UK) research group is studying Incompact3d-code, which is an in-house Computational Fluid Dynamics (CFD) code that provides the opportunity of using a high-order finite difference method for Direct Numerical Simulation (DNS) of incompressible flows in relatively complex geometries. In this project, the research group checks and evaluates the potential of the code on thousands of processors on low-frequency cores with a small amount of memory available. Moreover, the group investigates if the domain decomposition strategy, based on global operations, is suitable when thousands of cores are used.

The group will use 1 900 000 code hours on the FZJ IBM BlueGene/P prototype (Germany).



Porting of GADGET2 to GPUs

Carsten Frigaard's (Mergeit Aps, Denmark) optimizes GADGET2, an astrophysical code, using GPUs as co-processors. Frigaard has himself developed the code. He aims at evaluating the performance of GADGET2 with GPUs compared to a pure CPU simulation. The goal of this project is to support users of GADGET2, enabling them to run the code on the GPU system. GADGET2 is part of an open source package aimed for the scientific community.

Frigaard will use 3100 core hours on CEA GPU clusters (France) and 3100 core hours on HLRS GPU clusters (Germany).

More information about PRACE prototypes: <http://www.prace-project.eu/prototype-access>

About PRACE: The Partnership for Advanced Computing in Europe prepares the creation of a persistent pan-European HPC service, consisting of several tier-0 centres providing European researchers with access to capability computers and forming the top level of the European HPC ecosystem. PRACE is a project funded in part by the EU's 7th Framework Programme. The PRACE project receives funding from the European Community's Seventh Framework Programme (FP7/2007-2013) under grant agreement n° RI-211528.

