Press release

For release: 15/10/09

# Six Projects granted Access to the PRACE Prototype Systems - 4.5 Million Core Hours

Six projects, three from Ireland, two from France and one from Spain, have been granted access to the PRACE (Partnership for Advanced Computing in Europe) prototype systems. These projects will spend a total of 4 449 713 core hours on the PRACE prototypes.

In 2008, PRACE selected six promising architectures for Petaflop-class systems to be deployed from 2010 on. 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.

**Fluid mechanics for very high Reynolds flows on complex geometries**

**Remi Abgrall'**s (INRIA and Institute Polytechnique de Bordeaux, France) research group is studying a class of schemes for hyperbolic problems with the fluid mechanics code FluidBox. The main goals of this study are to test how very large-scale clusters may help the research group to check their conjectures about scalability and to test the portability of the FluidBox code on one of the PRACE prototypes, namely on CSC/CSCS's (Finland/Switzerland) joint prototype Cray XT5. Code-scaling experiments up to 4935 core hours are planned.

**Porting the molecular dynamics code Desmond to two different platforms**

**Damien Thompson'**s (Tyndall National Institute, University College Cork, Ireland) research group works on biomolecule-functionalised nanomaterials. The group will test the molecular dynamics code Desmond on two different PRACE prototype architectures, namely on the FZJ (Germany) IBM BlueGene/P and the NCF/SARA (The Netherlands) IBM Power 6 systems, to enable more accurate calculations which better match experimental conditions. The group expects to spend 11 237 core hours on each platform. The tests will enable a cross-code and cross-architecture evaluation of portability and scalability for different classes of problems.

The group will test the Desmond molecular dynamics code at different levels of theory, for a range of problem sizes, over a range of processor numbers on the FZJ and NCF/SARA architectures. The group intends also to benchmark the new data against existing data for the alternative NAMD code on both PRACE architectures and also the group's own scaling tests for NAMD (already available) and Desmond (to be performed) on the ICHEC IBM BlueGene/P.

**Tests of the astrophysics code HERACLES on three PRACE platforms**

The objectives of **Edouard Audit**'s research group (CEA, France) are to port, test and examine the scalability and I/O performances of the HERACLES (Eulerian multi-physics) code on three PRACE prototypes. The code is used for a large number of astrophysics related applications (interstellar medium turbulence, jets from young stellar objects, accretion disk dynamics and laser experiments). Porting HERACLES on the future Petascale machines will provide HERACLES users with a code that is ready to perform challenging numerical simulations on these machines.

HERACLES will be ported and tested on the following platforms: the Cray XT5 at CSC/CSCS (Finland/Switzerland): 45 000 core hours; CEA/FZJ (France/Germany) Bull Intel Xeon Nehalem 80 000 core hours and NCF/SARA (The Netherlands) IBM Power 6: 17 000 core hours.

**Electronic structure computations with the Monte Carlo Configuration Interaction method**

**James (Jim) Greer'**s (Tyndall National Institute, University College Cork, Ireland) research group is using the Monte Carlo Configuration Interaction (MCCI) method to calculate electronic structures. In this project the group is seeking to explore how this type of novel electronic structure computation scales in massively parallel processing environments. The group's initial tests suggested that the coupled Monte Carlo search/matrix diagonalisation technique can be combined to study problems believed to be "computationally intractable". The research group aims to find optimal control parameters for running the program in massively parallel environments. From the tests, the group seeks to understand where efforts at code porting optimisation should be focused to develop an efficient massively parallel version of the program. A primary goal of this research is to identify the ultimate scaling limits for the MCCI algorithm.

The tests will be made on FZJ (Germany) IBM BlueGene/P, 44 032 core hours and on NCF/SARA (The Netherlands) IBM Power 6, 22 016 core hours.

**Comparison of three task attribution policies on four different platforms**

**Gary McGuire**'s (University College Dublin, Ireland) research group aims at evaluating the suitability of different task distribution policies, depending on the machine architectures and environments. The test data consists of a large number of independent instances of the hitting set problem (also known as set covering problem). The group intends to use a task farming-like approach based on a classical master-slaves MPI parallelisation. The group will test three different tasks attribution policies, which will be compared on the various machines and batch environments.

The tests will be run on four different platforms: FZJ (Germany) IBM BlueGene/P (3 900 000 core hours), CSC/CSCS (Finland/Switzerland) CrayXT5 (13 632 core hours), CEA-FZJ (France/Germany) Bull Intel Xeon Nehalem (261 696 core hours) and NCF/SARA (The Netherlands) IBM Power 6 (32 928 core hours).

**Shallow water simulations on Cell processors**

**Basilio Rodriguez**'s **(**University of A Coruña, Spain) research group works on shallow-water systems. The group's simulator works on systems where a layer of fluid rests atop a fixed arbitrarily shaped bottom, and simulates the variations occurring on the surface due to diverse forces, as well as the variation of the concentration of a contaminant along the fluid.

The tests on the BSC (Spain) IBM Cell will allow the simulation of bigger and more geographically accurate systems in a reasonable time. Besides the scalability of the solver, also the performance of the solver with double precision floating point data and double precision operations with the Cell processors can be tested. The tests offer also the chance of parallelizing the solver among several Cell processors with shared memory. The group will use 6 000 core hours on the IBM Cell platform.

**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.