

First projects granted access to the PRACE Prototype systems - 4.4 Million Core hours to 3 projects

Three projects, two from Ireland and one from France, have been granted access to the PRACE prototype systems. 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/s Infrastructure. The evaluation process has therefore focused on technical feasibility and the expected benefits both for PRACE and the users.

Simulation of interfaces of biological systems

The aim of this feasibility study by **Niall English** (University College Dublin) is to test new approaches in applying Carr-Parrinello Molecular Dynamics (CP-MD) methods to simulate interfaces of biological systems with nanomaterials. In particular, the detailed mechanisms of protein and dye binding and adsorption to metal and metal oxide surfaces raise interesting and unresolved questions which only fully dynamic, electronic simulations by CP-MD methods can answer at the present time.

More specifically, the goals of this feasibility study are to assess how these methods may be applied efficiently on PRACE-provided HPC architectures, in particular the IBM BlueGene/P at Jülich, Germany, the Cray XT5 at CSC/CSCS (Finland/Switzerland), and the Intel Nehalem cluster at CEA/Jülich (France/Germany). Code-scaling experiments up to 16.384 cores are planned.

Porting the astrophysical fluid code HYDRA to two different platforms

The code to be used in this project, HYDRA, by **Turlough Downes** (Dublin City University) is an astrophysical fluid code which incorporates the effects of magnetic fields and, most interestingly, multi fluid effects. In astrophysics many fluids, such as molecular clouds, are only partially ionised. It is widely accepted within the astrophysics community that multi fluid simulations will be essential to the continuing development of our understanding of many important phenomena such as turbulence and dynamo action. Until recently it has been difficult to perform such simulations on massively parallel architectures due to a lack of efficiently parallel algorithms with appropriate stability properties. Novel algorithms to overcome these issues were developed and implemented in a production code, HYDRA, by the Project Leader and collaborators. This code has been shown to scale well to tens of thousands of cores on a BlueGene/P system.

The goal of this project is to port HYDRA to two of the prototype platforms (Cray XT5 and the Bull Nehalem systems) and compare its performance across these platforms and the BlueGene/P platform to which it has already been ported, thus using three systems in total. This comparison will be performed in terms of scalability, time-to-solution and cash cost.

From the point of view of the proposers of this project, the main results will be a code which has been tested and proven on several different architectures. This will then serve as a basis for applications for full production access to massively parallel machines both within Europe and internationally.

It is planned to make scaling experiments exploring the full size of the prototypes, on the Jülich BlueGene/P this involves all 294.912 cores.

Development of X10 environment on a parallel machine

The project by **Marc Tajchman** (CEA) aims at exploring the performance of the X10 environment on a parallel machine, i.e. IBM Power6, for numerical simulations. X10 is a new PGAS (Partitioned Global Address Space) programming language from IBM. PGAS languages represent a new programming paradigm designed for creating scalable applications for large parallel computers and are also being assessed by PRACE. The project will also evaluate mixed X10 C/C++/Fortran source code. A comparison of the traditional MPI programming paradigm with the X10 PGAS language and mixed mode programming is planned on the IBM Power 6 Prototype at SARA, the Netherlands.

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.

