

PRACE Investigated Application Requirements

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PRACE, the Partnership for Advanced Computing in Europe, investigated application requirements for European Petaflop systems. The investigation work consists of an analysis of the behaviour of a set of applications on current hardware platforms, and a survey of key users.

PRACE investigated the applications and other software that will run on future European Petaflop systems. The application codes analysed are those selected earlier by PRACE as representative of the likely load on European Petaflop/s systems and which are candidates for inclusion in a benchmark suite to help select such systems.

The applications analysed are covering molecular dynamics and quantum chemistry (NAMD, CPMD, CP2K, GROMACS, GPAW, VASP), atomic physics (HELIUM), cosmology (GADGET), computational fluid dynamics (CODE_SATURNE, N3D, ALYA), plasma physics (TORB, PEPC), particle physics (QCD) and earth system modeling (NEMO, ECHAM5).

Each of the applications was run on one of the classes of architectures identified by PRACE as suitable prototypes for future Petascale systems. The appropriate data sets for each application were selected and profiling data on production-scale runs was collected so that the requirements of each application could be identified.

In addition, PRACE complemented this data by the results of a survey of many of the major HPC (High Performance Computing) users in Europe. A survey was sent to the major HPC users in most PRACE countries asking for their input on future applications requirements. This survey included questions about the user, usage patterns, HPC infrastructure, upcoming algorithms and general comments about future Petascale systems. Almost 70 responses were received and analysed by PRACE.

PRACE Work Package 6, which has been leading this investigation work has so far investigated the usage of most major HPC systems across Europe, the key applications and algorithms used, the performance of these applications on key architectures and the views of major users on emerging applications requirements. This provides a full picture of the requirements of current applications and identifies how these would translate to future Petaflop systems.

This work is essential for later tasks in PRACE which will involve optimising and petascaling these applications and packaging them into a benchmark suite to be used in future Petaflop procurements.

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Further information:

<http://www.prace-project.eu>