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Partnership for Advanced Computing in Europe

Selection of a Unified European Application Benchmark Suite

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Abstract

This White Paper reports on the selection of a set of application codes taken from the existing PRACE and DEISA application benchmark suites to form a single Unified European Application Benchmark Suite (UEABS).

The selected codes are: **QCD, NAMD**, **GROMACS**, **Quantum Espresso**, **CP2K**, **GPAW**, **Code_Saturne**, **ALYA**, **NEMO**, **SPECFEM3D**, **GENE**, and **GADGET**.

This work was undertaken as the first stage of creating a "Unified European Applications Benchmark Suite for Tier-0 and Tier-1" in the PRACE Second Implementation PHASE (PRACE-2IP) project. The publication of this White Paper addresses a Milestone of the project "Identification of applications for unified benchmark suite".

The main purposes of the unified benchmark suite are the following:

- To provide a resource of application codes and datasets that PRACE partners can draw on for procurement purposes.
- To provide performance data on existing PRACE systems to assist users when choosing which system to apply for time on.
- To provide data for "currency conversion" of CPU hours between PRACE systems.

Please note that there is no obligation for PRACE partners to use all or any of the codes for national procurements. Furthermore, it is not intended that inclusion of a given code in UEABS (or otherwise) should influence peer review decisions concerning access to PRACE systems, or the internal selection of optimisation and scaling projects.

The first stage of the process was to produce a short list, by considering the 29 distinct application codes that are contained in the existing PRACE [1] and DEISA [2] benchmark suites. The codes were evaluated against the following criteria:

- The code must be publically available, either unlicensed or with a suitable open license agreement.
- Suitable datasets must be publically available.
- The code must not have any significant barriers to portability.
- The code must demonstrate good scalability.
- The code must have active support by the developers.

It was decided at this stage not to consider accelerator-enabled versions of codes, since there is currently no widely adopted vendor-neutral programming model for these devices.

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This process resulted in a short list of 15 application codes that met the above criteria. A consultation process was then undertaken to take into account the relevance of the shortlisted codes to PRACE partners and their respective user communities, as well the coverage of scientific areas by the list of codes. This process resulted in a final list of 12 codes to form the initial version of UEABS, which (listed by scientific area) are:

Particle Physics:	QCD
Classical MD:	NAMD, GROMACS
Quantum MD:	Quantum Espresso, CP2K, GPAW
CFD:	Code_Saturne, ALYA
Earth Sciences:	NEMO, SPECFEM3D
Plasma Physics:	GENE
Astrophysics:	GADGET

Details of these application codes can be found in [1] and [2].

For the remainder of the PRACE-2IP project, the following work is planned:

- Collect new versions of the 12 selected codes where required.
- Identify suitable datasets for Tier-0 and Tier-1 systems.
- Make the codes and datasets publically available on the PRACE-RI web site.
- Run the benchmarks on a selection of relevant Tier-0 and Tier-1 systems, and report the results in the public deliverable (D7.4) in July 2013.

Support of the benchmark suite will also continue in PRACE-3IP, and it is envisaged than an annual review of the contents of the suite take place, to allow the possibility of updating code versions and datasets, removing obsolete codes and admitting new codes, for example from emerging science areas.

References

[1] PRACE Preparatory Phase Deliverable D6.3.2 **"**Final benchmark suite", available at http://www.prace-ri.eu/IMG/pdf/D6-3-2-extended.pdf

[2] DEISA Benchmark Suite: http://www.deisa.eu/science/benchmarking

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