



PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE

Identification and Categorisation of Applications
and Initial Benchmarks Suite

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Software Enabling for Petaflop/s Systems

The Work Package Consists of Six Tasks:


1. Identification and Characterisation of Applications
2. Application Requirements Capture
3. Performance Analysis and Benchmark Selection
4. Petascaling
5. Optimisation
6. Software Libraries and Programming Models

Aim of Task 6.1

- Identification and categorisation of applications and initial benchmarks suite
- Create a list of *potential* applications for benchmarking suite
- Understand the HPC background to make quantitative statements about any application list
- Weight the list accordingly
- Led by EPCC



Method



PRACE WP6.1 Systems Survey

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Please fill in the information below to the best of your knowledge
Note required fields are denoted by a * symbol

About you

Name: *

Institution: *

Email address: *

PRACE partner name: *

Survey period

Start Date (dd-mm-yyyy): *

End Date (dd-mm-yy): *

Machine details

Please select your system from the following list. If your system is not on the list, please email [Jon Hill](#), who will add the system and let you know when this has happened, so you may complete the survey.

Name: *


Hardware architecture

Machine name:

Manufacturer:

Model:

Processor type:



PRACE WP6.1 Applications Survey

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Name: *

About the application

Name

What is the application's name:

Current workload

Scientific Area	Area/Dwarf	Dense linear algebra	Spectral methods	Structured grids	Sparse linear algebra	Particle methods	Unstructured grids	Map reduce methods
		Astronomy and Cosmology	0	0	0	0	0	0
Computational Chemistry	15.35	26	"Seven Dwarves" →					12.98
Computational Engineering	0						2.8	
Computational Fluid Dynamics	0	1					0	
Condensed Matter Physics	9.10	15					5.70	
Earth and Climate Science	0	2.03	5.83	1.33	0	0.26	0	
Life Science	0	4.72	0.94	0.13	0.94	0.28	3.46	
Particle Physics	12.50	0	4.59	0.92	0.10	0	89.27	
Plasma Physics	0	0	1.33	1.33	3.55	0.42	0.63	
Other	0	0	0	0	0	0	0	

Method used

Application List

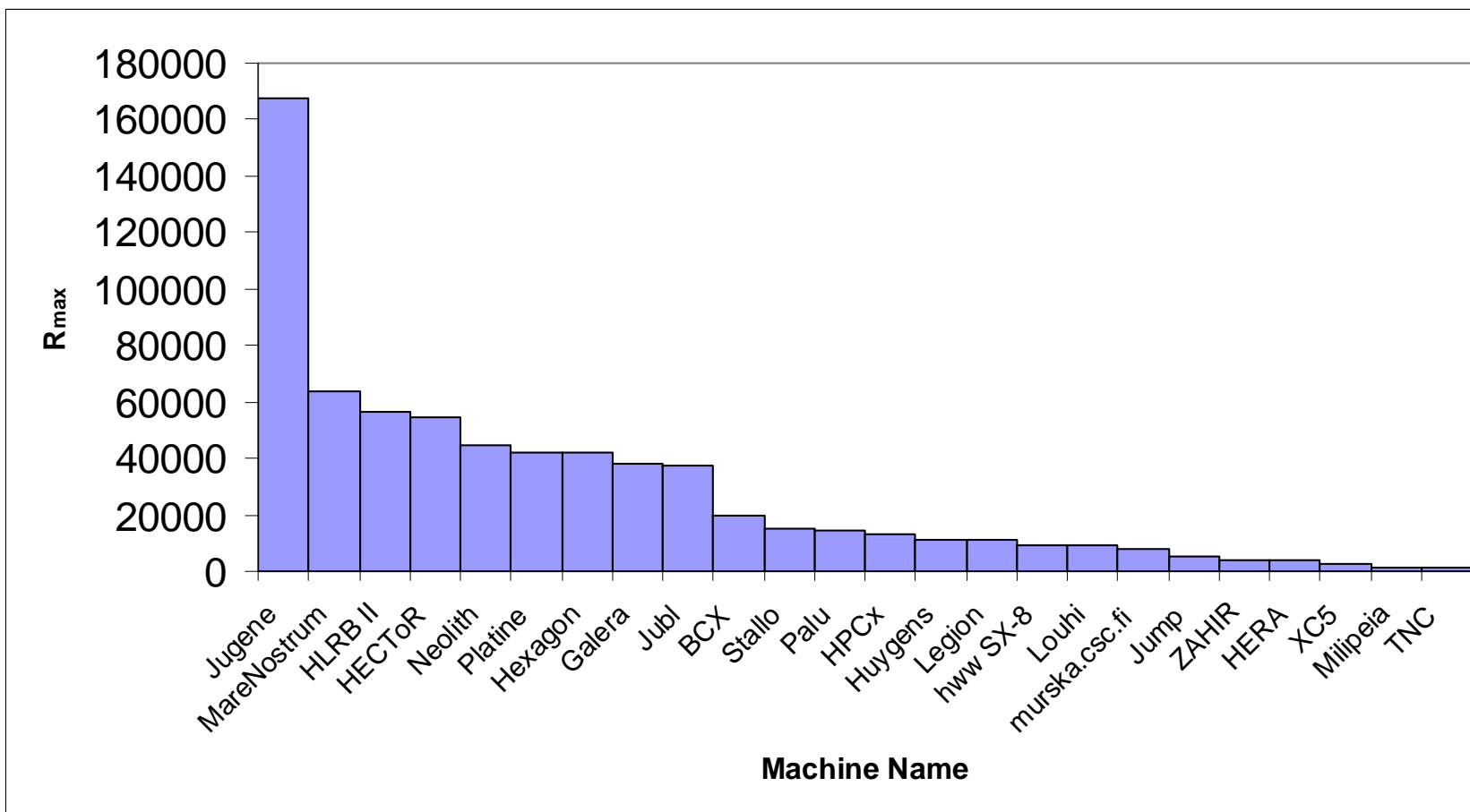
1. VASP
2. CHROMA
3. SIESTA



Area/Dwarf	Dense linear algebra	Spectral methods	Structured grids	Sparse linear	Particle	Unstructured	Map reduce
Astronomy and	0	0	379629	379654	0	0	0
Computational	936689.31	1515643.517	115331.1667	120077.9767	43264.35	57167.2	158113.7
Computational	0	0	56173.33333	56173.33333	0	56173.33333	294910
Computational Fluid	0	136663.63	17550	199100	21730.63	216660	0
Condensed Matter	199100	452944	0	0	61601.5	0	231320
Earth and Climate	0	132733.3333	453697.3333	132733.3333	0	26112	0
Life Science	0	0	0	13120.32	0	0	82126
Particle Physics	1866500	0	262357	200376	0	0	3006312
Plasma Physics	0	0	132733.3333	132733.3333	198060.8333	44415	65327.5
Other	0	0	0	0	0	0	0

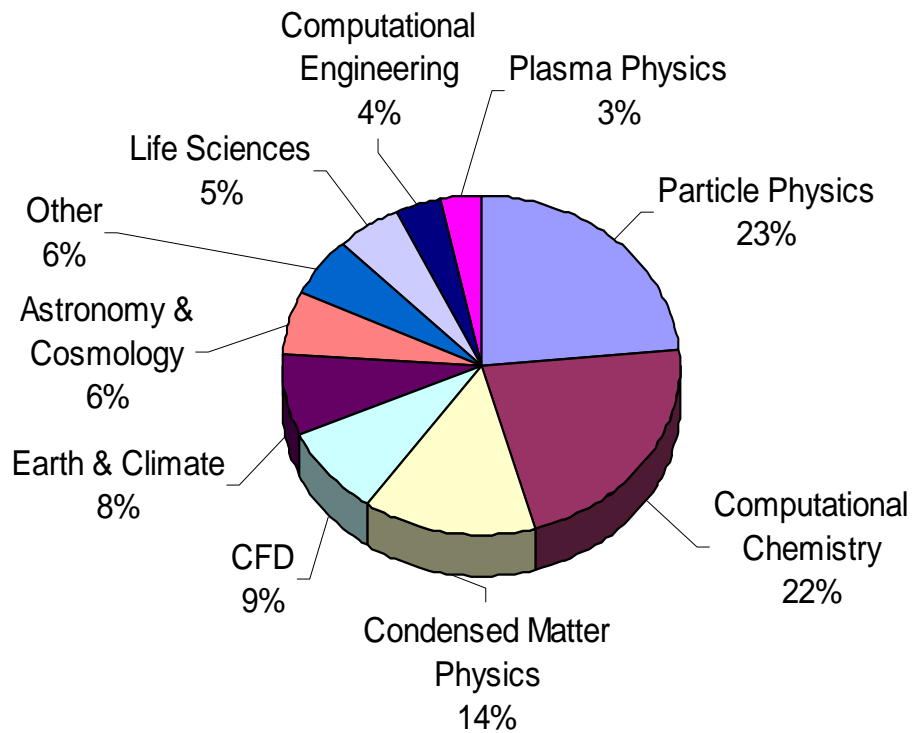


System results

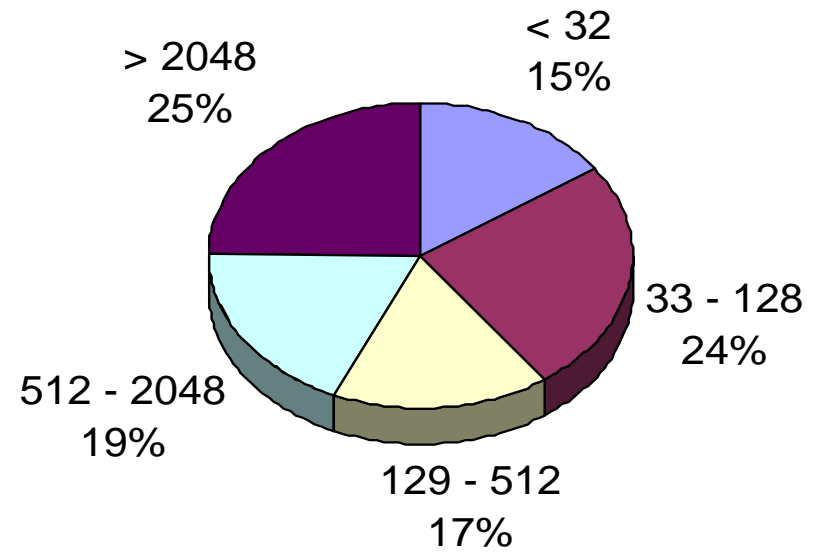


System results

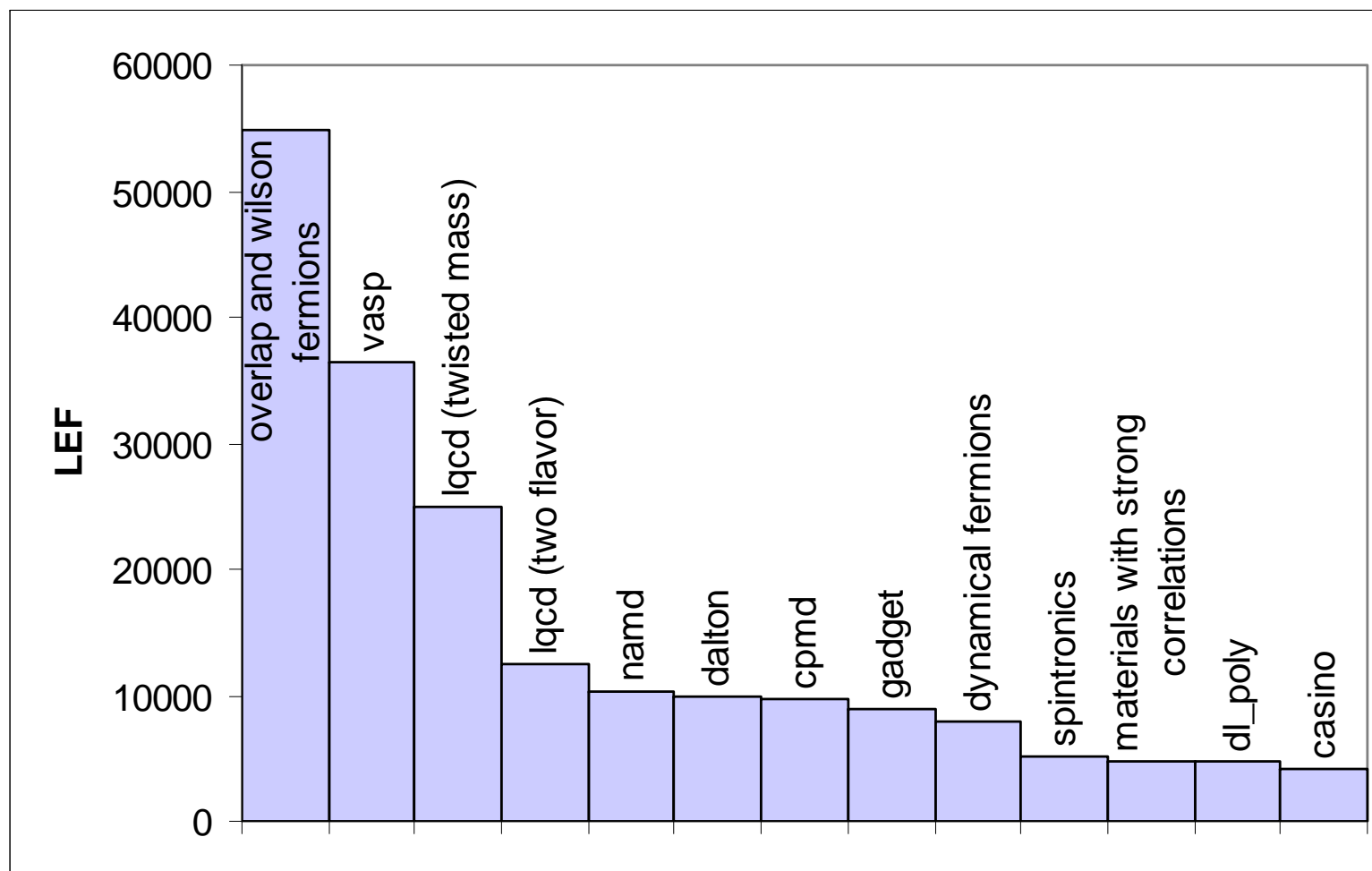
Scientific Area



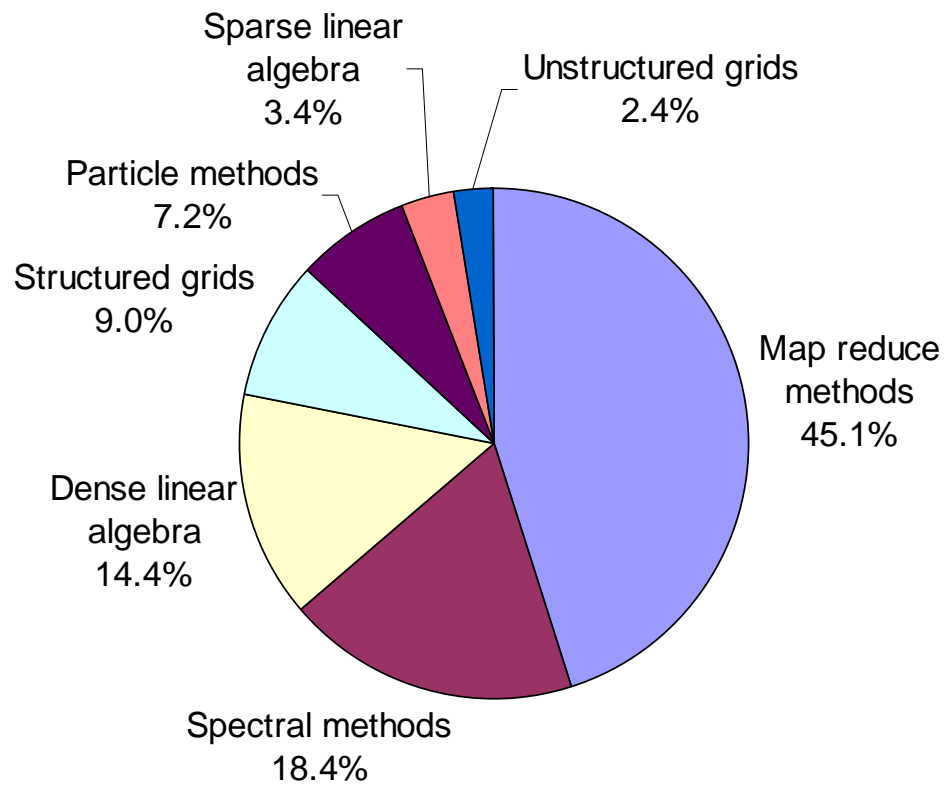
Job size



Applications results



Applications results: Dwarves



List of representative applications

- QCD benchmark – Particle Physics
- VASP – Comp. Chem. & Condensed Matter Physics
- NAMD – Comp. Chem. & Life Sciences
- CPMD – Comp. Chem. & Condensed Matter Physics
- Code_Saturne - CFD
- Gadget – Astronomy & Cosmology
- TORB – Plasma Physics
- Echem5 – Atmospheric Modelling
- NEMO – Ocean Modelling

Extensions

- Avbp - CFD
- Cp2k – Comp. Chem.
- Gromacs – Comp. Chem.
- Helium - Other
- Smmp – Life Science
- Tripoli4 - Engineering
- Pepc – Plasma Physics
- Ramses – Astronomy & Cosmology
- Cactus - Astronomy & Cosmology
- N3D - CFD

Future

- The benchmark applications will now be:
 - Analysed
 - Optimised
 - Peta-scaled
- Used to form a benchmark suite for procurement
- Enable research into how to petascale applications



About PRACE

- The aim of PRACE is to provide scientists in Europe with unlimited and independent access to fast supercomputers and competent support. PRACE prepares the creation of a persistent pan-European HPC service, consisting 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 following countries collaborate in the PRACE project: Germany, UK, France, Spain, Finland, Greece, Italy, Ireland, The Netherlands, Norway, Austria, Poland, Portugal, Sweden, Switzerland and Turkey. The PRACE project is coordinated by the Gauss Centre for Supercomputing (Germany), which bundles the activities of the three HPC centres in Jülich, Stuttgart, and Garching.
- <http://www.prace-project.eu/>
- The PRACE project receives funding from the EU's Seventh Framework Programme (FP7/2007-2013) under grant agreement n° RI-211528.