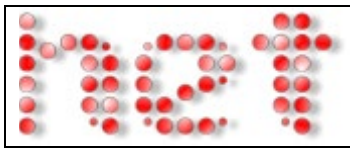

HPC in Europe Taskforce
Towards a new level of High Performance Computing facilities for Europe

18.1.2007

Towards a Sustainable High-Performance Computing Ecosystem through Enabling Petaflop Computing in Europe

1 Introduction

The High-Performance computing in Europe Taskforce (HET) has developed a strategy for boosting European computational science infrastructure and services with a focus on the creation and operation of European centers with an extreme computing capability reaching the petaflop performance. HET is a temporary taskforce established in June 2006 with a target to complete the strategy, including recommendations for developing the European HPC ecosystem, in a 6 month period. The outcome of this work will be available in January 2007.

The HET strategy includes this summary paper and four documents describing four key areas in more detail: scientific case for high-end computing, sustainable HPC ecosystem, funding and utilization model and a peer review process.

The taskforce has focused on the high end of the performance pyramid and the strategic issues enabling the best possible usage of such resources. Through the intense work of HET members the challenge of building an extreme computing facility has been accepted to the ESFRI roadmap among the 34 projects of major European scientific impact.

It is important to note that the infrastructure for high-end computing capability is just one of the necessary instruments in computational science. In order to gain the most benefit out of such a resource, it needs to be integrated with the rest of the available computing services, each covering various levels of performance.

2 Executive summary for building a sustainable HPC ecosystem

HET, the High Performance Computing in Europe Taskforce, was established in June 2006 by eleven countries aiming at more intense collaboration in providing competitive resources for computational science in Europe. The target of HET was to propose a strategy and actions to develop a sustainable HPC Ecosystem in Europe which takes into account the main elements required such as top-class supercomputers, existing national computing infrastructures, software development and need for competence development for computational science. The HET work has included the development of a European scientific case for high-end computing (developed during 2005 – 2006), which demonstrates a strong need for computational resources with a performance far beyond the currently available systems.

At the moment there is no major European resource which could match the capability computing performance of the USA or Japan. This is an intolerable situation for the competitiveness of European computational science. The scope of the HET work focused both on the top of the computing performance pyramid, e.g. systems with a petaflops (10^{15} calculations in second) capability, and activities enabling utilization of such an extreme computing power system efficiently. It is important to note that the computing hardware alone is inadequate in solving scientific problems – petaflop systems need also petaflop software, scalable algorithms and competent scientists. Also any petaflop system needs to be integrated with the national computing centers who provide the majority of computing resources to the many science problems that do not require the most capable and expensive systems. That is the main reason why instead of considering only top end resources, HET discussed the whole HPC ecosystem.

The basic element of the HPC ecosystem is the performance pyramid. At the top we propose a small number of supercomputer systems which would be funded through national sources, with additional funding at a European level. The middle layer consists of a number of national and regional supercomputers, which should have a high enough performance to be capable of running most of the computing load below petaflop and in addition serving as a development platform for the most scalable code directed to the petaflop systems. The bottom of the pyramid represents the local level of activity including the development of a strong competence base of scientists in multiple European countries, the renewal and development of new skills through local education and increasing the visibility of scientific computing so to attract new users. In addition to the

well defined roles in each level of the pyramid, the transparent interaction between the layers is a major requirement.

The European Research Grid, the well connected infrastructure of all e-resources integrated at the hardware, software and communication level and the services utilizing them to benefit the research community at large (from purely scientific to applied or even commercial research) *is* the e-resources eco-system. The supercomputers, top or lower level, need to be integrated in the European Research Grid as any other resources. Through tight integration and optimal utilisation of distributed resources and skills in European countries it is possible to achieve high efficiency for the operations.

Due to international competition, the quality of infrastructure available for research plays a major role. Computing performance is one important factor in achieving competitiveness, thus establishing a sufficiently powerful European infrastructure is a necessity. In order to close the gap currently existing between European resources and the more advanced systems available in the USA and Japan, additional competitive tools need to set in place, such as investments in scientific software development and code optimisation, middleware development, data repositories and efficient networking. With the right support, competence in designing petascale software could become a competitive advantage for Europe.

A sustainable HPC ecosystem for Europe is a target which can be achieved gradually. EU FP7 provides one tool to develop HPC in Europe further. During the FP7 the European HPC ecosystem can be established based on the existing national infrastructures and active participation of other stakeholders for funding and using the HPC services. The stakeholders include – in addition to scientists using the services, nations funding computing infrastructure and computing centers providing services – European industry as a user and producer for parts of the computing environment, European Union and current EU supported Grid projects. Open questions, to which HET targeted efforts to propose solutions, included funding models, peer review processes and organisation of the European level resources.

One of the major issues for the HET work is how to ensure sustainability of such an ecosystem, including a strong base but also a sufficient top to the ecosystem pyramid. The following issues will contribute to increasing the life-time of the collaborative infrastructure:

- Integration and compatibility with national infrastructures
- Building on the current HPC-related work, such as a successful European research infrastructures projects
- An appropriate level of communication, experience and skill sharing between the national centres
- Co-ordination by an European group with a strong mandate
- Financial support from the European Union
- Acknowledgement of the importance and contribution of computational resources in increasing the output of a number of science areas

- Creating sustainable research groups in HPC based both on current experienced ones, and establishing new ones
- Creating sustainable application development and optimization groups based on both current experienced ones, and establishing new ones

3 HET Recommendations

Recommendation for the development and operation of a "top end" infrastructure

HET recommends establishment of a small number of European HPC facilities to provide extreme computing power – exceeding petaflop capability – for the most demanding computational tasks. In addition, a funding model based on national investments with an additional European share and a possible new collaborative entity governing it is recommended. Construction principles for European facilities are proposed to include tight integration in existing infrastructure targeting sustainability, optimal synergy and efficiency in operations.

The European extreme computing facility is listed in ESFRI Roadmap (European HPC Service).

Remarks:

- The motivation for investments is proven by the *HET Scientific case* document
- According to the scientific case Europe has a number of world-class computational research groups, which can efficiently benefit from petaflop performance
- The usage of the European share of the facility needs to be allocated to the most important research proposals, a proposal for evaluation of such proposals is presented in the *HET peer review process* document

Recommendation for developing the full European ecosystem

HET recommends increased emphasis on the development of the full HPC ecosystem, including the local infrastructure, national and regional facilities, top-level European computing capabilities and the interoperability of their services.

HET recommends growing investments on the different levels of the computational pyramid with a target to provide services in each level in a balanced way: few facilities dedicated to providing the extreme resources for top of the pyramid with a

strong base of medium-size systems and integration with local infrastructures and competencies.

Remarks:

- Some of the important scientific problems never need the top resources of the computational pyramid, but can utilize a lot of the medium level computing
- Since one system or architecture does not serve all users efficiently, through collaboration and resource sharing mechanisms it is possible to optimize European usage
- All the performance steps in between are required in order to utilize the top resources efficiently, since scalable code development advances gradually

Recommendation to enable petascale computing by supporting the development of novel software architectures

HET recommends starting a range of activities aimed at addressing the key issues in building software that allows exploiting the performance potential of petascale machines in a coherent, efficient, scalable and sustainable manner.

Remarks:

- Hardware for the top of the pyramid alone will not be sufficient to bring petascale performance to bear on any given scientific problem.
- In order to run such large (and potentially heterogeneous) machines new operating system solutions will be required to address the problems related to scheduling, address space management, communication, fault tolerance, extensibility, reconfiguration etc.
- In addition, novel programming models, compiler techniques and runtime systems are needed in order to cope with task parallelism beyond 10^6.
- Mathematical models of most scientific problems have to be adapted in order to scale to the level provided by petaflop machines.
- All these measures are essential for utilizing petascale hardware, and Europe can legitimately claim a substantial advantage in those software-related developments.

Recommendation to implement an efficient and highly reliable infrastructure for storing large amounts of data

HET recommends increasing emphasis on permanent and persistent data repositories as a part of the HPC ecosystem.

Remarks:

- Computational science is – in large parts – driven by data and producing data.
- The amount of digitally stored scientific data has been doubling every year for a couple of decades now, and the end of this exponential growth does not seem to be near.
- Because of the huge amounts of data involved (many petabytes, approaching the exabyte range) large scale replication is not an option.
- On the other hand, most of these sensor data cannot be reproduced in case of a loss, so systematic measures against failures (including disasters) have to be implemented.
- Because of the heterogeneity of data sources semantic integration needs to be addressed, too.
- Because of issues related to IP, ownership, privacy etc. elaborate security measures have to be implemented.

Recommendation to support competence development in computational science through extensive training and education activities

HET recommends supporting extensive training and education activities which focus on enabling more efficient and higher quality use of the top-end facilities in the long run, activities such as computer-based modeling, scalable code development, integration work for the existing national infrastructures and training effort for competence development in computational sciences in general.

Remarks:

- Computational science will substantially change the way science is performed in basically all fields.
- In order to use this new paradigm of doing science, massive educational efforts have to be launched.
- Scientists have to be enabled to cast their investigations into computational models, exploiting the massive amounts of data being gathered by an ever-increasing number of sensors.
- Those models have to be turned into high-quality, scalable code to run on the fastest machines available.
- Code development, as well as running high-end systems, requires an increasing number of competent people.
- Existing national infrastructures work as the essential development platforms in designing scalable code for the top end systems.

Recommendation to raise the visibility of HPC

HET recommends strong activities to increase the visibility and improve the publicity of computational science in order to highlight the strategic impact and need of numerical simulation for most areas of science and engineering

Remarks:

- The strategic contribution of computing services has been highlighted in various high-level reports during the last two years, but this contribution is often still not recognized by the wider community
- Increasing visibility of HPC for society in general is important
- Funding of the research projects seldom include a significant contribution to computing infrastructure
- European HPC service as a mature ESFRI list entry is an excellent start for promoting higher visibility

Recommendation to boost collaboration

HET recommends support for collaborative actions with a target to link the major players in HPC Ecosystem – existing grid and HPC projects, national and regional centers, main computational research groups, funding organizations and potential new planned FP7 efforts – in order to maximize synergy for actions

Remarks:

- Number of major actors in the HPC arena is limited – results require often collaboration
- Existing EU Research Infrastructure projects, such as Geant2, Deisa or EGEE, have already developed a number of high-quality results
- Similar systems and processes are designed in parallel in different locations all the time
- A large number of ESFRI roadmap projects would benefit from IT-related collaboration

Recommendation to support European industry

HET recommends support for collaborative efforts with European industrial HPC users and European HPC industry at large – from hardware and software R&D to product design and manufacturing.

Remarks:

- Currently industrial users are a minority group compared with academic users in most of the HPC facilities, more collaborative projects with longer term targets searching for radical impacts are needed
- While investing in HPC facilities in Europe, efforts collaborating with the European HPC industry can be considered as long as they do not endanger the competition between the HPC vendors
- Increasing the volume of European R&D activities of non-European companies, such as software development or manufacturing plants placed in Europe, is beneficial

4 Scientific case for petascale computing

The Scientific Case for European Petascale Computing has been produced between August 2005 and April 2006 by an international scientific panel, put together by cooperation between Finland, France, Germany, Italy, the Netherlands, Spain and the United Kingdom. The origin of this endeavour was the recognition of the strategic role of High Performance Computing (HPC) at the leading edge, so-called "Leadership-Class Supercomputing", for European Science and Economy. The conviction that isolated European countries would not be able to provide their researchers and engineers with resources competitive on the world stage lay at the heart of the HPCEUR and HET initiatives.

In focusing on the requirements for the successful exploitation of Leadership-class Supercomputing – the provision of the order of 1 Petaflop/s peak performance around 2009 – the panel emphasised that the exploitation of such a resource demands an associated computational infrastructure. We envisage *one or more general purpose, Pflop-class machine operating at the apex of a wide pyramid of computational resources that embrace national, regional and thematic centres, accessible through a data network or grid, with appropriate user support organizations dedicated to ensuring maximum exploitation throughout the entire European community*. Europe has been very successful in establishing various elements of this resource and performance pyramid, notably through the GEANT2 network and its high throughput optical interconnections, and with the DEISA supercomputer grid. A compelling scientific leadership position for Europe's Computational Science and Scientific-Based Engineering Science demands such a strong and sustained commitment to high-end computing.

The report has been prepared by five thematic panels:

1. Weather, climatology and earth sciences
2. Astrophysics, HEP and plasma physics
3. Materials science, chemistry and nanoscience
4. Life sciences
5. Engineering

The full report is available in HET Web pages: www.hpcineuropetaskforce.eu

5 Funding and utilization model

Establishing an internationally competitive European HPC infrastructure with a small number of European level petaflop centres requires continuous funding of both hardware procurement and support structures. The funding has to be provided by several sources, primarily the member states and associate states, which host the infrastructure, and, in addition, the European Commission. While the allocation of resources to research

projects should follow scientific criteria, the funding organisations also have legitimate interests of their own. The different interests of science and the associated funding agencies have to be brought together, in order to create a world-leading petaflop infrastructure within the European e-Science ecosystem.

The proposed funding and utilization model is based on strong investments from the hosting countries with additional investment from European Commission allowing an "European portion" of the computing cycles.

The more detailed proposal for a funding and utilization model of European petaflop resources is available in HET Web pages: www.hpcineuropetaskforce.eu

6 Peer review process

The HET has been setup with the objective to contribute towards the improvement of the European Research Infrastructure in the area of scientific computing and data handling. It has clarified the requirement to make competitive world class supercomputers available for researchers involved in large size simulation and modeling, and has put forward a scientific case for such.

The requirements for the top-of-the-pyramid resources have been defined taking into account the principles of subsidiarity with existing national and thematic resources, and ensuring the most relevant scientific contribution. It is expected that scientists using the top-of-the-pyramid resource are to contribute in advancing science through numerical simulation. This calls for an evaluation process based on peer review to allocate computer resources. Since the optimal utilization of highly parallel systems, such as the petaflop computers, is challenging, a two-level review evaluating both scientific excellence and efficiency of the application code is required.

The more detailed proposal for a peer-review process is available in HET Web pages: www.hpcineuropetaskforce.eu.

7 More information about HET

HET Web pages contain the most accurate data, including the above mentioned documents: www.hpcineuropetaskforce.eu

The following draft documents are available:

1. European scientific case for high-end computing
2. A sustainable High Performance Computing Ecosystem for Europe
3. Peer-review process

4. Funding and utilization model

The current members of HET are (in alphabetic order of country)

* Jens Volkert (Austria)
* Dieter Kranzlmüller (Austria)
* Kimmo Koski (Finland) - chair
* Leif Laaksonen (Finland) - secretary
* Alain Kavenoky (France)
* Alain Lichnewsky (France)
* Achim Bachem (Germany)
* Helmut Löwe (Germany)
* Andreas Reuter (Germany)
* Andy Shearer (Ireland)
* Thibaut Lery (Ireland)
* Fabio Schifano (Italy)
* Piero Vicini (Italy)
* Patrick Aerts (The Netherlands)
* Peter Michielse (The Netherlands)
* Francesc Subirada (Spain)
* Felipe Lozano (Spain)
* Lennart Johnsson (Sweden)
* Marie-Christine Sawley (Switzerland)
* Jane Nicholson (United Kingdom)
* James Penman (United Kingdom)
* Hugh Pilcher-Clayton (United Kingdom)

8 Terminology

HPC
High Performance Computing

HET
High Performance Computing in Europe Taskforce, established in June 2006 with a mandate to draft a strategy for European HPC ecosystem

Petaflop/s
Performance figure: 10^{15} floating point operations (calculations) in second

Petascale
Systems or applications capable of petaflop/s computing performance

ESFRI
European Strategy Forum on Research Infrastructures. The role of ESFRI is to support a coherent approach to policy-making on research infrastructures in Europe, and to act as an incubator for international negotiations about concrete initiatives. In particular, ESFRI is preparing a European Roadmap for new research infrastructures of pan-European interest.

HPCEUR
Project aiming at establishing European high-end supercomputer installations was run until June 2006, after which the project was formally ended and the remaining work transferred to HET

DEISA
Distributed European Infrastructure for Supercomputing Applications. DEISA is a consortium of leading national supercomputing centers that currently deploys and operates a persistent, production quality, distributed supercomputing environment with continental scope.

EGEE-II
Enabling Grid for E-sciencE. The project provides researchers in academia and industry with access to a production level Grid infrastructure, independent of their geographic location.

GÉANT2
Seventh generation of pan-European research and education network