Building the European High-Performance Computing Ecosystem

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Topics

1. Background, terminology and definitions
2. Petaflop computing
   - Partnership for Advanced Computing in Europe (PRACE)
3. Middle layer HPC
   - DEISA
   - EGI/EGEE
4. ESFRI
5. New HPC Ecosystem
6. Case CSC
7. Some conclusions
Some background data

Me
- Born 1964, married and three daughters
- Dissertation on Metacomputing Technologies 1996 (Technical University of Helsinki)
TALKS ABOUT THE FINNS’ EMOTIONAL COLDNESS ARE NONSENSE. HERE ARE EXAMPLES OF PASSIONATE FEELINGS.

1. FURIOUS DELIGHT
2. ENDLESS LAUGH
3. ENORMOUS JOY
4. SMARTING FRUSTRATION
5. DEEP SORROW
6. BITTER ANGER
Terminology and pointers

- **HPC**
  - High Performance Computing

  - 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

  - e-Infrastructure Reflection Group. e-IRG is supporting the creation of a framework (political, technological and administrative) for the easy and cost-effective shared use of distributed electronic resources across Europe - particularly for grid computing, storage and networking.

  - 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.

- **RI**
  - Research Infrastructure
Terminology and pointers (cont.)

- **PRACE**
  - Partnership for Advanced Computing in Europe
  - EU FP7 project for preparatory phase in building the European petaflop computing centers, based on HET work

- **DEISA**, [https://www.deisa.org/](https://www.deisa.org/)
  - 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.

  - 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.

  - An effort to establish a sustainable grid infrastructure in Europe

  - Seventh generation of pan-European research and education network

- **NDGF**, [www.ndgf.org](http://www.ndgf.org)
  - Nordic Data Grid Facility
Performance Pyramid

- European HPC center(s) - TIER 0
- National/regional centers, Grid-collaboration - TIER 1
- Local centers - TIER 2
- Capability Computing
- Capacity Computing
Need to remember about petaflop/s...

- **What do you mean with petaflop/s?**
  1. Theoretical petaflop/s?
  2. LINPACK petaflop/s?
  3. Sustained petaflop/s for a single extremely parallel application?
  4. Sustained petaflop/s for multiple parallel applications?

- **Note that between 1 and 4 there might be several years**

- **Petaflop/s hardware needs petaflop/s applications, which are not easy to program, or not even possible in many cases**
  - Do we even know how to scale over 100000 processors …
Computational science infrastructure
Main players in European HPC Ecosystem

- ESFRI Roadmap and 35 new research infrastructures
- PRACE – Petaflop computing centers
- EU-supported infrastructure projects, such as EGEE, DEISA, GEANT2 and OMII-Europe
- European Grid Initiative, EGI
- Policy groups, such as ESFRI and e-IRG
- Regional activities, such as NDGF
- National Infrastructures
- International centers, such as CERN, EBI and ECMWF
- User communities with HPC requirements, such as fusion or climate
Petaflop/s computing
High-Performance Computing in Europe Taskforce (HET) outcome

- Entry in ESFRI list for petaflop computing
- Papers:
  - Scientific case for European HPC (most work done by previous HPCEUR project)
  - Proposal for funding models
  - Proposal for peer review process
  - Views for HPC Ecosystem
  - Summary paper with recommendations
- Good team spirit with a common approach
- Basis for practical implementation
  - Consortium for ESFRI Preparatory phase
  - Memorandum of Understanding for European Tier 0 HPC service
HET Scope: HPC Ecosystem

- The upper layers of the pyramid
  - HPC centers / services
  - European projects (HPC/Grid, networking, …)

- Activities which enable efficient usage of upper layers
  - Inclusion of national HPC infrastructures
  - Software development and scalability issues
  - Competence development

- Interoperability between the layers
What is going to happen with PRACE?

- Project will start 1.1.2008
- Consortium partners (14 countries)
  - Austria, Finland, France, Germany, Greece, Italy, Norway, Poland, Portugal, Spain, Sweden, Switzerland, The Netherlands, United Kingdom
- Two years, 10+10 MEUR volume
- Prototypes for petaflop computing during 2008-2009
- Target to have the first center operational in 2009-2010
- Open issues to be solved during the preparatory phase:
  - Which companies to prototype and where to place them?
  - Who will host the petaflop centers?
  - Who will pay for construction?
  - Who can use the resources and under which conditions?
  - How to link with other projects, for example DEISA?
PRACE preparatory phase

- FP7 Call for Research Infrastructure
  - Awaiting signature, starts 1/1/08, 2 years
  - Coordinator A. Bachem, FZ Jülich

Tasks summary (WPs):
- Management
- Organisational concept of RI
- Dissemination, training & outreach
- Distributed system management
- Deployment of prototype systems
- Petascaling & Benchmarking of appls.
- Petaflop/s system for 2010
- Future HPC technologies beyond 2010
Partners of the PRACE RI

- **Principal Partner**
  - Willing and able to host one of the 3-5 key facilities/sites
  - Adequate funding capability for investment and running costs

- **General Partner**
  - Important contribution to the RI
  - Help relate the RI, the research communities and the HPC ecosystem

- **Scientific Partner**
  - Contributes to progress of European science or industry by using the RI
  - World class modeling, simulation and computation
Middle layer HPC

National/regional centers, Grid-collaboration
DEISA – Distributed European Infrastructure for Supercomputing Applications

- A consortium of leading national supercomputing centres deploying and operating a persistent, production quality, distributed supercomputing environment with continental scope
- Grid-enabled FP6 funded Research Infrastructure
- A 4-year-project started on May 2004
- Total budget is 37,1 M€ (incl. DEISA and eDEISA contracts), EU funding - 20.9 M€
EGEE-II Applications Overview

- >200 VOs from several scientific domains
  - Astronomy & Astrophysics
  - Civil Protection
  - Computational Chemistry
  - Comp. Fluid Dynamics
  - Computer Science/Tools
  - Condensed Matter Physics
  - Earth Sciences
  - Fusion
  - High Energy Physics
  - Life Sciences
- Further applications under evaluation

Applications have moved from testing to routine and daily usage
- ~80-90% efficiency
Goal:
• Long-term sustainability of grid infrastructures in Europe

Approach:
• Establishment of a new federated model bringing together NGIs to build the EGI Organisation

EGI Organisation:
• Coordination and operation of a common multi-national, multi-disciplinary Grid infrastructure
  – To enable and support international Grid-based collaboration
  – To provide support and added value to NGIs
  – To liaise with corresponding infrastructures outside Europe

EGI Objectives:
– Ensure the long-term sustainability of the European e-infrastructure
– Coordinate the integration and interaction between National Grid Infrastructures
– Operate the European level of the production Grid infrastructure for a wide range of scientific disciplines to link National Grid Infrastructures

EGI Vision:
http://www.eu-egi.org/vision.pdf
EGI Preparation Team

Members:
- Johannes Kepler Universität Linz (GUP)
- Greek Research and Technology Network S.A. (GRNET)
- Istituto Nazionale di Fisica Nucleare (INFN)
- CSC - Scientific Computing Ltd. (CSC)
- CESNET, z.s.p.o. (CESNET)
- European organisation for Nuclear Research (CERN)
- Verein zur Förderung eines Deutschen Forschungsnetzes - DFN-Verein (DFN)
- Science & Technology Facilities Council (STFC)
- Centre National de la Recherche Scientifique (CNRS)

Work Packages
- **WP1**: EGI Project Management (Dieter Kranzlmuller, GUP)
- **WP2**: EGI Requirements Consolidation (Fotis Karayannis, GRNET)
- **WP3**: EGI functionality definition (Laura Perini, INFN)
- **WP4**: Study of EGI legal and organisational options (Beatrice Merlin, CNRS)
- **WP5**: Establishment of EGI (Jürgen Knobloch, CERN)
- **WP6**: EGI Promotion and Links with Other Initiatives (Per Öster, CSC)
ESFRI
ESFRI

- Strategy Forum with a consulting role to EU
- Wide representation of scientists in various disciplines
- Roadmap process for major new European research infrastructures (range of 10-1000 MEUR for an infrastructure)
- Roadmap published in 2006
  - 35 projects labeled mature
  - One of the projects European HPC Service
- Preparatory projects for each project
  - 1-4 years
  - Deadline for project call was May 2nd, 2007
Impact of ESFRI

- Rising a lot of interest
  - Scientific communities
  - EU
  - National priorities
- Preparatory phase call by EU
- National funding
- Political and non-political discussions for hosting of ESFRI infrastructures
- Obvious need for prioritising

- NOTE: ESFRI list includes only the new infrastructures. The existing ones have development plans, too
ICT infrastructure and ESFRI

- Only one of the projects is from ICT sector
  - PRACE for petaflop computing
- All of the projects need ICT infrastructure at some level
  - Computing, data handling, software development, networks, …
  - Will this be properly understood is a good question
- Need for a strong horizontal ICT infrastructure to avoid overlapping work

- And the ESFRI-list is being updated just now
  - Should there be more ICT entries in the updated list?
  - Data handling and software development would be good candidates…
ESFRI infrastructures and other infrastructures require professional services for computing, data handling, networks, software development, parallel computing skills, knowledge for computational methods etc.

These tasks do not necessarily vary much between sciences and should not be done separately to each research infrastructure.
New HPC Ecosystem is being built...
European HPC after FP6

- Multiple Grid projects with varying results – learning for collaboration
- Early experiences about interoperability between national HPC centers
- Communities start to form, in various levels
- Research community more active in computational science domain
- European Union targets in creating sustainable infrastructures

- Petaflop computing raised to European agenda, scientific case for high-end computing available
Targets for European HPC collaboration 2007 onwards

- Continuation of existing grid projects (DEISA, EGEE ...) and development in GEANT2 network infrastructure
- Building European petaflop computing services integrated in the full HPC ecosystem according to the performance pyramid model (PRACE)
- Maximal synergy between PRACE and DEISA (integration after some time?)
- Interoperability between PRACE and EGI/EGEE
- Building up research infrastructure services for ESFRI roadmap
- Target to establish an active European community for HPC: infrastructure, resource sharing, communication and collaboration over country borders
Some Key Issues

- **Sustainability**
  - EGEE and DEISA are projects with an end
  - PRACE and EGI are targeted to be sustainable with no definitive end

- **ESFRI and e-IRG**
  - How do the research side and infrastructure side work together?
  - Two-directional input requested

- **Requirement for horizontal services**
  - Let’s not create disciplinary IT silos
  - Synergy required for cost efficiency and excellence

- **ICT infrastructure is essential for research**
  - The role of computational science is growing

- **Renewal and competence**
  - Will Europe run out of competent people?
  - Will training and education programs react fast enough?
New market for European HPC

- 35 ESFRI list new research infrastructure projects, most of them starting a preparatory phase project late 2007
  - 1-4 years
  - 1-7 MEUR * 2 (petaflop computing 10 MEUR * 2)
- Successful new research infrastructures start construction 2009-2011
  - 10-1000 MEUR per infrastructure
- Existing infrastructures are also growing

Results:
- Growing RI market, considerably rising funding volume
- Need for horizontal activities (computing, data, networks, computational methods and scalability, application development,…)
- Real danger to build disciplinary silos instead of searching IT synergy
What needs to be done?

- **From Egosystem to Ecosystem**
  - Europe doesn’t afford not to collaborate
- **Focus on infrastructure and synergy**
  - Avoid running out of resources – hw nor competent labor
- **Remember the Enablers**
  - Utilisation of existing infrastructures
  - Scalable software development
  - Competence development
- **Understand the roles of different levels of the pyramid**
  - Not competing with each other, but completing each other
- **Get governments interested**
  - The impact for Europe is high when considering the whole ecosystem (not only hw): high level competence, more jobs, R&D in Europe etc.
- **And it would not harm to get industry interested either…**
  - But by switching the focus from quarterly benefits to longer term
Case CSC
Operated on a non-profit principle

All shares to the Ministry of Education of Finland in 1997

Reorganized as a limited company, CSC-Scientific Computing Ltd. in 1993

Founded in 1971 as a technical support unit for Univac 1108

CSC Turnover in 2006
15.6 M€, 150 employees

Since March 2005, facilities in Keilaniemi, Espoo

First supercomputer Cray X-MP/EA 416 in 1989

Funet started in 1984
VISION 2012:
CSC – a leading center of excellence in information technology for science in the European research area

MISSION:
CSC, as a part of the Finnish national research structure, develops and offers high quality information technology services
CSC Fields of Services

- UNIVERSITIES
- POLYTECHNICS
- RESEARCH INSTITUTES
- COMPANIES

- FUNET SERVICES
- COMPUTING SERVICES
- DATA SERVICES
- APPLICATION SERVICES
- INFORMATION MANAGEMENT SERVICES
Supercomputer as a part of Finnish Science Policy

- Finland has a strong base for computational science: first centralized resources available already in mid 80’s
- The impact of computational science is constantly growing: supercomputers are used increasingly often, and in new scientific disciplines
- The preconditions for using HPC capacity are strong in Finland: even if it is possible to purchase a supercomputer in less than one year, building up a competence center such as CSC takes easily 10 years
- Efficient computing environment attracts international top quality research and eases the collaboration possibilities of Finnish scientists
CSC’s supercomputers

**Cray Hood**
- 6736 processor cores
- 6.7 TB memory
- 70 Teraflops peak computing power
- 70 TB disk space

**HP ProLiant cluster**
- 2048 processor cores
- 4 TB memory
- 10 Teraflops peak computing power
- 98 TB disk space

**Sun Fire 25K**
- 192 processor cores
- 384 GB memory
Examples of computational challenges

2. Connected models: Forests and nanoscale aerosols, factors for our future climate
3. How do cell membranes function
4. Development of more efficient drugs against cancer
5. New environmentally friendly pulp bleaching chemicals
6. Better, faster, cheaper with the aid of computational fluid dynamics
7. Accurate quantification of the age and composition of the universe using satellite observations
8. New type of solar cells
9. Quantum dots and wells as nano-electronics solutions
10. Computational modelling of fusion reactors
CSC involvement (examples)

- CSC is the largest national IT center in northern Europe
  - Supercomputing environment: over 70 Tflop/s Cray capability system installed 2007-2008, 10.6 Tflop/s HP system early 2007, other systems
  - Staff of 160 with wide variation of competence: multi-disciplinary computational science, networks, information management, software development, …
  - Hosting over 200 commercial scientific applications and over 60 databases
- International collaboration: PRACE, DEISA, EGEE II, Embrace, HET chair, e-IRG chair, ESFRI-roadmap projects, other projects
- Scientific software development: in-house products from various projects (modeling, workflows and user interfaces etc.)
- Finnish University and Research Network (FUNET)
- Hosting the computing systems of the Finnish scientific libraries
Some conclusions

- HPC Ecosystem has a lot of acronyms 😊

- ESFRI Roadmap projects will have a major impact requiring horizontal (IT-infrastructure) services
  - ‘Research Infrastructure Market’ will burst in two years

- Interoperability between different European projects or infrastructures is said to be crucial, but this is not a technical challenge

- Collaboration has to develop in all levels, for example between different disciplines, between research communities and centers, between European projects and infrastructures, and between countries