Welcome to the 2011 PRACE Scientific Seminar, February 21 - 23

Lennart Johnsson
Professor
School of Computer Science and Communications
Director, PDC
Cullen Distinguished University Chair
University of Houston
Director, Texas Learning and Computation Center
Outline

- Stockholm
- KTH
- PDC
- PRACE
Stockholm

- Metro area has a population of 2.1 million (22% of 9.4 million) 2010
- Metro area responsible for 28% of GDP
- About 45% of companies with >200 employees has HQ in Stockholm
- About 21.7 million passengers from four airports (Arlanda 17 million)
- 2010 European Green Capital Award by the EU Comission
- 2006 Most Innovative City by the Maastricht Economic Research Institute on Innovation and technology (MERIT) and the Joint Research Centre's Institute for the Protection and the Security of the Citizen of the European Commission
- 2008 most competitive region outside the US and 6th in the world by the Center for International Competitiveness (UK)
- 2010 23rd most Global City (8th European most Global City) by the US Foreign Policy Magazine.
Stockholm

- Nobel Prizes in Physics, Chemistry and Nobel Memorial Prize in Economics are awarded by the Royal Swedish Academy of Sciences, the Nobel Prize in Medicine is awarded by the Nobel Assembly at the Karolinska Institute and Literature Prize is awarded by the Swedish Academy. The Nobel Banquet is held in Stockholm City Hall with about 1,300 guests.

- Stockholm Marathon, best Marathon in the World according to “The Ultimate Guide to International Marathons” had a total of 20,136 (15,441 men, 4,695 women) entrants, 15,468 starters (11,999 men, 3,469 women) and 14,715 finishers (11,436 men, 3,279 women)
Stockholm’s Top 10 companies by revenue

- **Ericsson**: Worlds leading mobile telecom equipment supplier with 35% market share. Revenue 206B SEK 2009.

- **Vattenfall**: 6th largest Global Electric Utility company (according to Platts ranking). Revenue 205B SEK 2009.


- **Skanska**: No 1 European and 4th global pulp and paper and a leading consumer goods manufacturer, Europe’s largest private land owner with 2.6M hectares (larger than Vermont), Revenue 111B SEK 2009.

- **TeliaSonera**: Europe’s no 1 and fastest growing IP backbone and no 1 Nordic and Baltic fixed-voice, broadband, and mobile operator by revenue and customer base, and 10th-largest global mobile group with 150M customers. Revenue 109B SEK 2009.
Stockholm’s Top 10 companies by revenue

**Electrolux**
- Worlds 2nd largest home appliance maker. One of the worlds 5 top durable goods maker according to Forbes Magazine.
- Revenue 109B SEK 2009.

**H&M**
- Worlds most valuable retailer according to Interbrand with 2,200 stores in 38 countries. Revenue 101B SEK 2009.

**ICA**
- The largest Nordic retailer. Revenue 95B SEK 2009.

**Nordea**
- The largest Swedish bank operating in 19 countries. Revenue 94BSEK 2009.

**Atlas Copco**
- Worlds leading manufacturer of air compressors and the first company to get a compressor certified for 100 percent energy recovery. Revenue 64B SEK 2009.
KTH

- Sweden’s largest Technical University
- Responsible for 1/3rd of technical research and education
- 13,000+ undergraduate students
- 1,500 PhD students
- 2,900 employees
- ~322M€/yr budget (2009)
- 18 National Research Centers
- Organized as 10 Schools
  - Architecture
  - Biotechnology
  - Computer Science and Communications
  - Electrical Engineering
  - Industrial Engineering and Management
  - Information and Communication Technology
  - Chemical Science and Engineering
  - Technology and Health
  - Engineering Sciences
PDC’s Mission

Infrastructure (PDC-HPC)

Operation of a high-end infrastructure for HPC, data services, user support and training for Swedish research on behalf of the Swedish National Infrastructure for Computing (SNIC), collaborative international and national consortia, and research groups at KTH and Stockholm University

Research

Conduct world-class research and education in parallel and distributed computing methodologies and tools
SNIC

- Organized within the Swedish Research Council
- Mission:
  - Provide funding for computing resources in Sweden
  - Coordinate investments and competence
  - Allocate resources to users (SNAC committee)
  - Fund and coordinate development projects
  - Host the Swedish National Graduate School in Scientific Computing (NGSSC)
- Means:
  - Work by the six SNIC centers
  - A board and a very small executive organization
  - Strategic plan: The SNIC Landscape Document
PDC Computing Resources

Key - HP SMP
32 Cores, 256 GB memory

Povel
Prace Prototype (energy efficiency)
4320 cores (180 4x6core AMD nodes)
36 TF theoretical peak performance
5.76 TByte memory

Ferlin and SweGrid - Dell Cluster
SNIC Foundation Level Service
32 nodes with Infiniband
6120 cores (765 nodes, 2 quad core Intel)
7 TByte memory

Ekman - Dell PowerEdge Cluster
Climate and Flow research
6120 cores (765 nodes, 2 quad core Intel)
7 TByte memory

Hebb - IBM Blue Gene/L
Stockholm Brain Institute, Mechanics, and IN
c
1024 nodes
6 TF theoretical peak performance
20 TByte memory

10,144 cores (1268 nodes, 2 quad core AMD)
89 TF theoretical peak performance
20 TByte memory

Lennart Johnsson
PRACE Scientific Seminar
Stockholm, 2011-02-21
PDC’s latest HPC system

- Cray XE6
- 1,516, dual-socket AMD 12-core, 2.1 GHz
  32 GB compute nodes (36,384 cores),
  305 TF TPP, 237 TF sustained (Linpack)
- Gemini 3D torus network
- SNIC PRACE system
- Would be Nr. 8 in Europe and Nr. 28 worldwide
  on the November 2010 Top500 list
# PDC’s Computational Resources

<table>
<thead>
<tr>
<th>System</th>
<th>Cores</th>
<th>TPP</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lindgren</td>
<td>36384</td>
<td>305 TF</td>
</tr>
<tr>
<td>Ekman</td>
<td>10,144</td>
<td>89 TF</td>
</tr>
<tr>
<td>Ferlin</td>
<td>5,360</td>
<td>58 TF</td>
</tr>
<tr>
<td>SweGrid</td>
<td>744</td>
<td>8 TF</td>
</tr>
<tr>
<td>Hebb</td>
<td>2,048</td>
<td>6 TF</td>
</tr>
<tr>
<td>Povel</td>
<td>4,320</td>
<td>36 TF</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td><strong>59,000</strong></td>
<td><strong>502 TF</strong></td>
</tr>
</tbody>
</table>
Storage

- **~20 TB disk**
  - Accessible via AFS

- **~900 TB disk**
  - Currently attached to individual systems
  - Lustre parallel file system
    - Site wide configuration planned

- **IBM tape robot**
  (~2900 slots, ~2.3 PB)
  - Accessible via HSM, TSM, and dCache (planned via NDGF)

Large datasets, e.g. Brain image database, Human Proteon Data,…
PDC Users

• Systems at PDC are used for a wide variety of scientific applications
• Over 500 time allocations by 400 PIs (past 4 years)
• Examples of these research areas include:
  • Quantum Chemistry
  • Climate Modeling
  • Neuroinformatics
  • Life Sciences
  • Physics
  • Computational Fluid Dynamics
Community Code Development

- **Gromacs**
  - GROMACS is a versatile package to perform molecular dynamics, i.e. simulate the Newtonian equations of motion for systems with hundreds to millions of particles
  - Head authors and project leaders: Erik Lindahl, KTH, David van der Spoel, Uppsala, Berk Hess, KTH
  - [http://www.gromacs.org/About_Gromacs](http://www.gromacs.org/About_Gromacs)

- **Dalton**
  - Dalton is a molecular electronic structure package with members of the KTH Theoretical Chemistry department being active contributors, especially Olaf Vahtras and Hans Agren
  - [http://www.daltonprogram.org/description.html](http://www.daltonprogram.org/description.html)
Education and Training

PDC Summer School since 1996
For many years now jointly with

Total 1996 – 2010: 834
Schools, examples

International Summer School on Grid Computing 2007
Gripsholmsviken, Mariefred, Sweden, 8 - 20 July

- EU
- Asia
- China
- USA
- Central South Am.
- South Am.
- Africa
- Russia
- Europe
- Austr.-alasia
- Other

2006
- Total 64 students
- EU 75% → 44%
- Other 20%

2007
Schools, examples

- 31 students (target 30)
- 14 PRACE partner countries represented
- 2 non-PRACE countries represented
- Access to Forschungs Zentrum Juelich’s BG/P
- Access to CSC’s Cray XT4
Workshops, examples

- 41 participants
- 3 PRACE partner countries represented
- 1 non-PRACE countries represented
- Access to AMD/ATI Radeon 5770 and 5870 GPUs
- Access to AMD/ATI Firestream 9270 GPUs
PDC Collaborations - Globus

GUSTO testbed for Grid applications demonstrated at the Supercomputing97 exhibit
PDC Collaborations - Alliance98
Interactive Collaborative Virtual Environment

www.pdc.kth.se/projects/alliance98/
PDC Collaborations

- The distributed interactive virtual reality demonstration needed high-bandwidth for real-time video and audio. This was accomplished through a dedicated connection to New York City, and a special connection from NYC to StarTap in Chicago arranged in collaboration between Sunet, Nordunet, Internet2, StarTap and NSF.

- This successful demo set-up motivated NORDUnet to become "the very first research network outside the United States to begin negotiations with Internet2 over a connection to Abilene, even before Abilene was put into operation." "The Abilene connection was implemented in 1999 as a 155 Mbps ATM link between a NORDUnet router and an Abilene router in the Teleglobe building in New York." Quotes from A History of International Research Networking: The People who Made it Happen, by Howard Davies, Beatrice Bressan, Wiley-VCH, April 2010.
1996 PDC Conference

Software for Parallel Computing

PDC invites you to the traditional December conference on parallel and high-performance computing. PDC is a national center for high-performance computing funded by the Swedish Council for High Performance Computing and KTH. The center operates an IBM SP system with 110 nodes, a Fujitsu VX/2 system, a Cray J932 system, mass storage facility and a visualization laboratory.
1999 PDC Conference

Simulation and Visualization on the Grid
Startap Annual Meeting 2001

About

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STAR TAP International Advisory Committee Meeting

INET 2001, Stockholm, Sweden
Tuesday, June 5, 2001

Handouts and Documentation

Meeting Agenda
Welcome and Introductions, Tom DeFanti
STARTAP_2001Mtq_DeFanti_Welcome.ppt (250KB)

STAR TAP Annual Update, Tom DeFanti
STARTAP_2001Mtq_DeFanti_STARТАPAnnualReport.ppt (3198KB)

STAR TAP Present and Future Applications, Maxine Brown
STARTAP_2001Mtq_Brown_Applications.ppt (1266KB)

Future Directions of the NSF ANIR, Tom Greene
STARTAP_2001Mtq_Greene.ppt (209KB)

STAR TAP's StarLight, Tom DeFanti
STARTAP_2001Mtq_DeFanti_StarLight.ppt (3229KB)

SURFnet's Connections to StarLight, Erik-Jan Bos
STARTAP_2001Mtq_Bos.ppt (968KB)

The Optical Network Evolution, Yves Poppe
STARTAP_2001Mtq_Poppe.ppt (3801KB)
Gelato Meeting 2003

The Stockholm meeting of the Gelato Federation Strategy Council--held October 13-15, was hosted by KTH, Sweden's Royal Institute of Technology. The meetings comprised formal technical presentations by the Gelato Focus Groups--Performance in a Box, Scalability in a Box (SIAB), Cluster Scalability and Performance, Compilers, and Parallel Filesystems--as well as in-depth discussions in the areas of Itanium hardware and the potential for future focus on grid computing.
Projects at PDC

Scala Life

DEISA

Baltic Grid

Enabling Grids for E-sciencE

PRACE

GRDI 2020

Virtual multidisciplinary Environments Using Cloud Infrastructures

NEON

Windows HPC Server 2008
PRACE
Partnership for Advanced Computing in Europe
PRACE Vision and Mission

- **Vision**: Enable and support European global leadership in public and private research and development.

- **Mission**: Contribute to the advancement of European competitiveness in industry and research through the provisioning of world leading persistent High-End Computing infrastructure
PRACE AISBL

- PRACE AISBL (Association International Sans But Lufratif) is a Belgian legal entity seated in Brussels formed April 23 2010 for providing a persistent pan-European Research Infrastructure for High-End Computing and associated services. Member countries currently are
  - Austria
  - Bulgaria
  - Cyprus
  - Czech Republic
  - Finland
  - France
  - Germany
  - Greece
  - Ireland
  - Italy
  - Netherlands
  - Norway
  - Poland
  - Portugal
  - Serbia
  - Spain
  - Sweden
  - Switzerland
  - Turkey
  - United Kingdom
Commitments to PRACE AISBL

- Hosting Partners: Germany, France, Italy, Spain
  - Binding commitments to contribute 100 M€ over 5 years in terms of Tier-0 cycles
  - Contribution measured by TCO
- All partners:
  - Binding commitment to share PRACE AISBL Head-Quarters costs equally
- EU Commission (expected)
  - 70 M€ in FP7

Note: GDP spread among PRACE partners a factor of ~200
Governance of the Association

- Modeled after successful examples of existing RIs
- Council as main decision making body
- Director with strong managing mandate
- Scientific Steering Committee and Access Committee to give scientific advice and to steer the Peer Review process
- Further committees will be instantiated by the Council as needed
PRACE Board of Directors (interim)

- **France**
  - Jean-Philippe Nominé (Financial Tasks, Dissemination)

- **Germany**
  - Thomas Eickermann (HQ-local Organizational Tasks, Legal Tasks)

- **Italy**
  - Sergio Bernardi (Legal Tasks, Peer Review, Business Plan)

- **Spain**
  - Sergi Girona, Chair (Business Plan, Peer Review)

- **Non-hosting partners (16)**
  - Lennart Johnsson (Dissemination, Financial Tasks)
Scientific Steering Committee

- The SSC is responsible for advice on all matters of a scientific and technical nature
  - Maximum of 21 members
  - Members appointed by Council based on a list of candidates prepared by the SSC
- Two year term (renewable twice)
- Propose the members of the Access Committee
- Resolutions by simple majority
Scientific Steering Committee

Appointed 2010-10-05

- Richard Kenway (chair) (UK, particle physics)
- Jose M. Baldasano (Spain, environment)
- Kurt Binder (Germany, statistical physics)
- Paolo Carloni (Italy, biological physics)
- Giovanni Ciccotti (Italy, statistical physics)
- Daan Frenkel (Netherlands, molecular simulations)
- Sylvie Joussaume (France, environment)
- Ben Moore (Switzerland, astrophysics)
- Gernot Muenster (Germany, particle physics)
- Risto Nieminen (Finland, materials)
- Modesto Orozco (Spain, life sciences)
- Maurizio Ottaviani (France, plasma physics)
- Michele Parrinello (Switzerland, chemistry)
- Olivier Pironneau (France, mathematics)
- Thierry Poinsot (France, engineering)
- Simon Portegies Zwart (Netherlands, astrophysics)
- Alfio Quarteroni (Italy, engineering)
- Kenneth Ruud (Norway, chemistry)
- Schroeder (Germany, engineering)
- Luis Silva (Portugal, plasma physics)
- Alfonso Valencia (Spain, bioinformatics)
Access Committee

Responsible for advice on the allocation of PRACE RI resources based on the Peer Review process

- Proposed by the SSC based on their personal experience in the areas of science
  - Appointed by the Council
  - Minimum of 5 members
  - Two years term (renewable once)
  - Half of the members shall be replaced every year
  - The Access Committee shall define its internal working rules
Access Committee

- **Kenneth Ruud** (Chair), Prof Dept of Chemistry, Dir., Center for Theoretical and Computational Chemistry, Univ of Tromsoe, http://www.ctcc.no/people/ruud
- **Roberto Capuzzo Dolcetta**, Prof Astronomy and Astrophysics, Dept of Physics, Univ of Rome, La Sapienza, Member of the Italian National Univ Council (Consiglio Universitario Nazionale), http://astro1.astro.uniroma1.it/dolcetta/dolcetta.html
- **Peter Nielaba**, Prof of Physics, Condensed Matter, Univ of Konstanz, http://cms.uni-konstanz.de/physik/nielaba/mitarbeiter/prof-dr-peter-nielaba
- **Manuel C. Peitsch**, Vice President, Biological Systems Research at Philip Morris International, Chair, Board of Directors, The Swiss Institute of Bioinformatics, Professor for Bioinformatics, University of Basel
- **Andreas Schaefer**, Institute of Theoretical Physics, University of Regensburg, http://homepages.uni-regensburg.de/~sca14496/schaefer.html
- **Hester Bijl**, Head of the Department of Aerodynamics, Wind Energy and Flight Performance and Propulsion, and Full Professor of Computational Fluid Dynamics in the Faculty of Aerospace Engineering, Delft Univ. of Technology, http://www.lr.tudelft.nl/live/pagina.jsp?id=cbaba9cd-db78-4675-8f07-3b2bef4d13ce&lang=en
PRACE RI Access

- Access strictly by PRACE peer review
- Free-of-charge for European scientific communities
- Three types of access
  - Preparatory access (Technical Review only)
    - Scalability, Code development, Code development with PRACE support
  - Project access – grant period ~1 year
    (Technical and Scientific Review)
  - Program access – resources managed by a community
    (Technical and Scientific Review)
- Early access call opened May 10 and closed June 10, 2010
- Start of provision: 1.8.2010
- 1st regular call opened June 15, closed August 15, 2010
- 2nd regular call opened November 1, 2010, closed January 11, 2011
- Further calls every 6 months
- 1st Preparatory Access call opened November 1, 2010
PRACE RI Review procedures for Project and Program proposals

- Technical peer review (system and code suitability) by hosting centre representatives
- Scientific peer review by 3 external reviewers
- Applicants may comment on the reviewers assessment; the comments are sent together with the reviewers assessment to the Access Committee
- The Council ratifies the prioritization list
- The Director informs (in writing) the applicants of the computing grants, on behalf of the Council
- Applicants have the right to appeal the decision of the Council
Early Access Call 324M core hours

- Belgium: 1
- Bulgaria: 2
- Denmark: 1
- Finland: 2
- France: 6
- Germany: 10
- Germany/UK: 1
- Greece: 2
- Ireland: 2
- Italy: 4
- Netherlands: 2
- Portugal: 4
- Spain: 13
- Sweden: 1
- Switzerland: 3
- UK: 12

- Astrophysics: 7
- Chemistry and Materials: 11
- Earth Sciences and Environment: 4
- Engineering and Energy: 15
- Fundamental Physics: 17
- Mathematics and Computing: 3
- Medicine and Life Sciences: 8

68 proposals from 15 countries
Scientific Review of 39 proposals
10 proposals granted access
Request 5x available resources
<table>
<thead>
<tr>
<th>Applicant</th>
<th>Organisation</th>
<th>Country</th>
<th>Title of project</th>
<th>Start date</th>
<th>Resource requested (cores)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dr Jochen Blumberger</td>
<td>University College London</td>
<td>UK</td>
<td>Simulation of electron transport in organic solar cell materials</td>
<td>1st Aug</td>
<td>24,660,000</td>
</tr>
<tr>
<td>Prof. Paolo Carloni</td>
<td>German Research School for Simulation Sciences GmbH</td>
<td>Germany</td>
<td>Excess proton at water/hydrophobic interfaces: A Car-Parrinello MD study</td>
<td>1st Aug</td>
<td>40,468,480</td>
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<tr>
<td>Prof Peter Coveney</td>
<td>University College of London</td>
<td>UK</td>
<td>Parallel space-time approach to turbulence: computation of unstable periodic orbits and the dynamical zeta function</td>
<td>1st Aug</td>
<td>17,000,000</td>
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<tr>
<td>Prof. Zoltán Fodor</td>
<td>Bergische Universitaet Wuppertal</td>
<td>Germany</td>
<td>QCD Thermodynamics with 2+1+1 improved dynamical flavors</td>
<td>1st Aug</td>
<td>63,000,000</td>
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<tr>
<td>Prof. Frank Jenko</td>
<td>Max Planck Institute for Plasma Physics (IPP)</td>
<td>Germany</td>
<td>Ab initio Simulations of Turbulence in Fusion Plasmas</td>
<td>1st Aug</td>
<td>50,000,000</td>
</tr>
<tr>
<td>Prof Harmen Jonker</td>
<td>Delft University</td>
<td>Netherlands</td>
<td>Providing fundamental laws for weather and climate models</td>
<td>1st Aug</td>
<td>35,000,000</td>
</tr>
<tr>
<td>Dr Nuno Loureiro</td>
<td>Instituto Superior Técnico</td>
<td>Portugal</td>
<td>Plasmoid Dynamics in Magnetic Reconnection</td>
<td>1st Dec</td>
<td>20,000,000</td>
</tr>
<tr>
<td>Prof. Dr. Dierk Raabe</td>
<td>Max-Planck-Institut für Eisenforschung</td>
<td>Germany</td>
<td>A dislocation dynamics study of dislocation cell formation and interaction between a low angle grain boundary and an in-coming dislocation</td>
<td>1st Aug</td>
<td>15,600,000</td>
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<tr>
<td>Dr Friedrich Roepke</td>
<td>Max-Planck-Gesellschaft</td>
<td>Germany</td>
<td>Type Ia supernovae from Chandrasekhar-mass white dwarf explosions</td>
<td>1st Dec</td>
<td>23,600,000</td>
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<tr>
<td>Prof. Silvano Simula</td>
<td>Sezione di Roma Tre</td>
<td>Italy</td>
<td>QCD Simulations for Flavor Physics in the Standard Model and Beyond</td>
<td>1st Dec</td>
<td>35,000,000</td>
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<tr>
<td><strong>Total</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td><strong>324,328,480</strong></td>
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# 1st Regular Access Call

363M core hours

<table>
<thead>
<tr>
<th>Country</th>
<th>Allocation</th>
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</thead>
<tbody>
<tr>
<td>Belgium</td>
<td>1</td>
</tr>
<tr>
<td>Bulgaria</td>
<td>1</td>
</tr>
<tr>
<td>Cyprus</td>
<td>2</td>
</tr>
<tr>
<td>Denmark</td>
<td>2</td>
</tr>
<tr>
<td>Finland</td>
<td>1</td>
</tr>
<tr>
<td>France</td>
<td>6</td>
</tr>
<tr>
<td>Germany</td>
<td>7</td>
</tr>
<tr>
<td>Greece</td>
<td>2</td>
</tr>
<tr>
<td>Hungary</td>
<td>1</td>
</tr>
<tr>
<td>Ireland</td>
<td>3</td>
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<tr>
<td>Italy</td>
<td>5</td>
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<tr>
<td>Netherlands</td>
<td>1</td>
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<tr>
<td>Poland</td>
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<tr>
<td>Portugal</td>
<td>2</td>
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<tr>
<td>Spain</td>
<td>10</td>
</tr>
<tr>
<td>Switzerland</td>
<td>1</td>
</tr>
<tr>
<td>UK</td>
<td>13</td>
</tr>
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</table>

- Astrophysics - 4
- Chemistry and Materials - 8
- Earth Sciences and Environment - 1
- Engineering and Energy - 6
- Fundamental Physics - 10
- Mathematics and Computing - 1
- Medicine and Life Sciences - 3

59 proposals from 17 countries
<table>
<thead>
<tr>
<th>Applicant</th>
<th>Organisation</th>
<th>Country</th>
<th>Title of project</th>
<th>Resource requested (cores)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dr J Bec</td>
<td>Observatoire de la Cote d'Azur</td>
<td>France</td>
<td>Droplet growth by coalescence in turbulent clouds: kinetics, fluctuations, and universality</td>
<td>50,000,000</td>
</tr>
<tr>
<td>Prof P Carloni</td>
<td>German Research School for Simulation Sciences GmbH</td>
<td>Germany</td>
<td>Ab initio molecular dynamics simulations of proton transport in a biological ion channel</td>
<td>48,758,784</td>
</tr>
<tr>
<td>Prof J Jimenez</td>
<td>Universidad Politecnica Madrid</td>
<td>Spain</td>
<td>Entrainment effects in rough-wall boundary layers</td>
<td>40,000,000</td>
</tr>
<tr>
<td>Dr S Katz</td>
<td>Eotvos University</td>
<td>Hungary</td>
<td>QCD Thermodynamics with Wilson fermions</td>
<td>72,000,000</td>
</tr>
<tr>
<td>Prof D Marx</td>
<td>Ruhr-Universitat Bochum</td>
<td>Germany</td>
<td>Investigating the effects of quantum nuclear motion in an enzyme that employs hydrogen tunnelling</td>
<td>32,000,000</td>
</tr>
<tr>
<td>Dr M van Reeuwijk</td>
<td>Imperial College London</td>
<td>UK</td>
<td>Turbulent entrainment due to a plume impinging on a density interface</td>
<td>30,000,000</td>
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<tr>
<td>Dr E Sanchez</td>
<td>EURATOM-CIEMAT Association</td>
<td>Spain</td>
<td>Non diffusive transport in ITG plasma turbulence</td>
<td>20,000,000</td>
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<tr>
<td>Dr L Silva</td>
<td>Instituto Superior Tecnico</td>
<td>Portugal</td>
<td>Predictive full-scale fast ignition with PW plasma amplified laser pulses</td>
<td>31,000,000</td>
</tr>
<tr>
<td>Prof F Toschi</td>
<td>Eindhoven University of Technology</td>
<td>Netherlands</td>
<td>Large scale high resolution blood flow simulations in realistic vessel geometrics</td>
<td>39,000,000</td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td></td>
<td></td>
<td>362,758,784</td>
</tr>
</tbody>
</table>
PRACE RI Systems

• 2010 1st PRACE System
  • BG/P by Gauss Center for Supercomputing at Juelich
    – 294,912 CPU cores, 144 TB memory
    – 1 PFlop/s peak performance
    – 825.5 TFlop/s Linpack
    – 600 I/O nodes (10GigE) > 60 GB/s I/O
    – 2.2 MW power consumption
    – 35% for PRACE
GENCI

- 2011 2nd PRACE system
  - Bull, 1.6PF, 92160 cores, 4GB/core
  - Phase 1, December 2010, 105 TF
    - 360 four Intel Nehalem-EX 8-core nodes, 2.26 GHz CPUs (11,520 cores), QDR Infiniband fat-tree
    - 800 TB, >30GB/sec, local Lustre file system
  - Phase 1.5 Q2 2011
    - Conversion to 90 16-socket, 128 core, 512 GB nodes
  - Phase 2, Q4 2011, 1.5 TF
    - Intel Sandy-Bridge
    - 10PB, 230GB/sec file system
HLRS

- 2011 3rd PRACE System
- Cray XE6 (Multi-year contract for $60+M)
  - Phase 0 – 2010
    10TF, 84 dual socket 8-core
    AMD Magny-Cours CPUs,
    1344 cores in total, 2 GHz,
    2GB/core,
    Gemini interconnect
  - Phase 1 Step 1 – Q3 2011
    AMD Interlagos, 16 cores, 1 PF
    2 – 4 GB/core
    2.7 PB file system, 150 GB/s I/O
  - Phase 2 – 2013
    Cascade, first order for Cray, 4-5 PF
LRZ

- 2011/12 4th PRACE system
- IBM iDataPlex (€83M including operational costs)
  - >14,000 Intel Sandy-Bridge CPUs, 3 PF (~110,000 cores), 384 TB of memory
  - 10PB GPFS file system with 200GB/sec I/O, 2PB 10GB/sec NAS
- Innovative hot water cooling (60C inlet, 65C outlet) leading to 40 percent less energy consumption compared to air-cooled machine.
BSC and CINECA

- 2012/2013 5th and 6th PRACE Systems

CINECA
Target ~2.5 PF

Computing Facility
10 MW 2013
Education and Training Highlights

- Petascale training and education needs surveyed Spring 2008
- First PRACE Summer School on Peta-scaling, KTH, Stockholm, August 2008. Platforms: IBM Blue Gene/P (FZJ) (65,536 cores) and Cray XT4 (CSC) (10,816 cores)
- First PRACE Winter School on Scalable Programming Models and Paradigms, GRNET, Athens, February 2009. Platforms IBM Power 6 (3,328 cores) and IBM Cell (1,152 SPE cores)
- Seven Code Porting Workshops in 2009

In total 270 participants in education and training events
PRACE Code Porting Workshops

- GPU and Hybrid system programming using CUDA and CAPS-HMPP, CEA, Paris, April 2009
- Porting and optimization techniques for PRACE applications, CSC, Helsinki, June, 2009
- Porting and optimization techniques for the CRAY XT5, CSCS, Manno, Switzerland, July, 2009
- Porting and optimization techniques for the Clearspeed/Petapath architecture, NCF/SARA, Amsterdam, October, 2009
- Porting and optimization techniques for the NEC/SX-9 (HLRS) and IBM BG/P (FZJ), Cyfronet, Cracow, October, 2009
- Porting and optimization techniques for the IBM Cell (BSC) and GPGPU systems, BSC, Barcelona, October, 2009
- Stream Programming with OpenCL, KTH, Stockholm, December, 2009
PRACE Access

- Next Regular Call expected in May 2011
- Preparatory Access any time

www.prace-ri.eu
DEISA-PRACE Symposium
April 13 – 14, 2011, Helsinki

• PRACE User Group Initiation Meeting