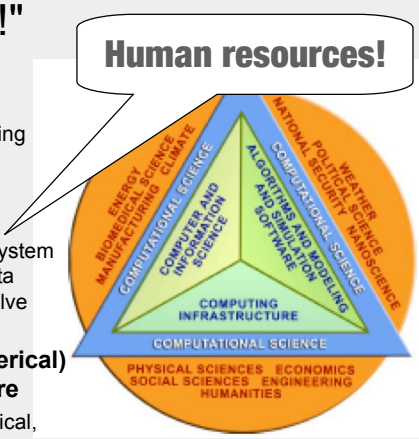
Supporting computational science

How to help both young and experienced researchers?

Juha Haataja
CSC - the Finnish IT Center for Science

What is computational science? — "It's all about software!"

- **Computing infrastructure**
  - supports both the science and engineering problem solving and the developmental computer and information science
- **Computer and information science**
  - develops and optimizes the advanced system hardware, software, networking, and data management components needed to solve computationally demanding problems
- **Algorithms (numerical and non-numerical) and modeling and simulation software**
  - developed to solve science (e.g., biological, physical, and social), engineering, and humanities problems



Picture from the PITAC report

Definition taken from the PITAC report:
Computational Science: Ensuring America's Competitiveness
(President's Information Technology Advisory Committee, 2005)



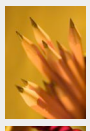
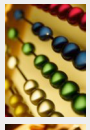
×  = const ?

Something different or more of the same?

CSC

Increasing requirements for HPC support

- **Many (not all) projects require extensive expert help from CSC**
  - high-performance, global-scale networking
  - middleware (grid platforms like DEISA, EGEE etc.)
  - high-performance computing services (special needs for scheduling, memory, I/O, tuning, parallelization etc.)
  - data management and analysis
  - improved interfaces and visualization services
  - algorithm and method development
- **Encouraging feedback from customers**
  - FinHPC: code optimization and parallelization
  - CoMS: coupled models systems for Earth Science
  - DECI: using the European supercomputing platform
  - MIKA/GPAW, NAMI, SOMA2, Elmer: scientific software development
- **Ministry of Education working group recommendations**
  - "Finnish eScience program"
  - "Developing computational science in Finland" (to appear)
- **Results from the CSC customer survey (end of 2006)**
- **Supporting the European HPC ecosystem**


CSC

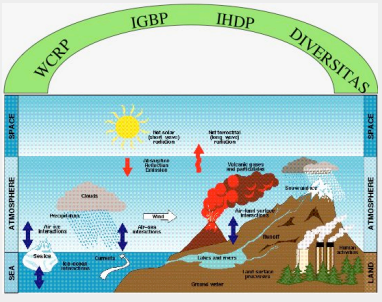
Code optimization and parallelization in the FINHPC project

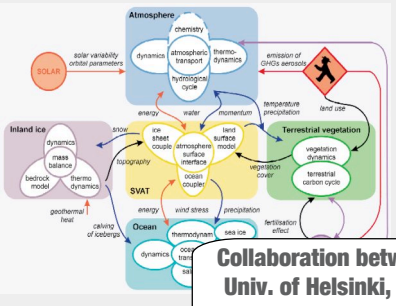
The software bottleneck — CSC has rewarding collaboration with Åbo Akademi

- **Funding from the Tekes MASI program**
  - Contact: Jussi Heikonen at CSC
- **Several codes have been treated, e.g.**
  - ELMFIRE (Tokamak fusion plasma simulation)
  - ProCon (Protein correlation analysis)
  - FIBER (Dynamics of complex elastic systems)
  - BioImageXD (Microscopy image analysis and processing)
  - A turbulence code
- **Performance of computational kernels can be doubled in many cases**
- **Greatest speed ups have been achieved by algorithmic optimization (up to order of 10000)**
- **Benchmark set was used in CSC's supercomputer procurement**

CSC

Coupled Model Systems in Earth Science





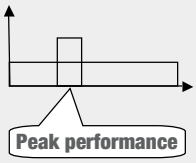
Collaboration between Univ. of Helsinki, FMI and CSC

- **CSC develops technology for coupling model systems**
  - CoMS project funded by Tekes (contact: Juha Lento at CSC)
- **Development based on Finnish expertise on modeling**
- **Coupler technology based on the international PRISM collaboration**

CSC

Plans for HPC support at CSC

- **Simplified quotas (no separate MPP and serial quotas)**
  - already implemented
- **New kinds of applications — "Grand Challenge Program"**
  - need for both human and software/hardware resources from CSC
  - currently no application process for human resources from CSC
  - *limited in time* (project duration, e.g., six months)
  - "peak resources" (cpu, I/O, network, disk), human support (software development, algorithmic expertise, code tuning, middleware or user interface development)
  - arranged as projects within the program (project management within CSC)
  - special application process, continous submitting of applications
  - focus on quality of service
  - first to be implemented in a test phase (1-2 years)
- **The normal resource allocation process will continue (and probably allocate most of cpu time)**
- **Contact at CSC: Juha Haataja, Juha Fagerholm**



CSC

Criteria for Grand Challenge Projects

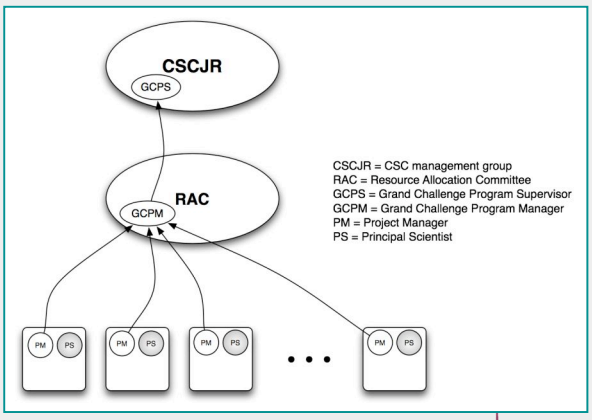
- **Scientific quality (main criteria)**
  - publications, patents etc.
  - group status (e.g., center of excellence)
- **Impact for the Finnish research community**
- **New and rising group or research area (future importance)**
- **Suitability for the CSC infrastructure**
  - hardware, software, expertise
  - working within the available resources (including human)
  - possibilities to apply for external funding?
- **Brokering to other channels possible (e.g., DECI, Nordic Grand Challenges, etc.)**



CSC

How support will be organized within CSC

- **Short applications**
- **Negotiations with the top candidates**
- **Reviewed by the Resource Allocation Committee**
- **Decisions by the CSC management group**
- **Based on principles given by the board of CSC**
- **For each project, a named contact person at CSC**



CSC

Supercomputing grants for young Finnish researchers

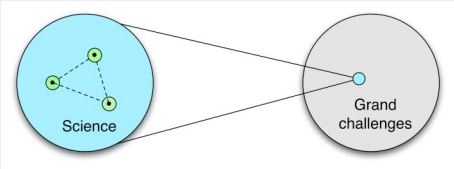
- **A call for proposals on computational science on Louhi (deadline April 30th)**
  - grants between 5 000 and 25 000 euros will be awarded to students and young researchers
- **Possible topics for the proposals include**
  - applying scalable and efficient computational tools to novel research problems
  - developing novel and efficient algorithms and their implementations in software
  - developing tools which suport software development and computational science
- **Requirements and criteria**
  - target platform: Cray XT4 with AMD processors
  - connection to research done at Finnish universities or polytechnics
  - scalability to hundreds or thousands of processors
  - projects based on open source software are especially welcome
- **CSC will support the selected projects with**
  - a named contact person
  - access to CSC experts on computational science
  - possibility to become a visiting researcher at CSC
- **The grants are sponsored by Cray, Inc. and AMD, Inc.**



CSC

From information deluge to unmapped seas

- **Information deluge**
  - Each researcher is like an island in a sea of information.
- **Grand challenges**
  - Science is a drop in the sea of the unknown.



- **Connecting**
  - Coordination, cross-disciplinary, IT skills, central data archives and computational resources, computer networking.
- **Pioneering**
  - New uses for HPC , data access, international services.

CSC