1971-2006
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HPC facilities at CSC

Juha Fagerholm

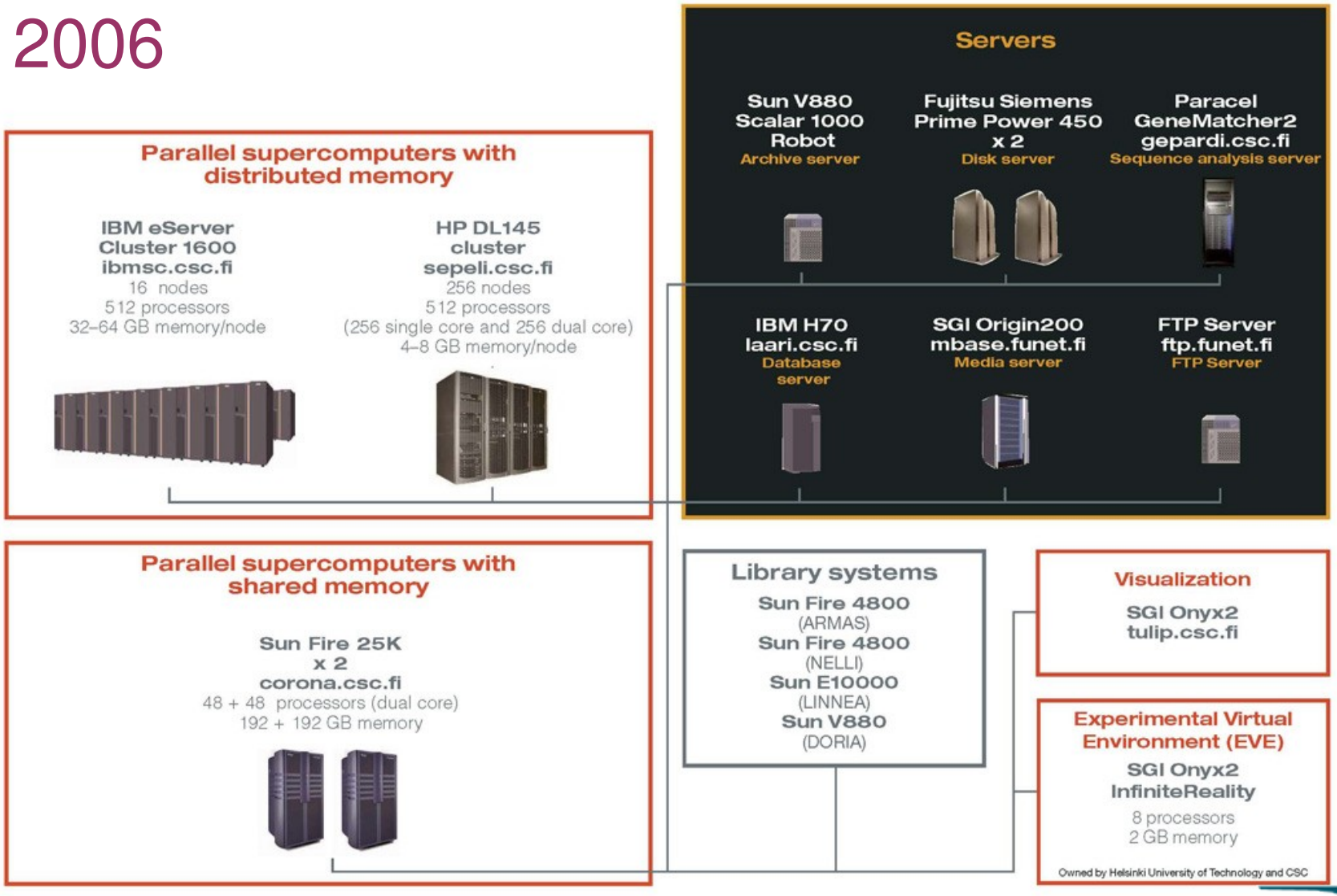
7th Annual Workshop on Linux Clusters for Super Computing, LCSC 2006

CSC

Topics to be covered

- **Computer environment at CSC**
- **Supercomputer procurement**
- **Data storage procurement**
- **Nordic Grand Challenge Survey**

CSC's Servers 2006



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IBMSC – IBM eServer Cluster 1600

- **First phase installed 2000**
- **Theoretical peak performance 2.2 Tflop/s**
- **512 CPUs and 672 GB memory**
  - 16 IBM p690 nodes each configured with 32 Power4 CPUs (1.1 GHz) and 32-64 GB of memory
- **IBM HPS Switch (”Federation”)**
- **Customers with efficiently parallelized codes are given priority**

Sepeli – HP ProLiant DL145 Cluster

- **Installed 2005**
- **Part of M-grid (Material Science Grid in Finland)**
- **Theoretical peak performance 3.1 Tflop/s**
- **772 cores and 1.6 TB memory**
  - 128 nodes with two AMD Opterons @ 2.2 GHz
  - 128 nodes with two dual-core AMD Opterons @ 2.2 GHz
  - GE network
  - ROCKS Cluster Mgmt System
- **Profiled for serial and at first up to 8-way parallel workloads**

CSC's Top500 computers 1993–2007

Supercomputer procurement in 2006

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- Grant of 10 M€ from Ministry of Education
- Grant was split to address different needs: capacity & capability computing, storage
- Benchmark seminar for users in October 2005
- Call for participation was out in February 2006 and RFP in June 2006
- Agreements were signed on 9th October 2006
- First installation of HP cluster at 4Q/2006: 10 TF peak
- First phase of Cray Hood at 1Q/2007: 10 TF peak
- Second and third phases of Cray Hood at 1H/2008 and 2H/2008: 70 TF peak
- Project manager Janne Ignatius

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Benchmarks

- **Application benchmarks for supercomputers:**
  - DALTON
  - GROMACS
  - HIRLAM
  - POLAR (user code)
  - SU3_AHIGGS (user code)
  - VASP
- **Application benchmarks for clusters:**
  - GROMACS
  - HMMER
  - POROUS (user code)
  - SU3_AHIGGS (user code)
- **HPC Challenge benchmarks**
  - HPL
  - PTRANS
  - FFT
  - RR latency, bandwidth
  - etc.
- **IOZONE, b_eff_io**
- **Intel MPI Benchmarks**

Software use

- Large computational projects use mainly their own codes or other academic codes for research:
  - VASP, SIESTA, Elmfire, Finger, Finflo, Aplac, Elmer, Mika, …
- 75% of the use of IBM SC is done with academic codes
- 25% of the use is done with commercial software
- The most popular application software on computational servers is (in CPUh):
  - Gromacs / molecular modeling
  - Gaussian03 / quantum chemistry
  - TURBOMOLE / quantum chemistry
  - BLAST / biosciences
  - POY / biosciences
  - Cerius2 / molecular modeling
  - FLUENT / computational fluid dynamics
  - ADF / quantum chemistry
  - NWChem / chemistry
  - Abaqus / structural analysis

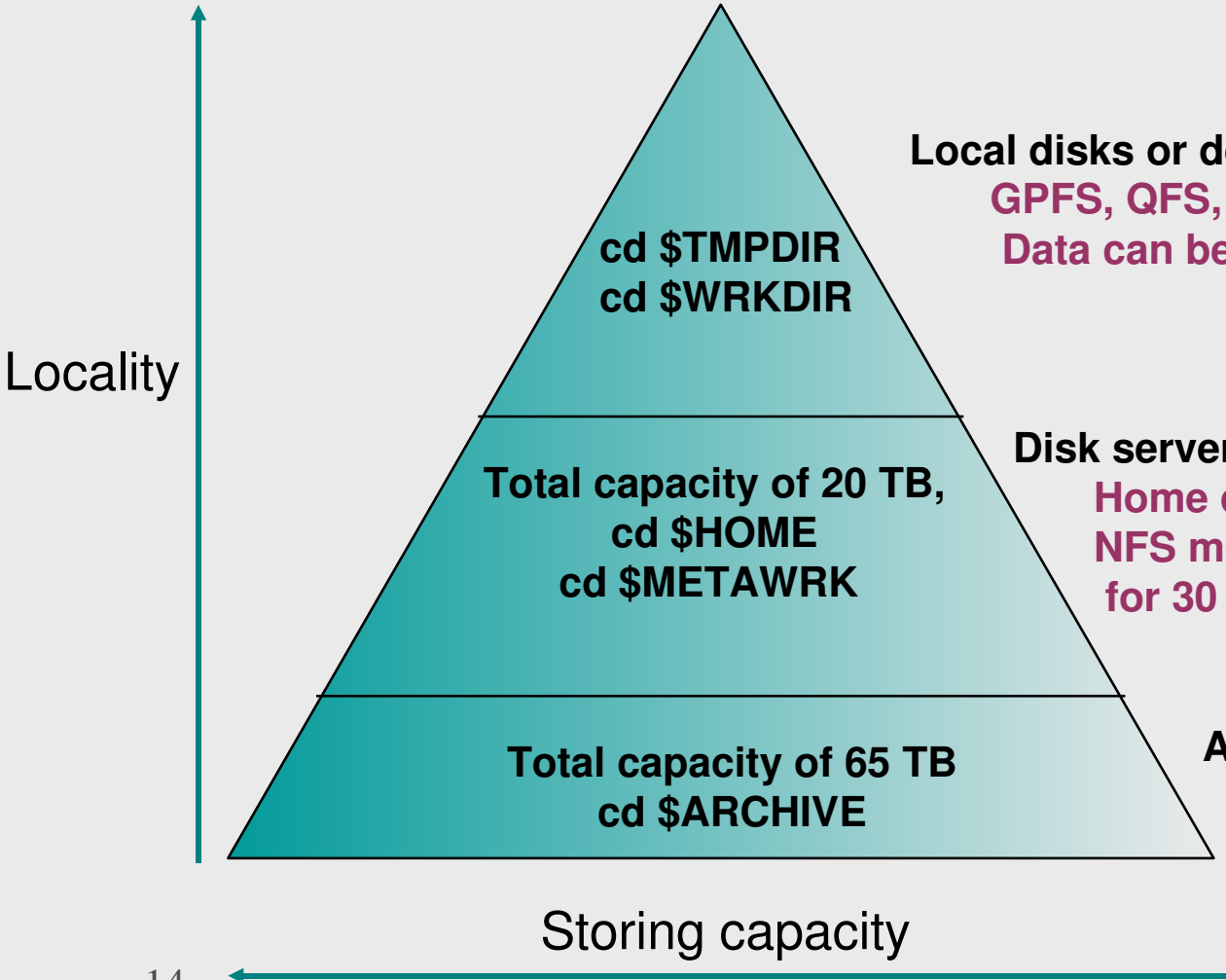
Cray Hood (XT4)

- 10.6 TF -> 70 TF peak
  (11 -> 18 cabinets)
- AMD Opteron Dual Core 2.6 GHz, Quad Core
- 1 GB/core memory
- Cray SeaStar 2 interconnect (3D torus)
- Unicos/lc (Linux, LWK Catamount in compute nodes)
- Lustre filesystem, 74 TB
- PGI compilers

HP CP4000BL Proliant

- 10 TF peak performance
- 2048 compute cores
- AMD Opteron Dual Core 2.6 GHz
- 4 TB memory
- Infiniband interconnect
- RH EL 4 (Linux)
- HP XC cluster software
- 100 TB file system (Lustre)

Data storage policy



Local disks or dedicated external disks
GPFS, QFS, Lustre
Data can be stored for 7 days

Disk server
Home directories, project directories,
NFS mounted work disk
for 30 days of storing

Archive server
Long term storage on tapes

Data storage procurement

- **Schedule: decision in 2006**
- **Disk arrays, administration software and tools**
- **Possibility for petabyte capacity in 2010**

Perspectives for resource allocations at CSC

- **Demand for other resources than CPU hours:**
  - data storage (=mainly disk space)
  - application optimization, visualization
- **Demand for really large projects that have an important scientific goal**
- **Part of the capacity of CSC's Cray will be admitted based on the Nordic Grand Challenge Survey**

Nordic Computational Grand Challenge Survey

- **The four Nordic countries Denmark, Finland, Norway and Sweden are carrying out a survey to determine scientific problems that are of high interest to the research community in the Nordic countries and whose solution requires the availability of large-scale e-Infrastructure.**
- **This survey is part of a larger study that also addresses the current status of the largest computational projects and the (need for) resource sharing policies in the Nordic countries.**
- **The survey is commissioned by the Danish Agency for Science, Technology and Innovation, the Finnish IT center for Science, the Research Council of Norway, and the Swedish Research Council.**

Objectives of the survey

- **Aim: To find out the ongoing computational grand challenges or the ones emerging during the next 10 years in Nordic countries.**
  National level
  - To increase the visibility of computational science
  - Indications for needed resources; more balanced HPC infrastructure
- **Nordic level**
  - synergistic effects for Nordic research
  - strengthen cooperation
  - efficient use of resources
  - Funding in the Nordic level (Nordforsk etc.)
  - mechanism for finding and putting through grand challenges
- **EU level**
  - Funding and policy making (roadmaps etc.)
  - ESFRI, e-IRG…
- **Global**
  - To increase the visibility of Nordic research in an European and global context
  - enable participation in international grand challenges

Criteria for grand challenges

- **International interest and relevance**
  - will increase the research profile of the Nordic region
- **Scientific problem that requires large scale (in Nordic level) HPC resources**
- **Long-term project**
- **Need for cooperation among research teams and communities**
- **Should consist of intermediate goals**
- **Widely recognized as a grand challenge**
- **Gives an answer for a fundamental scientific question.**
- **Industrial grand challenges will not be included in the survey, unless they come to light through academic world**

Conducting the survey

- **Scientific community is asked to submit grand challenge proposals**
  - Dealt with both locally and on the Nordic level.
  - Deadline for proposals 31.10.2006
  - Proposal www-page: www.notur.no/gcs
  - Project group:
    - Jacko Koster, UNINETT Sigma AS
    - Sinisa Krajnovic, SNIC
    - Kurt V. Mikkelsen, DCSC
    - Jura Tarus, CSC
- **A report with recommendations will be written and published (beginning of 2007)**

Summary

- **Finnish capacity will be competent again**
  - Cray Hood
  - HP cluster
  - disk array system
- **EU procurement hard to carry out**
  - Important to have users involved (benchmarks)
- **Resource allocations will change**
  - Nordic Grand Challenges Survey
  - data resources