CSC resources intro:

most powerful computational resources in Finland

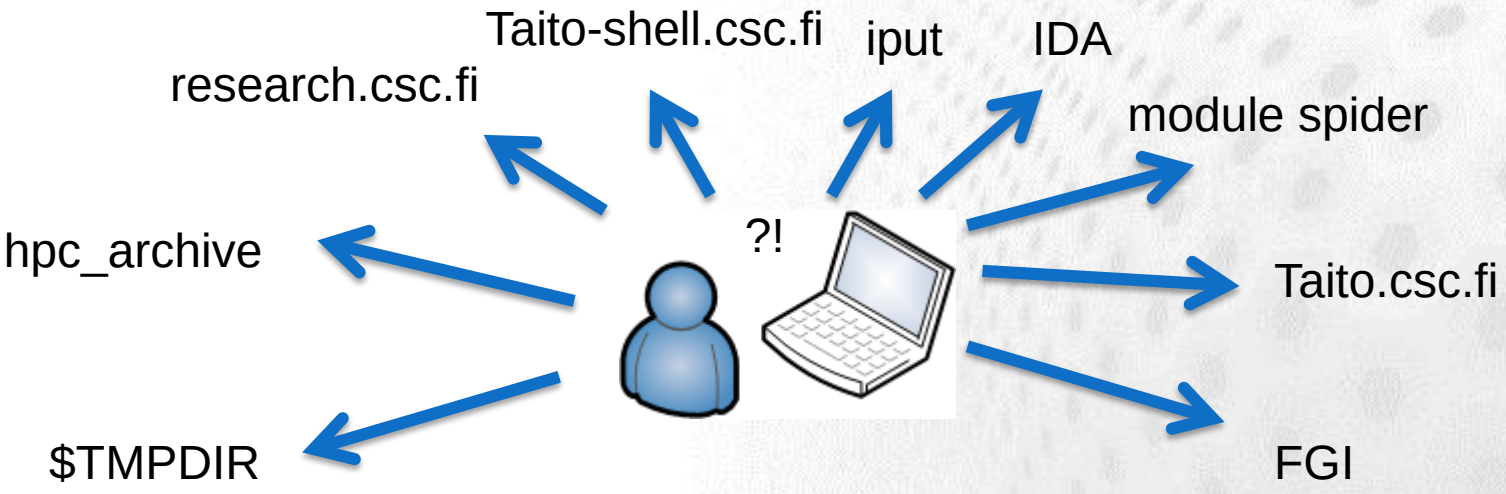
Tomasz Malkiewicz
CSC – IT Center for Science Ltd.

Outline

- Intro
  - Why supercomputers?
  - CSC at glance
  - Kajaani Datacenter
- Finland's supercomputers
  - *Sisu* (Cray XC30)
  - *Taito* (HP cluster)
- ***Live demos/hands-on 1 (Taito)***
- CSC resources available for researchers
- ***Live demos/hands-on 2 (Taito)***

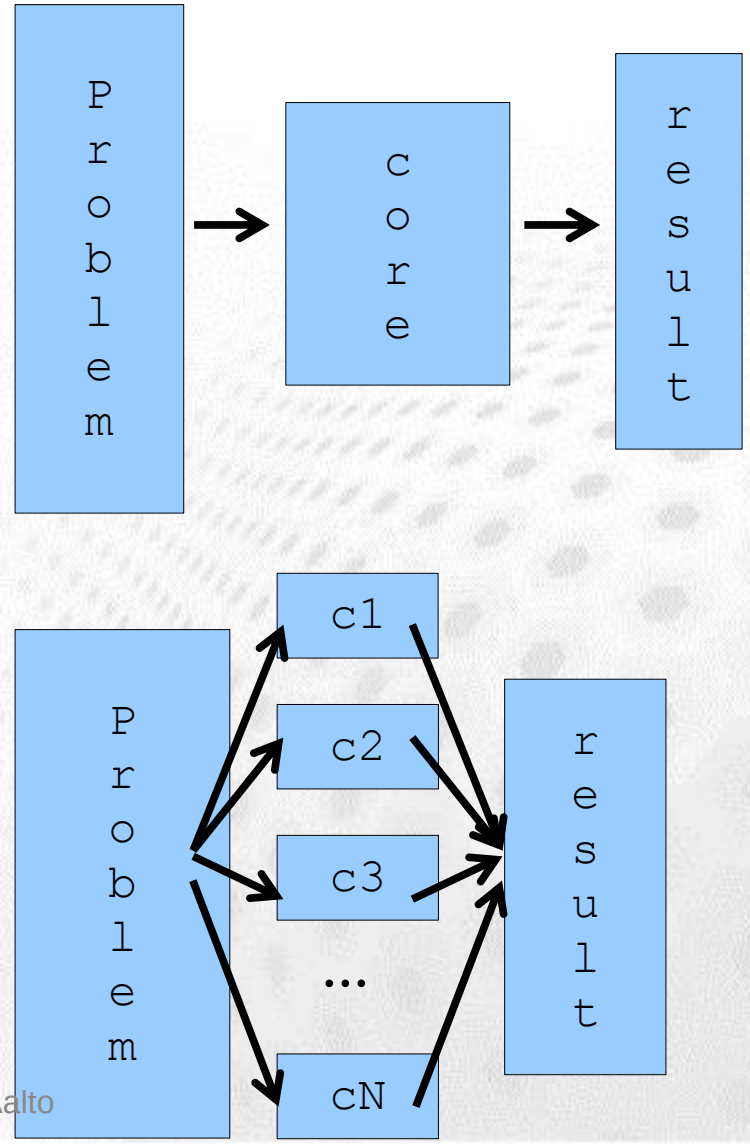
Learning targets

- Be able to use Taito supercluster
  - Create a batch job script, submit a job and view the results
- Get acquainted with what is available
  - Know how to choose right server (resource)



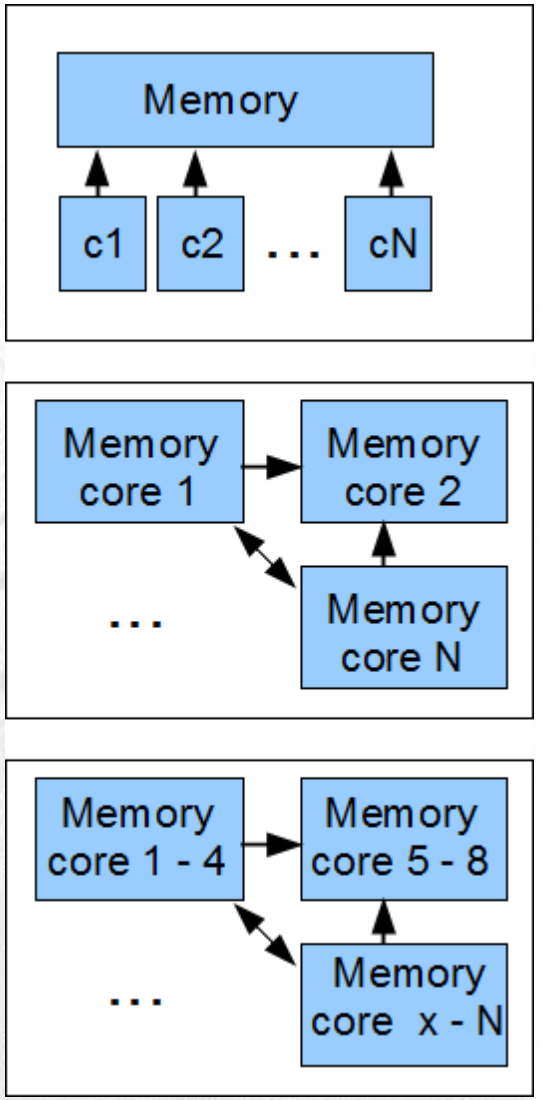
Supercomputing: serial and parallel processing

- Serial computing
  - single processing unit (core) is used for solving a problem
  - single task performed at once
- Parallel computing
  - multiple cores are used for solving a problem
  - problem is split into smaller subtasks
  - multiple subtasks are performed simultaneously



Types of parallel computers

- Shared memory
  - all the cores can access the whole memory
- Distributed memory
  - all the cores have their own memory
  - communication is needed in order to access the memory of other cores
- Current supercomputers combine the distributed memory and shared memory approaches

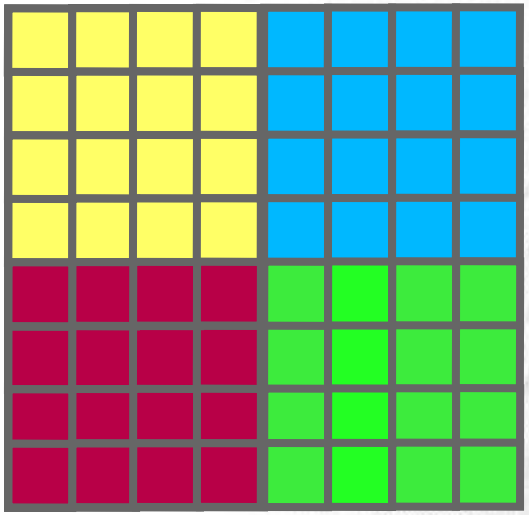


Data parallelism

- Data is distributed to processor cores
- Each core performs (nearly) identical tasks with different data
- Example: summing the elements of a 2D array

core 1: ∑=

core 2: ∑=



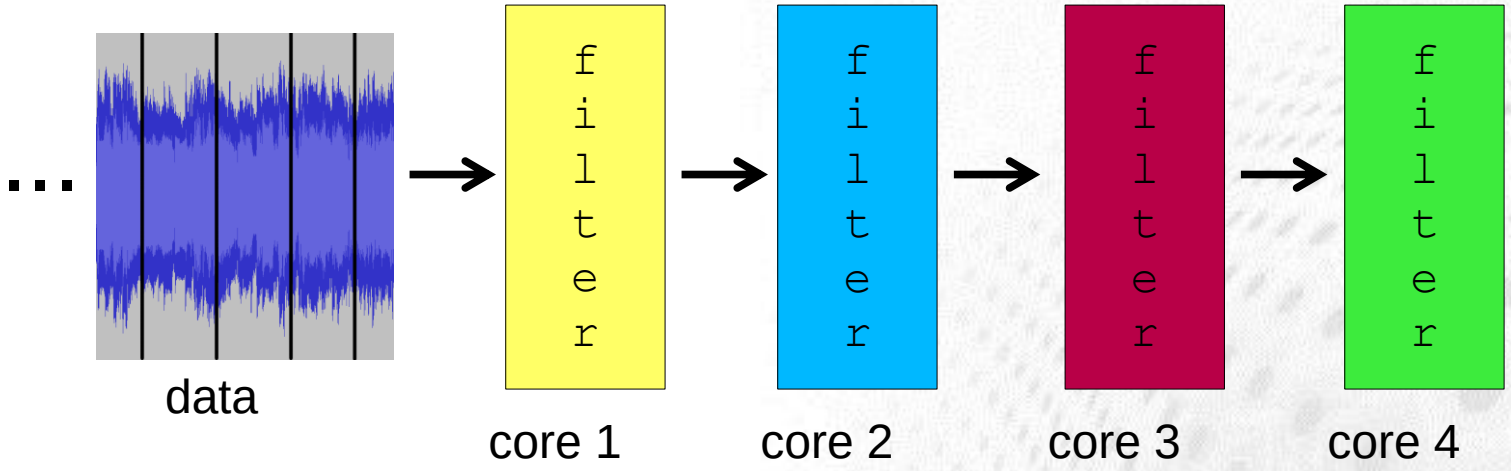
core 3: ∑=

core 4: ∑=

- Each core sums it's part of the array
- The individual sums have to be combined in the end

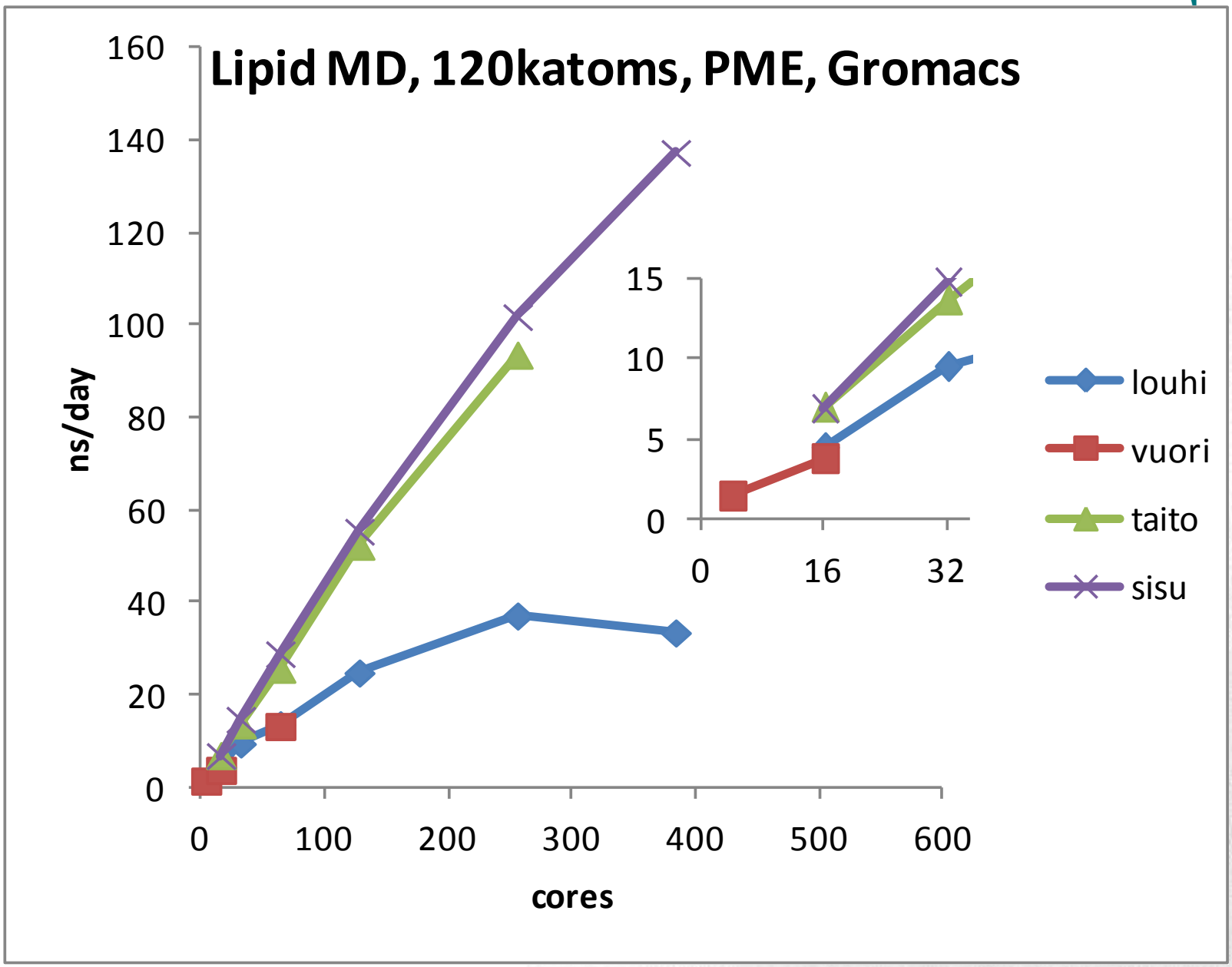
Task parallelism

- Different cores perform different tasks with the same or different data
- Example: signal processing, four filters as separate tasks

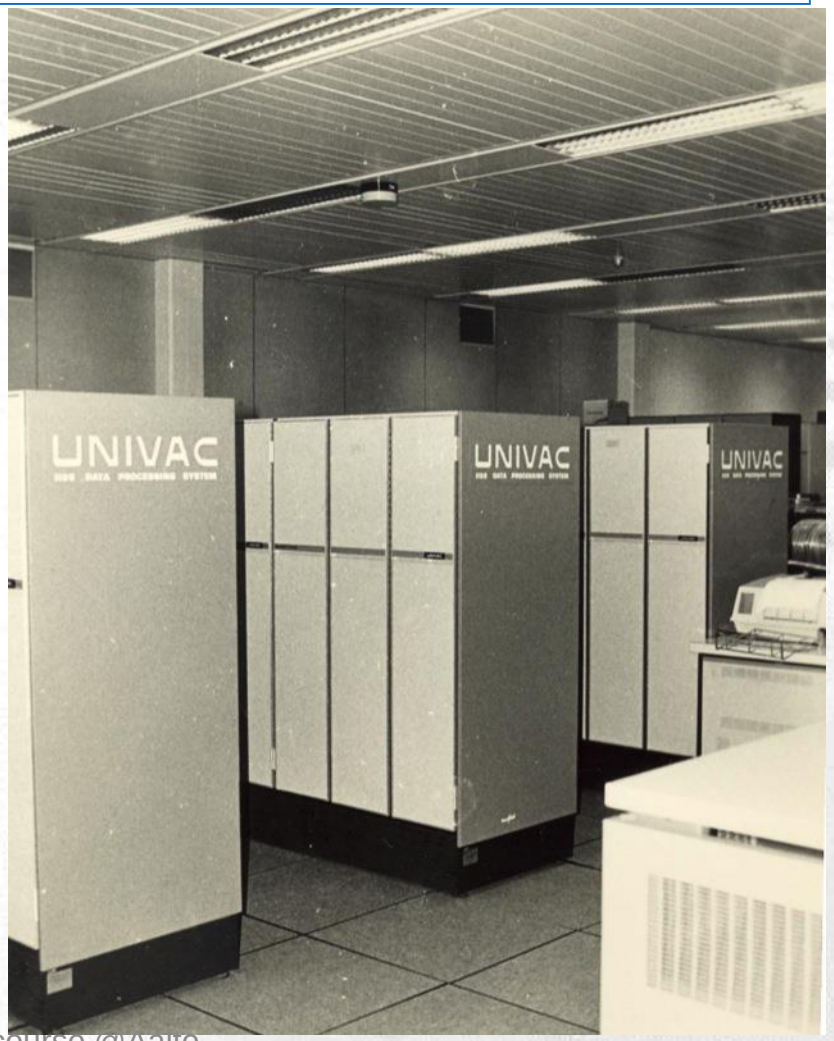


- Data is processed as segments
- Core 2 obtains a segment after core 1 has processed it; core 1 starts to process a new segment
- When the first segment gets to core 4, all cores are busy

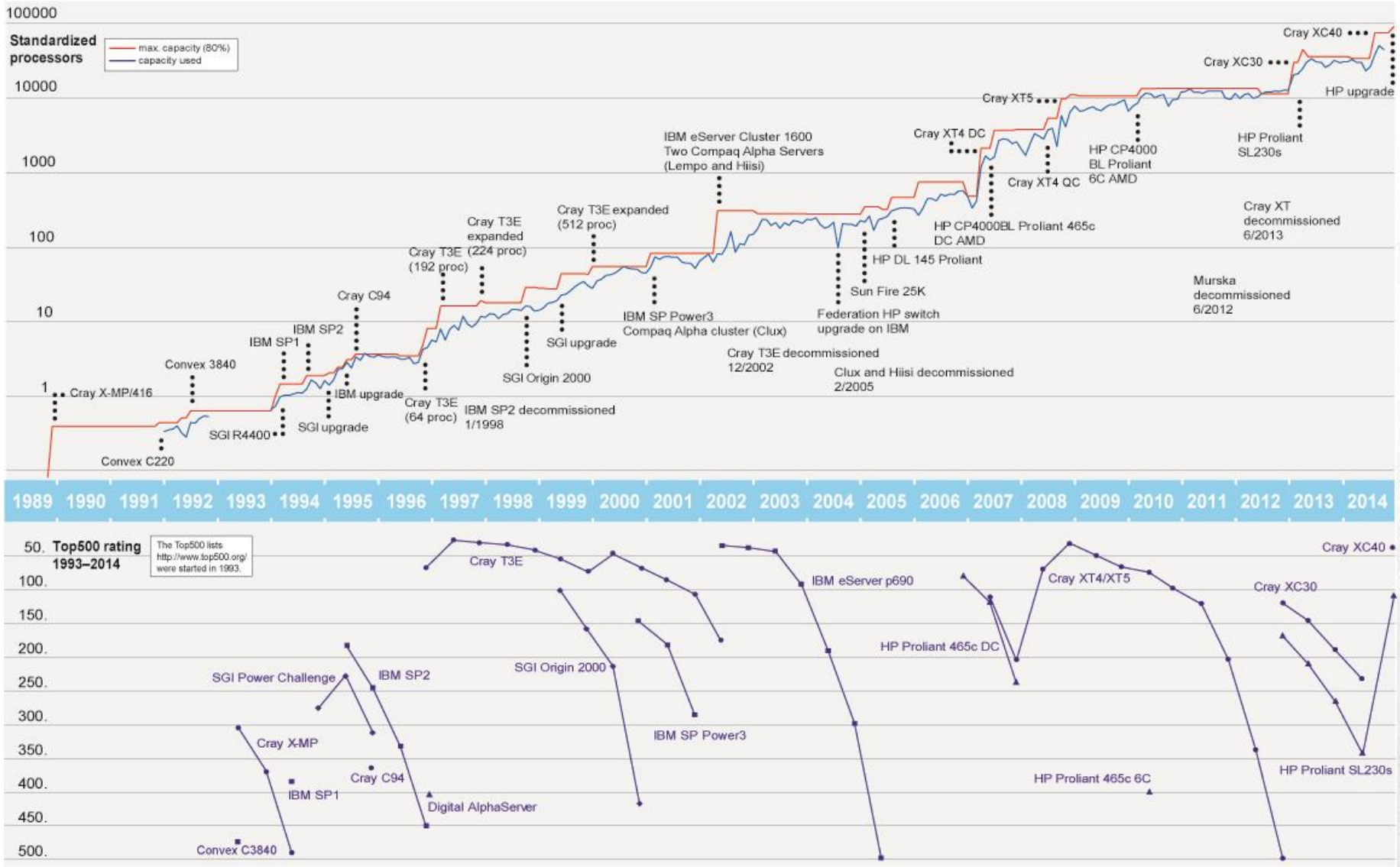
Why supercomputers?



CSC and High Performance Computing



CSC Computing Capacity 1989–2014

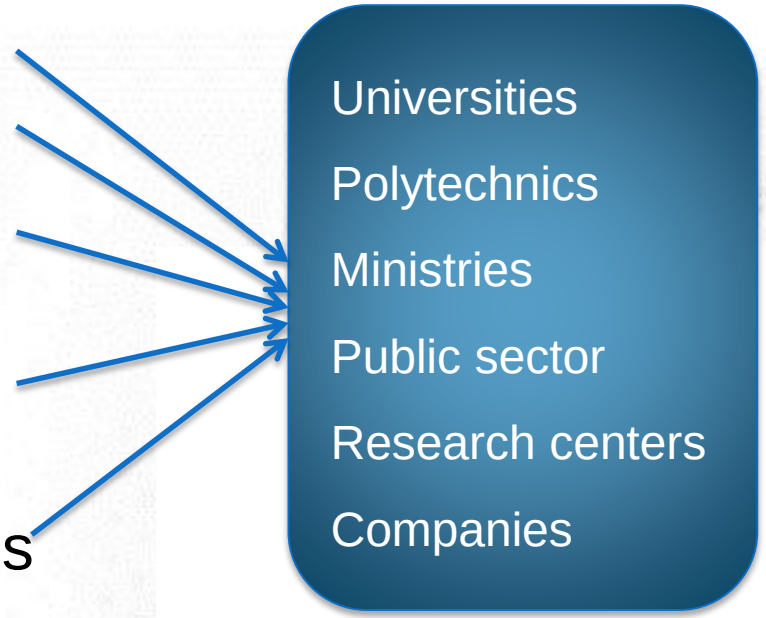


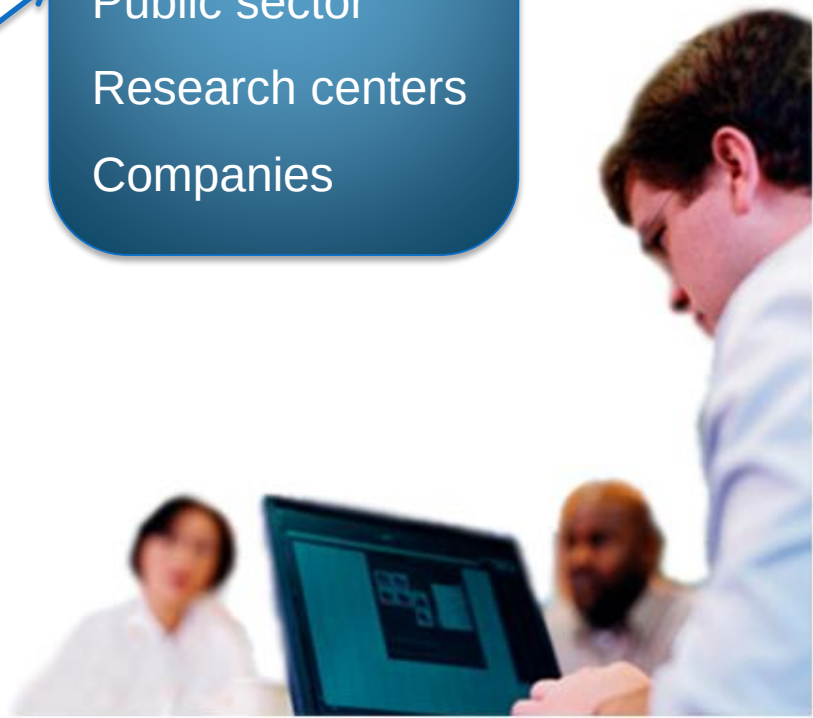
CSC at glance

- Founded in 1971
  - technical support unit for Univac 1108
- Connected Finland to Internet in 1988
- Reorganized as a company, CSC – Scientific Computing Ltd. in 1993
- All shares to the Ministry of Education and Culture of Finland in 1997
- Operates on a *non-profit* principle
- Facilities in Espoo and Kajaani
- Staff ~270 people

CSC's Services

- FUNET Services
- Computing Services
- Application Services
- Data Services for Science and Culture
- Information Management Services





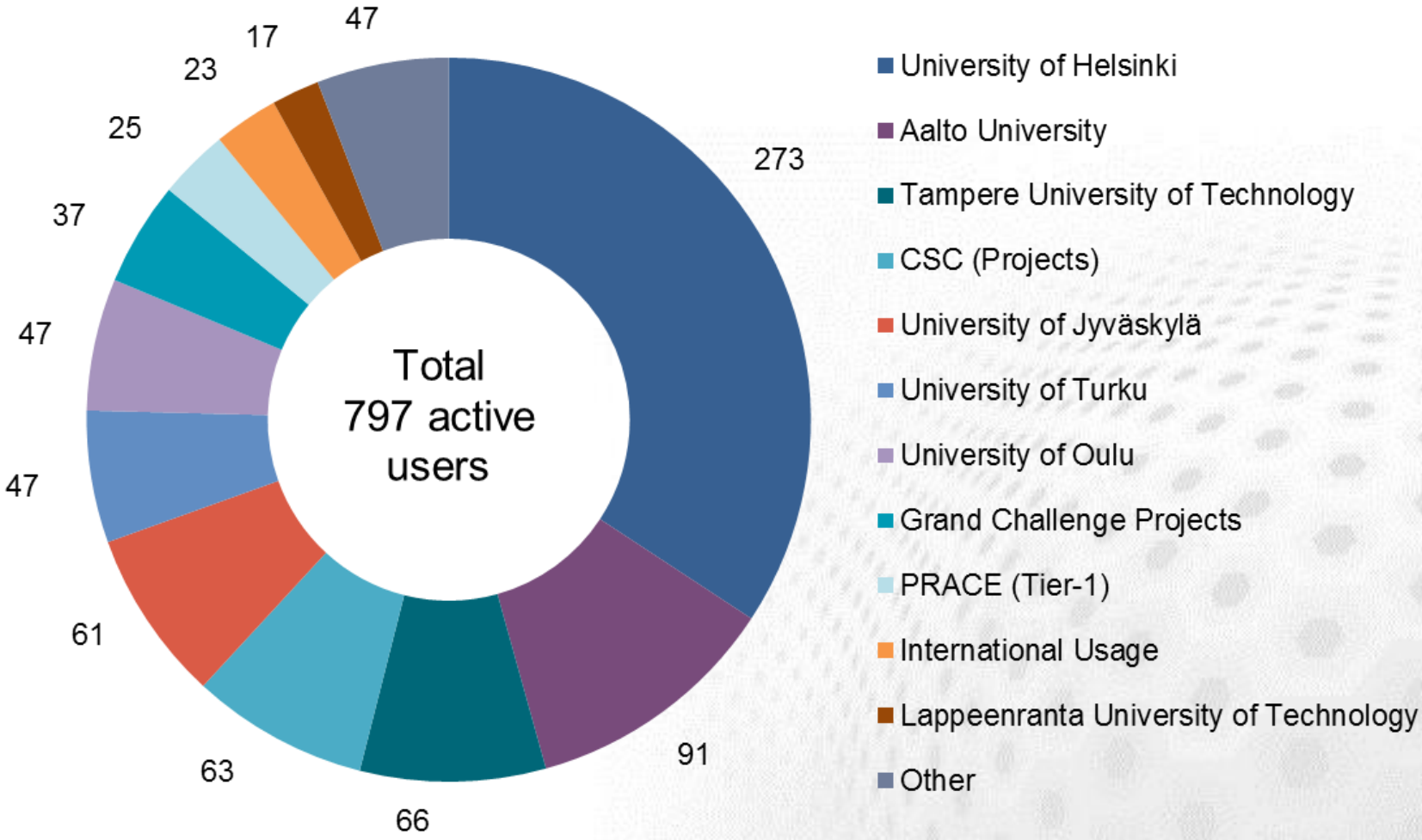
FUNET and Data services

- ***FUNET***
  - Connections to all higher education institutions in Finland
  - Haka-identity Management
  - Campus Support
  - The NORDUnet network
- ***Data services***
  - Digital Preservation and Data for Research
    - Data for Research (TTA), National Digital Library (KDK)
  - Database and information services
    - nic.funet.fi – freely distributable files with FTP since 1990
  - Memory organizations (Finnish university and polytechnics libraries, Finnish National Audiovisual Archive, Finnish National Archives, Finnish National Gallery)

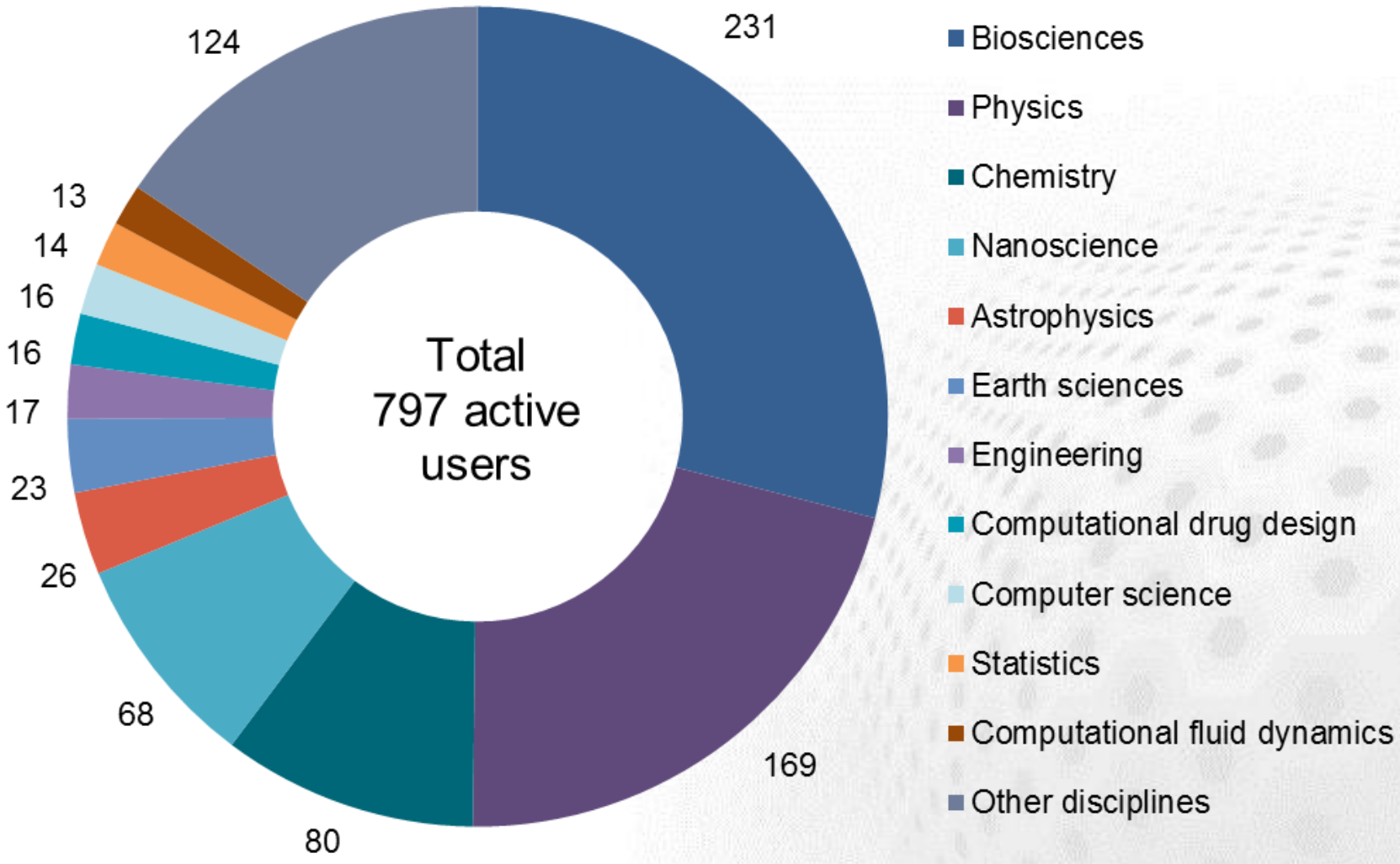
Users

- About 700 active computing projects
  - 3000 researchers use CSC's computing capacity
  - 4250 registered customers
- Haka-identity federation covers all universities and higher education institutes (287 000 users)
- Funet - Finnish research and education network
  - Total of 370 000 end users

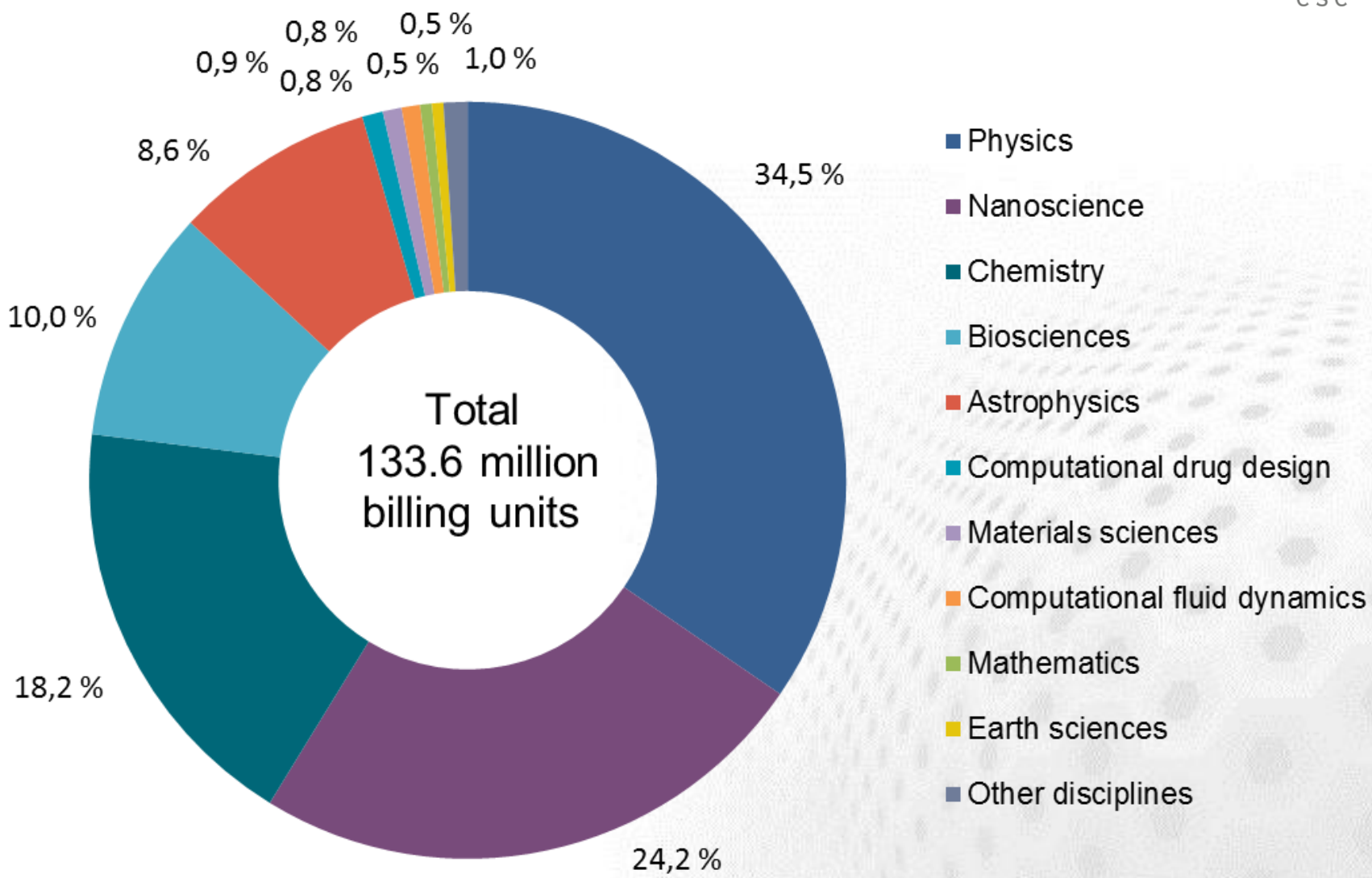
Users of computing resources by organization 1Q/2015



Users of computing resources by discipline 1Q/2015

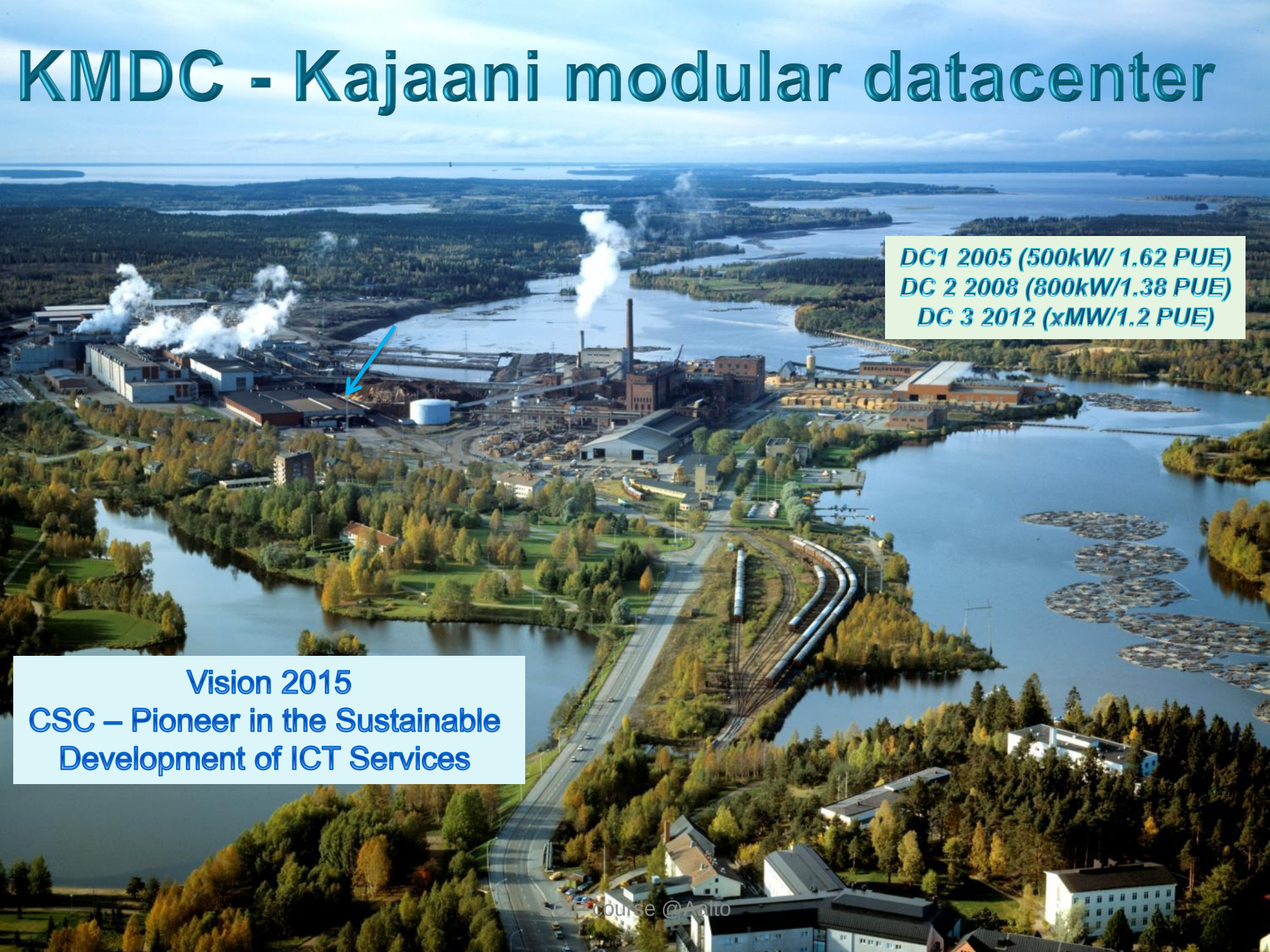


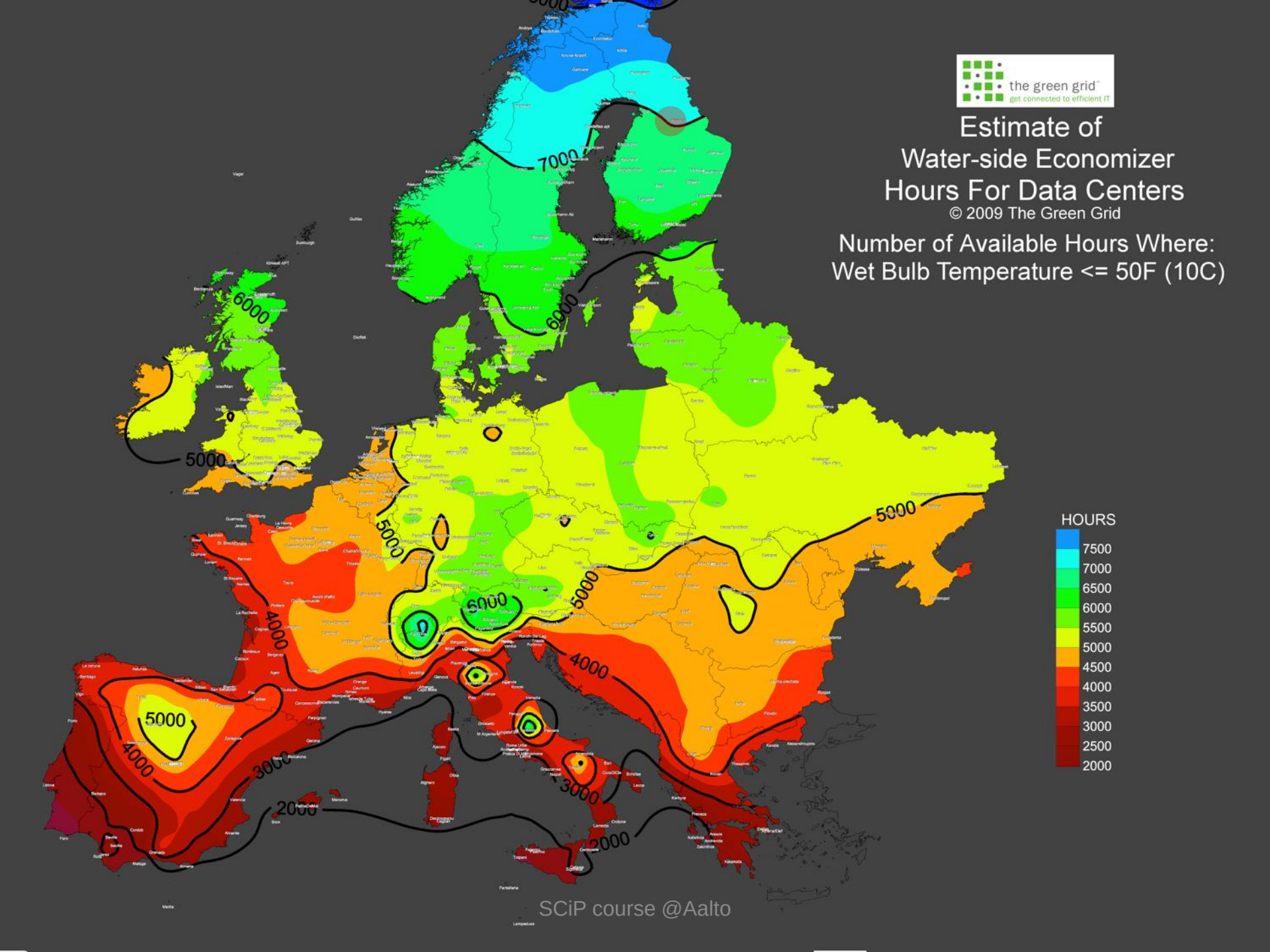
Computing usage by discipline 1Q/2015



THE KAJAANI DATACENTER

KMDC - Kajaani modular datacenter




the green grid
get connected to efficient IT
Estimate of
Water-side Economizer
Hours For Data Centers
© 2009 The Green Grid
Number of Available Hours Where:
Wet Bulb Temperature <= 50F (10C)
HOURS
7500
7000
6500
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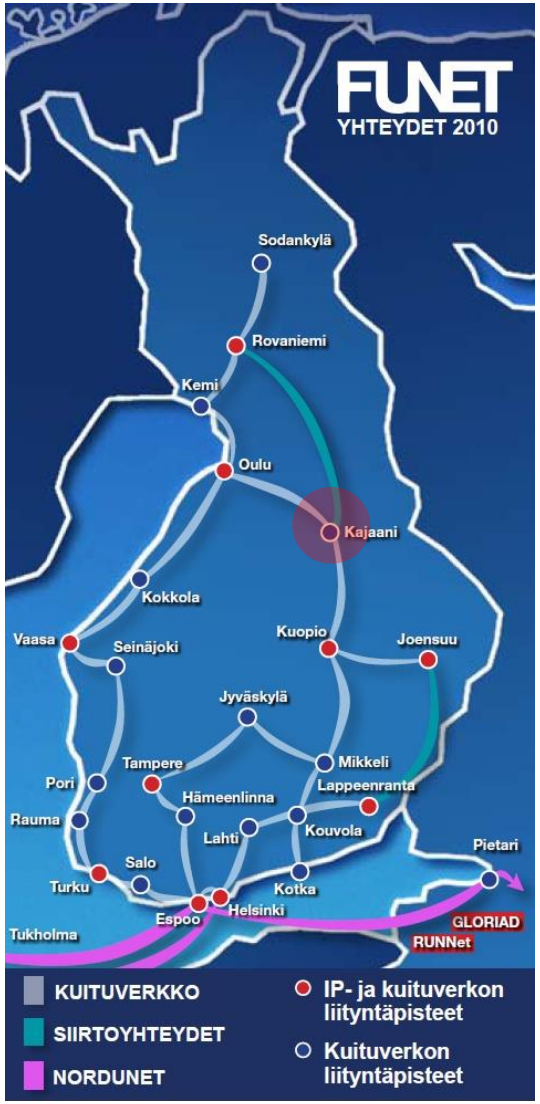
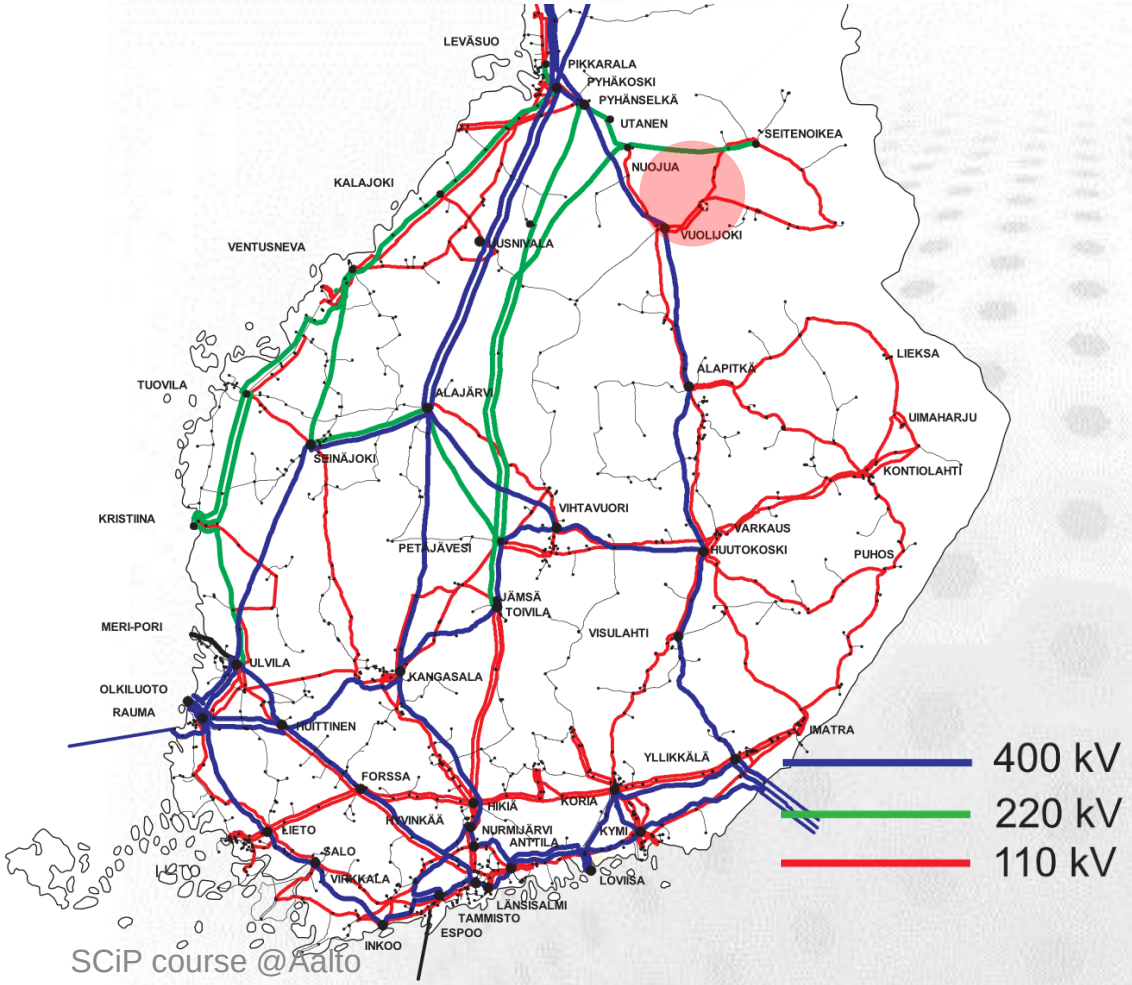
Power distribution (FinGrid)



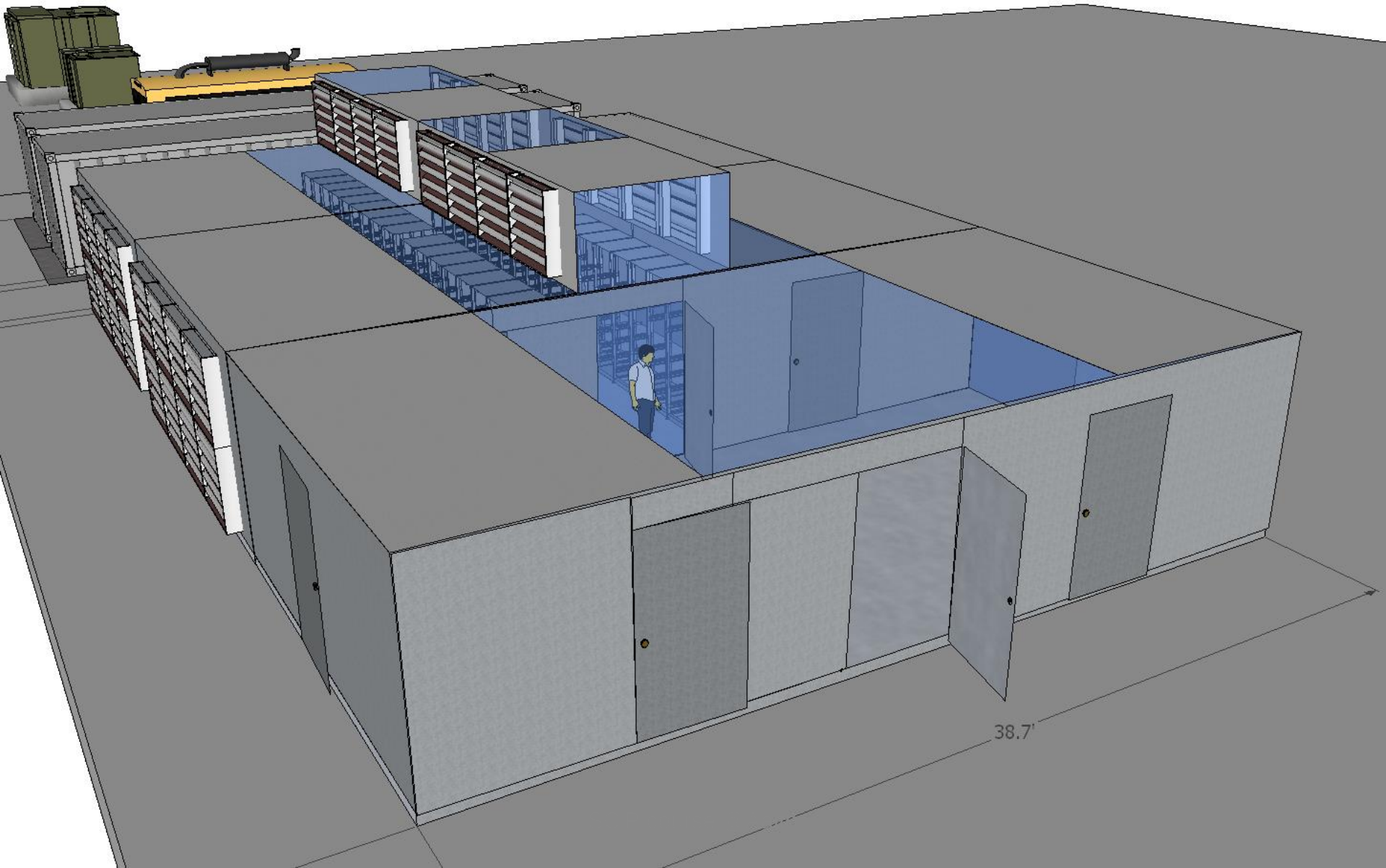


Kajaani site

Sisu

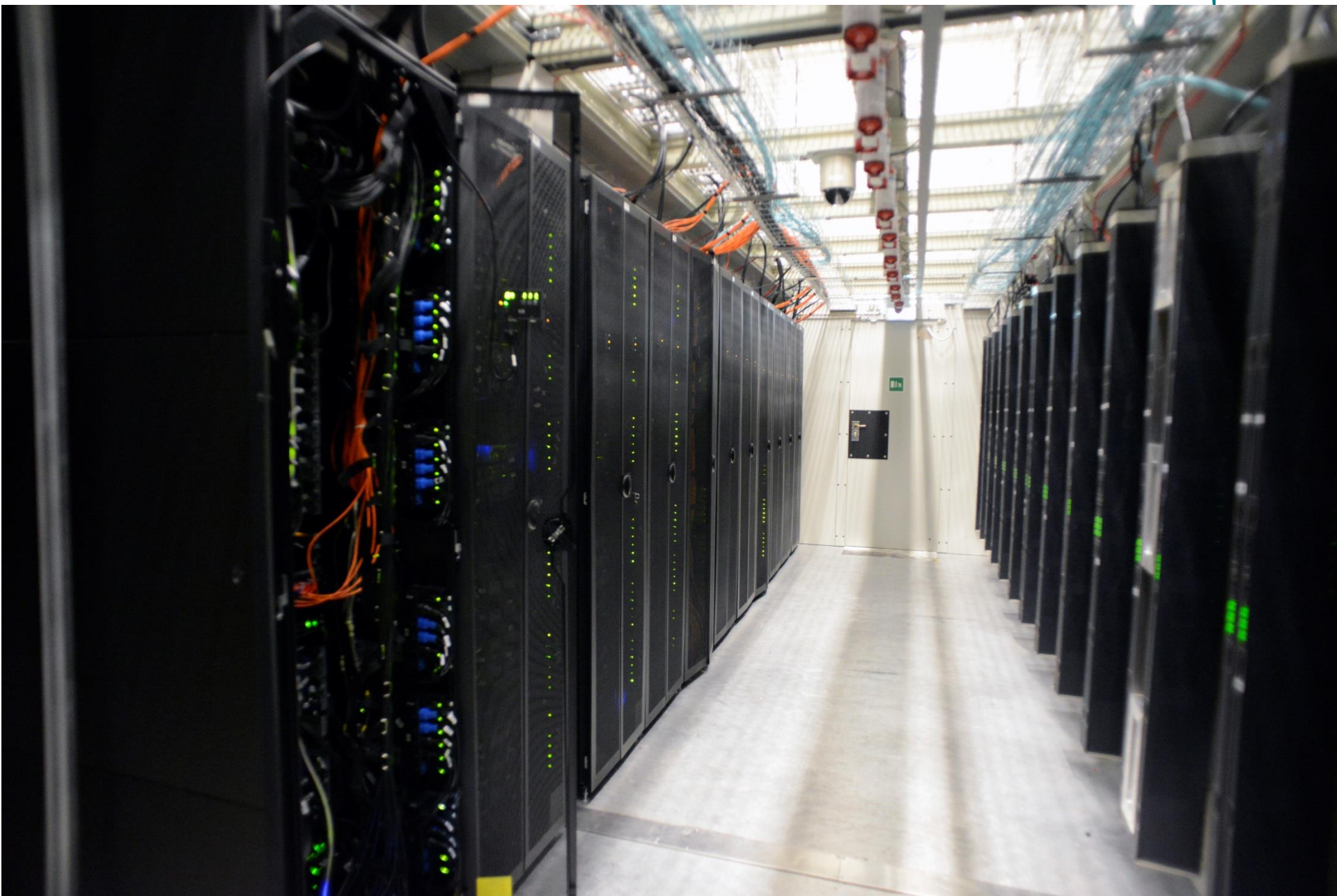
Sisu rear view

Taito (HP) hosted in SGI Ice Cube R80



SGI Ice Cube R80

Taito now



Data center specification

- 2.4 MW combined hybrid capacity
- 1.4 MW modular free air cooled datacenter
  - Hosting e.g. Taito
  - Upgradable in 700 kW factory built modules
  - Order to acceptance in 5 months
  - 35 kW per extra tall racks – 12 kW common in industry
  - PUE < 1.08 ($pPUE_{L2,YC}$)
- 1MW HPC datacenter
  - Optimised for Cray super & T-Platforms prototype
  - 90% Water cooling

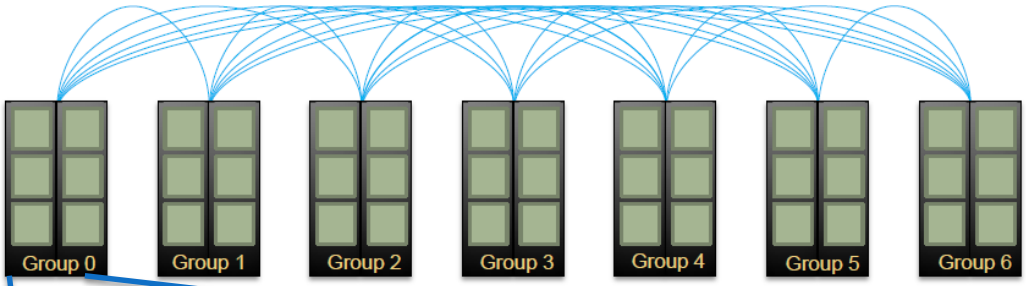
CSC SUPERCOMPUTERS

Main Computing capacity: Sisu,Taito, FGI

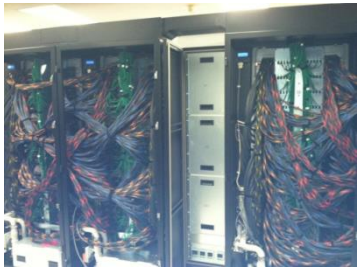
	Sisu (Phase 2)	Taito (Phase 2)	FGI	Taygeta
Availability	2014-	2015-	2012-	2012-
CPU	Intel Haswell and Sandy Bridge, 2 x 12 and 2 x 8 cores, 2.6 GHz, Xeon E5-2690v3 and E5-2670		Intel Xeon, 2 x 6 cores, 2.7 GHZ, X5650	
Interconnect	Aries	FDR IB	QDR IB	
Cores	40512	9768+9216	7308	360
RAM/node	64 GB	64/128/256/ 1536** GB	24/48/ 96 GB	48 GB
Tflops	1688	515	95	4
GPU nodes	-	38	88	-
Disc space	4 PB	4 PB	1+ PB	0.8 TB

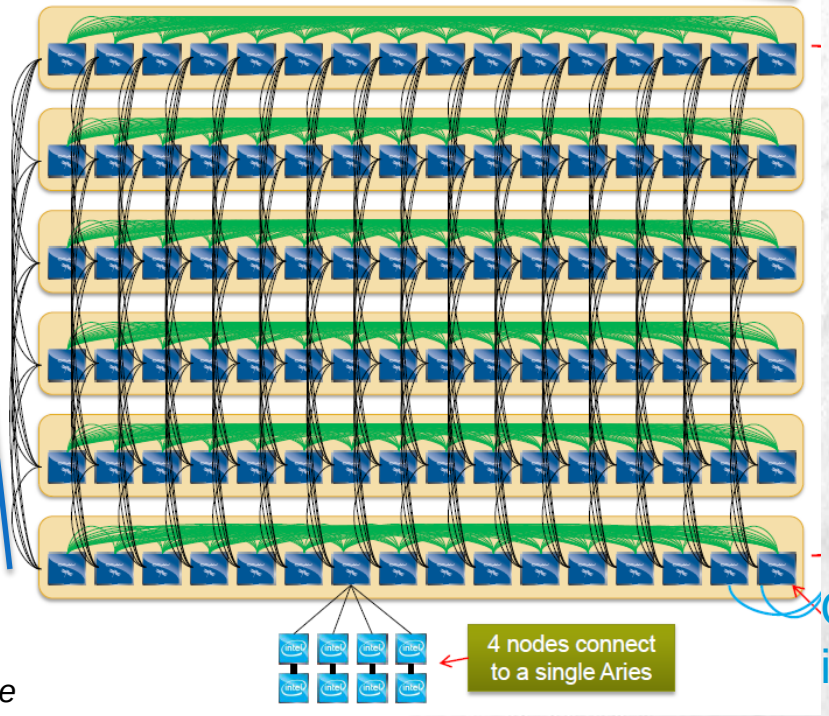
*) 2 nodes a 32 cores with 1,5 TB RAM/node (hugemem-queue)

Cray Dragonfly Topology



All-to-all network between groups





2 dimensional all-to-all network in a group

Optical uplinks to inter-group net

Source:
Robert Alverson, Cray
Hot Interconnects 2012 keynote

Cray environment (Sisu)

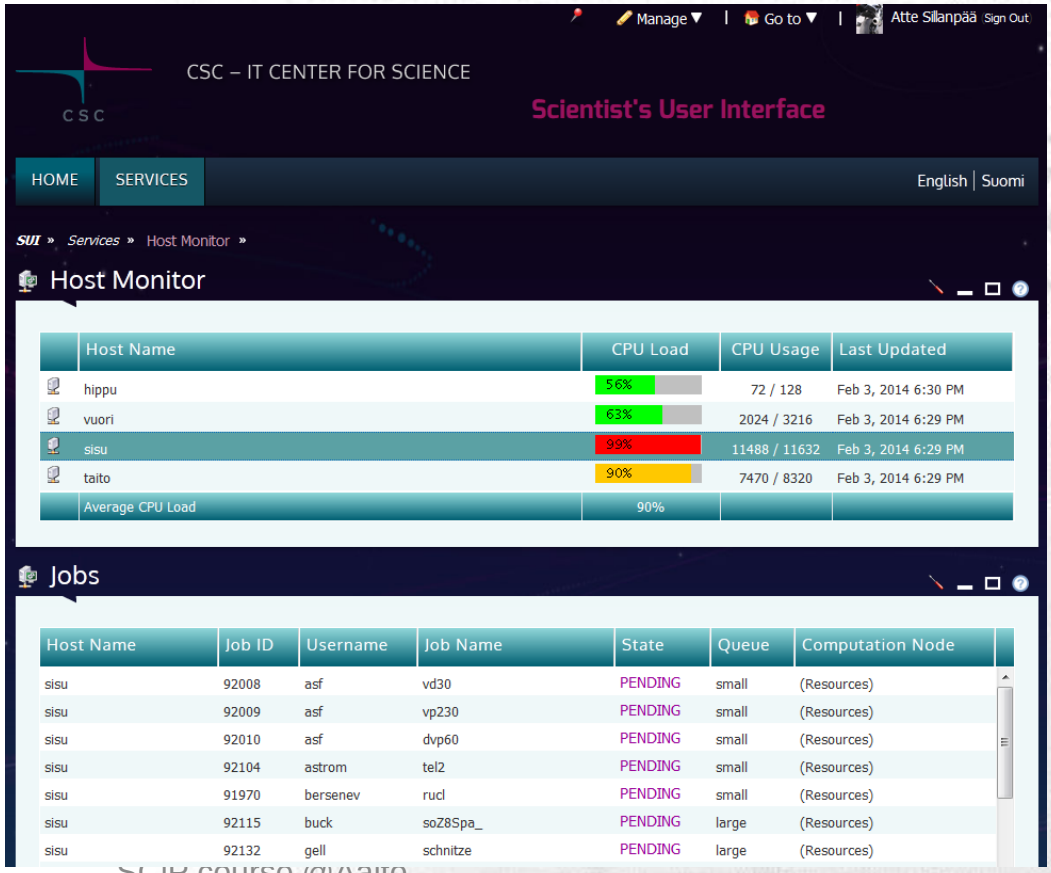
- Typical Cray environment
- Compilers: **Cray**, Intel and GNU
- Cray mpi, Cray tuned versions of all usual libraries
- SLURM
- Default shell: ***bash*** (previously tcsh)
- Character encoding: UTF-8

HP Environment (Taito)

- Compilers: **Intel**, GNU
- MPI libraries: Intel, mvapich2, OpenMPI
- Batch queue: SLURM
- Robust module system
  - Only compatible modules shown with *module avail*
  - Use *module spider* to see all
- Default shell: ***bash*** (used to be tcsh)
- Character encoding: UTF-8

How to get access to CSC supercomputers?

- sui.csc.fi (HAKA authentication)
  - Sing up



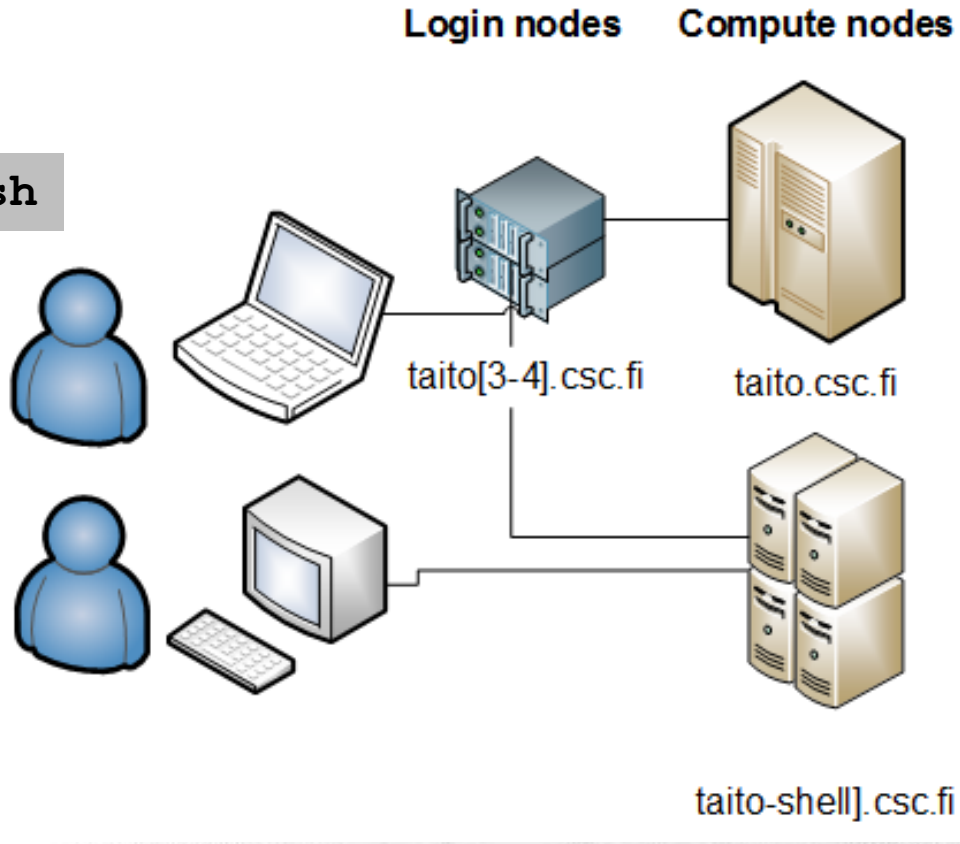
Preparing for demo/hands-on

- Prerequisite:
  - Batch queueing system
  - Module system

Compute nodes are used via queueing system

```
$ sbatch job_script.sh
```

```
$ ./my_prog &
```



Modules

- Some software installations are conflicting with each other
  - For example different versions of programs and libraries
- Modules facilitate the installation of conflicting packages to a single system
  - User can select the desired environment and tools using module commands
  - Can also be done "on-the-fly"

Taito module system

- ***module avail*** shows only those modules that can be loaded to current setup (no conflicts or extra dependencies)
  - Use ***module spider*** to list all installed modules and solve the conflicts/dependencies

Live demo/hands-on (Taito)

- ***ssh*** trng86 - trng135 ***@taito.csc.fi***

  (e.g. ssh trng100@taito.csc.fi)

- To be on the safe side:

  mkdir own_username

  cd own_username

- ***module avail***

Live demo/hands-on (1) cont.

- ***nano test_hostname.sh***

```
#!/bin/bash -l
#SBATCH -J print_hostname
#SBATCH -o output.txt
#SBATCH -e errors.t
#SBATCH -t 00:01:00
#SBATCH -p test
#
echo "This job runs on the host:"; hostname
```

CTRL+O; CTRL+X to exit

- ***sbatch test_hostname.sh***

Live demo/hands-on (1) cont.

- Check out the output:
  - ***less output.txt*** (type ***q*** to quit)
  - ***less errors.t*** (type ***q*** to quit)

- More examples:

  https://research.csc.fi/taito-constructing-a-batch-job-file

Taito is a heterogeneous cluster

- Different jobs need different resources
  - Bulk Sandy Bridge compute nodes
  - Largemem Sandy Bridge compute nodes
  - Hugemem Sandy Bridge compute nodes (***1.5 TB*** memory)
  - Bulk Haswell compute nodes
  - Taito-shell (Sandy Bridge) for interactive work

- Choosing between Haswell and Sandy Bridge nodes
  - --constraint=snb or =hsw
    - snb: **16**, hsw: **24**
  - Sandy Bridge: 64 GB memory nodes, Haswell: 128 GB memory in most nodes + 10 with 256 GB
  - More details:
    - *https://research.csc.fi/taito-constructing-a-batch-job-file#3.1.4*

- Local */tmp* disk 2 TB on each node

→ reserve only what you need

Preinstalled modules: optimizations

What architectures a code has been optimized for

- (h) only Haswell → runs only on Haswell
- (sh) Haswell and Sandy Bridge → runs optimally on both
- (g) GPGPU aware → needs to be run on taito-gpu.csc.fi
- No entry → optimized for Sandy Bridge: should run on both SB/H, but not optimally on Haswell (or even SB)

```
[GPU-Env ~]$ module avail

------------------------------ /appl/gpu_modulefiles/Compiler/gcc/4.8.2 ------------
   intelmpi/4.1.3        mkl/11.1.1              openblas/0.2.8
   magma/1.4.1    (g)    mvapich2/2.0-GDR (g)    openmpi/1.8.1  (g)

------------------------------ /homeappl/appl_taito/gpu_modulefiles/Core -------------
   StdEnv      cuda/6.0        gcc/4.8.2 (D)    intel/14.0.1    pgi/14.4
   cuda/5.5    cuda/6.5 (D)    gcc/4.9.1        pgi/14.3        pgi/14.7 (D)

------------------------------ /homeappl/appl_taito/gpu_modulefiles/Linux --------------
   amber-env/14-cuda      (g)    namd-env/2.10b1-cuda (g)        totalview/8.13.0-0
   git/1.9.2                     python-env/2.7.6         (D)    totalview/8.14.0-21  (D)
   gromacs-env/4.6.6-cuda (g)    python-env/3.4.1

  Where:
   (g):  built for GPU
   (D):  Default Module
```

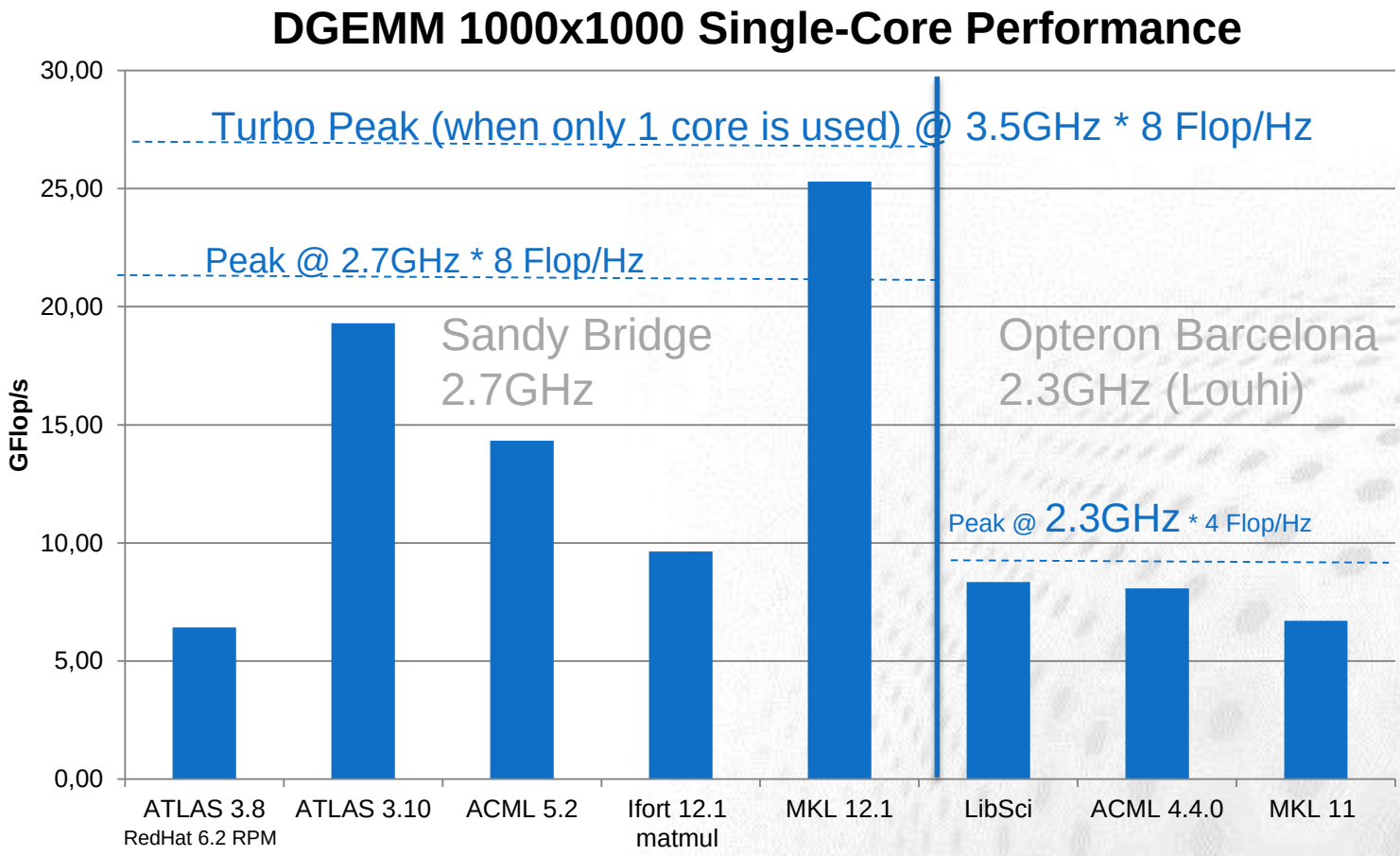
SLURM configuration: Fair usage

- SLURM uses fair share: the highest priority jobs go into execution next
  - Priority is decreased by the total amount of resources used in last 2 weeks per user
  - Priority is increased by time spent queueing
  - Backfiller will try to put small jobs into gaps due to current available resources and highest priority job
  - Jobs labeled ”Association limit” are not eligible to run (due to too many jobs in queue by the user)
- *Due to abuse, a maximum limit of jobs in queue now enforced*
- Chain jobs (--dependency –flag for SLURM) if you need long running time
- Don’t overallocate memory (add this command to your batch script `used_slurm_resources.bash` will print requests vs. used at stdout)
  - If you request a full node (-N 1), use –mem=55000 instead of –mem-per-cpu=something)
  - If you see abuse or think that the setup is unfair, contact *servicedesk@csc.fi*
- SUI has a monitoring tool for your jobs and used resources (*Services -> eServices -> My Project*)

Core development tools

- Intel XE Development Tools
  - Compilers
    - C/C++ (icc), Fortran (ifort), Cilk+
  - Profilers and trace utilities
    - Vtune, Thread checker, MPI checker
  - MKL numerical library
  - Intel MPI library (only on HP)
- Cray Application Development Environment
- GNU Compiler Collection
- Tokens shared between HP and Cray
- TotalView debugger

Performance of numerical libraries



MKL the best choice on Sandy Bridge, for now.

(On Cray, LibSci a good alternative)

CSC RESOURCES AVAILABLE FOR RESEARCHERS

Server use profiles

- Taito (HP)
- Serial and parallel upto 448/672 cores
- Huge memory jobs
- Lots of preinstalled software

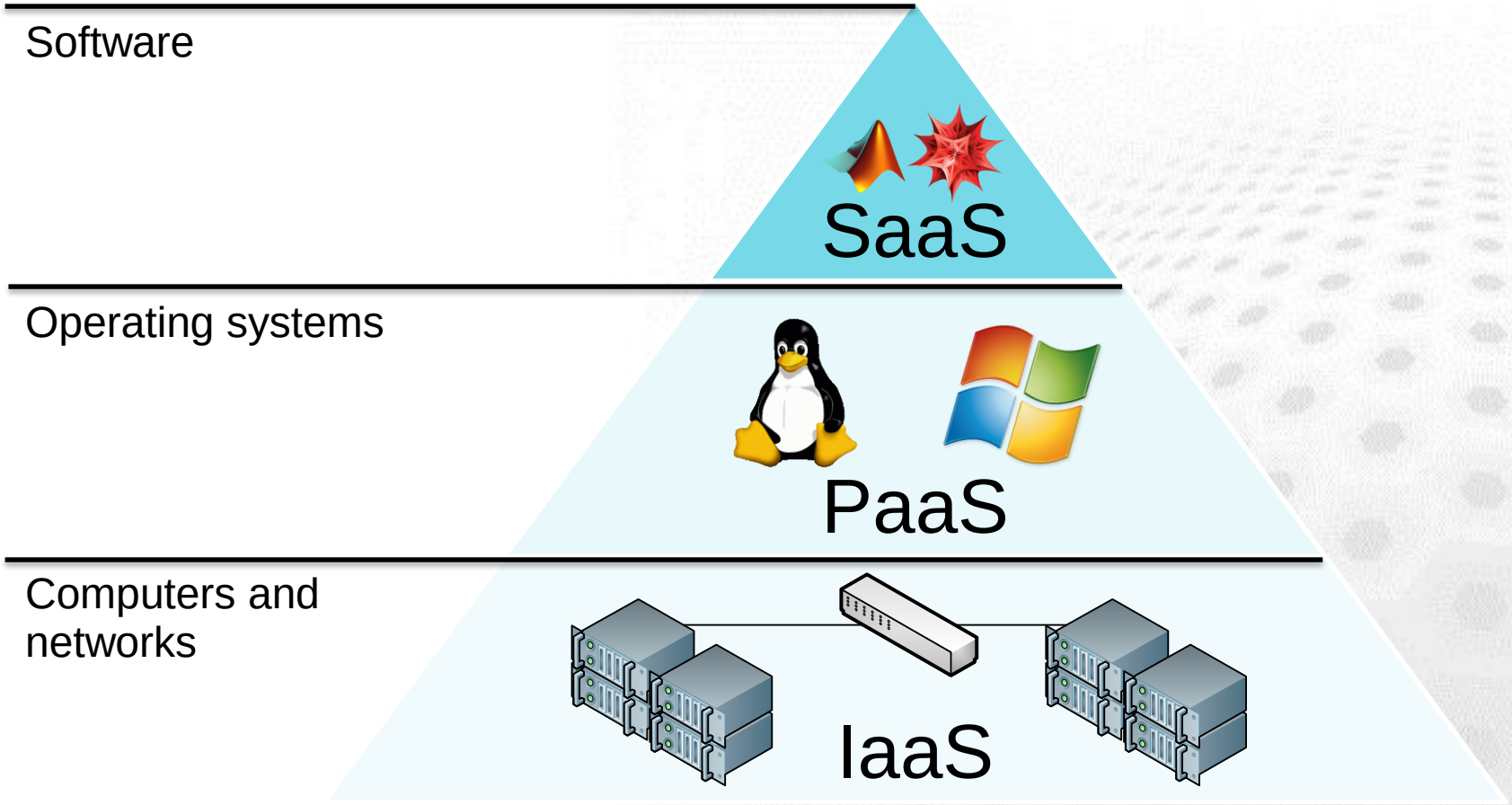
- Taito-shell (HP)
- Interactive jobs
- Very long jobs
- Automatic queue, shared resources

- Sisu (Cray XC40)
- Parallel from 72 up to thousands of cores
- Scaling tests 1008+

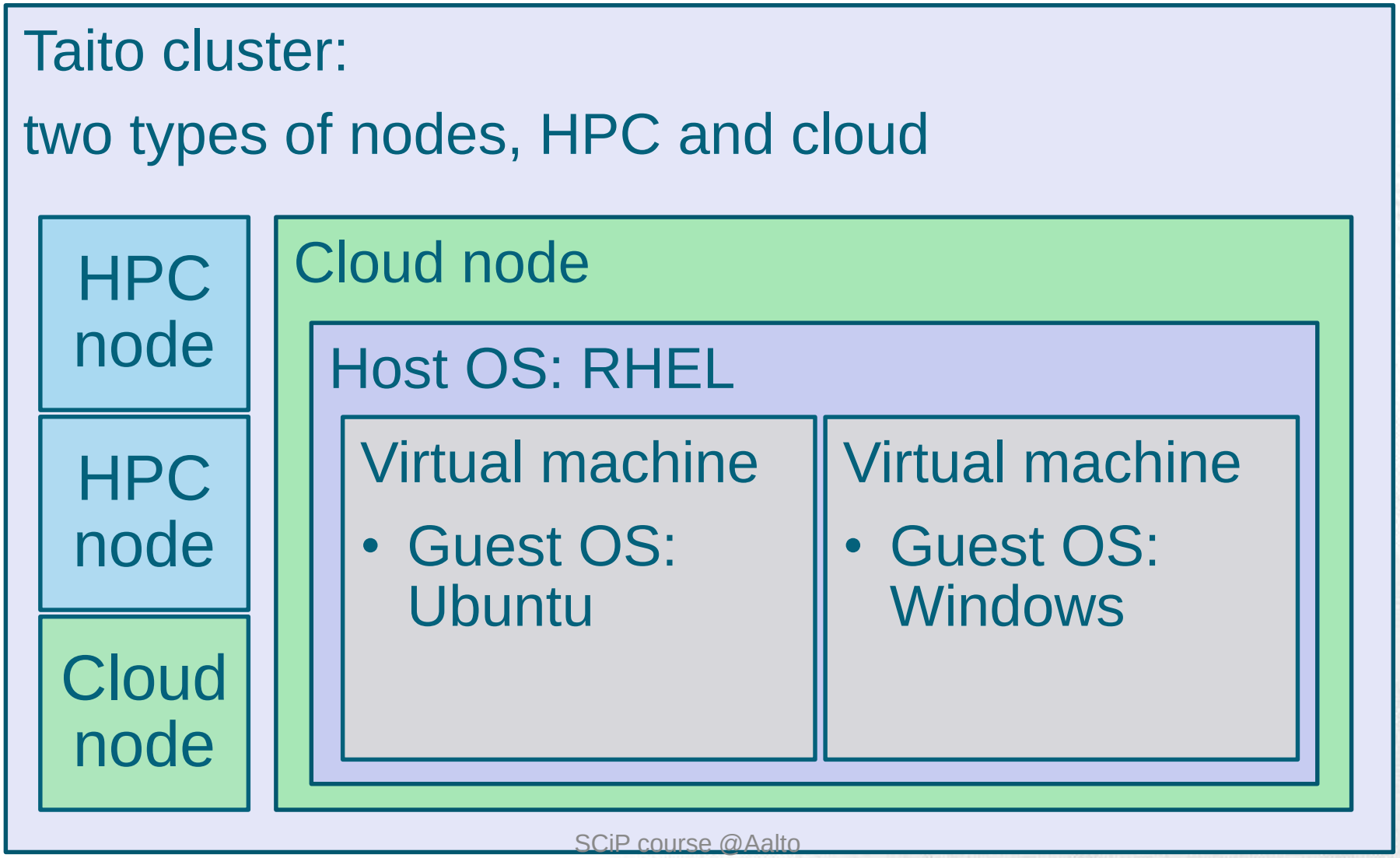
- cPouta (HP) Cloud
- Serial and parallel upto 16 cores

- FGI (HP)
- Serial and parallel (16)

Three service models of cloud computing



Example: Virtualization in Taito



Bull

- 38 NVIDIA K40 nodes (76 gpus)
  - 12 GB memory per card
- 45 Intel Xeon Phi nodes (90 Xeon Phis)
  - 16 GB memory per card
- Energy efficient CPU’s

How to access Bull

- **Accessing the resources**
  - **Intel Xeon Phi:**
    ssh taito-mic.csc.fi
    (*from taito.csc.fi*)
  - **NVIDIA K40:**
    ssh taito-gpu.csc.fi

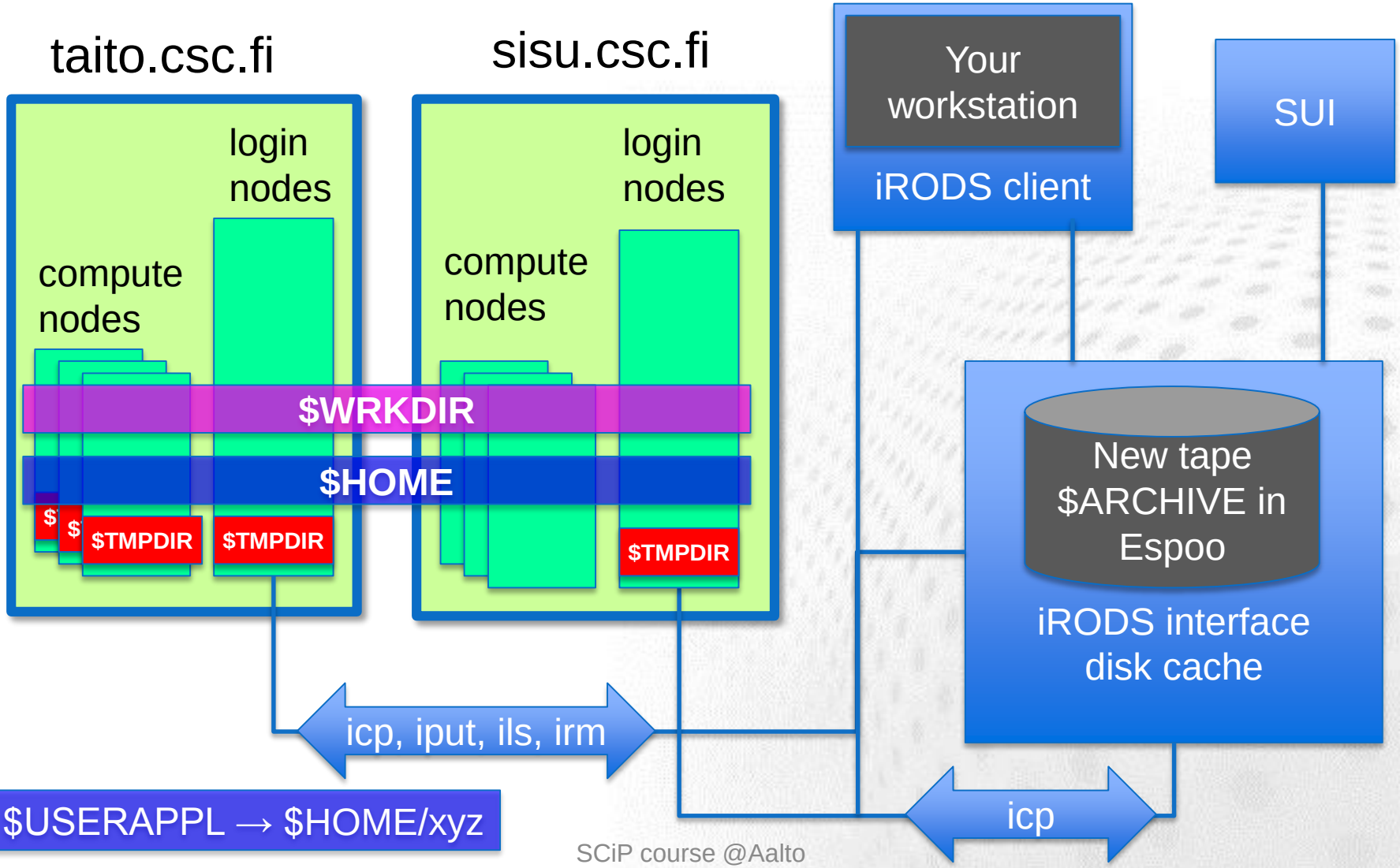
IDA storage service

- Intended for storing research data, the ultimate goal being to facilitate the exploitation of electronic data in research.
- Secure and user-friendly storage service for data and the associated metadata.
- The integrity of the data to be stored is secured by managing copies and their integrity.

Becoming an IDA user

- Universities: Please contact your local IDA contact person (*http://www.tdata.fi/en/idan-kayttajaksi*)
- Universities of applied science: Please contact contact@csc.fi
- Academy of Finland: please contact contact@csc.fi

Disks space


taito.csc.fi
sisu.csc.fi
Your workstation
iRODS client
SUI
login nodes
compute nodes
login nodes
compute nodes
$WRKDIR
$HOME
$TMPDIR
$TMPDIR
$TMPDIR
New tape $ARCHIVE in Espoo
iRODS interface disk cache
icp, iput, ils, irm
icp
$USERAPPL → $HOME/xyz

Disks space cont.

- 4.8 PB on DDN
  - New $HOME directory (on Lustre)
  - $WRKDIR (*not backed up*), soft quota: 5 TB
- HPC_ARCHIVE
  - 5 TB / user, common between Cray and HP
- Disk space through IDA
  - 1 PB for Univerisities
  - 1 PB for Finnish Academy (SA)
  - 1 PB to be shared between SA and ESFRI
  - more could be requested

Directories at CSC Environment (1)

Directory or storage area	Intended use	Default quota/user	Storage time	Backup
$HOME [1]	Initialization scripts, source codes, small data files. Not for running programs or research data.	50 GB	Permanent	Yes
$USERAPPL [1]	Users' own application software.	50 GB	Permanent	Yes
$WRKDIR [1]	Temporary data storage.	5 TB	Until further notice.	No
$TMPDIR [3]	Temporary users' files.	-	~2 days	No
Project [1]	Common storage for project members. A project can consist of one or more user accounts.	On request.	Permanent	No
HPC Archive [2]	Long term storage.	2 TB	Permanent	Yes
IDA [2]	Sharing and long term storage	several TB	At least -2017	Yes

[1]: Lustre parallel ([3]:local) file system in Kajaani [2]: iRODS storage system in Espoo

Moving files, best practices

- tar & bzip first
- rsync, not scp
  - `rsync -P username@hippu1.csc.fi:/tmp/huge.tar.gz .`
- Blowfish may be faster than AES (CPU bottleneck)
- Funet FileSender (max 50 GB)
  - *https://filesender.funet.fi*
  - Files can be downloaded also with wget

- Consider: SUI, IDA, iRODS, batch-like process, staging
- CSC can help to tune e.g. TCP/IP parameters
  - *http://www.csc.fi/english/institutions/funet/networkservices/pert*
- FUNET backbone 10-100 Gbit/s

ARCHIVE, dos and don'ts

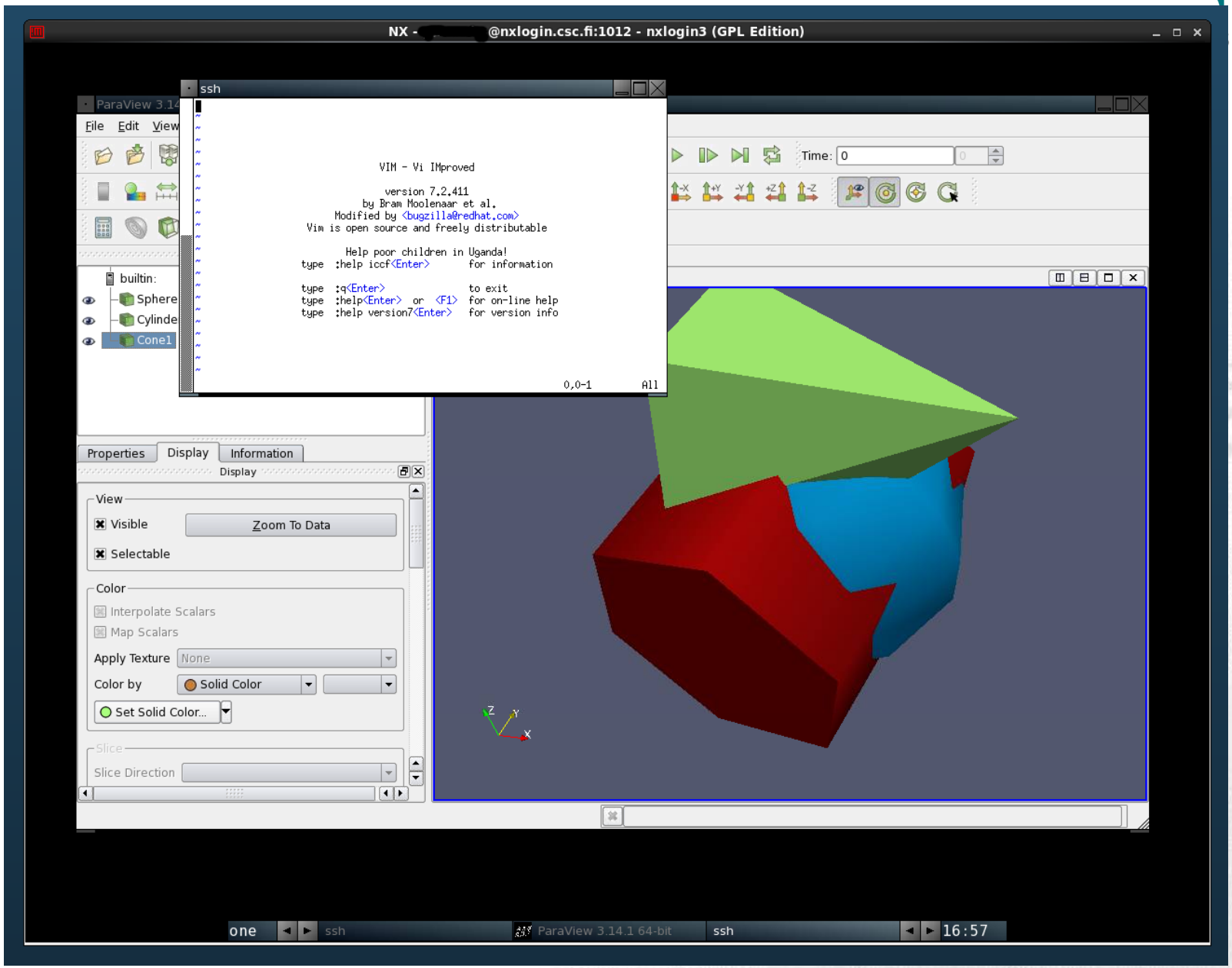
- Don't put small files in HPC ARCHIVE
  - Small files waste capacity
  - Less than 10 MB is small
  - Keep the number of files small
  - Tar and bzip files

- Don't use ARCHIVE for incremental backup (store, delete/overwrite, store, …)
  - Space on tape is not freed up until months or years!
- Maximum file size 300 GB
- Default quota 5 TB per user

Grand Challenges

- Normal GC *(in half a year / year)*
  - new CSC resources available for a year
  - no bottom limit for number of cores
- Special GC call (mainly for Cray) *(when needed)*
  - possibility for short (day or less) runs with the whole Cray
- Remember also PRACE/DECI
  - *www.prace-ri.eu/DECI-11-Call*

NX screenshot



Demo / hands on (2)

- Transpose a matrix, e.g. 3X3, by running a batch job of *Matlab* on Taito

Demo / hands on (2) cont.

- Create a matlab file, called e.g. *transpos.m*, which may look like this:

a=[1 2 3;4 5 6;7 8 9];

% non-conjugate transpose of matrix a

b2=transpose(a)

Demo / hands on (2) cont.

- Create a batch job script (e.g. *matlab_transpos.sh*), which will submit it to the queue in a row (non-interactive) mode, e.g. like this (everything in one line, without the "\" character)

srun -v matlab -r "transpos;exit" -no display \ -nosplash -nodesktop –nojvm

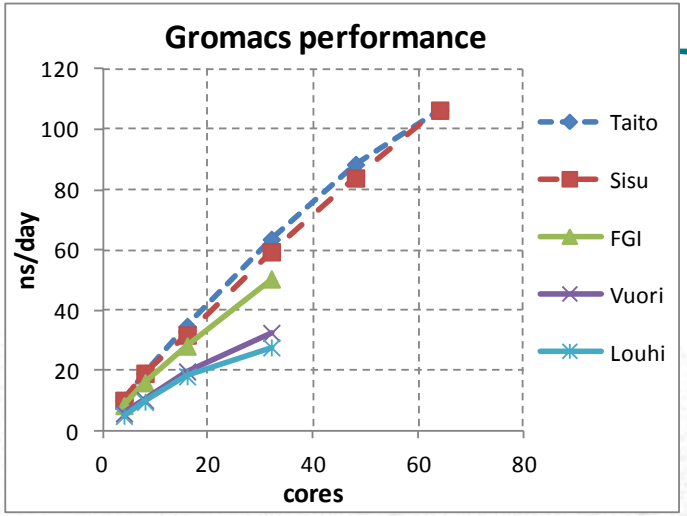
- Remember to load Matlab module before the srun command in the batch script:

module load matlab

Courses at CSC

- **CSC courses**: *http://www.csc.fi/courses*
  - Introduction to Linux and Using CSC Environment Efficiently
  - Pouta training
  - CSC HPC Summer School
  - Spring, Autumn, Winter Schools
  - Parallel Programming
  - Some courses have possibility for remote participation
  - Course materials often available from event website for self study

Summary



- ***Sisu*** *supercomputer*
  - *Fastest in Finland*
- ***Taito*** *supercluster*
  - *Serial & parallel jobs + large memory*
- ***Taito-shell*** *environment*
- ***Pouta Cloud***
  - *cPouta*
  - *ePouta*
- ***Bull*** system
- ***DDN*** HPC storage system