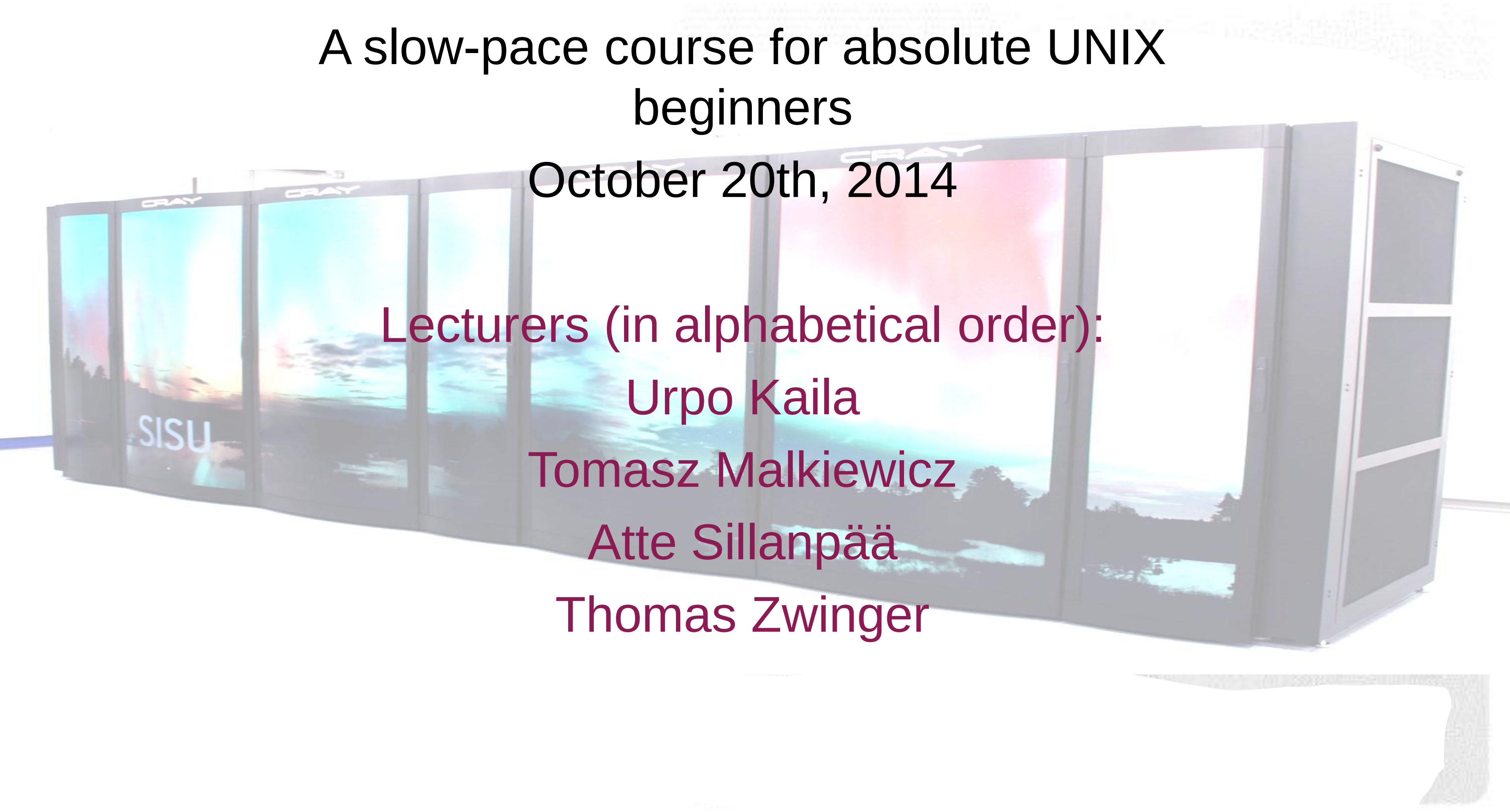
Introduction to Linux and Using CSC Environment Efficiently

October 20 - 21, 2014
CSC, Espoo

Introduction UNIX

A slow-pace course for absolute UNIX beginners

October 20th, 2014



Lecturers (in alphabetical order):

Urpo Kaila

Tomasz Malkiewicz

Atte Sillanpää

Thomas Zwinger

Program

09:45 – 10:00 Morning coffee + registration

10:00 – 10:15 Introduction to the course (whereabouts, etc.)

10:15 – 10:45 What is UNIX/Linux?: history and basic concepts (multi-user, multi-tasking, multi-processor)

10:45 – 11:15 Linux on my own computer: native installation, dual-boot, virtual appliances

11:15 – 12:15 A first glimpse of the shell: simple navigation, listing, creating/removing files and directories

12:15 – 13:15 lunch

13:15 – 13:30 Text editors: vi and emacs

13:30 – 14:15 File permissions: concepts of users and groups, changing permissions/groups

14:15 – 14:30 coffee break

14:30 – 14:45 Linux security

14:45 – 15:15 Job management: scripts and executables, suspending/killing jobs, monitoring, foreground/background

15:15 – 15:45 Setup of your system: environment variables, aliases, rc-files

15:45 – 16:45 A second look at the shell: finding files and contents, remote operations, text-utils, changing shells

16:45 – 17:00 Troubleshooter: Interactive session to deal with open questions

How we teach

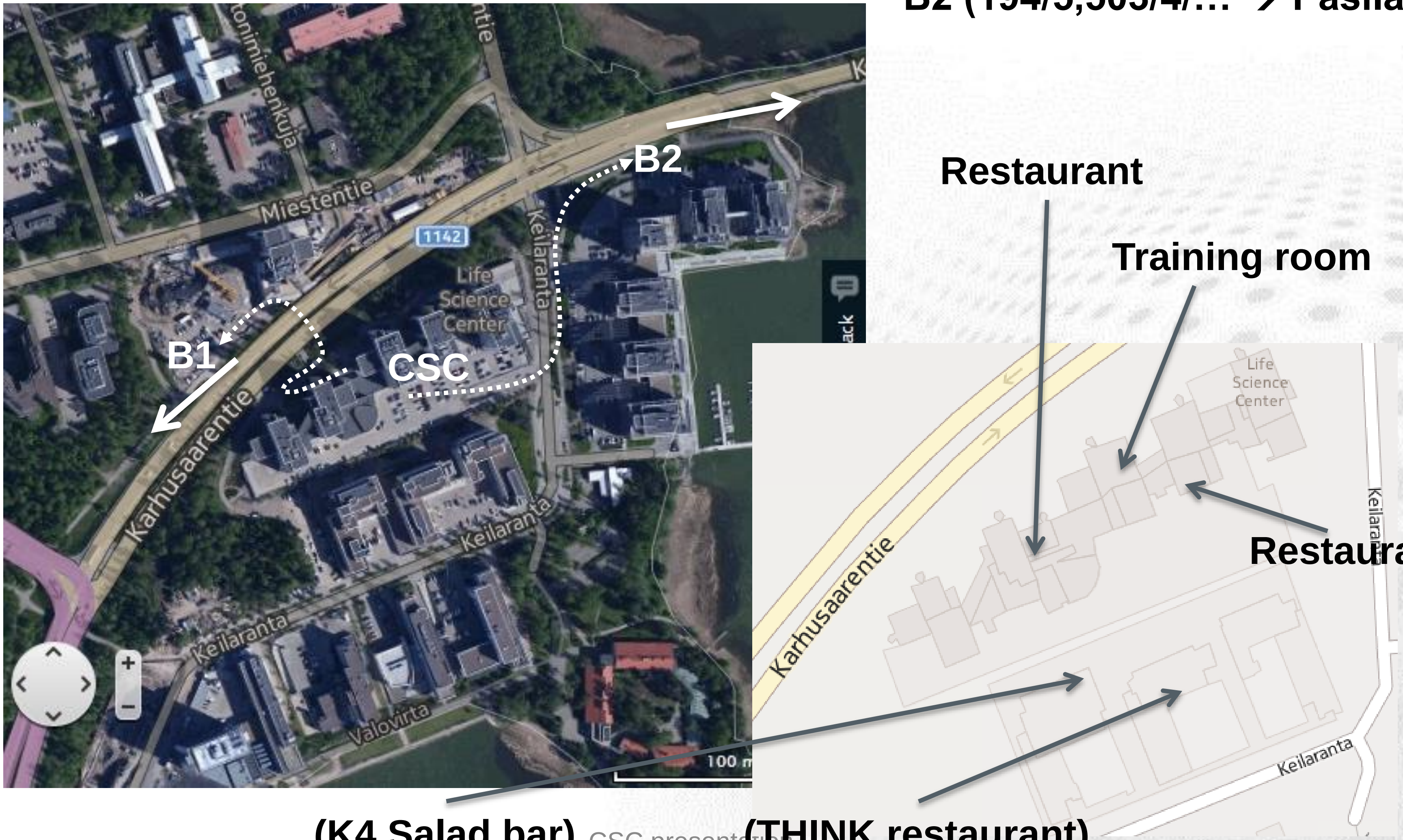
- All topics are presented with interactive demonstrations
  - Please, indicate immediately, if pace is too fast. We want to have everyone with us all the time
- Additionally, exercises to each of the sections will be provided
- The *Troubleshooter* section is meant for personal interaction and is (with a time-limit to 17:00) kept in an open end style

Practicalities

- Keep the name tag visible
- Lunch is served in the same building
- Toilets are in the lobby
- Network:
  - WIFI: eduroam, HAKA authentication
  - Ethernet cables on the tables
  - CSC-Guest accounts upon request
- Bus stops
  - Other side of the street (102,103) -> Kamppi/Center (note, underpass)
  - Same side, towards the bridge (194,195,503-6) -> Center/Pasila
  - Bus stops to arrive at CSC at the same positions, just on opposite sides
- *If you came by car: parking is being monitored - ask for a temporary parking permit from the reception (tell which workshop you're participating)*
- Visiting outside: doors by the reception desks are open
- Room locked during lunch
  - lobby open, use lockers
- Username and password for *workstations*: given on-site

Around CSC

B1 (102,103)→ Kamppi
B2 (194/5,503/4/… → Pasila,…



Restaurant

Training room

Restaurant

(K4 Salad bar)

(THINK restaurant)

What is UNIX/Linux: history and basic concepts

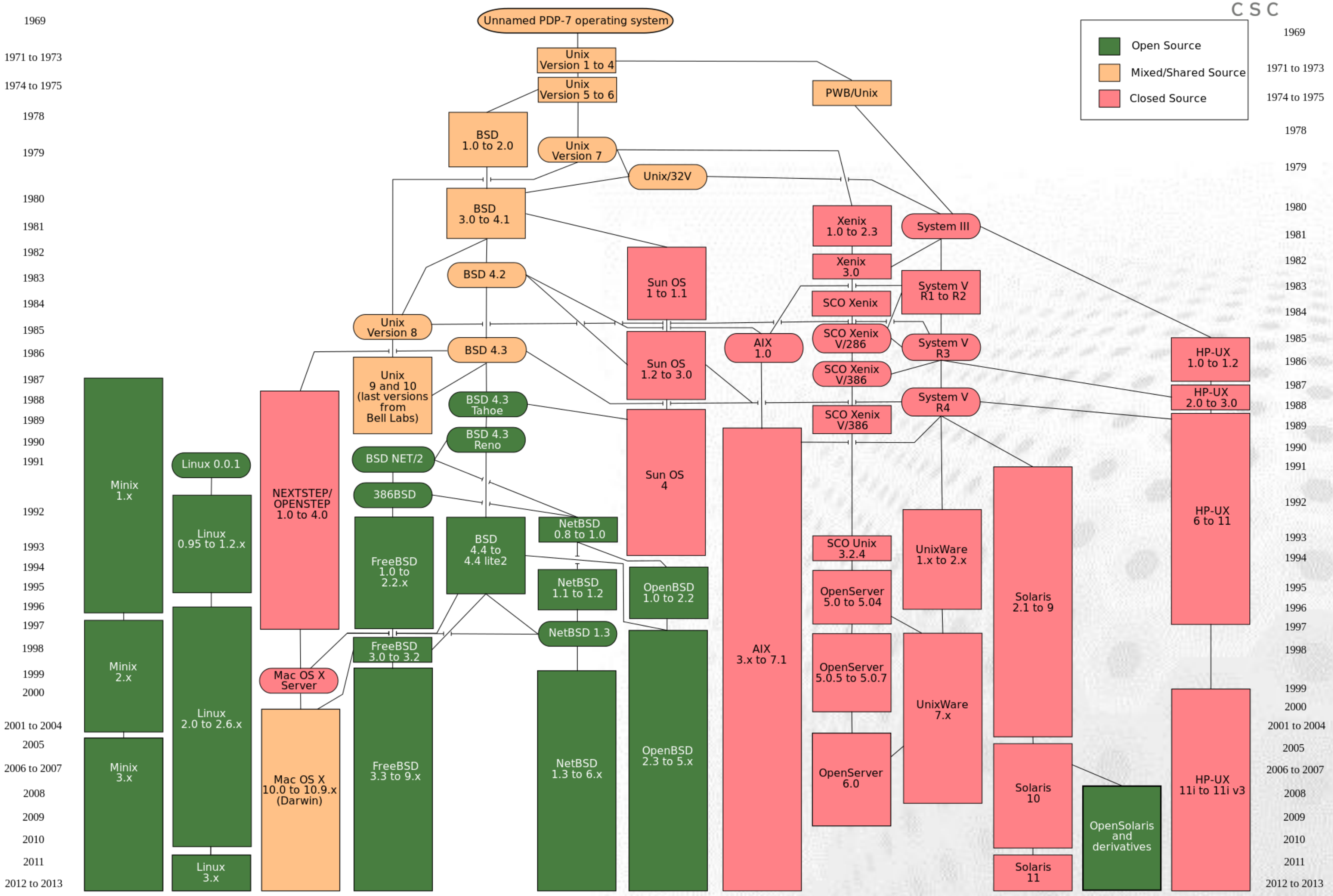
From a technical point of view

- UNIX and Linux are:
  - Operating systems
  - Multi-user systems (esp. servers)
  - Multitasking systems
- UNIX has a large commercial branch:
  - AIX®
  - HP-UX ®
  - SCO ®, SGI-IRIX ®, Solaris®, Digital-UNIX ®
- But also open source:
  - E.g., Open-Solaris, Open-BSD

From a technical point of view

- Linux is not UNIX
  - They share a common interface POSIX (Portable Operating System Interface) that is standardized by IEEE
  - They diverge in their code-base:
    - Unix was developed at AT&T in the early 70’s (Thompson, Ritchie)
    - Linux started in the 90’s just 6 km from here in Computational Science Institute (Univ. Helsinki): Linus Torvalds
    - MINIX is a second open source UNIX-like operating system (some parallels to Linux)

A short history



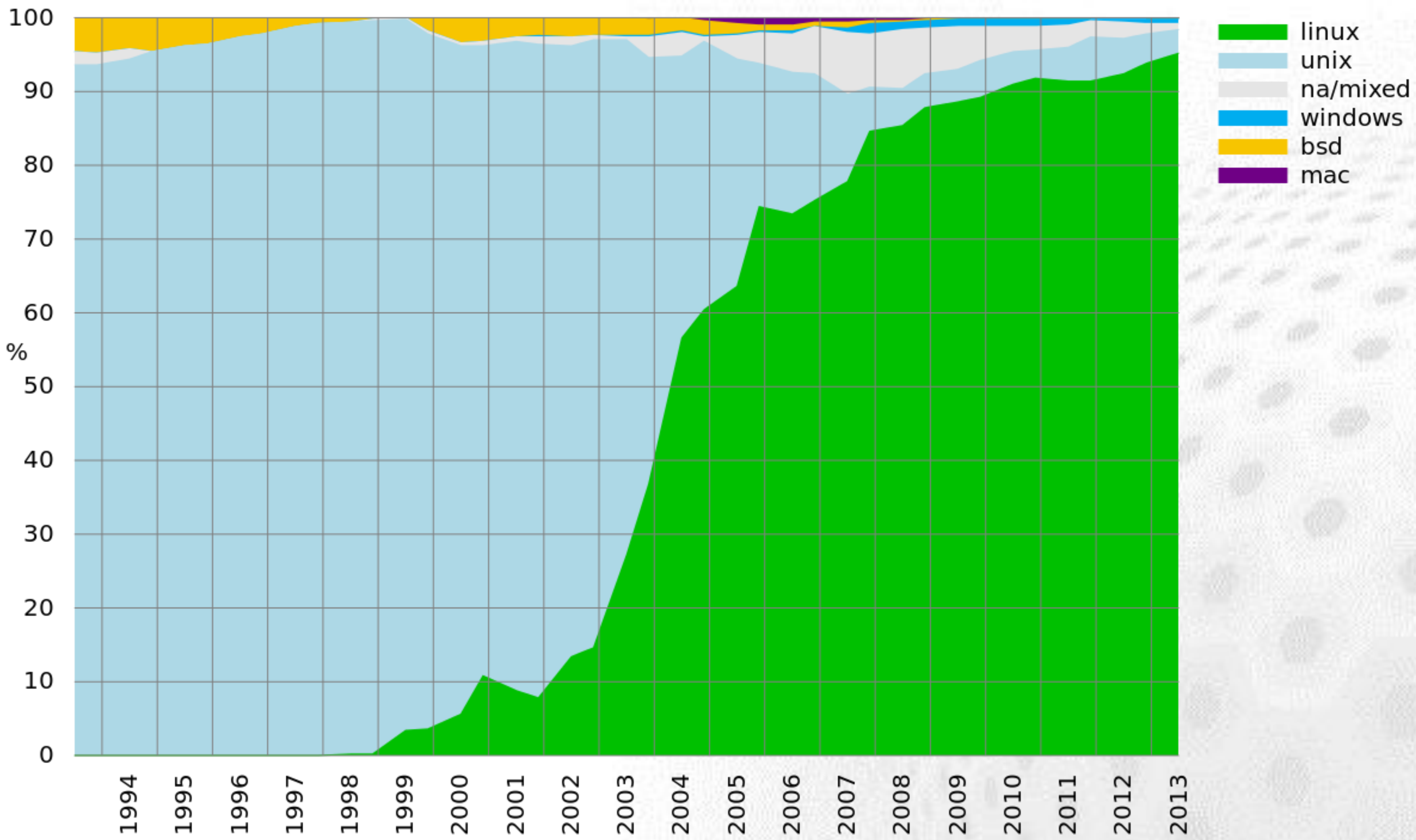
From http://en.wikipedia.org/wiki/File:Unix_history-simple.svg (see license there)

OS shares

Category	Source	Date	Linux based	Other Unix	In-House	Windows	Other
Desktop, laptop, netbook	Net Applications[34]	Jan-14	1.60% (Ubuntu)	7.68% (OS X)		90.72% (XP, 7, Vista, 8)	
Smartphone, tablet	StatCounter Global Stats[35]	Jan-14	44.95% (Android)	33.70% (iOS)		1.79% (WP8, RT)	19.46 %
Server (web)	W3Techs [36][24]	Jan-14	34.62% (Debian, CentOS, RHEL)	32.48% (BSD, HP-UX, Aix, Solaris)		32.90% (W2K3, W2K8)	
Supercomputer	TOP500 [33]	Nov-13	96.4% (Custom)	2.4% (UNIX)		0.4%	0.8%
Mainframe	Gartner[31]	Dec-08	28% (SLES, RHEL)				72% (z/OS)
Gaming console	Nintendo, Sony, Microsoft, Ouya [37]	Jun-13	0% (SteamOS, Android)	29.6% (PS3)	40.9% (Wii)	29.5% (Xbox)	
Embedded	UBM Electronics [38]	Mar-12	29.44% (Android, Other)	4.29% (QNX)	13.5%	11.65% (WCE 7)	41.1%

Source: http://en.wikipedia.org/wiki/Usage_share_of_operating_systems

OS shares: TOP500



Source:
http://en.wikipedia.org/wiki/File:Operating_systems_used_on_top_500_supercomputers.svg

Common features

- File system:
  - Supporting: files, directories, device files
  - latter added: sockets (API's for inter-process communication) and symbolic links [1)]
  - Similar layout (see next slide): *directory tree*
  - Mounted (=external) devices appear within the same tree under *mount points,* e.g., /media/usb1
    - This is contrary to common default on Windows®, where different physical disks usually have different letters (C:, D:, etc.)

[1)] Comparable to shortcuts in Windows GUI

Directory tree

`/`	Root-tree
`/etc`	System wide configuration
`/boot`	Boot configuration, kernel image
`/dev`	Device files

`/home`
`    /userid`
	Users’ home directories

`/root`	Root (=system administrator user) home
`/usr`	Distribution application
`    /lib`	libraries
`    /include`	library headers
`    /bin`	executable
`/usr/local`	Similar than **`usr`** with **`lib`**, **`include`** and **`bin`** for additional applications
`/opt`	Locally installed packages
`/media`	Often default where external disks are mounted (also **`/mnt`**)

Linux distributions

- Incredibly fast development
- Main trees:
  - Slackware/ Suse
  - RedHat/Fedora
  - Debian/ Ubuntu
- Countless spin-offs

Graphics on UNIX/Linux

- X11 or X-Windows:
  - Common window system
  - Incompatible with Windows (needs emulator)
  - Possible on OS X as additional package (Mac)
  - Not efficient, if exported over low-bandwidth connections (use remote desktop, instead)
- Graphical User Interface (GUI):
  - X11 itself needs a window manager on top of it
  - Versatile GUI’s: Gnome, KDE
    - Linux is possible to be deployed as a desktop OS

Linux on my own computer

Running your own Linux

- Basically, three options:

1. Run native Linux on you computer
   - Includes the option of *dual boot* (two OS's side-by-side, but optionally booting into one of them)
   - Not recommended: run as live-system (boot from USB/CD)
2. Run it inside a Virtual Machine
3. Run it remotely over the network
   - Includes remote login and remote desktops
   - Depends on network connection

Dual boot

- Boot loader in the beginning gives choice of which OS to load
- Pros:
  - native Linux works faster and all resources of computer are dedicated to a single OS
  - Windows file-system can be mounted
- Cons:
  - changing between OS’s needs reboot of machine
  - Mounting of Linux/Unix file-systems on Windows at least problematic

Dual boot

- I have a Windows machine, what do I have to do to install Linux parallel (as dual boot) to it?:
  1. Provide a separate disk(-partition) on computer
     - It is possible (e.g., in Ubuntu) to install into existing Windows system, but you loose performance
     - Some installation medias allow for live-mode (Linux running from USB/CD) and have a repartitioning program within (always backup your data!)
  2. Download the image of your favorite Linux distribution (see later)
  3. Installation generally guides you also through boot-loader configuration

Virtual machines

- Running an application inside your native OS that emulates hardware on which you can install another OS
- Pros:
  - Seamless integration of Linux (guest) in host system
  - Data exchange between guest and host
  - Suspend system (no new boot, leave applications open)
  - Backup and portability (copy to new computer)
- Cons:
  - Performance loss of guest system (SW layer between)
  - Shared resources between guest and host

Virtual machines

- I have a Windows computer. How can I install Linux running in a Virtual Machine (VM)?
  1. Make sure you have the hardware to support a VM (CPU, memory > 2GB, disk-space)
  2. Download a VM software (see next slide) and install it
  3. Download an image of your favorite Linux distribution (see later)
  4. Mount the medium in your VM and install as if it would be a normal computer
  5. Instead of 3+4: Download a ready made virtual appliance (~virtual computer system)

Virtual machines

- Two main vendors for VM packages:
  - VMware™ Player (free-of-charge)
    - Only max 4 cores supported in VM
  - Oracle (former Sun) VirtualBox (open-source)
    - Supports even Vmware virtual disks
- Usually, additional tools (Vmware-tools) have to be installed
- Important to know the hardware, especially CPU type (32- or 64bit)
  - Might need adjustments in BIOS
- Virtual Appliances: Google or FUNET

Remote connection

- From OS X:
  - – ssh and X available – like from a Linux machine
- From Windows ®:
  - – Needs a ssh client: e.g. PuTTY
  - – If graphics, needs a X11-emulator: e.g. Xming
- Remote desktops:
  - – Needs a server running
  - – Certain software (client + server)
  - – CSC is maintaining such a service (see tomorrow): NoMachine, NX

A first glimpse of the shell

Contents

- What is a shell?
- What is a command?
- Listing of directories
- Contents of a file
- Moving around
- Directories
- Files

What is a shell?

- “*A **shell** in computing provides a user interface for access to an operating system's kernel services.*” (Wikipedia)
- Remote login:
  - Normally no GUI (Graphical User Interface)
  - Text shell: Terminal with a set of commands
- Different flavours:
  - **bash** (default), tcsh (old default), zsh, corn-shell, …

What is a command?

- A command is a small program provided by the shell
- The over-all structure of a command is:

```
command -option [optional input]
```

- Example:

```
     ls    -lsh     /etc/init.d
```

(we will see later)

- Case sensitive? Try: `Ls -lsh /etc/init.d`
- How to find a command? `apropos list`
- How to find all options? `man ls`

Listing of directories

- Prints contents of a directory or information on a file
- Detailed list of directory:

```
ls -lthr /etc/
```

`-l` displays additional information (detailed list in Windows)

`-h` displays size in human readable format

`-t` orders by date (use `-r` to reverse order, i.e., oldest first)

`-d` keeps from going into sub-directories

- Only print directory/filenames matching a wildcard expression: `ls -d /etc/*.d`
- Only print directory/filenames with a 4 char suffix: `ls -l /etc/*.????`

Contents of a file

- Prints contents of file to screen:

```
cat /etc/group
```

- `-n` to precede lines with line numbers

What if the file doesn’t fit on the screen?:

- Open a scrollable view of a file:

```
 less /etc/group
```

- Press **q** to quit
- **/** to search forward, **?** to search backwards
- **n** to find the next match, **N** for previous

Moving around in directrories

- change directory: `cd /etc/`
- print work directory: `pwd →/etc`
- go to subdirectory: `cd ./init.d`

  `pwd → /etc/init.d`
- Relative path: `cd ../`

  `pwd -> /etc`
- Absolute path: `cd /etc/init.d`
- Combination: `cd ../../usr`

  `pwd -> /usr`
- Where is my home?: `cd` or `cd ~/`

Creating and (re-)moving directories

- **M**a**k**e a new **dir**ectory: `mkdir test1`
- Relative to (existing) path:

```
mkdir test1/anotherone
```

- Recursively: `mkdir -p test2/anotherone`
- **M**o**v**ing a directory: `mv test2 test3`
- **Re**mo**v**ing a **dir**ectory:

```
cd test1
rmdir anotherone
cd ..
rmdir test1
rmdir test3
```

- Recursively: `rmdir -p test3/anotherone`

Creating/copying/(re-)moving files

- In UNIX: everything is text
- Redirecting output of command/programs into files:

```
echo “hello world” > mytest.txt
```

- Important: if file exists, it will be overwritten!
- Appending to existing files:

```
echo “hello again” >> mytest.txt
cat mytest.txt
cat mytest.txt > othertest.txt
```

Creating/copying/(re-)moving files

- **C**o**p**y a file: `cp mytest.txt othertest2.txt`
- Same with directory:

```
mkdir -p test/anotherone
cp -r test test2
```

- **M**o**v**e a file (renaming):

```
mv mytest.txt othertest3.txt
mv othertest3.txt test2/anotherone
```

- **R**e**m**ove file(s): `rm -f mytest.txt`
- Remove recursively: `rm -r test2`

Further resources

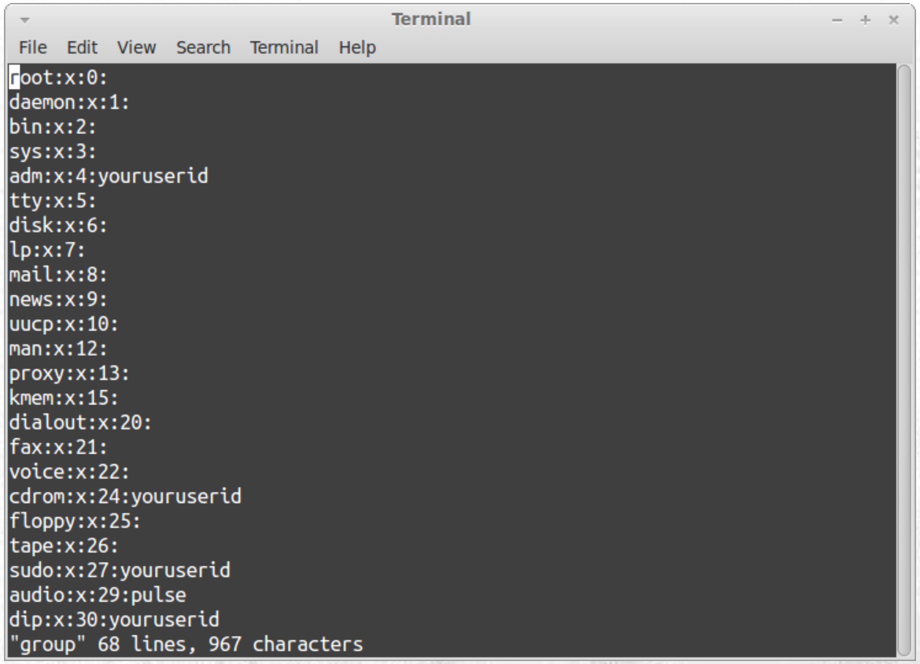
- CSC’s online user guide: http://research.csc.fi/csc-guide
- All the man-pages of the commands mentioned in these slides
- The UNIX-wiz sitting by your side
- Else:
  - http://www.ee.surrey.ac.uk/Teaching/Unix/index.html
  - http://en.wikipedia.org/wiki/List_of_Unix_utilities

Text editors

Texteditors: vi

- Default on each system:

```
mkdir test
cd test
cp /etc/group lala
vi lala
```



```
root:x:0:
daemon:x:1:
bin:x:2:
sys:x:3:
adm:x:4:youruserid
tty:x:5:
disk:x:6:
lp:x:7:
mail:x:8:
news:x:9:
uucp:x:10:
man:x:12:
proxy:x:13:
kmem:x:15:
dialout:x:20:
fax:x:21:
voice:x:22:
cdrom:x:24:youruserid
floppy:x:25:
tape:x:26:
sudo:x:27:youruserid
audio:x:29:pulse
dip:x:30:youruserid
"group" 68 lines, 967 characters
```

- Delete char: **X**
- Delete line: **dd**
- Insert-mode: **i**
- New line above (below): **O** (**o**)
- Exit insert.mode: **ESC**
- Undo: **u**

-Search: **/** and **n** to continue

- Write and quit: **:wq**

Texteditors: emacs

- Almost on any system
- More WYSIWYG
- Menu-buttons

  `emacs lala`

  – Delete char: **DEL**

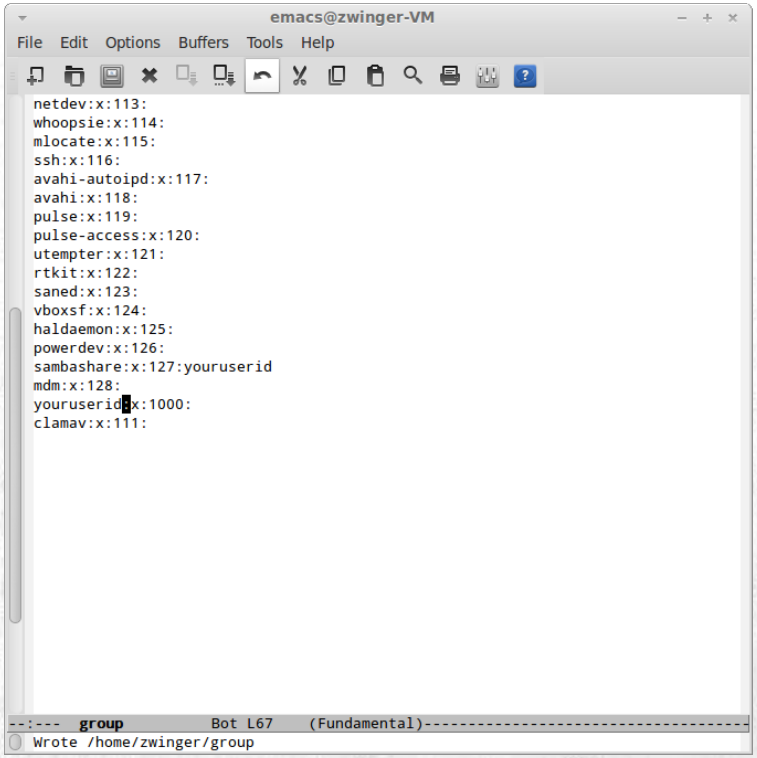
  – Delete line: **CTRL** + **K**

  – Query-replace: **ESC** + **%**
  then enter expressions
  press **!** for auto replace

  – Search: **CTRL** + **S**

  – Save: **CTRL** + **X** followed by **CTRL** + **S**

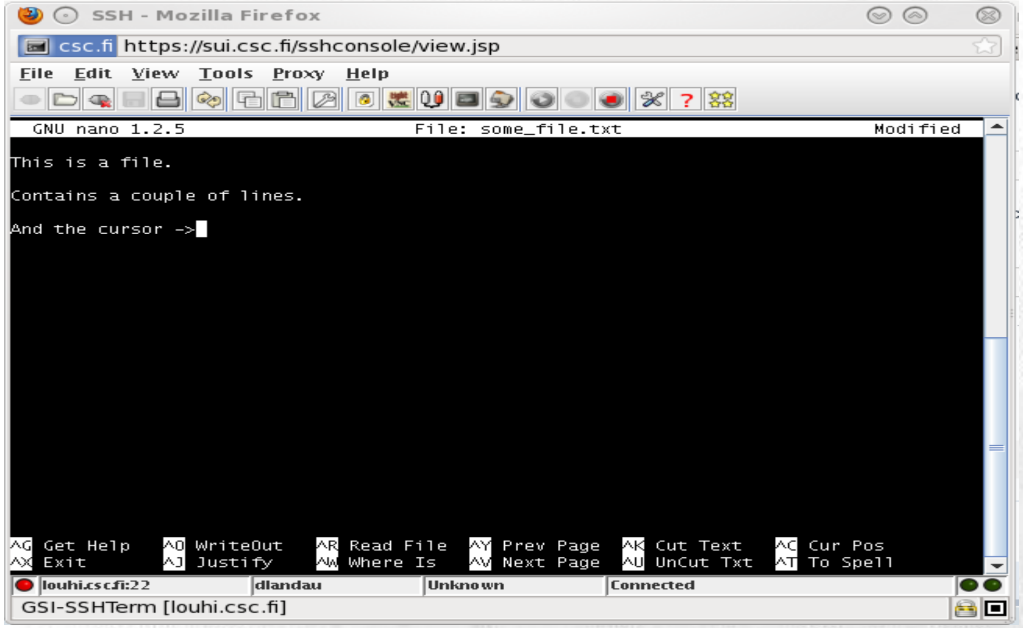
  – Exit: **CTRL** + **X** followed by **CTRL** + **C**



```
netdev:x:113:
whoopsie:x:114:
mlocate:x:115:
ssh:x:116:
avahi-autoipd:x:117:
avahi:x:118:
pulse:x:119:
pulse-access:x:120:
utempter:x:121:
rtkit:x:122:
saned:x:123:
vboxsf:x:124:
haldaemon:x:125:
powerdev:x:126:
sambashare:x:127:youruserid
mdm:x:128:
youruserid:x:1000:
clamav:x:111:

--:---  group          Bot L67    (Fundamental)----------------------------------
Wrote /home/zwinger/group
```

Texteditors: nano

- ^x (Ctrl-x) to exit (prompts for save)
- ^o to save without exiting
- Depending on the system, you may want to use other editors: gedit, ed, …


SSH - Mozilla Firefox
csc.fi https://sui.csc.fi/sshconsole/view.jsp
File Edit View Tools Proxy Help
louhi.csc.fi:22
dlandau
Unknown
Connected
GSI-SSHTerm [louhi.csc.fi]

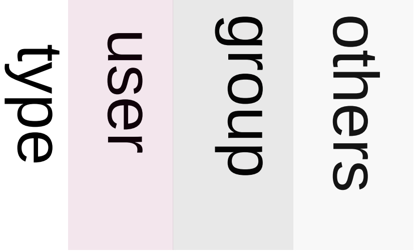
```
  GNU nano 1.2.5                    File: some_file.txt                     Modified

This is a file.

Contains a couple of lines.

And the cursor ->

^G Get Help   ^O WriteOut   ^R Read File  ^Y Prev Page  ^K Cut Text   ^C Cur Pos
^X Exit       ^J Justify    ^W Where Is   ^V Next Page  ^U UnCut Txt  ^T To Spell
```

File permissions

File permissions

- UNIX distinguishes between users, groups and others
  - Check your groups: **`groups`**
- Each user belongs to at least one group
- **`ls -l`** displays the attributes of a file or directory

```
-rw-r--r-- 1 userid groupid 0 Jan 29 11:04 name
```



r = read, **w**=write, **x**=execute

The above configuration means: user can read + write, group and all others only read

File permissions

- Changing permissions with **chmod**

```
> ls -l lala
> rw-r--r-- 1 userid groupid 0 Jan 29 11:04 lala
> chmod o-r,g+w,u+x lala
> ls -l lala
> rwxrw---- 1 userid groupid 0 Jan 29 11:04 lala
> chmod u-xrw lala
> less lala
```

- Changing group **chgrp** and user **chown**

```
> chgrp othergrp lala
> chown otherusr lala
> ls -l name
> rwxrw---- 1 otherusr othergrp 0 Jan 29 11:04 lala
```

File permissions

- You can make a simple text file to be executed – **your first script**
- Open file **`befriendly.sh`** and insert following lines:

```
#!/bin/bash
echo "Hello and welcome"
echo "today is:"
date
echo "have a nice day"
```

- Change to executable:

Execute:
```
> chmod u+x befriendly.sh
> ./befriendly.sh
```

Introduction to Linux Security

Introduction to Linux and Using CSC Environment Efficiently course
Oct 20-21, 2014

Urpo Kaila <urpo.kaila@csc.fi>

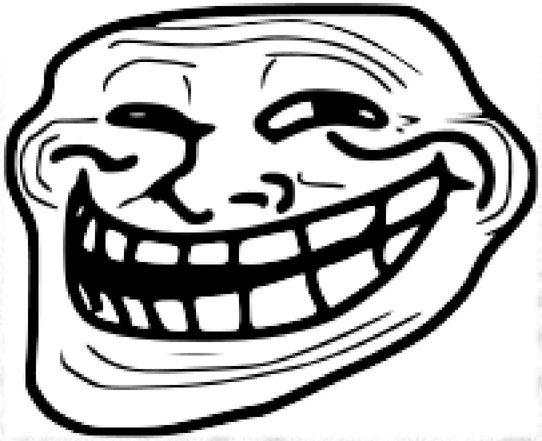
What is Security actually?

- Security is a set of appropriate procedures to protect your resources (your data, your account, your services and your reputation) against **ris**

- The main aspects of security are
  - <u>Confidentiality</u> (don’t let others access or forward your confidential data, such as passwords, personal data, business secrets)
  - <u>Integrity</u> (don’t let others change your data without permission, beware of malware and hackers)
  - <u>Availability</u> (keep your data and services available for yourself and those who should have access to it)

Security Risks and Compliance

- Typical risks for Linux users:
  - Compromised account (#1!)
  - System compromise and spying
  - Denial of Service
  - Surveillance
  - Infrastructure related issues
  - Bad user and system administration
  - Legal issues



- You must comply with laws and Terms of Use
  - Do not endanger other users or the Infrastructure
  - Protect personal data and other confidential information
  - As a User, you are responsible to protect your account

Security related obligations in CSC General Terms of Use (1/2)

Do not:

- Share your credentials, leave them for others to see, or neglect any security responsibilities defined in the service description.
- Misuse or abuse any CSC or third party service or property, including intellectual property. Obviously breaking the law is considered misuse.

- Misuse or abuse Users Content, credentials or other confidential information.
- Send or transmit harassing, abusive, libellous, obscene or unsolicited (spam) communications.

Security related obligations in CSC General Terms of Use (2/2)

Do not:

- Tamper with or deliberately disrupt system resources or network traffic to the Services.
- Users agree to notify CSC promptly if their account has been used without permission or if their credentials have been lost or stolen
- Users are liable, even after the user account has been terminated, for any damage and costs CSC incurs as a result of violating these terms.

How to protect yourself?

- Compromised account
  - Use only good passwords (hard to guess, easy to remember)
  - 8 chars min, (large alphabet, no dictionary worlds), use password managers (such as KeePass)
  - Be careful with public systems and services (never recycle passwords)
  - User keys instead of passwords (but protect your keys too!)
- System compromise
  - Patch your own system regularly, keep firewall (iptables, ufw) on, use only necessary services
- Denial of Service
  - Offer only the necessary services to others

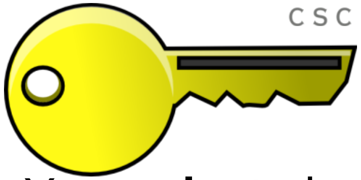
- Surveillance
  - Don’t store any confidential information on cloud services
- Bad user and system administration
  - Beware of forgotten test accounts, patch your system regularly

Patch and secure your own computer!

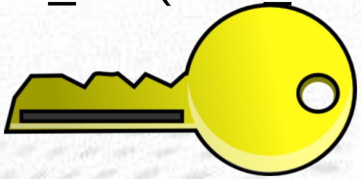
- Install patches regularly:
  - Debian: apt-get update && apt-get uppgrade
  - RHEL/Centos: yum update
  - GUI and scheduled
- Do not run any unnecessary services
  - Email, WWW, SMB
- Anti-virus on windows computers
- Enable local firewall
  - Iptables, yum
    - ufw enable
    - ufw allow ssh, ufw default deny incoming
- Do not keep test accounts with bad passwords
  - Systems are continuously scanned by intruders

Create and use ssh-keys

```
cscuser@algol ~]$ ssh-keygen
Generating public/private rsa key pair.
Enter file in which to save the key (/home/cscuser/.ssh/id_rsa):
Enter passphrase (empty for no passphrase):
Enter same passphrase again:
Your identification has been saved in /home/cscuser/.ssh/id_rsa.
Your public key has been saved in /home/cscuser/.ssh/id_rsa.pub.
The key fingerprint is: 57:2b:b3:c8:f1:3d:46:10:... cscuser@algol.csc.fi
The key's randomart image is:
+--[ RSA 2048]----+
| ...oE  . .      |
...
[cscuser@algol ~]$ scp .ssh/id_rsa.pub  user@sisu.csc.fi:.ssh/authorized_keys
Password:
id_rsa.pub
cscuser$ ssh sisu.csc.fi
+-[Welcome]-----------------------------------------------------------+
|        CSC - Tieteen tietotekniikan keskus - IT Center for Science        |
..
```



Your **private** key:
Id_rsa (or id_dsa)

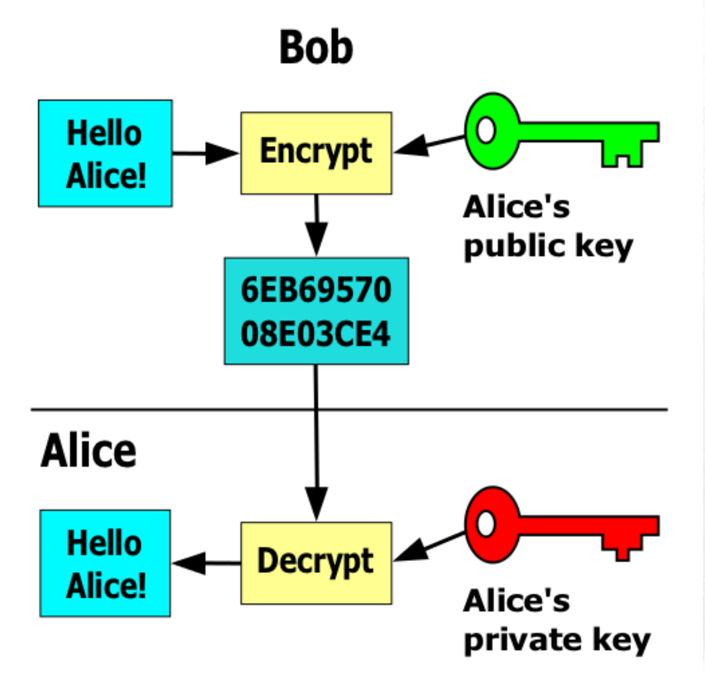


Your **public** key
Id_rsa.pub
On you local **and**
on your remote host

Bonus for the smart & lazy user: **ssh-agent (if you want to log in many times per day)**

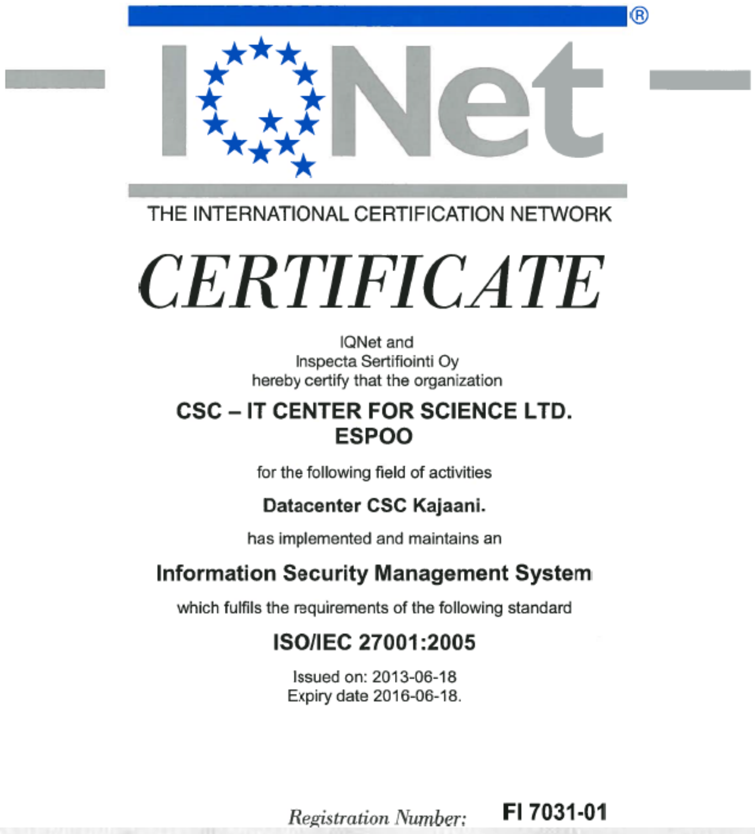
Encrypt your data

- Use native encryption on your workstation
  - Available for Windows, Linux and Mac
  - Improves basic protection
- Encrypt confidential email with PGP/GnuPG
  - Can be a little bit difficult to implement for non-technical people
  - No centralised key-management
  - Plug-ins for email clients
- Encrypting cloud content
  - Some solutions available



CSC is a Reliable Partner

- CSC complies to requirements and best practices on Information Security
  - – National requirements (Raised Information Security Level)
    - Audited several times
  - – International Standards
    - ISO 27001:2005 Certification for CSC Datacenters in Espoo and in Kajaani
    - 100+ manadatory controls
- Peering with national and international security partners
- In case of security incidents or other infosec matters, contact security@csc.fi



IQNet

THE INTERNATIONAL CERTIFICATION NETWORK

CERTIFICATE

IQNet and
Inspecta Sertifiointi Oy
hereby certify that the organization

CSC – IT CENTER FOR SCIENCE LTD.
ESPOO

for the following field of activities

Datacenter CSC Kajaani.

has implemented and maintains an

Information Security Management System

which fulfils the requirements of the following standard

ISO/IEC 27001:2005

Issued on: 2013-06-18
Expiry date 2016-06-18.

Registration Number: **FI 7031-01**

Job management (in shell)

Managing jobs

- By default commands (jobs) are run in foreground `> emacs newfile`
- Try to enter something in your shell
  - does not respond
  - emacs blocks the shell as long as you do not quit it
- Killing a job: in shell press **Ctrl** + **C**
  - That is not recommended
  - Usually only when program hangs

Managing jobs

- Launch again into foreground

```
> emacs newfile
```

- Type something into emacs
- Suspending a job: in shell press **Ctrl + Z**
  - Shell reports on stopped job
  - type a command into the shell: > `ls -ltr`
  - Try to type something into emacs
  - The process of emacs is suspended, hence does not accept any input

Managing jobs

- Sending to background: `> bg`
  - type a command into the shell: `> ls -ltr`
  - type something into emacs
  - It works now
- Fetching back to foreground:
  - Shell is blocked again
  - emacs accepts input (but exit)
- Launching directly into background:

```
> xterm -T "no 1" &
> xterm -T "no 2" &
```

Managing jobs

- Listing jobs of shell: `> jobs`

```
[1] -  Running                    xterm -T "no 1" &
[2]+  Running                    xterm -T "no 2" &
```

- Explicitly bring to foreground: `> fg %2`
  - Send it back again: **Ctrl** + **Z** `> bg`
- Killing job: `> kill -9 %2`

  `> jobs`

```
[1] -  Running                    xterm -T "no 1" &
[2]+  Killed                   xterm -T "no 2"
```

Setup of system

Environment variables

- Concept of global information, accessible within the shell
- Most of those variables are being set by the system
- How can I show them?

```
> printenv > myvariables.txt
> less myvariables.txt
```

search for **`HOME`** (using **`/HOME`**)

Environment variables

- `HOME` is the environment variable that contains the path to your home-directory
- How to refer to the contents of an environment variable?

  `> echo $HOME`

  `> cd $HOME` (is the same as `cd ~/`)
- How to set my own variable:
  - (ba)sh: `export MYVARIABLE=“whatever you like"`
  - (t)csh[1]: `setenv MYVARIABLE “whatever you like"`

[1] in tcsh a simple setenv (without further arguments) displays all environment variables that have been set

Environment variables

- Important variables [1] :
  - **`HOME`** contains the path to your home-directory
  - **`USERNAME`** contains your login ID
  - **`PATH`** contains all search-paths for executables
  - **`PWD`** contains current directory (same as **`pwd`** command would display)
  - **`LD_LIBRARY_PATH`** contains search-paths for shared objects (runtime libraries)

[1] Default settings can vary between distribution and installations

How to change shell

- If installed, it usually is enough to just type the command of the shell: `> tcsh`
- See what shell is running:
  - If default shell is used: `> echo $SHELL`
  - If one is loaded upon: `> ps`

```
  PID TTY          TIME CMD
26111 pts/4    00:00:00 bash
26703 pts/4    00:00:00 tcsh
26778 pts/4    00:00:00 ps
```

- Exit a currently loaded shell: `> exit`
- How to find one’s default shell:

  `> less /etc/password` (search for user-ID)

System initialization

- Usually done by special files:
  - System wide setup files in `/etc` (don’t touch ‘em)
  - Files in your `$HOME`-directory (they are at your service)
  - So, where are they? `> ls -d .*`

```
.bashrc              .config
.emacs               .emacs.d
.local               .profile
.ssh
```

  - The preceding dot hides them from normal `ls` (option `–a` reveals hidden files)
  - Exact list depends on Linux distribution

Creating your own command

- You can define your own command using an alias, either directly in the shell:

  ```
  > alias hello='echo "hello world"'
  > hello
  ```

- Or put the line into `.bashrc`
  - Next time you open a new bash-shell you will have the new command
  - Suggestion for something more useful:

    ```
    > alias ltr='ls -ltrh'
    > ltr
    ```

Creating your own command

- You can execute scripts and executables
- Earlier we created the file **befriendly.sh**

```
> mkdir bin
> mv befriendly.sh bin
```

- If you now want to run the script:

```
> bin/befriendly.sh
```

- That is complicated, hence

```
> export PATH="$PATH:$HOME/bin"
> echo $PATH
```

A second look at the shell

Finding stuff (1)

- The hard way: `cd` yourself through the tree and `ls`
- The elegant way:

```
> find /etc -name "*.conf" -print
```

  – Finds all config file in the `/etc`-tree

- The alternative:

```
> locate *.conf
```

Finding stuff (2)

- Finding expressions inside files:
  - For instance, we want to know all files in the directory `/etc/init.d` that contain keyword "network": `> grep network /etc/init.d/*`
  - Or recursively: `> grep -r network /etc`
  - Getting rid of noise:

```
> grep -r network /etc 2> /dev/null
```

- Piping of output:
  - Instead of re-directing into files, output can be piped in a chain of commands:

```
> grep -r network /etc 2> /dev/null| grep start| less
```

Managing space

- How much space is left on my filesystem?

```
> df -h
```

```
Filesystem          Size  Used Avail Use% Mounted on
/dev/sda5            22G   20G  903M  96% /
/dev/sda1           447M   27M  396M   7% /boot
.host:/              12G  8.0G  4.1G  66% /mnt/hgfs
```

- What are the sub-directories that consume the most disk-space?

```
> du -sh ./*
```

```
1.4M    bin
6.3M    core
44K     Desktop
696M    Documents
1.2G    Downloads
…
```

Login

- Only secure connections (no telnet, rlogin) are recommended
- Secure Shell (SSH):

```
ssh name@target.computer.fi -X
```

`-X` tunnels the graphical output

e.g. `ssh trgnXX@taito.csc.fi -X`

- More details in tomorrow’s course

Remote copying

- `scp` is like `cp`, but used for remote transfer

```
> scp lala user@taito.csc.fi:'$HOME'
```

Quotes are important here

- `rsync` works local as well as remotely and helps to keep two (remote) directories in sync:

```
> mv lala test
> rsync -avt test/ test2
```

This syncs everything in `test` with `test2`

Important: Do not drop trailing `/`

– Remotely:

```
> rsync -avt test user@taito.csc.fi:'$HOME'
```

Remote download

- scp works also with remote computer as source:

```
> scp user@taito.csc.fi:'$HOME/lala' .
```

Here is a space

- If you know a source (=URL) on the internet[1)]:
  - Usually: Open browser and download
  - Not possible/recommended to use a graphical browser on a remote system
  - Elegantly from the shell:

```
> wget http://ftp.gnu.org/gnu/hello/hello-2.7.tar.gz
```

[1)] Be sure you can trust the contents of the source – there is malware also in UNIX!

(De-)compressing files

- Storage and copying of large files: make them smaller
- Several formats supported:
  - `gzip` (GNU zip): `.gz`
  - `zip`: `.zip`
  - `bzip2`: `.bz2, .bz`

(De-)compressing files

- GNU zip:

```
Inflate:     > ls -l *.gz

             > gunzip hello-2.7.tar.gz
             > ls -l *.tar
Compress:  > gzip hello-2.7.tar
             > ls -l *.gz
```

- ZIP:

```
Compress:  > zip myvar.zip myvariables.txt
Directories: > zip -r test.zip test
Listing:   > unzip -l myvar.zip
Inflate:     > unzip myvar.zip
```

- BZIP: `Bzip2:   bzip2, bunzip2` (`-t` for testing)

Archives of files

- Most common: tar (tape archive)
  - Take whole sub-tree and make a single compressed file

```
> tar cvzf myfirsttarfile.tar /etc/init.d
```

- c create new archive
- v verbosity
- z gzip simultaneously
- f target file

  - Check contents (and simultaneously gzip):

```
> tar tvzf hello-2.7.tar.gz
```

  - Unpack (and simultaneously gzip):

```
> tar xvzf hello-2.7.tar.gz
```

More tools (discussed tomorrow)

```
head, tail, wc, which,
time, ps, top
```

```
sed, sort, uniq, cut,
paste, awk, alias
```

Troubleshooter: Interactive session to deal with open questions and specific problems

Using CSC Environment Efficiently

October 21st, 2014

Lecturers:

Tapani Kinnunen

Tomasz Malkiewicz

Ari-Matti Saren

Atte Sillanpää

Thomas Zwinger

Program

09:00 - 09:10 Welcome
09:10 - 09:15 CSC at a glance
09:15 – 09:45 How to connect: how to access CSC's computers
09:45 – 10:00 *Coffee break*
10:00 - 10:30 Installation session: helping with installation of NX client, PuTTy, ...
10:30 - 11:15 Scientist's User Interface (SUI): introduction to web-based access to CSC's services
11:15 - 12:15 Linux on supercomputers: a basic guide to use the shell
12:15 - 13:15 *Lunch*
(**12:50-13:15** ***Supercomputer's tour for those who are interested***)
13:15 - 13:45 CSC's computing environment: different platforms, module system
13:45 - 14:15 *Coffee break*
14:15 - 15:00 Running your jobs: resource-management (a.k.a. batch job) systems
15:00 - 15:30 Compiling your program (writing makefile, linking, debugging)
15:30 - 15:45 Science services at CSC: a short introduction
15:45 - 16:15 Troubleshooter: Interactive session to deal with open questions and specific problems

Practicalities

- Keep the name tag visible
- Lunch is served in the same buildingToilets are in the lobby
- Network:
  - WIFI: eduroam, HAKA authentication
  - Ethernet cables on the tables
  - CSC-Guest accounts upon request
- Bus stops
  - Other side of the street (102,103) -> Kamppi/Center (note, underpass)
  - Same side, towards the bridge (194,195,503-6) -> Center/Pasila
  - Bus stops to arrive at CSC at the same positions, just on opposite sides
- *If you came by car: parking is being monitored - ask for a temporary parking permit from the reception (tell which workshop you're participating)*
- Visiting outside: doors by the reception desks are open
- Room locked during lunch
  - lobby open, use lockers
- Username and password for *workstations*: given on-site

CSC at a Glance

CSC?

- Non-profit company owned by Ministry of education and culture
- Services mainly free (*as in beer*) for researchers
- 4250 registered users (2012)
- Applications, computational capacity, user support, FUNET, information management services, data services
- Participating in 18 EU projects

Internationally competitive research environments and e-Infrastructures

Collaboration with majority of European computing centers

- International research network organizations:
  - *NORDUnet, TERENA, GÉANT (GN3)*
- European research infrastructures and supporting projects:
  - *ELIXIR, CLARIN, ENVRI*
- International HPC projects and GRID-organizations:
  - *Nordic e-Infrastructure Collaboration (NeIC), PRACE, EGI-Inspire, HPC-Europa2*
- European e-Infrastructure policy initiatives :
  - e-Infranet, e-Infrastructure Reflection Group (e-IRG)

CSC

EU Projects 2012

EUDAT

egi

ODE
Opportunities for Data Exchange

APARSEN
Alliance Permanent Access to the Records of Science in Europe Network

SIM4RDM
SUPPORT INFRASTRUCTURE MODELS FOR RESEARCH DATA MANAGEMENT

ENVRI

ALLBIO
BIOINFORMATICS

e-InfraNet

GÉANT

PRACE

HPC-Europa2
Pan-European Research Infrastructure on High Performance Computing

e-IRG
e-Infrastructure Reflection Group

ice2sea

MMM@HPC

elixir Data for Life

BioMedBridges

SVALI

NDGF
Nordic DataGrid Facility

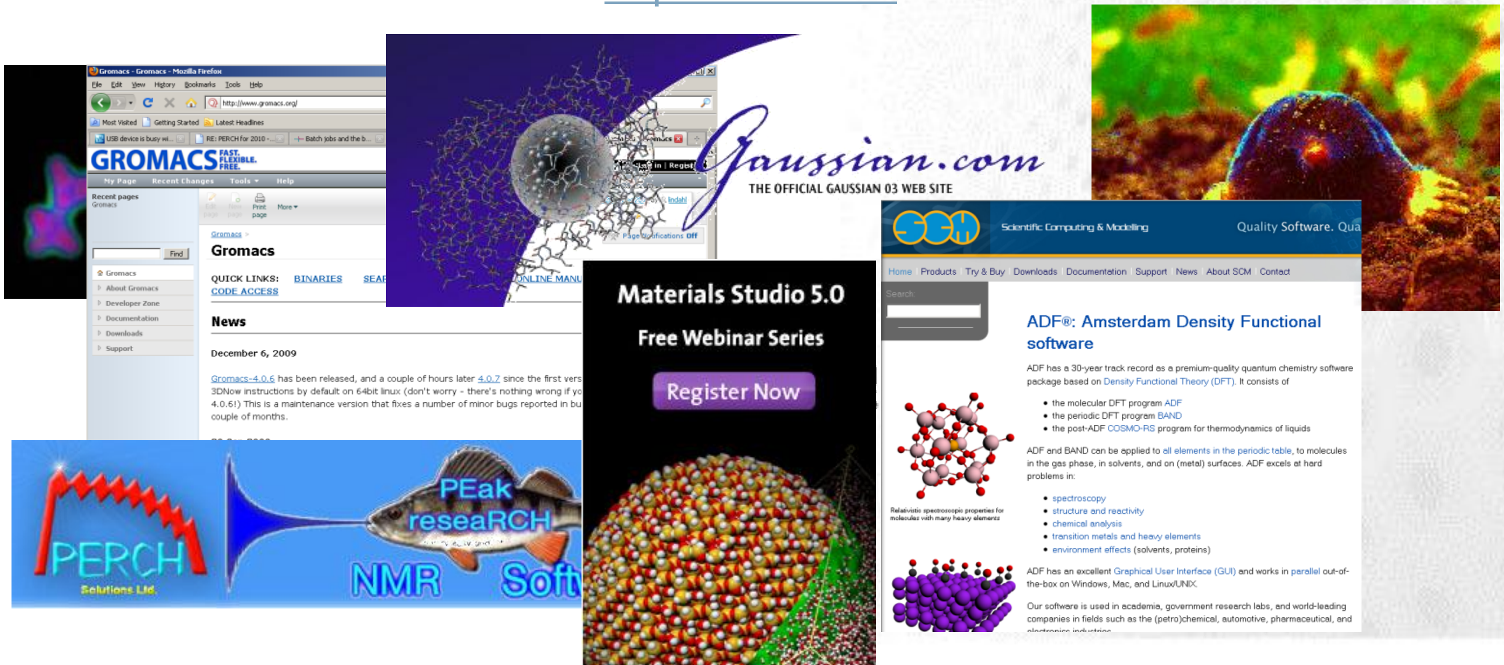
CRESTA
COLLABORATIVE RESEARCH INTO EXASCALE SYSTEMWARE, TOOLS & APPLICATIONS

Datacenter CSC Kajaani

- CSC’s modular Data Center in Kajaani. Modern and reliable infrastructure (national power grid, roads, airline connections, data networks)
- The Funet Network ensures excellent networking capabilities around the world
- Place for CSC’s next supercomputers with other CSC customer systems
- Cost-Efficient Solution – Sustainable and Green Energy Supply

Software offered by CSC

- Large selection (200+) of scientific software and databases https://research.csc.fi/software
- Selection based on researchers’ needs
- Majority available for no additional cost – others: consortia
- Benefits from centralization (license costs, maintenance, training, continuity – one access point)
- NoMachine remote desktop
- Scientist’s User Interface: https://sui.csc.fi



Gromacs

QUICK LINKS: BINARIES SEAR ONLINE MANU CODE ACCESS

News

December 6, 2009

Gromacs-4.0.6 has been released, and a couple of hours later 4.0.7 since the first vers 3DNow instructions by default on 64bit linux (don't worry - there's nothing wrong if yo 4.0.6!) This is a maintenance version that fixes a number of minor bugs reported in bu couple of months.

ADF®: Amsterdam Density Functional software

ADF has a 30-year track record as a premium-quality quantum chemistry software package based on Density Functional Theory (DFT). It consists of

- the molecular DFT program ADF
- the periodic DFT program BAND
- the post-ADF COSMO-RS program for thermodynamics of liquids

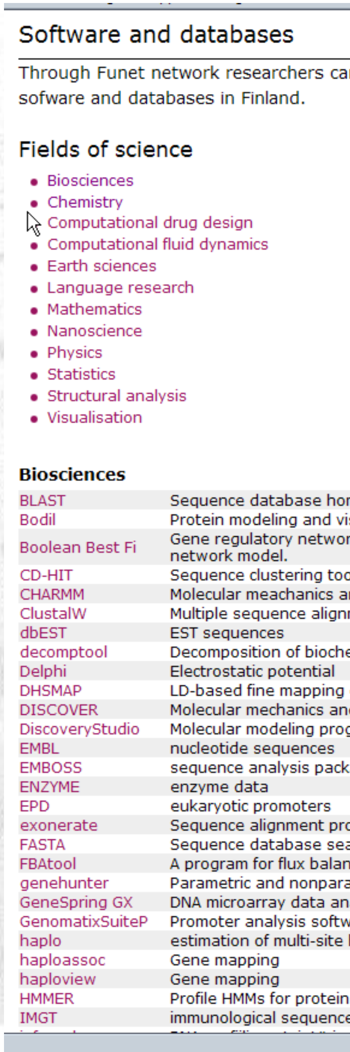
ADF and BAND can be applied to all elements in the periodic table, to molecules in the gas phase, in solvents, and on (metal) surfaces. ADF excels at hard problems in:

- spectroscopy
- structure and reactivity
- chemical analysis
- transition metals and heavy elements
- environment effects (solvents, proteins)

Relativistic spectroscopic properties for molecules with many heavy elements

ADF has an excellent Graphical User Interface (GUI) and works in parallel out-of-the-box on Windows, Mac, and Linux/UNIX.

Our software is used in academia, government research labs, and world-leading companies in fields such as the (petro)chemical, automotive, pharmaceutical, and electronics industries.



Software and databases

Through Funet network researchers ca
sofware and databases in Finland.

Fields of science

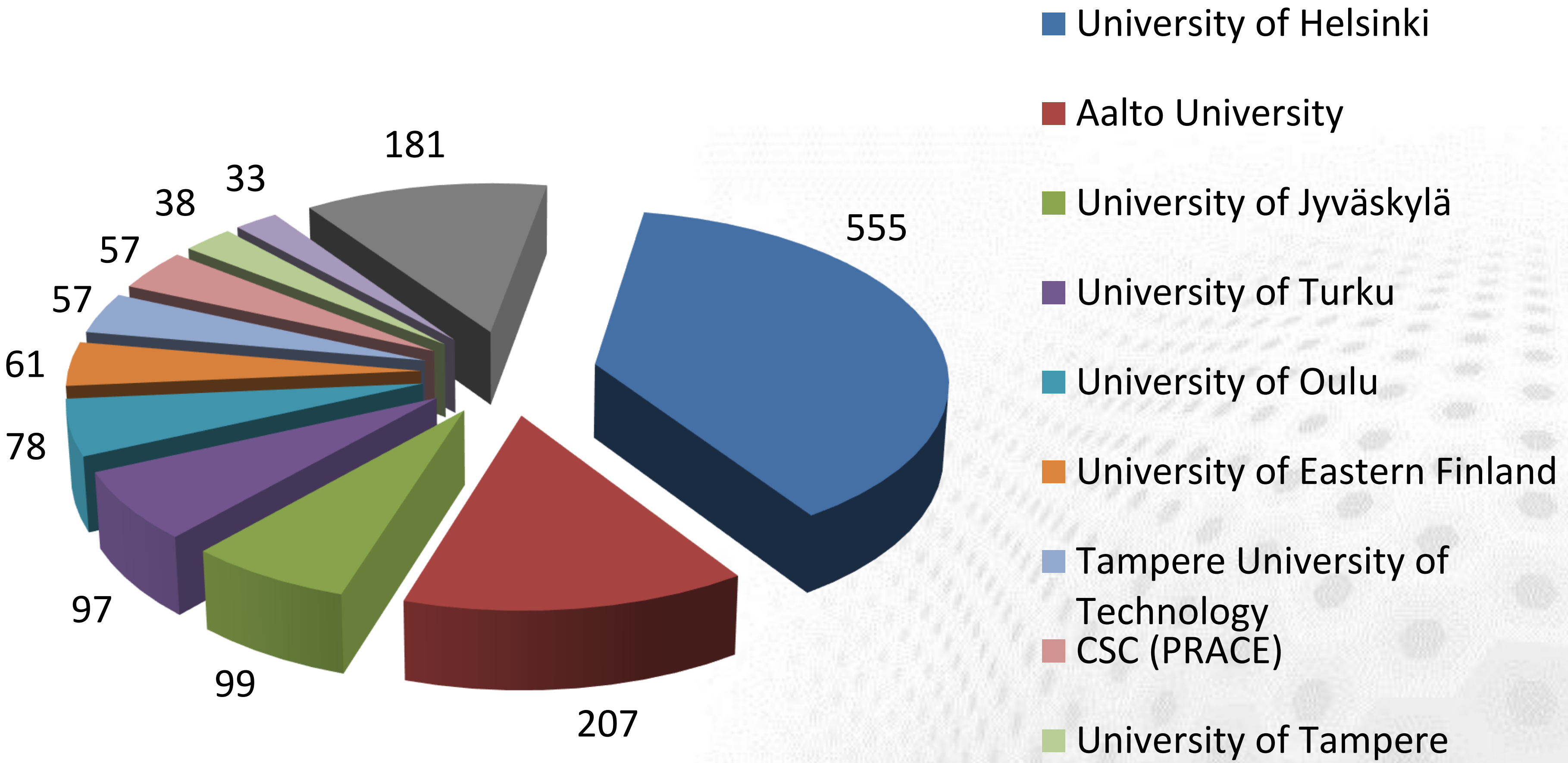
- Biosciences
- Chemistry
- Computational drug design
- Computational fluid dynamics
- Earth sciences
- Language research
- Mathematics
- Nanoscience
- Physics
- Statistics
- Structural analysis
- Visualisation

Biosciences

BLAST	Sequence database hor
Bodil	Protein modeling and vi
Boolean Best Fi	Gene regulatory networ network model.
CD-HIT	Sequence clustering too
CHARMM	Molecular meachanics ar
ClustalW	Multiple sequence alignr
dbEST	EST sequences
decomptool	Decomposition of bioche
Delphi	Electrostatic potential
DHSMAP	LD-based fine mapping
DISCOVER	Molecular mechanics an
DiscoveryStudio	Molecular modeling prog
EMBL	nucleotide sequences
EMBOSS	sequence analysis pack
ENZYME	enzyme data
EPD	eukaryotic promoters
exonerate	Sequence alignment pro
FASTA	Sequence database sea
FBAtool	A program for flux balan
genehunter	Parametric and nonpara
GeneSpring GX	DNA microarray data an
GenomatixSuiteP	Promoter analysis softw
haplo	estimation of multi-site
haploassoc	Gene mapping
haploview	Gene mapping
HMMER	Profile HMMs for protein
IMGT	immunological sequence

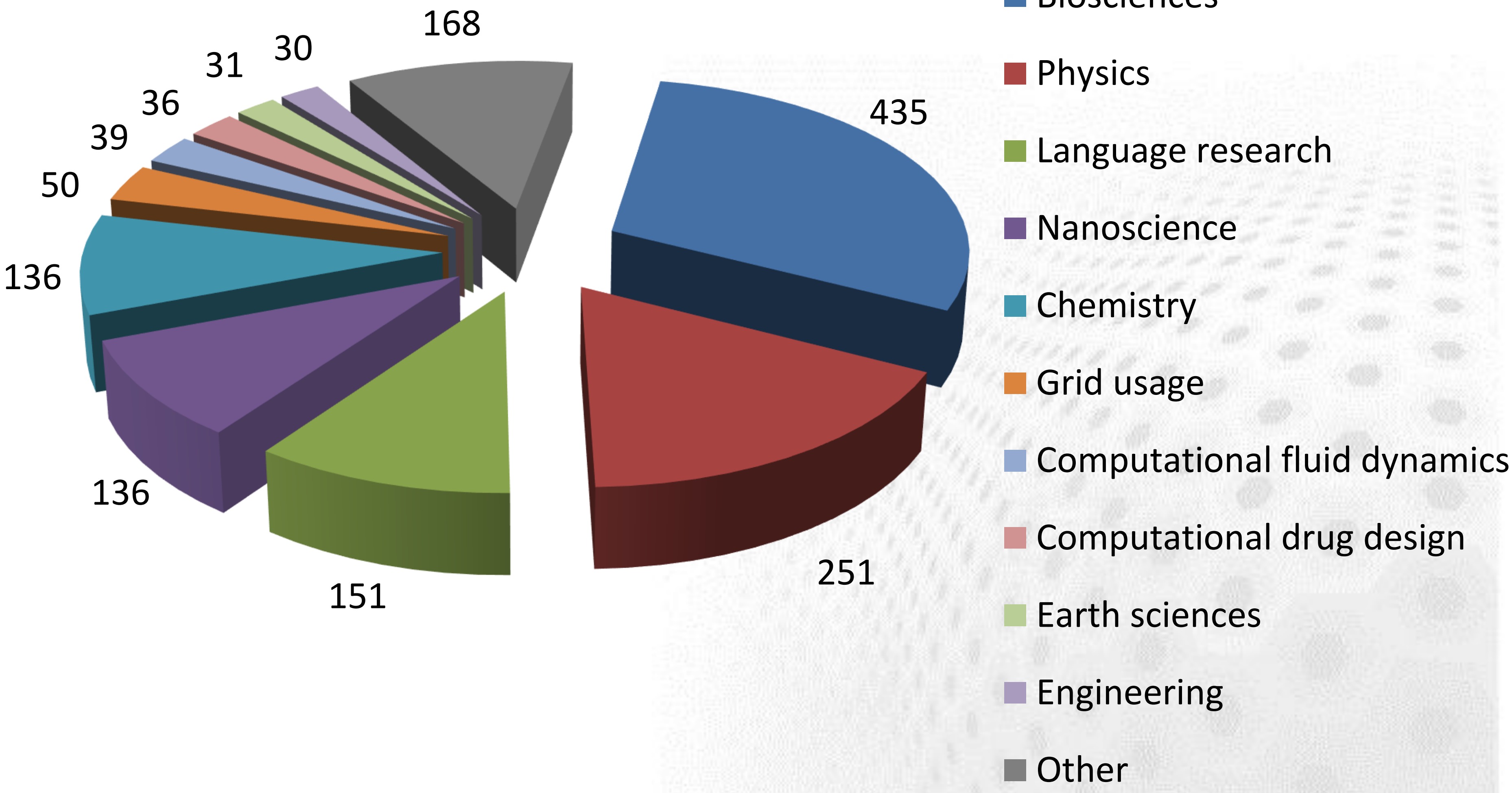
Users of computing servers by organization 2012

(total 1463 users)



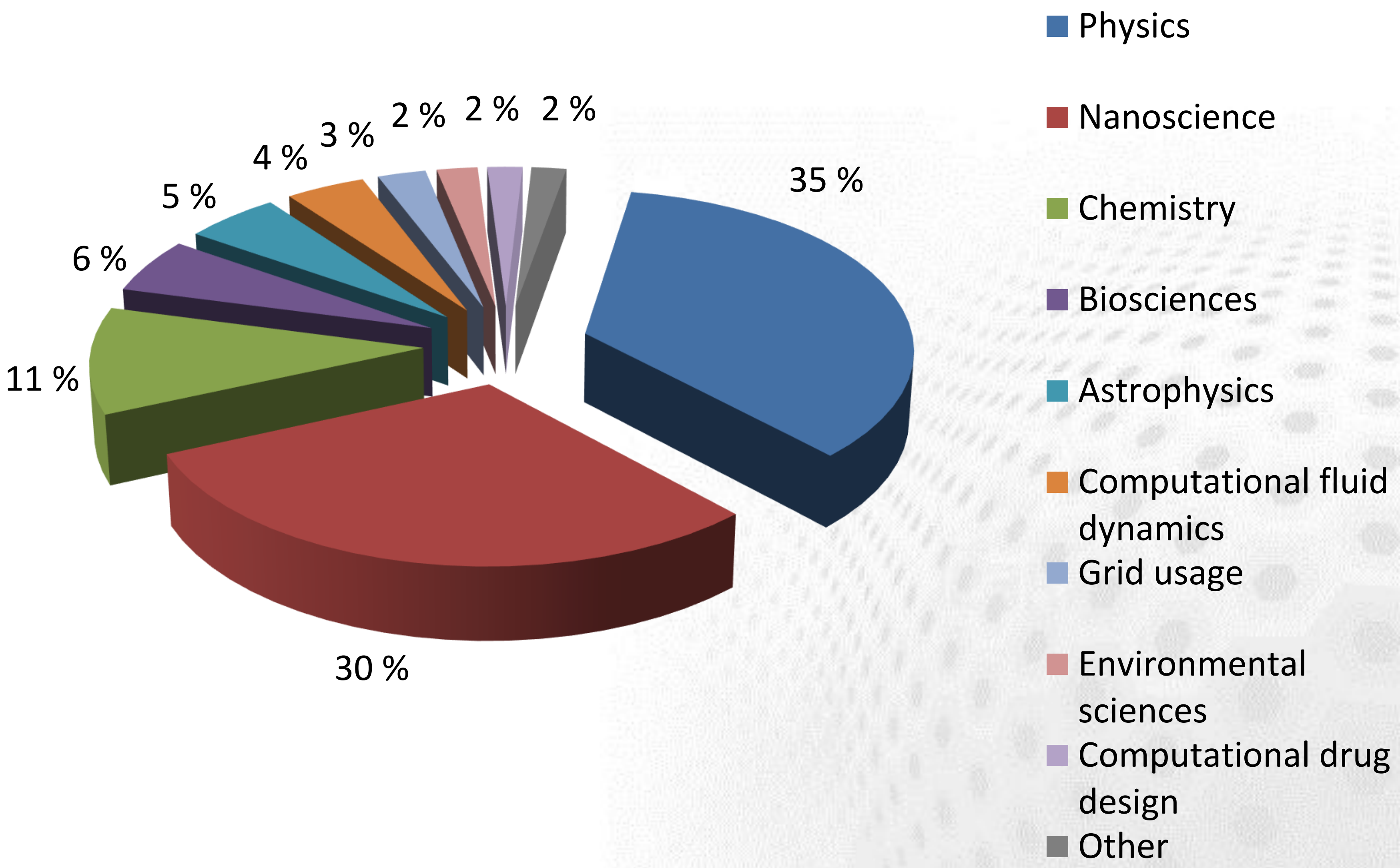
Users of computing resources by discipline 2012

(total 1463 users)



Usage of processor time by discipline 2012

(total 96.5 million core hours)

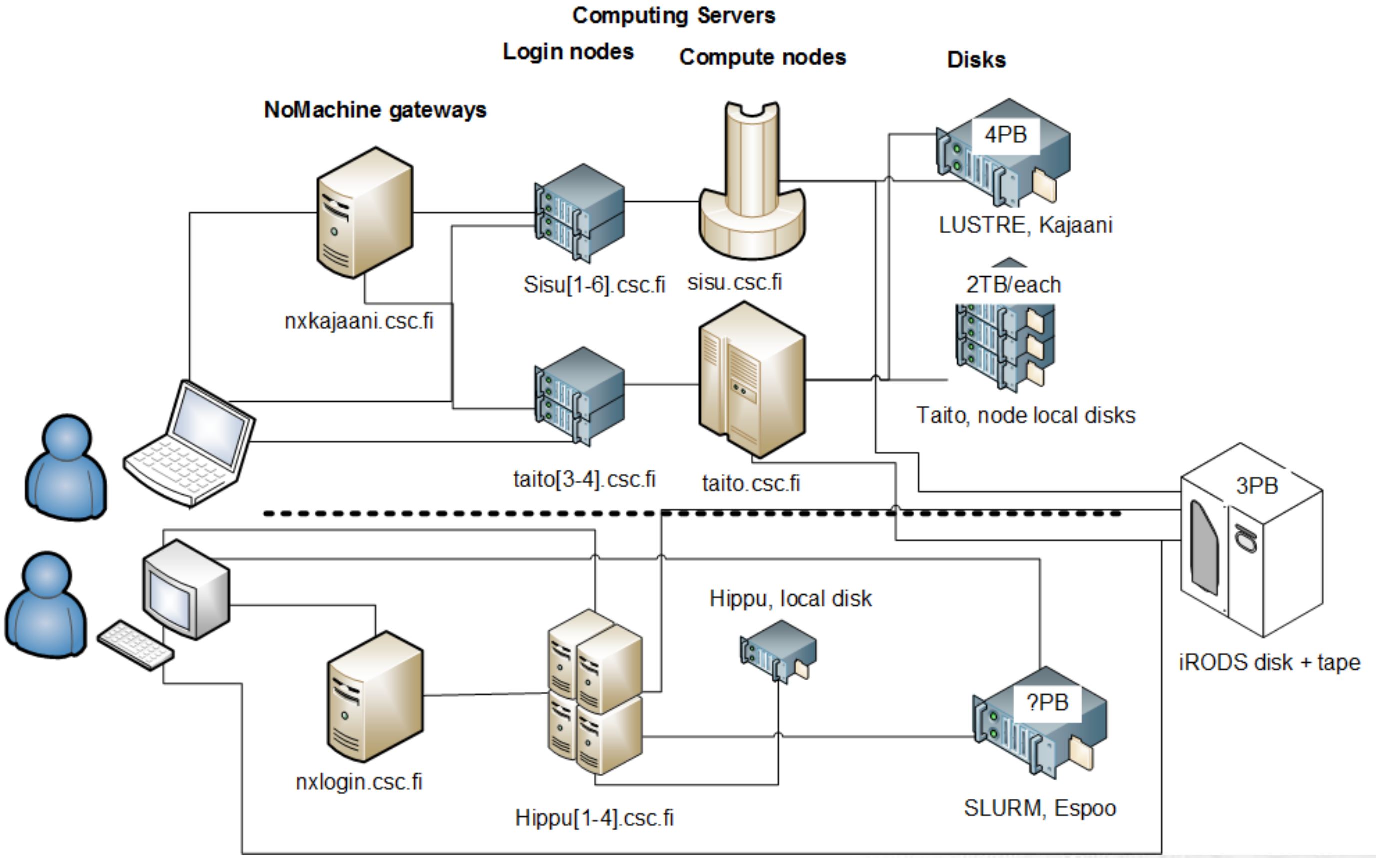


Connecting to CSC

Learning targets

- Be aware of different ways of accessing CSC resources

The (almost) Complete Picture



Access via any of:

- Ssh
- NoMachine
- Browser (SUI)
- Tunneling
- ARC (FGI)
- HAKA
- iRODS

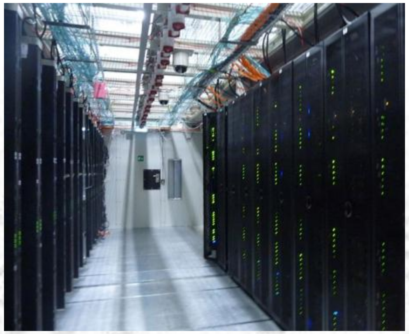
Computing servers

Sisu: Cray XC30

- 1688 x 24 Intel 2.6 GHz = 40512 cores
- 2.7 GB mem / core
- Aries interconnect
- Massively parallel jobs

Taito: HP ProLiant SL 230s

- 1152 x 16 Intel 2.6 GHz = 9216 cores
- 4/16/48 GB memory / core (64/256/1536 GB / node)
- FDR Infiniband
- Serial and parallel jobs
- Very large memory jobs



Hippu3,4: HP ProLiant DL580 G7 servers

- 2 x 32 Xeon X7560 2,26 GHz = 64 cores
- 1 TB memory/ node
- Interactive and very long jobs

To be decommissioned

Vuori: HP CP4000 BL Proliant supercluster

- 240 x 2 x 6 AMD 2.6 GHz = 2880 cores (+ 24 x 2 x 6 Intel X5650 2.6 GHz = 288 cores)
- 8 GPGPU nodes
- 96/32/16 GB memory / node

Decommissioned

+ FGI

Direct ssh connection – Unix/Linux

- From UNIX/Linux/OSX command line
- Use –X (or –Y) to enable remote graphics*

```
ssh –X yourid@taito.csc.fi
```

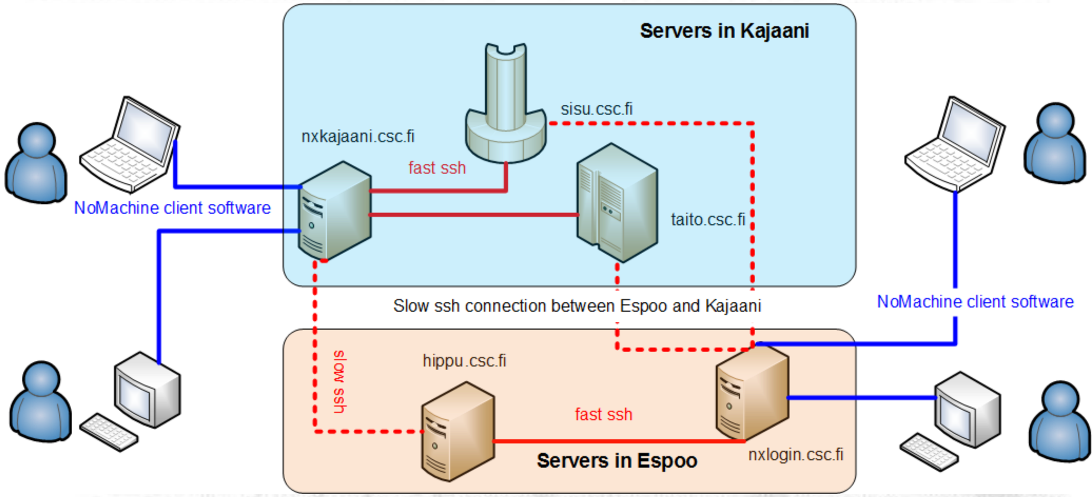
```
ssh -l yourid –X taito.csc.fi
```

```
login as: asillanp
Last login: Tue Sep 24 13:12:21 2013 from php.csc.fi
┌─ Welcome ───────────────────────────────────────────────────────────────────┐
│         CSC - Tieteen tietotekniikan keskus - IT Center for Science         │
│                  HP Cluster Platform SL230s Gen8 TAITO                      │
├─ Contact ───────────────────────────────────────────────────────────────────┤
...
```

* In Windows you'd also need a windows emulator, but there is a better way

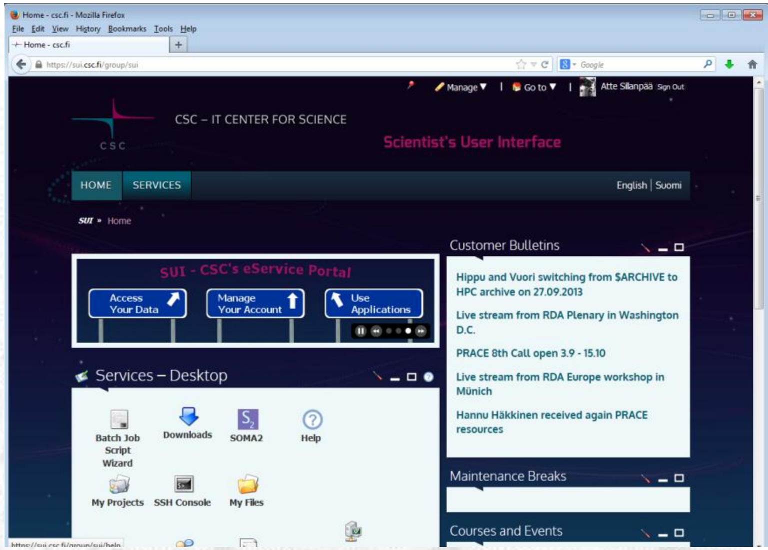
NoMachine Remote Desktop

- Client connection between user and gateway
- Good performance even with slow network
- Ssh from gateway to server (fast if local)
- Connect to right gateway
  - nxkajaani.csc.fi
  - nxlogin.csc.fi
- Persistent connection
- Suspendable
  - Continue later at another location
- Read the instructions…
  - ssh-key, keyboard layout, mac specific workarounds, …
- Choose an application or server to use (right click)



Scientist’s User Interface - SUI

- Access with browser
  - HAKA or CSC password
- File manager, Downloads, Batch job script wizard, Own projects and batch jobs, ssh-client, Host-monitor, My certificates, …
- Note: if you don’t have a CSC account you’ll only see a subset of services. To make services available with the HAKA authentication, login with the the CSC username at least once (and pair the accounts, will prompt for it).



Hippu and Vuori switching from $ARCHIVE to HPC archive on 27.09.2013

Live stream from RDA Plenary in Washington D.C.

PRACE 8th Call open 3.9 - 15.10

Live stream from RDA Europe workshop in Münich

Hannu Häkkinen received again PRACE resources

HAKA federation

- HAKA is the identity federation of the Finnish universities, polytechnics and research institutions.
- 280000 users
- HAKA authentication gives access with your university account and password to:
  - SUI
  - Eduroam
  - …

Access with scientific software

- Some software can be configured to use CSC servers directly, e.g.
  - TMolex, ADF, Maestro
- The GUIs can be used to create and submit jobs directly to the Taito queueing system

Finnish Grid Infrastructure - FGI

- Distributed computing capacity
- 9 universities + CSC
- Requires a certificate
- Lots of preinstalled software
- Access with ARC –client
- From your own computer or e.g. hippu

```
arcproxy
arcsub jobscript.xrsl
arcget gsiftp://usva.fgi.csc.fi:2811/jobs/12465133890987654
```

- FGI guide

Oulu
Kuopio
Joensuu
Jyväskylä
Tampere
Lappeenranta
Turku
Espoo
Åbo
Helsinki

Cloud services

- For biomedical research (Elixir BMI)
  - Extend your capacity with cloud resources
  - Aimed for IT administrators
  - More information:
    - BMI: virtualized hosting for biomedical research
- Pouta is the CSC main IaaS service
  - https://research.csc.fi/pouta-user-guide
  - high performance computing
  - Available for any CSC user
  - Limited assistance with configurating your VM

Summary: How to access resources at CSC

- Ssh terminal connection to CSC (+ X-term emulator for win)
- Installation at your own computer, license from CSC
  - Materials Studio, Discovery Studio, Ansys, …
- GUI at your own computer, computation at CSC (ssh pipe)
  - Tmolex, ADFgui, Discovery Studio
- GUI at your own computer, input files to CSC by hand, jobs launched from command prompt
- Scientist's User Interface (www based) sui.csc.fi
  - File manager, certificates, terminal, software distribution, …
- SOMA2: www based workflow manager, available in SUI
  - Docking, Gaussian, …
- ARC (Nordugrid) middleware to run jobs in FGI
- NoMachine Remote desktop (etätyöpöytä)
  - Client installed at your own computer, working with graphics at CSC
- Cloud services: Elixir BMI or pouta.csc.fi
  - Lots of freedom/flexibility and hence administration and configuration work

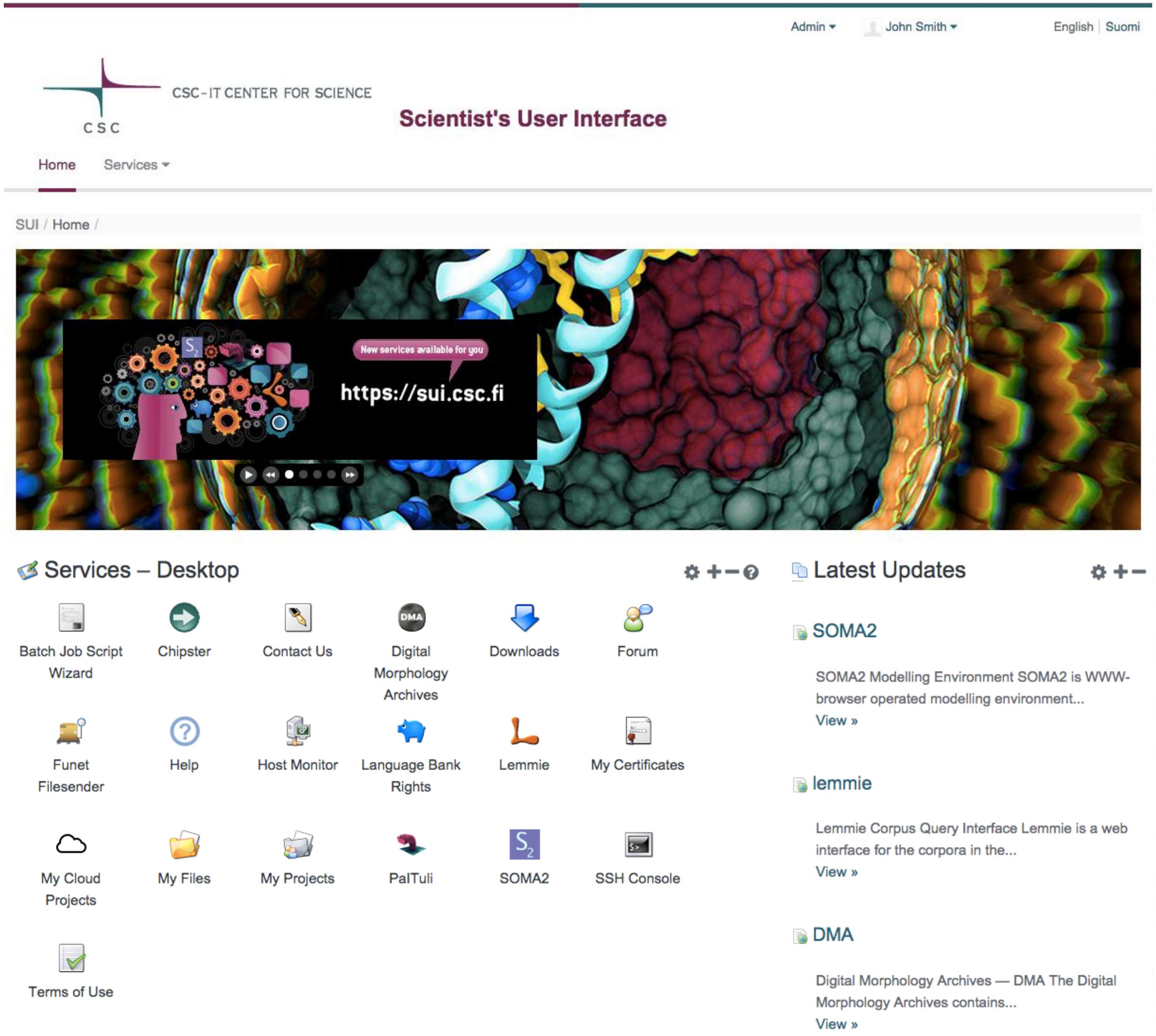
Installation session: installation/configuration of NX client

Scientist's User Interface (SUI)

Scientist's User Interface (SUI)

WWW-portal for all CSC users – https://sui.csc.fi

- Sign up as customer
- Manage your account
- Access your data
- Download material
- Watch videos
- Submit jobs
- Monitor hosts and jobs
- Use applications
- Personalize your use
- Participate
- + **more**



Admin ▾ John Smith ▾ English | Suomi

CSC - IT CENTER FOR SCIENCE

Scientist's User Interface

Home Services ▾

SUI / Home /

Services – Desktop

Batch Job Script Wizard
Chipster
Contact Us
Digital Morphology Archives
Downloads
Forum
Funet Filesender
Help
Host Monitor
Language Bank Rights
Lemmie
My Certificates
My Cloud Projects
My Files
My Projects
PalTuli
SOMA2
SSH Console
Terms of Use

Latest Updates

SOMA2

SOMA2 Modelling Environment SOMA2 is WWW-browser operated modelling environment...
View »

lemmie

Lemmie Corpus Query Interface Lemmie is a web interface for the corpora in the...
View »

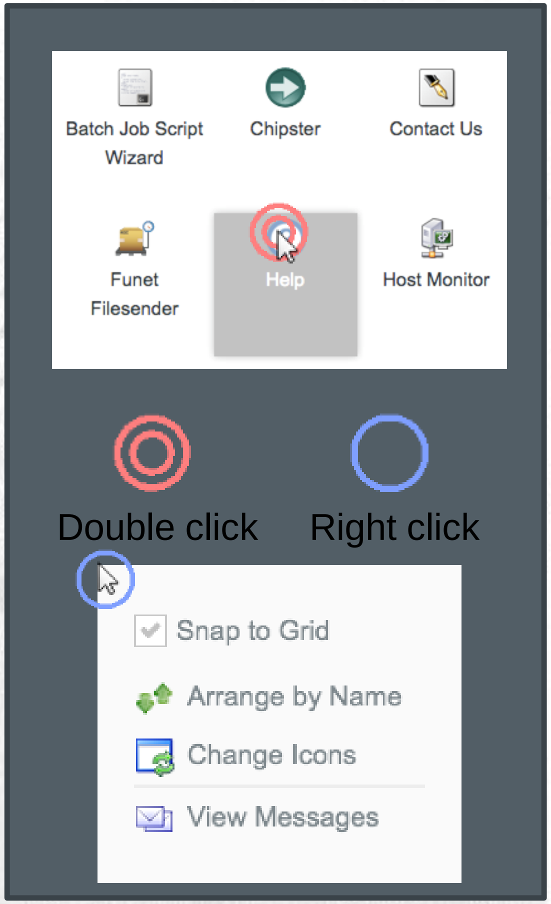
DMA

Digital Morphology Archives — DMA The Digital Morphology Archives contains...
View »

Scientist’s User Interface (SUI)

Easy to use services with rich user experience

- CSC’s services integrated under one access point
- Improved user experience – more than just a UNIX shell
- Look & feel like in desktop applications
  - Select, double click, context menus by right click, drag & drop, etc.
- Help is always near – click ? -icon
  - Help as a separate portal service
  - Help modes of individual applications



Scientist's User Interface (SUI)

Use case – run job via SUI-portal

Generate and store suitable job script with **Batch Job Script Wizard**

Open terminal connection to Taito with **SSH Console** and submit job

or

Submit job with **My Files**

Monitor your job on Taito with **Host Monitor**

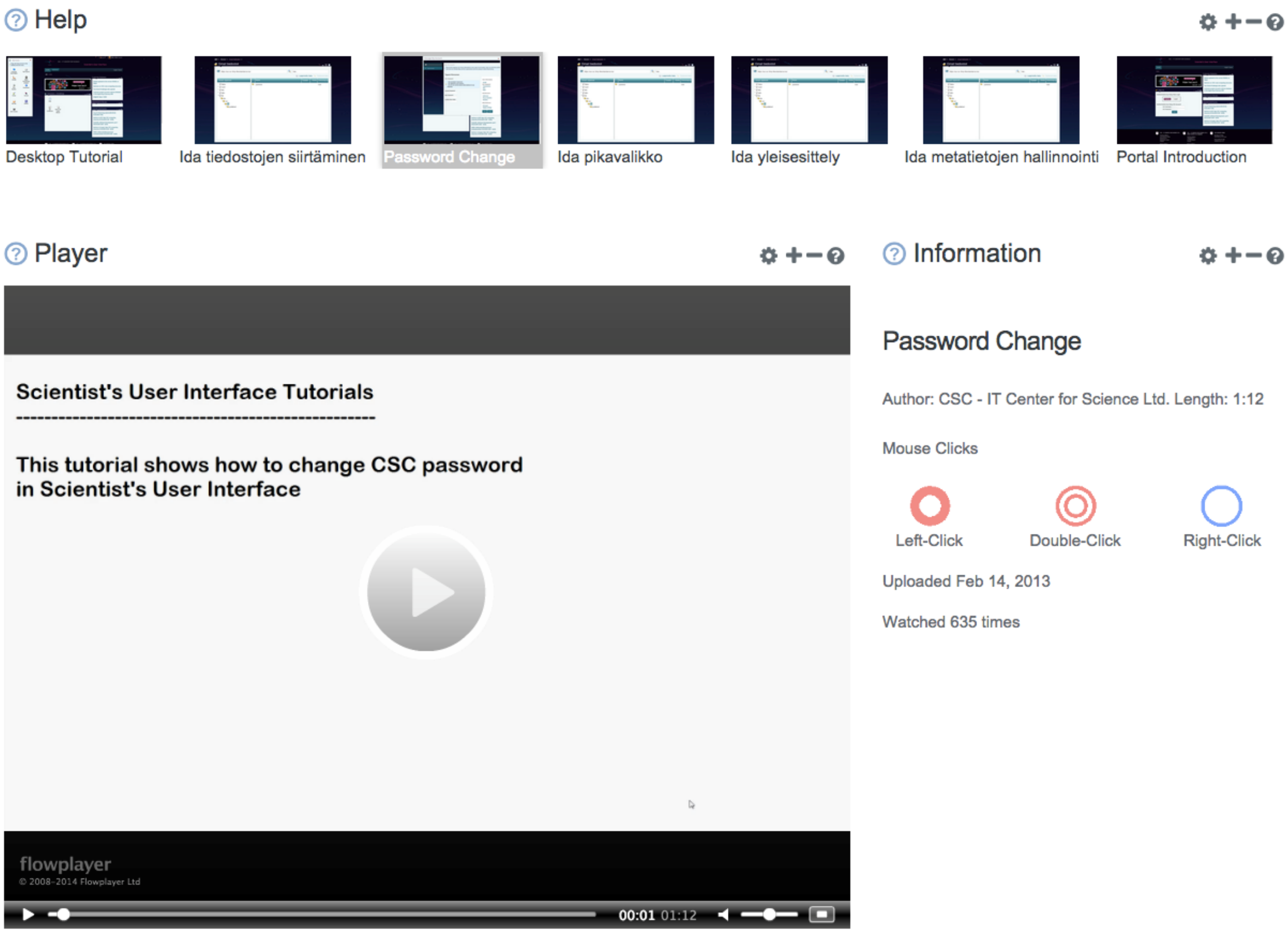
Examine and download results with **My Files**

Monitor your project's resource usage with **My Projects**

Scientist's User Interface (SUI)

Help

- **Watch** SUI portal's tutorial videos
- **Learn** how to use SUI's services



Scientist's User Interface Tutorials

This tutorial shows how to change CSC password in Scientist's User Interface

Password Change

Author: CSC - IT Center for Science Ltd. Length: 1:12

Mouse Clicks

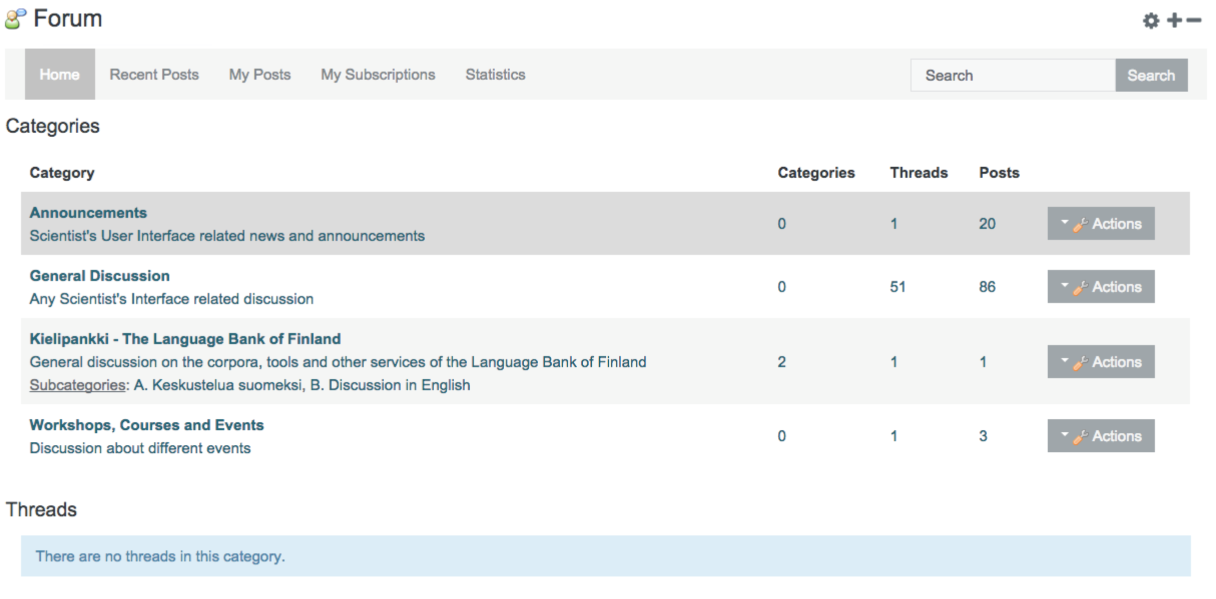
Uploaded Feb 14, 2013

Watched 635 times

Scientist's User Interface (SUI)

Forum

- **Participate** in discussion on forum
- Quick way to find information of SUI, ask questions or **give feedback** to developers
- **Share ideas** for new services



Categories

Category	Categories	Threads	Posts	
Announcements Scientist's User Interface related news and announcements	0	1	20	Actions
General Discussion Any Scientist's Interface related discussion	0	51	86	Actions
Kielipankki - The Language Bank of Finland General discussion on the corpora, tools and other services of the Language Bank of Finland Subcategories: A. Keskustelua suomeksi, B. Discussion in English	2	1	1	Actions
Workshops, Courses and Events Discussion about different events	0	1	3	Actions

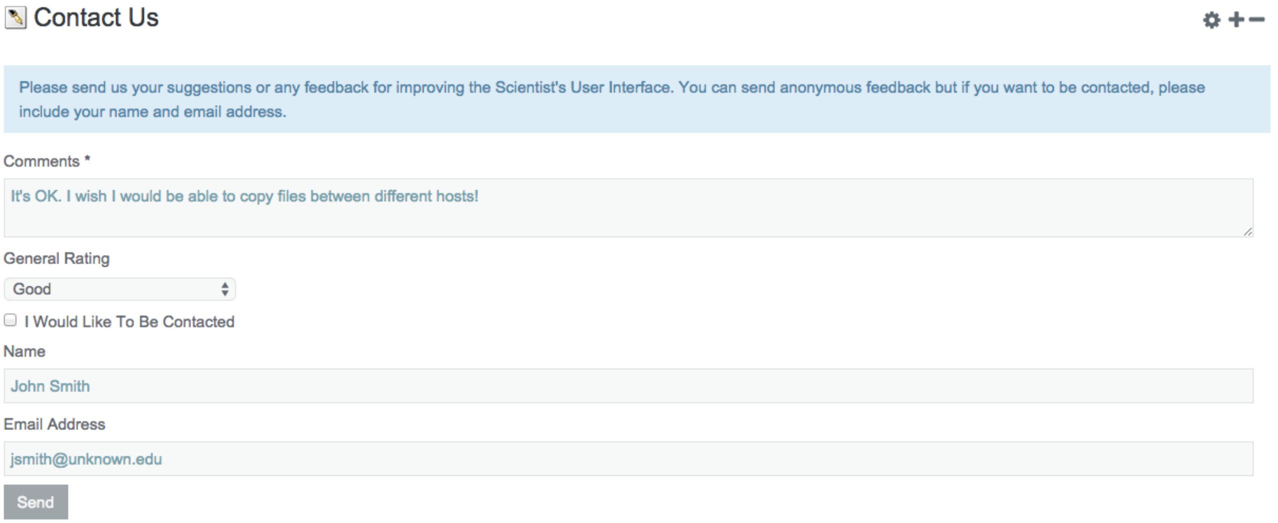
Threads

There are no threads in this category.

Scientist's User Interface (SUI)

Contact Us

- Another way to **contact** or **give feedback**
- Direct feedback can be sent privately and anonymously



Contact Us

Please send us your suggestions or any feedback for improving the Scientist's User Interface. You can send anonymous feedback but if you want to be contacted, please include your name and email address.

Comments *

It's OK. I wish I would be able to copy files between different hosts!

General Rating

Good

□ I Would Like To Be Contacted

Name

John Smith

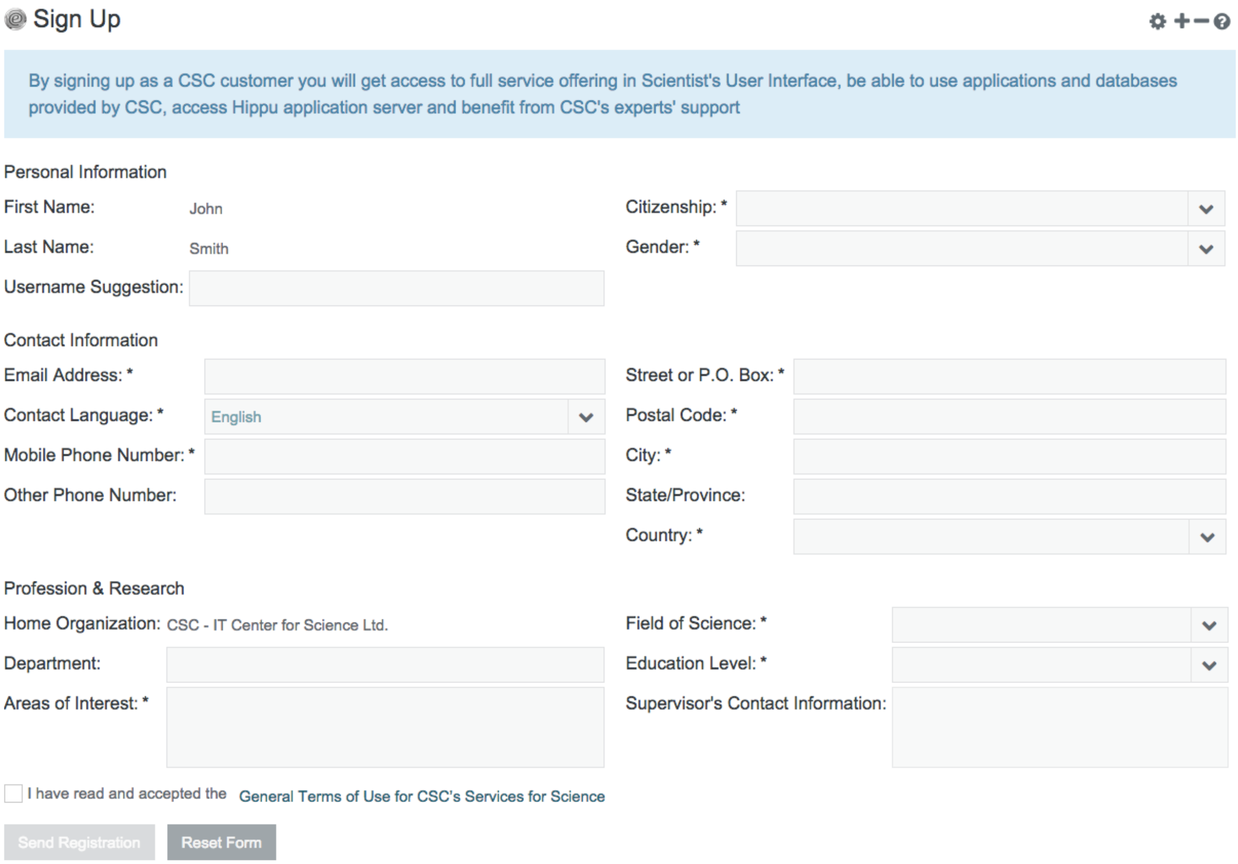
Email Address

jsmith@unknown.edu

Scientist’s User Interface (SUI)

Sign Up

- Quick and easy way to **Sign up** as CSC customer
- Available for all users by **Haka login**
- By signing up you can access all SUI’s services, applications and databases, Hippu application server + more



Sign Up

By signing up as a CSC customer you will get access to full service offering in Scientist's User Interface, be able to use applications and databases provided by CSC, access Hippu application server and benefit from CSC's experts' support

Personal Information

First Name: John
Last Name: Smith
Username Suggestion:
Citizenship: *
Gender: *

Contact Information

Email Address: *
Contact Language: * English
Mobile Phone Number: *
Other Phone Number:
Street or P.O. Box: *
Postal Code: *
City: *
State/Province:
Country: *

Profession & Research

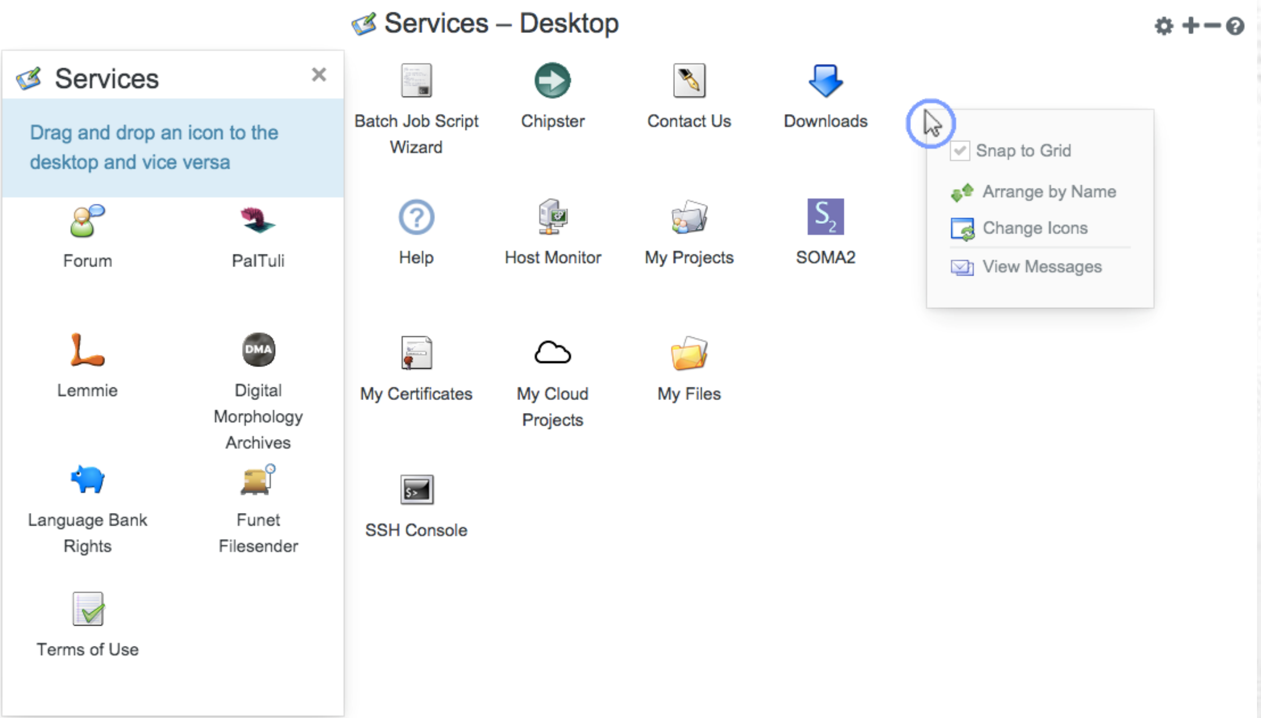
Home Organization: CSC - IT Center for Science Ltd.
Department:
Areas of Interest: *
Field of Science: *
Education Level: *
Supervisor's Contact Information:

□ I have read and accepted the General Terms of Use for CSC's Services for Science

Scientist’s User Interface (SUI)

Services - Desktop

- **Personalize** your desktop by selecting your favorite services
- Sort/arrange by using drag&drop
- See messages



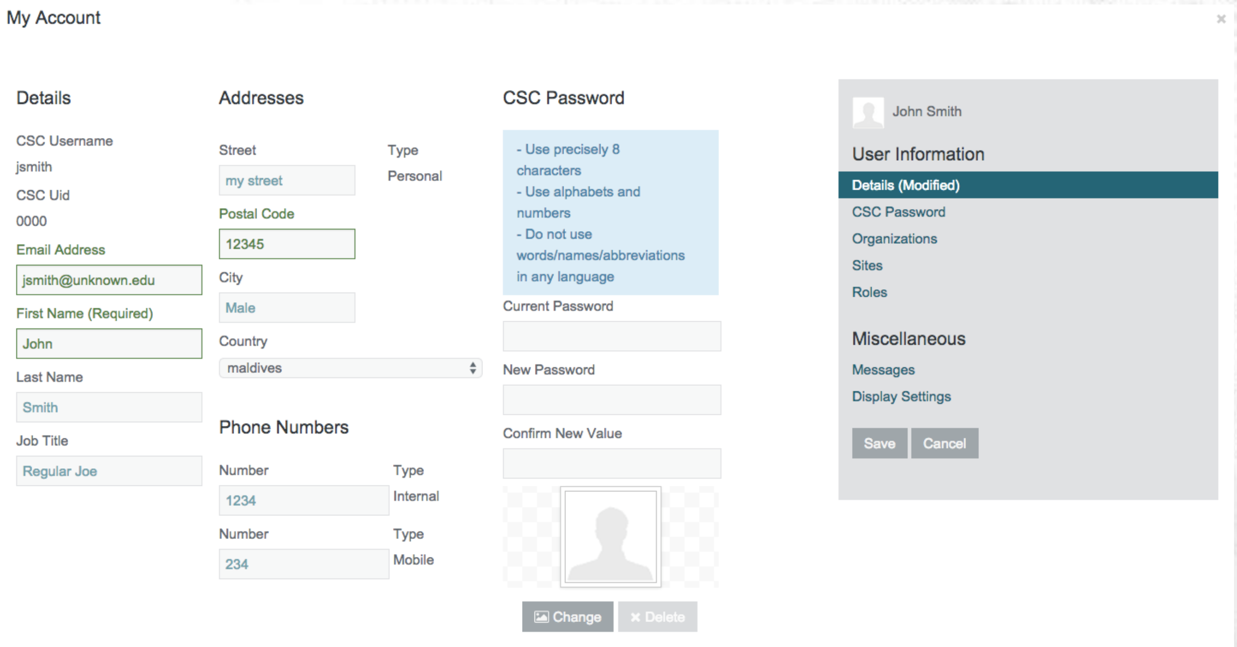
Services

Drag and drop an icon to the desktop and vice versa

Scientist’s User Interface (SUI)

My Account

- **Maintain** your account information
- **Change password** for CSC environment
- **Define** your personal settings



My Account

×

Details

CSC Username
jsmith

CSC Uid
0000

Email Address
jsmith@unknown.edu

First Name (Required)
John

Last Name
Smith

Job Title
Regular Joe

Addresses

Street	Type
my street	Personal

Postal Code
12345

City
Male

Country
maldives

Phone Numbers

Number	Type
1234	Internal

Number	Type
234	Mobile

CSC Password

- Use precisely 8 characters
- Use alphabets and numbers
- Do not use words/names/abbreviations in any language

Current Password

New Password

Confirm New Value

John Smith

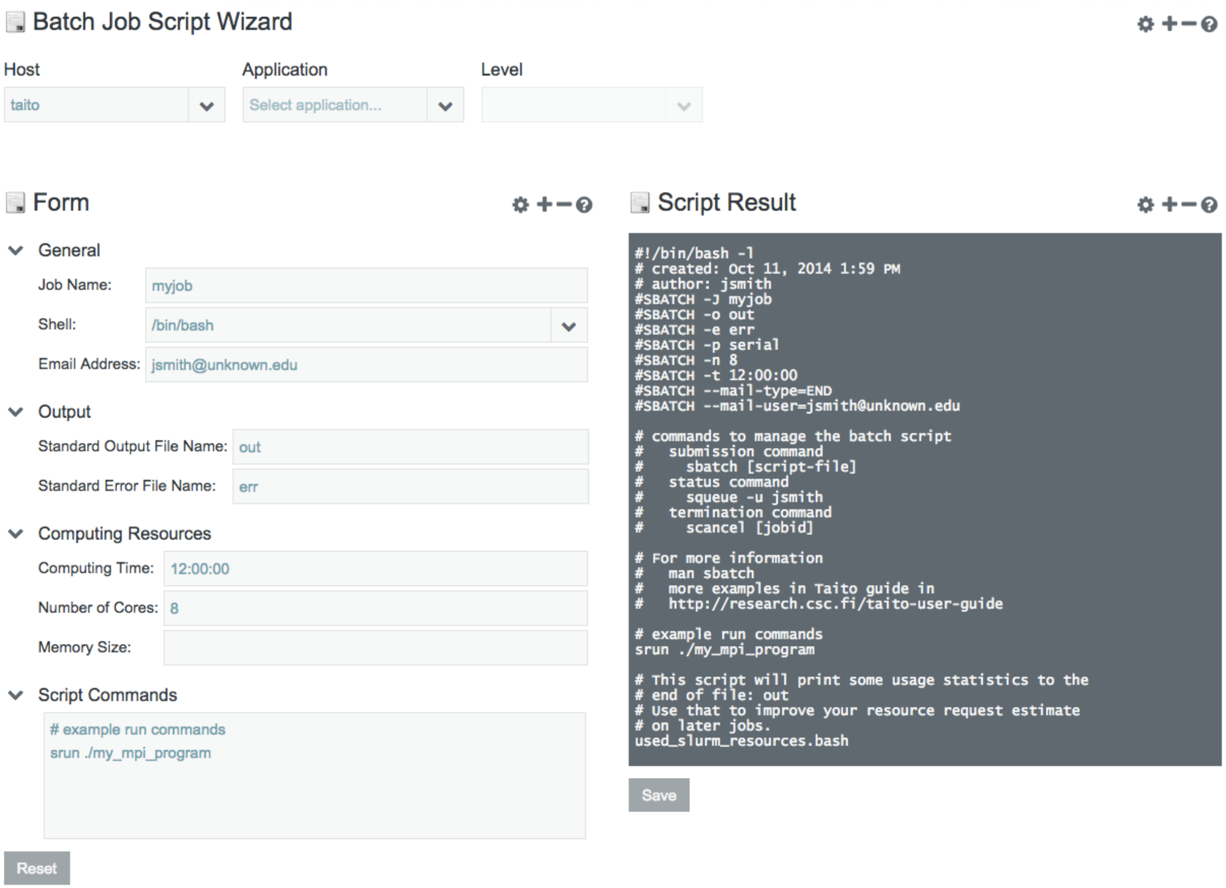
User Information

Miscellaneous

Scientist's User Interface (SUI)

Batch Job Script Wizard

- **Create job scripts** with easy to use forms
- **Save scripts** locally or in CSC $HOME
- Instructions of how to submit and monitor



Batch Job Script Wizard

Host: taito

Application: Select application...

Level:

Form

General

Job Name: myjob

Shell: /bin/bash

Email Address: jsmith@unknown.edu

Output

Standard Output File Name: out

Standard Error File Name: err

Computing Resources

Computing Time: 12:00:00

Number of Cores: 8

Memory Size:

Script Commands

```
# example run commands
srun ./my_mpi_program
```

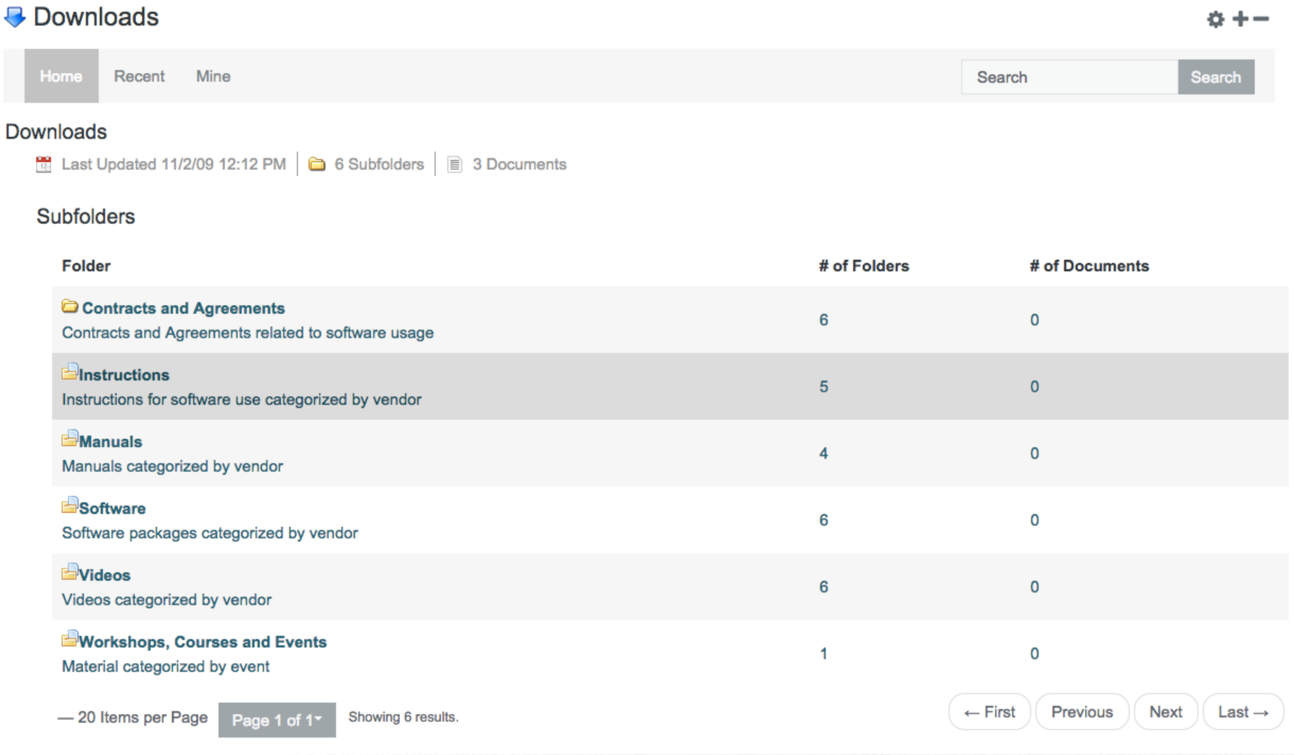
Script Result

```
#!/bin/bash -l
# created: Oct 11, 2014 1:59 PM
# author: jsmith
#SBATCH -J myjob
#SBATCH -o out
#SBATCH -e err
#SBATCH -p serial
#SBATCH -n 8
#SBATCH -t 12:00:00
#SBATCH --mail-type=END
#SBATCH --mail-user=jsmith@unknown.edu

# commands to manage the batch script
#   submission command
#     sbatch [script-file]
#   status command
#     squeue -u jsmith
#   termination command
#     scancel [jobid]

# For more information
#   man sbatch
#   more examples in Taito guide in
#   http://research.csc.fi/taito-user-guide

# example run commands
srun ./my_mpi_program

# This script will print some usage statistics to the
# end of file: out
# Use that to improve your resource request estimate
# on later jobs.
used_slurm_resources.bash
```

Scientist's User Interface (SUI)

Downloads

- **Access material** provided to you by CSC
- Software installation packages, manuals, videos etc.



Downloads

Last Updated 11/2/09 12:12 PM | 6 Subfolders | 3 Documents

Subfolders

Folder	# of Folders	# of Documents
Contracts and Agreements Contracts and Agreements related to software usage	6	0
Instructions Instructions for software use categorized by vendor	5	0
Manuals Manuals categorized by vendor	4	0
Software Software packages categorized by vendor	6	0
Videos Videos categorized by vendor	6	0
Workshops, Courses and Events Material categorized by event	1	0

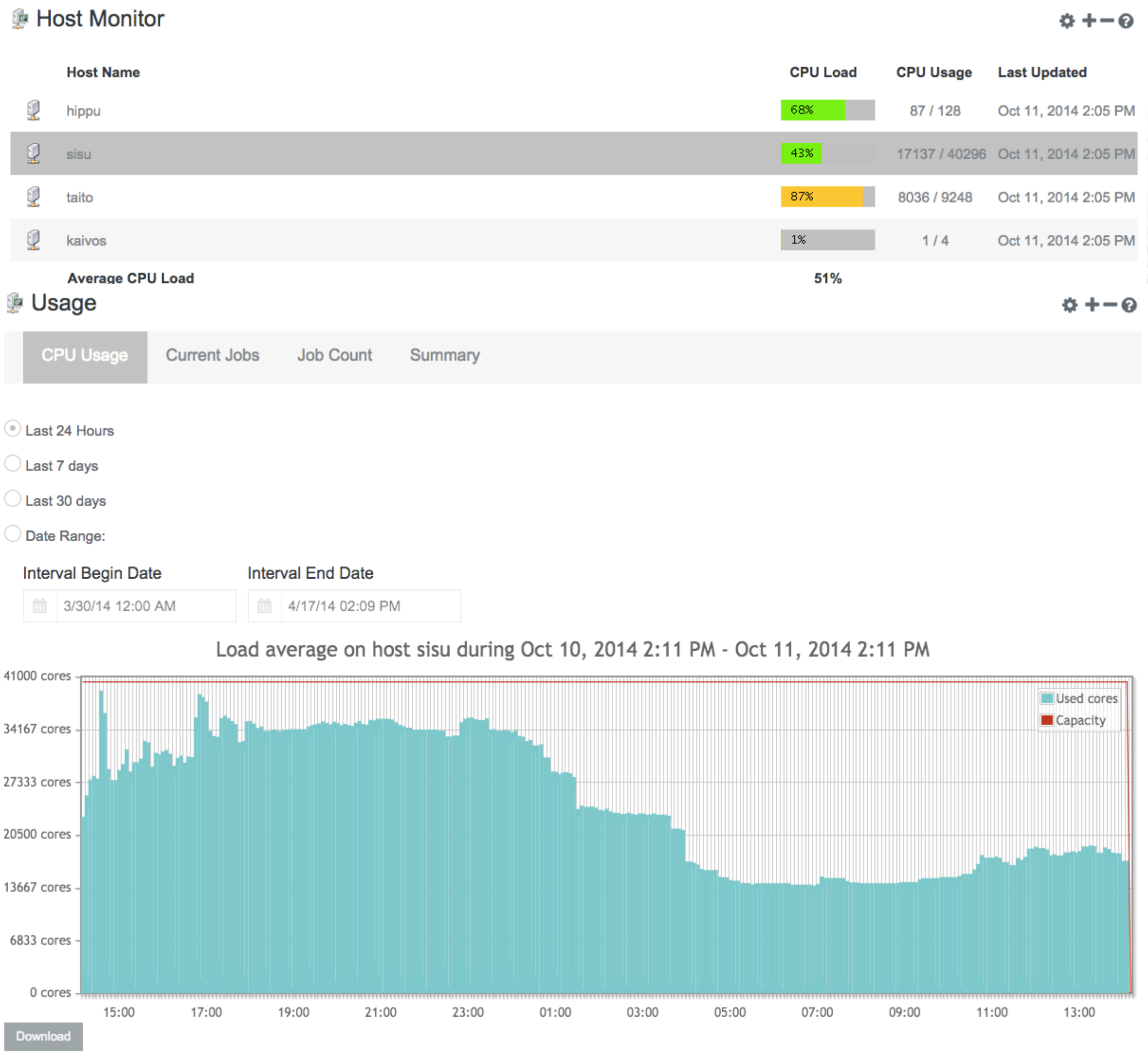
— 20 Items per Page | Page 1 of 1 | Showing 6 results.

Scientist's User Interface (SUI)

CSC

Host Monitor

- **View statuses and details** of CSC's computing servers and batch systems
- **Visualize history** of CPU usage and job count
- **Monitor jobs** in all hosts in single view
- **Control** your own jobs



Host Monitor

Host Name	CPU Load	CPU Usage	Last Updated
hippu	68%	87 / 128	Oct 11, 2014 2:05 PM
sisu	43%	17137 / 40296	Oct 11, 2014 2:05 PM
taito	87%	8036 / 9248	Oct 11, 2014 2:05 PM
kaivos	1%	1 / 4	Oct 11, 2014 2:05 PM
Average CPU Load	51%		

Usage

● Last 24 Hours

○ Last 7 days

○ Last 30 days

○ Date Range:

Interval Begin Date: 3/30/14 12:00 AM

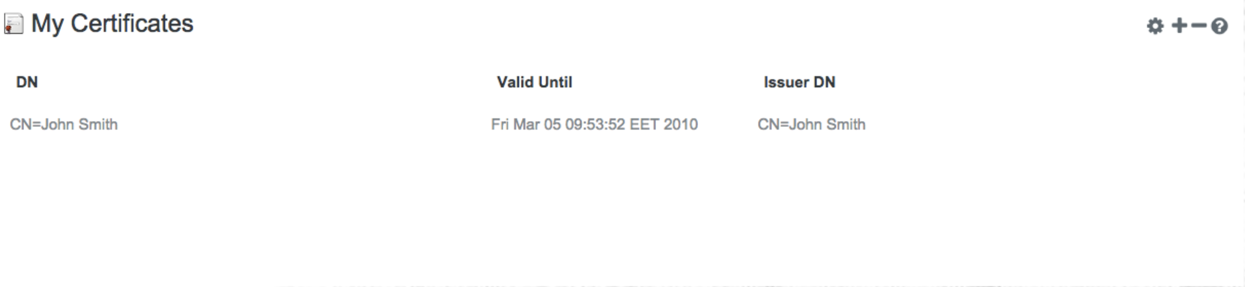
Interval End Date: 4/17/14 02:09 PM

Load average on host sisu during Oct 10, 2014 2:11 PM - Oct 11, 2014 2:11 PM

Scientist's User Interface (SUI)

My Certificates

- **Process** your X509 digital certificates
- Format conversions, export proxies, save locally or to your CSC $HOME
- **Setup grid usage** in CSC's computers



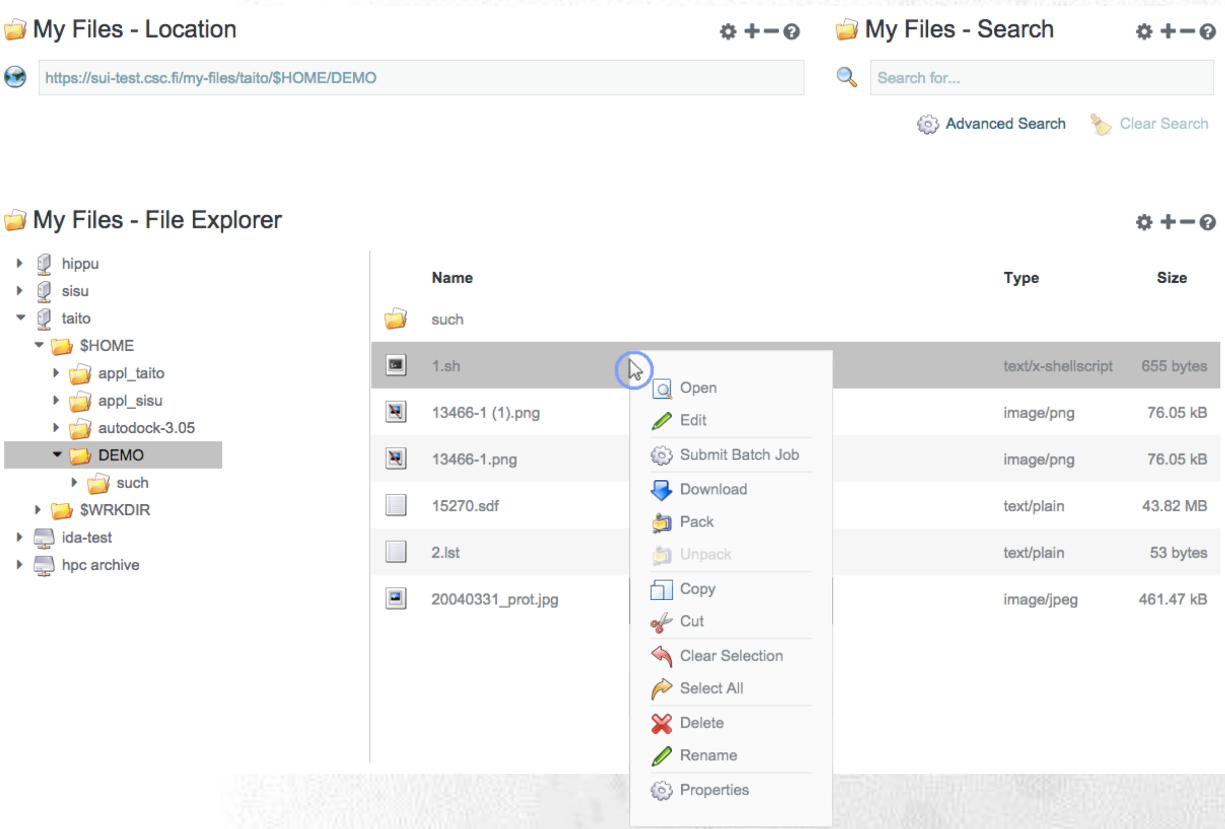
My Certificates

DN	Valid Until	Issuer DN
CN=John Smith	Fri Mar 05 09:53:52 EET 2010	CN=John Smith

Scientist's User Interface (SUI)

My Files

- **Access your data** in CSC's storage services in single view (computing servers, Ida and HPC Archive)
- Transfer files
- **Search** your data
- **Submit** jobs
- Typical folder and file operations are supported



My Files - Location

https://sui-test.csc.fi/my-files/taito/$HOME/DEMO

My Files - Search

Search for...

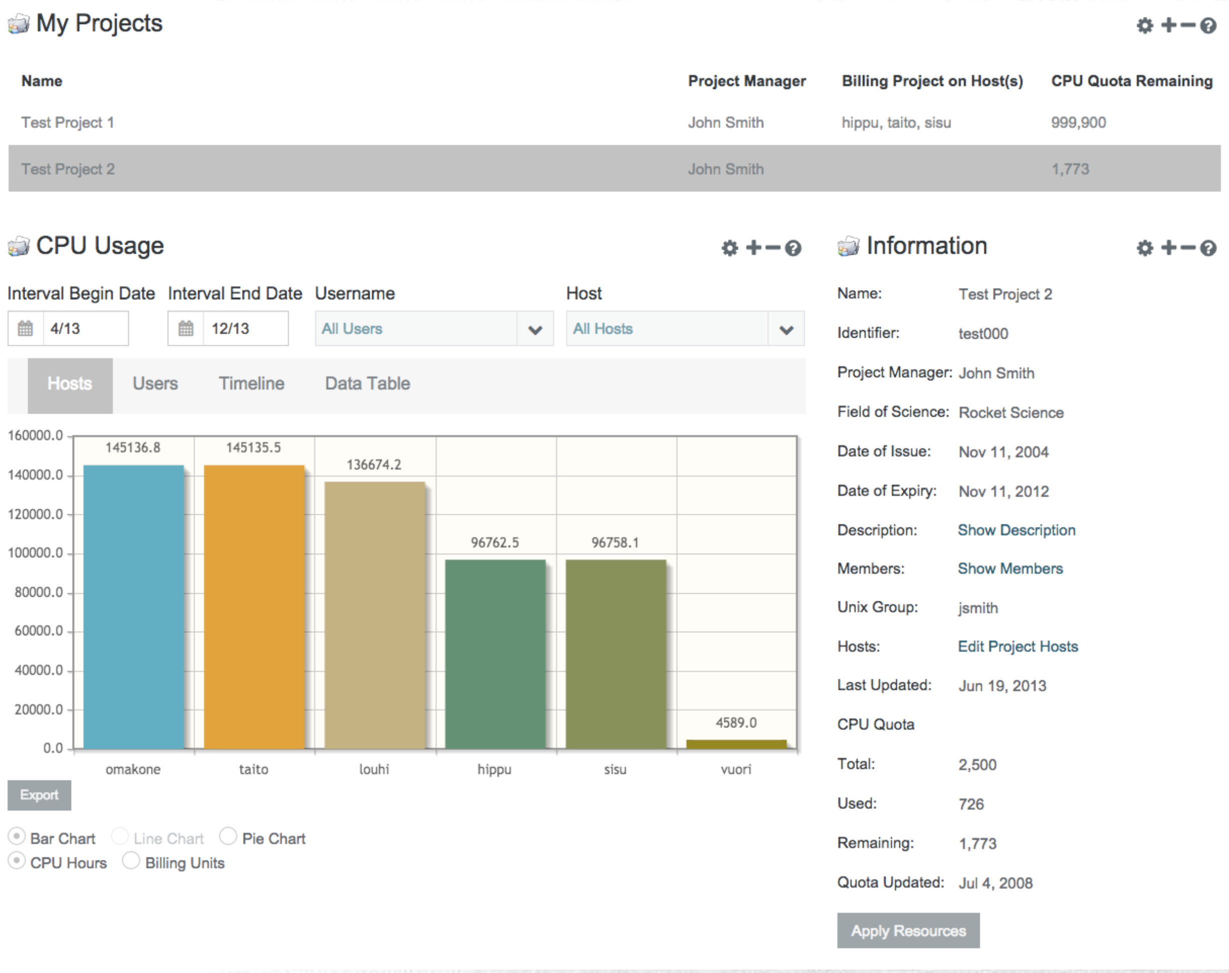
My Files - File Explorer

Name	Type	Size
such		
1.sh	text/x-shellscript	655 bytes
13466-1 (1).png	image/png	76.05 kB
13466-1.png	image/png	76.05 kB
15270.sdf	text/plain	43.82 MB
2.lst	text/plain	53 bytes
20040331_prot.jpg	image/jpeg	461.47 kB

Scientist's User Interface (SUI)

My Projects

- **View information and resource usage** of your CSC projects
- **Edit hosts** for projects
- **Apply resources** for your CSC customer project
- Resource usage presented by different kind of exportable graphs and data table



My Projects

Name	Project Manager	Billing Project on Host(s)	CPU Quota Remaining
Test Project 1	John Smith	hippu, taito, sisu	999,900
Test Project 2	John Smith		1,773

CPU Usage

Interval Begin Date: 4/13
Interval End Date: 12/13
Username: All Users
Host: All Hosts

● Bar Chart ○ Line Chart ○ Pie Chart
● CPU Hours ○ Billing Units

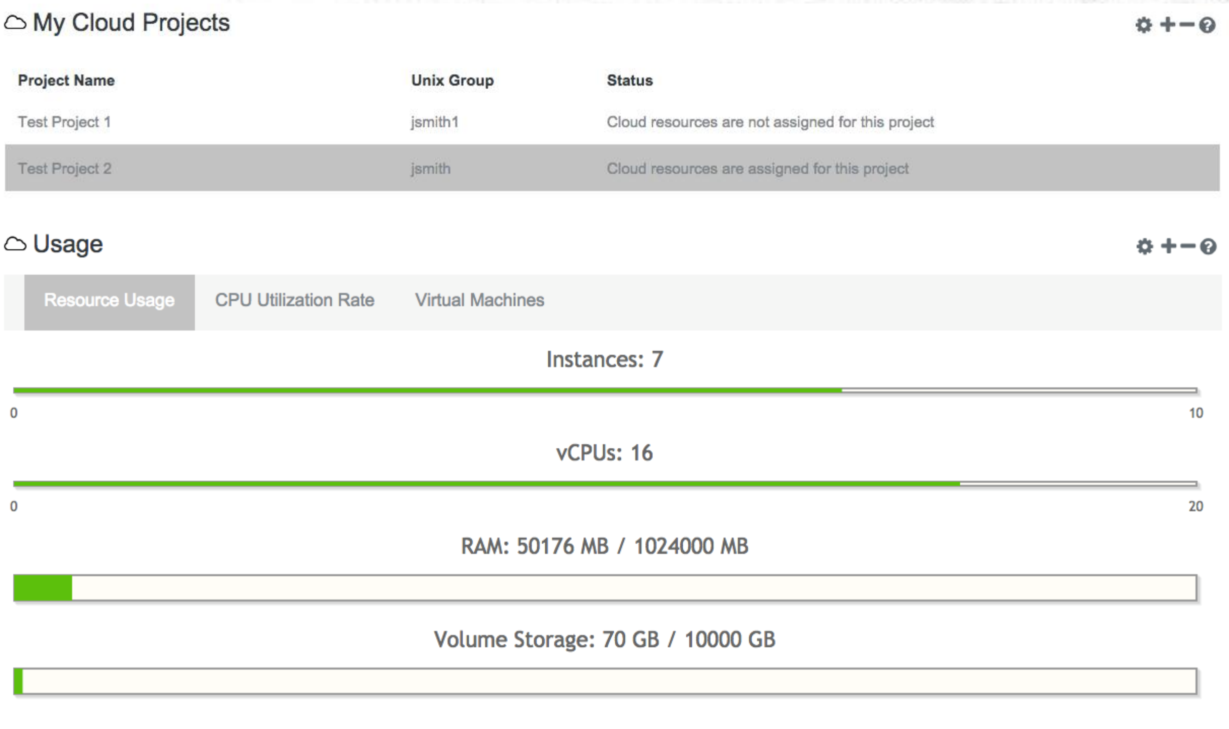
Information

Name:	Test Project 2
Identifier:	test000
Project Manager:	John Smith
Field of Science:	Rocket Science
Date of Issue:	Nov 11, 2004
Date of Expiry:	Nov 11, 2012
Description:	Show Description
Members:	Show Members
Unix Group:	jsmith
Hosts:	Edit Project Hosts
Last Updated:	Jun 19, 2013
CPU Quota	
Total:	2,500
Used:	726
Remaining:	1,773
Quota Updated:	Jul 4, 2008

Scientist’s User Interface (SUI)

My Cloud Projects

- **Apply cloud resources** for your CSC projects
- **View** information of cloud resource usage
- Resource usage presented by different kind of exportable graphs and data table



My Cloud Projects

Project Name	Unix Group	Status
Test Project 1	jsmith1	Cloud resources are not assigned for this project
Test Project 2	jsmith	Cloud resources are assigned for this project

Usage

Instances: 7

vCPUs: 16

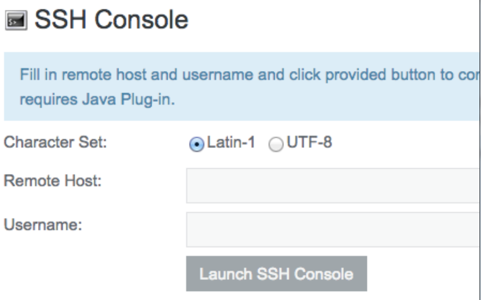
RAM: 50176 MB / 1024000 MB

Volume Storage: 70 GB / 10000 GB

Scientist’s User Interface (SUI)

SSH Console

- **Connect** to CSC’s computing servers
- UTF-8 character translation support

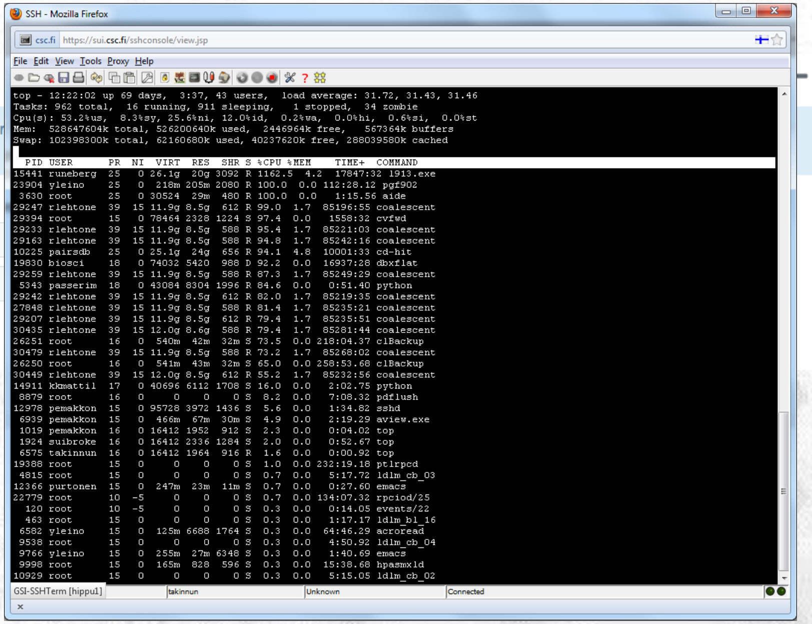


Fill in remote host and username and click provided button to co
requires Java Plug-in.

Character Set: ● Latin-1 ○ UTF-8

Remote Host:

Username:



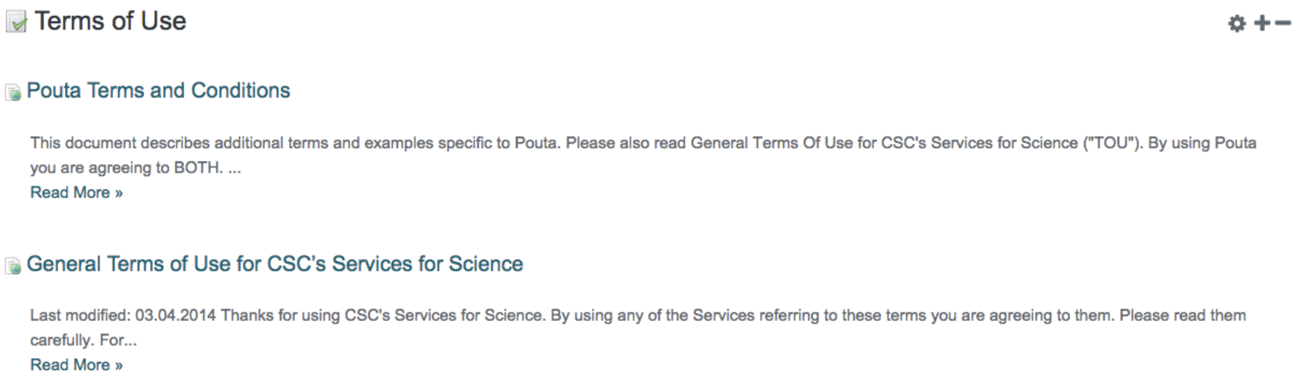
SSH - Mozilla Firefox
csc.fi https://sui.csc.fi/sshconsole/view.jsp
File Edit View Tools Proxy Help

```
top - 12:22:02 up 69 days,  3:37, 43 users,  load average: 31.72, 31.43, 31.46
Tasks: 962 total,  16 running, 911 sleeping,   1 stopped,  34 zombie
Cpu(s): 53.2%us,  8.3%sy, 25.6%ni, 12.0%id,  0.2%wa,  0.0%hi,  0.6%si,  0.0%st
Mem:  528647604k total, 526200640k used,  2446964k free,   567364k buffers
Swap: 102398300k total, 62160680k used, 40237620k free, 288039580k cached

  PID USER      PR  NI  VIRT  RES  SHR S %CPU %MEM    TIME+  COMMAND
15441 runeberg  25   0 26.1g  20g 3092 R 1162.5  4.2  17847:32 1913.exe
23904 yleino    25   0  218m 205m 2080 R 100.0  0.0 112:28.12 pgf902
 3630 root      25   0 30524  29m  480 R 100.0  0.0   1:15.56 aide
29247 rlehtone  39  15 11.9g 8.5g  612 R 99.0  1.7  85196:55 coalescent
29394 root      15   0 78464 2328 1224 S 97.4  0.0   1558:32 cvfwd
29233 rlehtone  39  15 11.9g 8.5g  588 R 95.4  1.7  85221:03 coalescent
29163 rlehtone  39  15 11.9g 8.5g  588 R 94.8  1.7  85242:16 coalescent
10225 pairsdb   25   0 25.1g  24g  656 R 94.1  4.8  10001:33 cd-hit
19830 biosci    18   0 74032 5420  988 D 92.2  0.0  16937:28 dbxflat
29259 rlehtone  39  15 11.9g 8.5g  588 R 87.3  1.7  85249:29 coalescent
 5343 passerim  18   0 43084 8304 1996 R 84.6  0.0   0:51.40 python
29242 rlehtone  39  15 11.9g 8.5g  612 R 82.0  1.7  85219:35 coalescent
27848 rlehtone  39  15 11.9g 8.5g  588 R 81.4  1.7  85235:21 coalescent
29207 rlehtone  39  15 11.9g 8.5g  612 R 79.4  1.7  85235:51 coalescent
30435 rlehtone  39  15 12.0g 8.6g  588 R 79.4  1.7  85281:44 coalescent
26251 root      16   0  540m  42m  32m S 73.5  0.0 218:04.37 clBackup
30479 rlehtone  39  15 11.9g 8.5g  588 R 73.2  1.7  85268:02 coalescent
26250 root      16   0  541m  43m  32m S 65.0  0.0 258:53.68 clBackup
30449 rlehtone  39  15 12.0g 8.5g  612 R 55.2  1.7  85232:56 coalescent
14911 kkmattil  17   0 40696 6112 1708 S 16.0  0.0   2:02.75 python
 8879 root      16   0     0    0    0 S  8.2  0.0   7:08.32 pdflush
12978 pemakkon  15   0 95728 3972 1436 S  5.6  0.0   1:34.82 sshd
 6939 pemakkon  15   0  466m  67m  30m S  4.9  0.0   2:19.29 aview.exe
 1019 pemakkon  16   0 16412 1952  912 S  2.3  0.0   0:04.02 top
 1924 suibroke  16   0 16412 2336 1284 S  2.0  0.0   0:52.67 top
 6575 takinnun  16   0 16412 1964  916 R  1.6  0.0   0:00.92 top
19388 root      15   0     0    0    0 S  1.0  0.0 232:19.18 ptlrpcd
 4815 root      15   0     0    0    0 S  0.7  0.0   5:17.72 ldlm_cb_03
12366 purtonen  15   0  247m  23m  11m S  0.7  0.0   0:27.60 emacs
22779 root      10  -5     0    0    0 S  0.7  0.0 134:07.32 rpciod/25
  120 root      10  -5     0    0    0 S  0.3  0.0   0:14.05 events/22
  463 root      15   0     0    0    0 S  0.3  0.0   1:17.17 ldlm_bl_16
 6582 yleino    15   0  125m 6688 1764 S  0.3  0.0  64:46.29 acroread
 9538 root      15   0     0    0    0 S  0.3  0.0   4:50.92 ldlm_cb_04
 9766 yleino    15   0  255m  27m 6348 S  0.3  0.0   1:40.69 emacs
 9998 root      15   0  165m  828  596 S  0.3  0.0  15:38.68 hpasmxld
10929 root      15   0     0    0    0 S  0.3  0.0   5:15.05 ldlm_cb_02
```

Scientist’s User Interface (SUI)

Terms of Use

- **Read** CSC’s services’ terms of use



Terms of Use

Pouta Terms and Conditions

This document describes additional terms and examples specific to Pouta. Please also read General Terms Of Use for CSC's Services for Science ("TOU"). By using Pouta you are agreeing to BOTH. ...

Read More »

General Terms of Use for CSC’s Services for Science

Last modified: 03.04.2014 Thanks for using CSC's Services for Science. By using any of the Services referring to these terms you are agreeing to them. Please read them carefully. For...

Read More »

Scientist’s User Interface (SUI)

Science Field Specific Application Environments

- Language Bank Rights
  - http://www.csc.fi/english/research/sciences/linguistics/index_html
- Lemmie – Corpus Query Interface
  - http://www.csc.fi/english/research/software/www-lemmie
- Digital Morphology Archives – DMA
  - http://www.csc.fi/english/research/software/dma

Scientist’s User Interface (SUI)

Science Field Specific Application Environments

- SOMA2 – Molecular Modeling Environment
  - http://www.csc.fi/soma
- PaITuli – Geospatial Data Service
  - http://www.csc.fi/paituli

Linux on supercomputers: a basic guide to use the shell

Contents

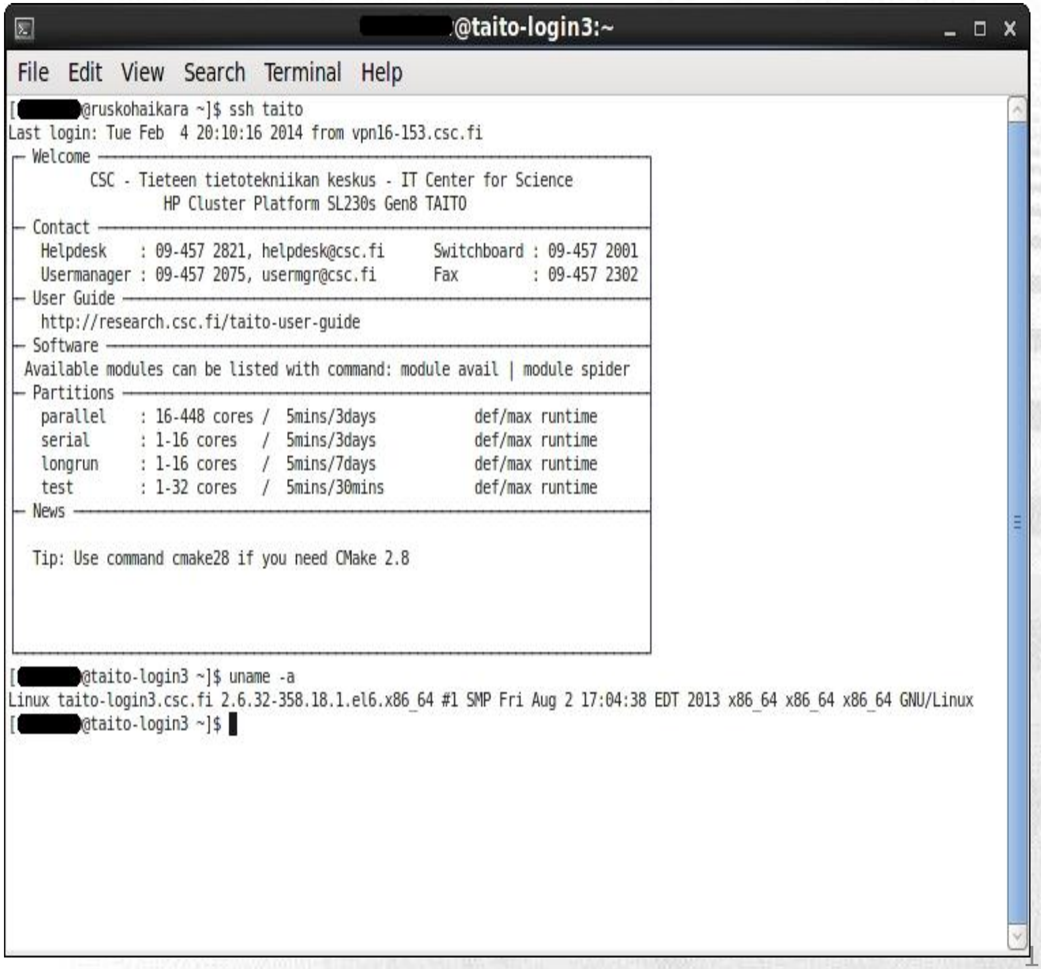
- Shells on CSC supercomputers
  - bash (recommended)
  - tcsh
- Shell commands
- Directories
- Files
- Programs
- Useful tools

What is shell?

- *A shell* is a program which provides the traditional, text-only user interface for Linux (and other Unix like systems)
- *Shell's* primary function is to read *commands* that are typed into a console or terminal window and then *execute* them.

What is shell cont., bash on Taito

- Text shell: Terminal with a set of commands
- Different flavors
  - **bash** (default)
  - tcsh (old default)
  - zsh,
  - corn-shell, …


[redacted]@taito-login3:~
File Edit View Search Terminal Help

```
[[redacted]@ruskohaikara ~]$ ssh taito
Last login: Tue Feb  4 20:10:16 2014 from vpn16-153.csc.fi
┌ Welcome ──────────────────────────────────────────────────────────────
│       CSC - Tieteen tietotekniikan keskus - IT Center for Science
│               HP Cluster Platform SL230s Gen8 TAITO
├ Contact ──────────────────────────────────────────────────────────────
│  Helpdesk    : 09-457 2821, helpdesk@csc.fi      Switchboard : 09-457 2001
│  Usermanager : 09-457 2075, usermgr@csc.fi       Fax         : 09-457 2302
├ User Guide ───────────────────────────────────────────────────────────
│  http://research.csc.fi/taito-user-guide
├ Software ─────────────────────────────────────────────────────────────
│ Available modules can be listed with command: module avail | module spider
├ Partitions ───────────────────────────────────────────────────────────
│  parallel    : 16-448 cores /  5mins/3days           def/max runtime
│  serial      : 1-16 cores   /  5mins/3days           def/max runtime
│  longrun     : 1-16 cores   /  5mins/7days           def/max runtime
│  test        : 1-32 cores   /  5mins/30mins          def/max runtime
├ News ─────────────────────────────────────────────────────────────────
│
│ Tip: Use command cmake28 if you need CMake 2.8
│
│
│
└───────────────────────────────────────────────────────────────────────
[[redacted]@taito-login3 ~]$ uname -a
Linux taito-login3.csc.fi 2.6.32-358.18.1.el6.x86_64 #1 SMP Fri Aug 2 17:04:38 EDT 2013 x86_64 x86_64 x86_64 GNU/Linux
[[redacted]@taito-login3 ~]$ █
```

bash and tcsh comparison

	bash	tcsh	invoking	bash output	tcsh output
Shell variables	x=2	set x = 2	echo $x	2	2
Env. variables	export z=3	setenv z 3	echo $z	3	3

PATH	export PATH=/a:/b	set path=(/a /b)	echo $path;
			echo $PATH;
				-
				/a:/b
					/a /b
					/a:/b

Aliases	alias ls="ls -l"	alias ls "ls -l"	ls	*same as ls -l*	*same as ls –l*
Command prompt	PS1=abc-	set prompt=abc-	[*ENTER*]	abc-	abc-
Redirection	prog > ofile 2> efile	(prog > ofile) >& efile	[*ENTER*]	*stdout -> ofile* *stderr -> efile*	*stdout -> ofile* *stderr -> efile*

Shell commands

- A *command* is an instruction given by a user telling a computer to do something, e.g.:
  - – run a single *program*
  - – run a group of *linked programs*
- Commands are generally issued by typing them in at the command line and then pressing the ENTER key, which passes them to the *shell*

Commands cont.

- Structure of a command:

  `command -`*`option`*` [`*`optional input`*`]`

- Examples
  - `apropos list`
  - `ls -l`
  - `clear`
  - `finger` *`username`* `(Taito)`
    - `finger -m` *`username`* `(Sisu)`

ls

- Prints names of files in current directory
- Prints contents of a directory, if given as *ls directory*
- Only print filenames matching a wildcard expression
  - *ls *.txt*
- Option *-l* gives more info
- May find useful on Taito and Sisu
  - *ls –lrt* (reverse time ordered)
  - *ls -d /* --color=tty* (list directories, colorize the output)

mkdir [directory]

- Make a new directory
- *-p* to not complain about already existing directory and to make missing parent directories as needed

cd [directory]

- Change the current working directory
- *cd ..* to go up a directory

mv [source] [dest]

- Moves files or directories
- Can also rename files

rm [file]

- Removes files (*be careful*!)
- *-r* to remove a directory recursively
- -f to force removal (*be supercareful*!)
- Sometimes, e.g., on Taito, alias: rm = ’rm –i’

find [directory] [options]

- Finds files in a directory and it's subdirectories that match the criteria given with the options
- Common use case, find files with certain names in the current directory:

```
find . -name '*.c’ -print
```

grep -e 'searchterm' [files]

- Search for matching lines inside files
- *-i* for case insensitive
- *-n* to print line numbers

pwd

- Print the current working directory

cat [file]

- Prints contents of file to screen
- cat -n to precede lines with line numbers

less [file]

- Opens a scrollable view of a file
- q to quit
- / to search forward, ? to search backwards
- n to find the next match, N for previous
- Some people prefer **more [file]**, it allows to scroll down, but not up

man [command]

- Show the manual of command in less

cp [source] [destination]

- Copy a file
- *-r* to copy recursively a directory and its contents
- *-v* for verbose

scp [source] [dest]

- Like cp, but used for remote transfer
- For example: scp my_file user@taito.csc.fi:’/absolute/path/to/dir’

rsync [source] [dest]

- Fast, versatile tool, remote and local usage
- E.g.: rsync my_file taito.csc.fi:

tar [commands] [file]

- Versatile tool used most in two ways
  - tar xvf some_file.tar
    - E**x**tracts from **f**ile some_file.tar the contents of the archive **v**erbosely
  - tar cvf my_files.tar my_dir/
    - **C**reates **v**erbosely a new archive in **f**ile my_files.tar from the directory my_dir/
  - tar cvzf my_files.tar.gz my_dir/
    - Apply g**z**ip (i.e., compress the tar archive)

wget *URL*

- Used to download files from the internet without a graphical browser such as Firefox or Chrome
- For example: wget http://ftp.gnu.org/gnu/hello/hello-2.7.tar.gz to download the gnu program hello

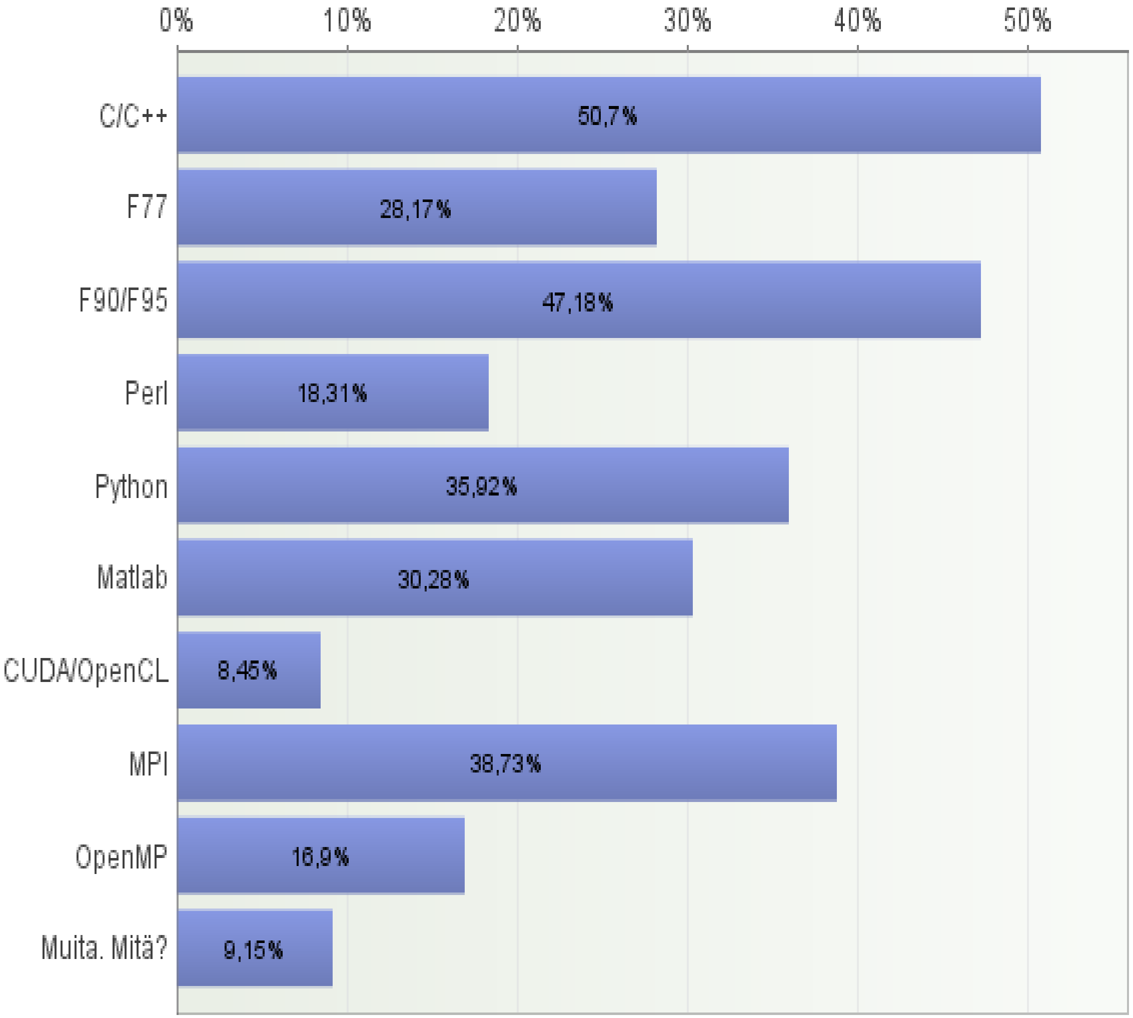
Selected Taito aliases

- Type *alias* to get the full list
  - alias chsh='/usr/alt/uadm2/bin/chsh'
  - alias mv='mv -i'
  - alias passwd='/usr/alt/uadm2/bin/passwd'
  - alias quota='/etc/profile.d/csc/csc-quota.bash'
  - alias sj='scontrol show job'
  - alias sn='scontrol show node'
  - alias vi='vim'

What is a program?

- A *program* is a sequence of instructions understandable by a computer’s central processing unit (CPU) that indicates which operations the computer should perform
  - Ready-to-run programs are stored as *executable* files
  - An executable file is a file that has been converted from source code into machine code, by a specialized program called a compiler

Programming languages at supercomputers



gcc [source files] [-o prog]

- Compiles C source files into a program
- *-o* to give the name of the program, defaults to a.out
- -c to compile into .o -files

Compiling and installing programs

- For most programs, the three commands to compile and install in directory /home/user/programs are:
  ./configure --prefix=/home/user/programs
  make
  make install
- *make* will be discussed in detail later today
- Common destination: *$USERAPPL*

More useful tools

- head
- tail
- wc
- which
- time
- ps
- top

- touch
- sed
- sort
- uniq
- cut
- paste
- awk

Use case: set command prompt on Taito

1) Edit your profile file, e.g., with *vi* or *nano*

- *vi .profile*

add:

- export PS1='\[\033[1;30m\]\u\[\033[0m\]@\[\033[1;34m\]\h\[\033[0m\]:[\w]# '

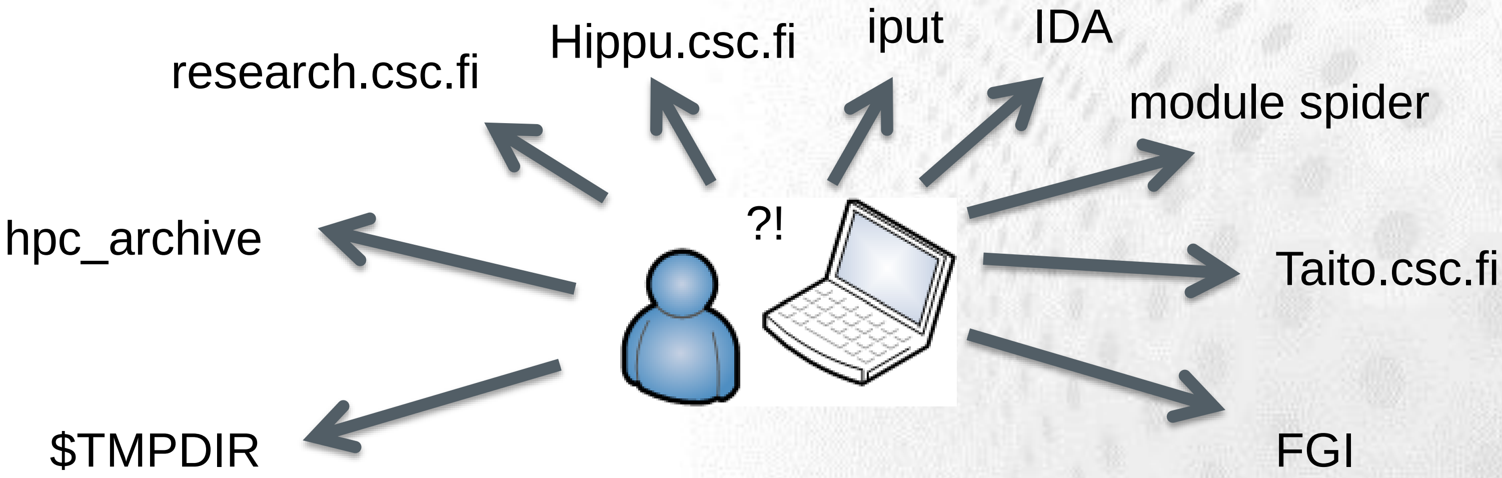
2) Apply changes

- *source .profile*

CSC Computing Environment

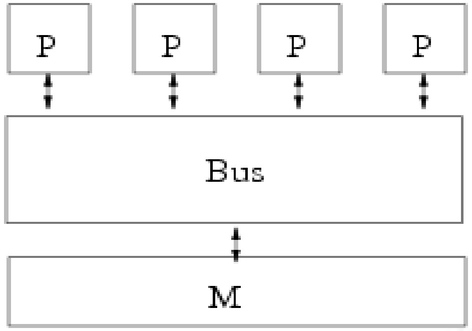
Learning target

- Know how to choose right server (resource)
- Know where to put your files
- Know how to setup and use preinstalled software

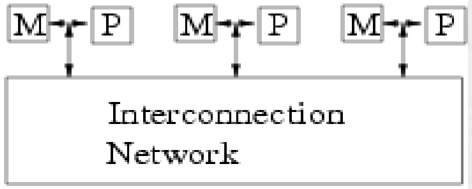


On Clusters and Supercomputers (1/2)

- Shared Memory Parallel (SMP):
  - All processors access (more or less) the same memory
  - Within node



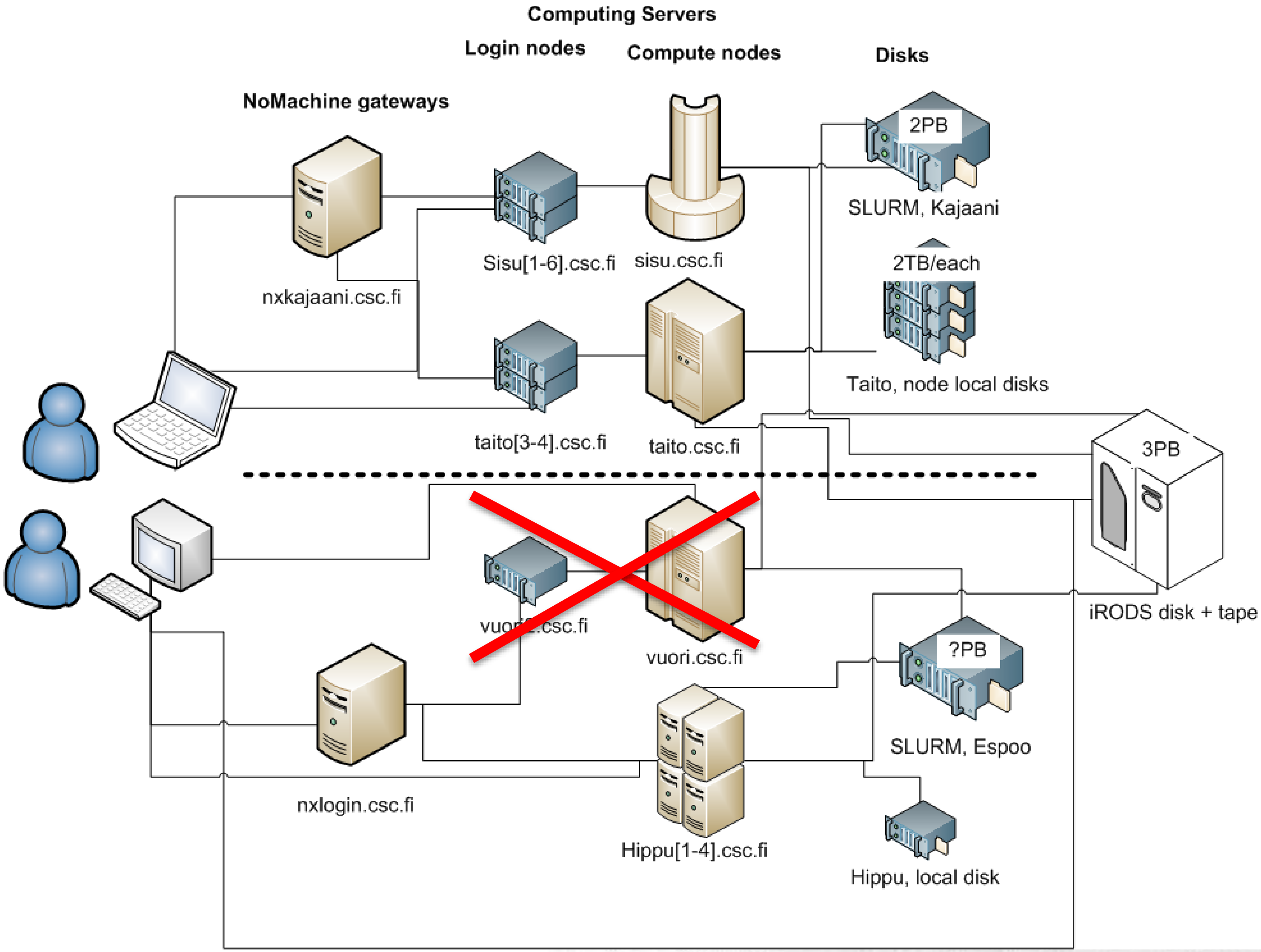
- Distributed Memory:
  - Reserved memory
  - Interconnection network for exchange
  - Between nodes



On Clusters and Supercomputers (2/2)

- A cluster is a connection of separate units (nodes) via a fast network
- –All larger CSC platforms (Sisu, Taito, FGI) are clusters in a general sense

The Complete Picture (apart from PRACE, FGI, Cloud)



Server use profiles

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

- Hippu (HP) (*to be decommissioned*)
- Interactive jobs
- Very large long jobs
- No queueing system

- Sisu (Cray XE30)
- Parallel from 72 up to thousands of cores
- Scaling tests 1008+

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

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

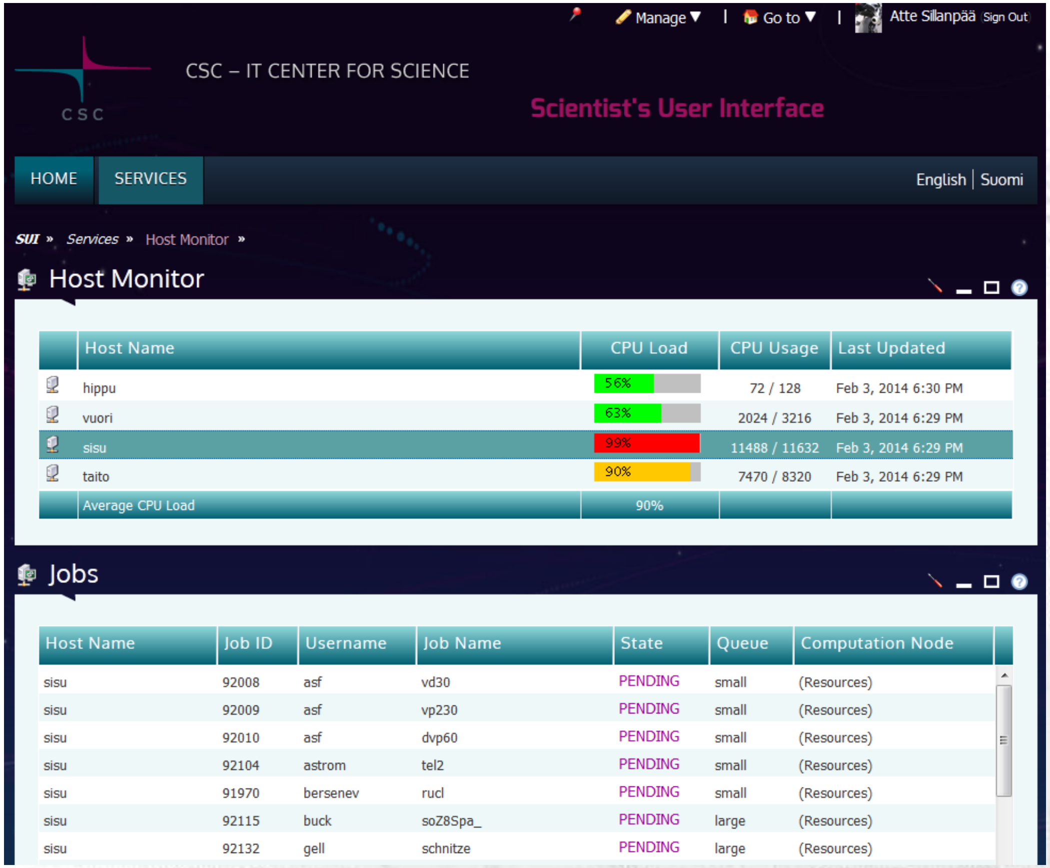
Main Computing capacity: Sisu,Taito,Vuori, FGI

	Sisu (Phase 2)	Taito (Phase 1)	FGI	Taygeta
Availability	2014-	2013-	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	9344	7308	360
RAM/core	2.67 GB	4/16/48 *) GB	2 / 4 / 8 GB	4 GB
Tflops	1688	180	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)

Host Monitor in SUI

- Load on servers
- Running jobs (`squeue`)
- sui.csc.fi



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CSC
CSC – IT CENTER FOR SCIENCE
Scientist's User Interface
HOME
SERVICES
English | Suomi
SUI » Services » Host Monitor »

Host Monitor

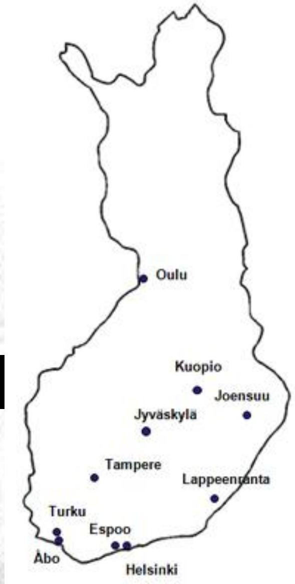
	Host Name	CPU Load	CPU Usage	Last Updated
	hippu	56%	72 / 128	Feb 3, 2014 6:30 PM
	vuori	63%	2024 / 3216	Feb 3, 2014 6:29 PM
	sisu	99%	11488 / 11632	Feb 3, 2014 6:29 PM
	taito	90%	7470 / 8320	Feb 3, 2014 6:29 PM
	Average CPU Load	90%		

Jobs

Host Name	Job ID	Username	Job Name	State	Queue	Computation Node
sisu	92008	asf	vd30	PENDING	small	(Resources)
sisu	92009	asf	vp230	PENDING	small	(Resources)
sisu	92010	asf	dvp60	PENDING	small	(Resources)
sisu	92104	astrom	tel2	PENDING	small	(Resources)
sisu	91970	bersenev	rucl	PENDING	small	(Resources)
sisu	92115	buck	soZ8Spa_	PENDING	large	(Resources)
sisu	92132	gell	schnitze	PENDING	large	(Resources)

FGCI – The Finnish Grid and Cloud Infrastructure

- Consortium of 9 Finnish Universities and CSC
- Infrastructure consists of 7368 cores and 100 GPU cards (+ Vuori)
- Accessed via ARC middleware
- Submit jobs from hippu/own workstation
- Preinstalled software
- More information: FGI webpages



Directories at CSC Environment (1)

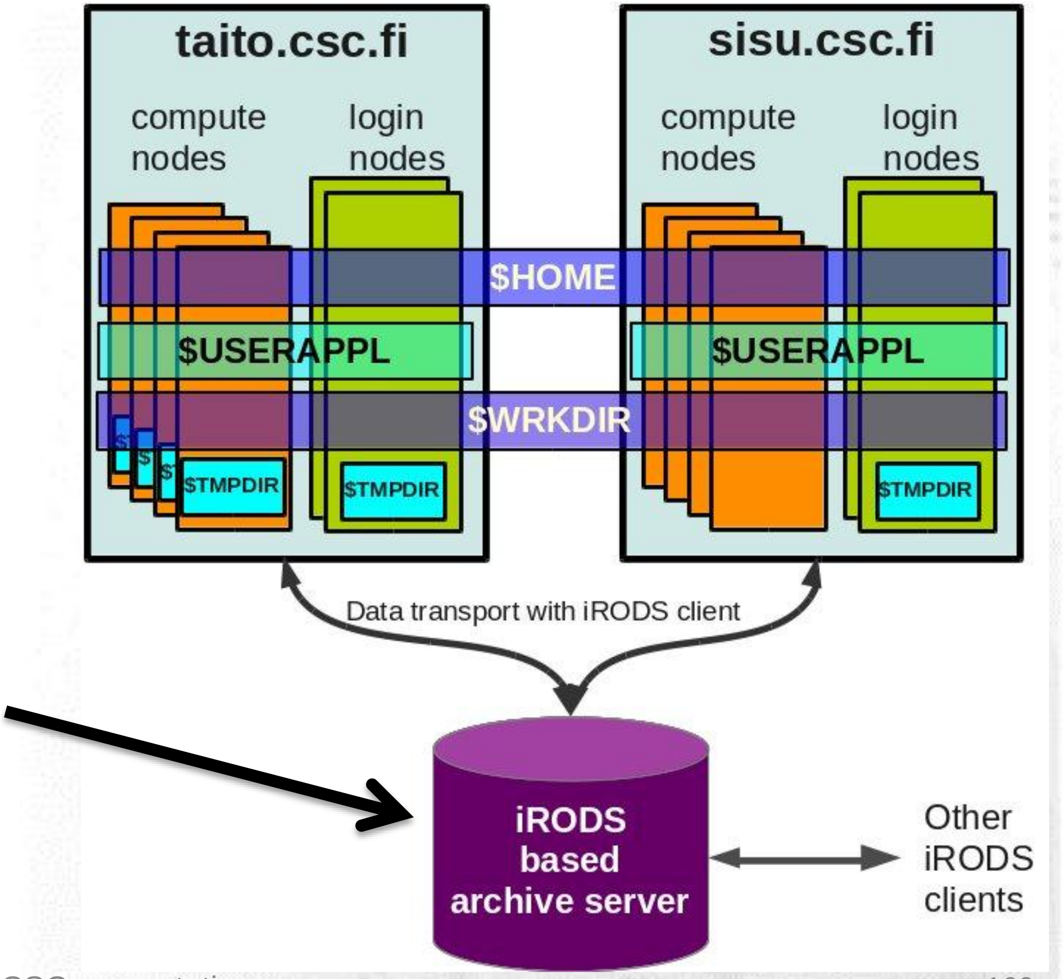
Directory or storage area	Intended use	Default quota/user	Storage time	Backup
$HOME [1]	Initialization scripts, source codes, small data files. Not for running programs or research data.	20 GB	Permanent	Yes
$USERAPPL [1]	Users' own application software.	20 GB	Permanent	Yes
$WRKDIR [1]	Temporary data storage.	5 TB	Until further notice.	No
$TMPDIR [1]	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 file system in Kajaani

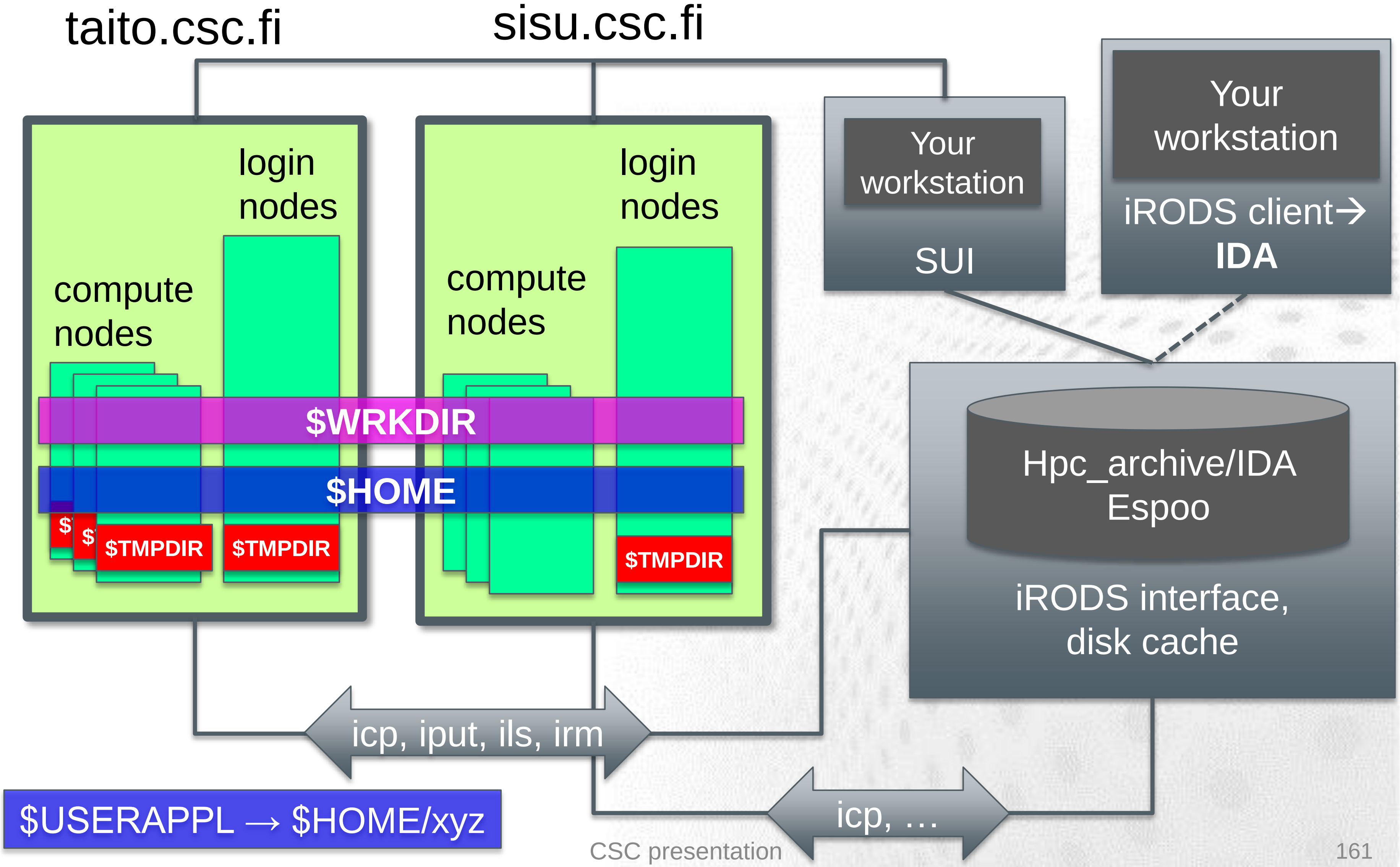
[2]: iRODS storage system in Espoo

Directories at CSC Environment (2)

- What can be seen from where
- Use **$TMPDIR** for fast/random file i/o
- IDA/hpc_archive accessed with i-commands



Directories at CSC Environment (3)



$USERAPPL → $HOME/xyz

Storage: hard disks

- 4 PB on DDN (Lustre), Sisu and Taito
  - $USERAPPL: *put your applications here*
  - /homeappl/home/username/app_taito
  - /homeappl/home/username/app_sisu
  - **/tmp** (Taito, ~2 TB) to be used for *e.g. compiling codes on the login nodes*
  - **$TMPDIR** on compute nodes: *for scratch files (accessed with $TMPDIR in batch script)*
  - **$HOME** for configuration files and misc. smallish storage
  - **$WRKDIR** for large data and during calculations. Avoid lots of small files.
- Lustre for Hippu and Vuori to be decommissioned in Espoo

Storage: disks and tape

- Disk/Tape space through IDA
  - Requires an application
  - 1 PB for Universities (local contacts at each university)
  - 1 PB for Finnish Academy (SA)
  - 1 PB for ESFRI and other needs (contact contact@csc.fi for more information)
  - Free of charge at least until 2017
  - Access with i-commands, webdav (mapped as network drive), SUI **also** from own computer
  - Described with metadata
  - Flexible sharing with colleagues/collaborators/public
- Tape (+ disk cache) as **hpc_archive**
  - Default long term storage
  - Access with i-commands from Sisu/Taito

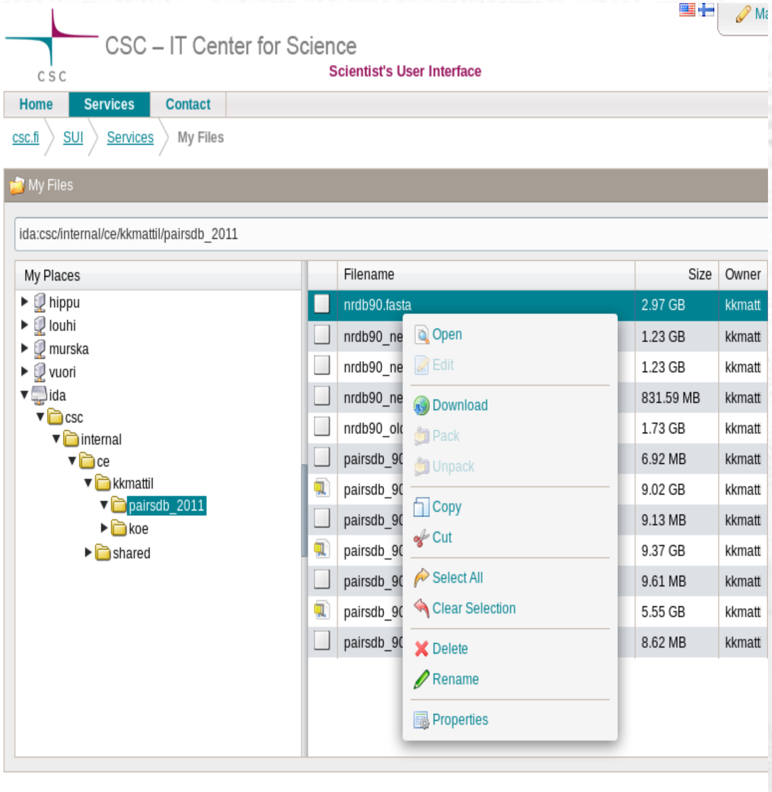
IDA interfaces at CSC

Some iRODS commands

● `iput` *`file`*	move file to IDA
● `iget` *`file`*	retrieve file from IDA
● `ils`	list the current IDA directory
● `icd` *`dir`*	change the IDA directory
● `irm` *`file`*	remove file from IDA
● `imv` *`file file`*	move file inside IDA
● `irsync`	synchronize the local copy with the copy in IDA
● `imkdir`	create a directory to IDA
● `iinit`	Initialize your IDA account

Tip: map IDA as a network drive (good for small files)

IDA in Scientist's User Interface



ida:csc/internal/ce/kkmattil/pairsdb_2011

	Filename	Size	Owner
□	nrdb90.fasta	2.97 GB	kkmatt
□	nrdb90_ne	1.23 GB	kkmatt
□	nrdb90_ne	1.23 GB	kkmatt
□	nrdb90_ne	831.59 MB	kkmatt
□	nrdb90_old	1.73 GB	kkmatt
□	pairsdb_90	6.92 MB	kkmatt
	pairsdb_90	9.02 GB	kkmatt
□	pairsdb_90	9.13 MB	kkmatt
	pairsdb_90	9.37 GB	kkmatt
□	pairsdb_90	9.61 MB	kkmatt
	pairsdb_90	5.55 GB	kkmatt
□	pairsdb_90	8.62 MB	kkmatt

Moving files, best practices

- tar & bzip first (bzip more error tolerant)
- rsync, not scp (when lots of/big files)
  - `rsync -P username@hippu1.csc.fi:/tmp/huge.tar.gz .`
- Blowfish may be faster than AES (if CPU bottleneck)
- Funet FileSender (max 50 GB [don't try this as an attachment])
  - *https://filesender.funet.fi*
  - Files can be downloaded also with **`wget`**

- iRODS, batch-like process, staging
- IDA: http://www.tdata.fi/ida
- CSC can help to tune e.g. TCP/IP parameters
  - http://www.csc.fi/english/institutions/funet/networkservices/pert
- FUNET backbone 10 Gbit/s
- More info in CSC computing environment Guide

The module system

- Tool to set up your environment
  - Load libraries, adjust path, set environment variables
  - Needed on a server with hundreds of applications and several compilers etc.
- Slightly different on Taito vs. other systems
- Used both in interactive and batch jobs

Typical module commands

`module avail`	shows available modules (compatible modules in taito)
`module spider`	shows all available modules in taito
`module list`	shows currently loaded modules
`module load <name>`	loads module <name> (default version)
`module load <name/version>`	loads module <name/version>
`module switch <name1> <name2>`	unloads module name1 and loads module name2
`module purge`	unloads all loaded modules

Taito has ”meta-modules” named e.g. gromacs-env, which will load all necessary modules needed to run gromacs.

Module example

- Show compatible modules on Taito

```
module avail
```

- Initialize Desmond

```
module load desmond
```

- Start Desmond via Maestro interface (see: research.csc.fi/-/maestro)
- It's better to run the GUI (and calculations) on a compute node (jobs that have used 1h of CPU on the login node will be killed automatically)
- For interactive work, use taito-shell.csc.fi

Learning targets achieved?

- How to choose right server (resource)?
- Where to put your files?
- How to setup and use preinstalled software/libraries/compilers?

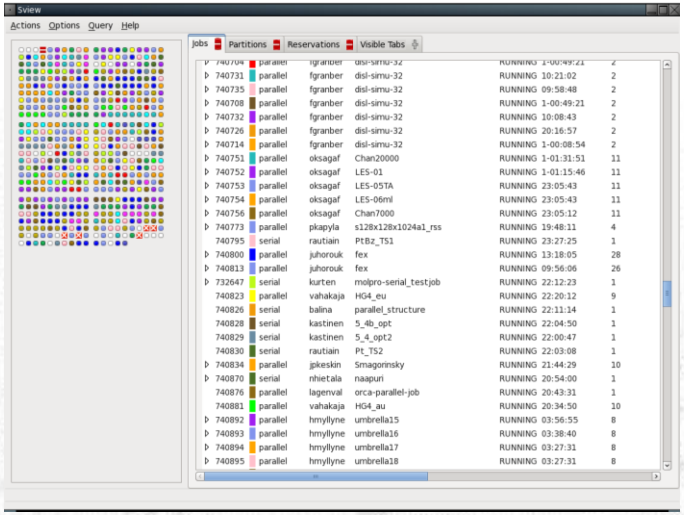
Running jobs at CSC

Batch jobs learning target

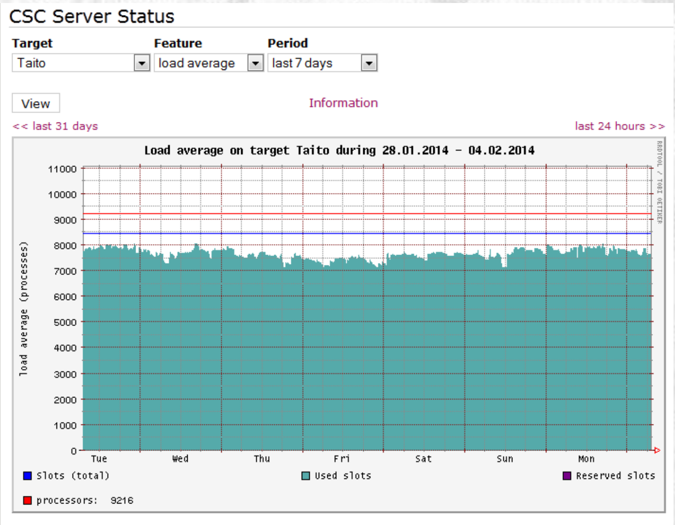
- Benefits of batch jobs for compute intensive jobs
  - Difference of login and compute node
- How to submit and monitor jobs
- Batch script contents i.e. requirements
- How to learn requirements of own jobs
- Be aware of batch script wizard in SUI
- Submit first job(s)
- Learn to read the the manual

What is a batch system?

- Optimizes resource usage by filling the server with jobs
- Cores, memory, disk, length, …
- Jobs to run are chosen based on their priority
- Priority increases with queuing time
- Priority decreases with recently used resources
- Short jobs with little memory and cores queue the least
- CSC uses SLURM (Simple Linux Utility for Resource Management)



740704	parallel	fgranber	disl-simu-32	RUNNING	1-00:49:21	2
740731	parallel	fgranber	disl-simu-32	RUNNING	10:21:02	2
740735	parallel	fgranber	disl-simu-32	RUNNING	09:58:48	2
740708	parallel	fgranber	disl-simu-32	RUNNING	1-00:49:21	2
740732	parallel	fgranber	disl-simu-32	RUNNING	10:08:43	2
740726	parallel	fgranber	disl-simu-32	RUNNING	20:16:57	2
740714	parallel	fgranber	disl-simu-32	RUNNING	1-00:08:54	2
740751	parallel	oksagaf	Chan20000	RUNNING	1-01:31:51	11
740752	parallel	oksagaf	LES-01	RUNNING	1-01:15:46	11
740753	parallel	oksagaf	LES-05TA	RUNNING	23:05:43	11
740754	parallel	oksagaf	LES-06ml	RUNNING	23:05:43	11
740756	parallel	oksagaf	Chan7000	RUNNING	23:05:12	11
740773	parallel	pkapyla	s128x128x1024a1_rss	RUNNING	19:48:11	4
740795	serial	rautiain	PtBz_TS1	RUNNING	23:27:25	1
740800	parallel	juhorouk	fex	RUNNING	13:18:05	28
740813	parallel	juhorouk	fex	RUNNING	09:56:06	26
732647	serial	kurten	molpro-serial_testjob	RUNNING	22:12:23	1
740823	parallel	vahakaja	HG4_eu	RUNNING	22:20:12	9
740826	serial	balina	parallel_structure	RUNNING	22:11:14	1
740828	serial	kastinen	5_4b_opt	RUNNING	22:04:50	1
740829	serial	kastinen	5_4_opt2	RUNNING	22:00:47	1
740830	serial	rautiain	Pt_TS2	RUNNING	22:03:08	1
740834	parallel	jpkeskin	Smagorinsky	RUNNING	21:44:29	10
740870	serial	nhietala	naapuri	RUNNING	20:54:00	1
740876	parallel	lagenval	orca-parallel-job	RUNNING	20:43:31	1
740881	parallel	vahakaja	HG4_au	RUNNING	20:34:50	10
740892	parallel	hmyllyne	umbrella15	RUNNING	03:56:55	8
740893	parallel	hmyllyne	umbrella16	RUNNING	03:38:40	8
740894	parallel	hmyllyne	umbrella17	RUNNING	03:27:31	8
740895	parallel	hmyllyne	umbrella18	RUNNING	03:27:31	8



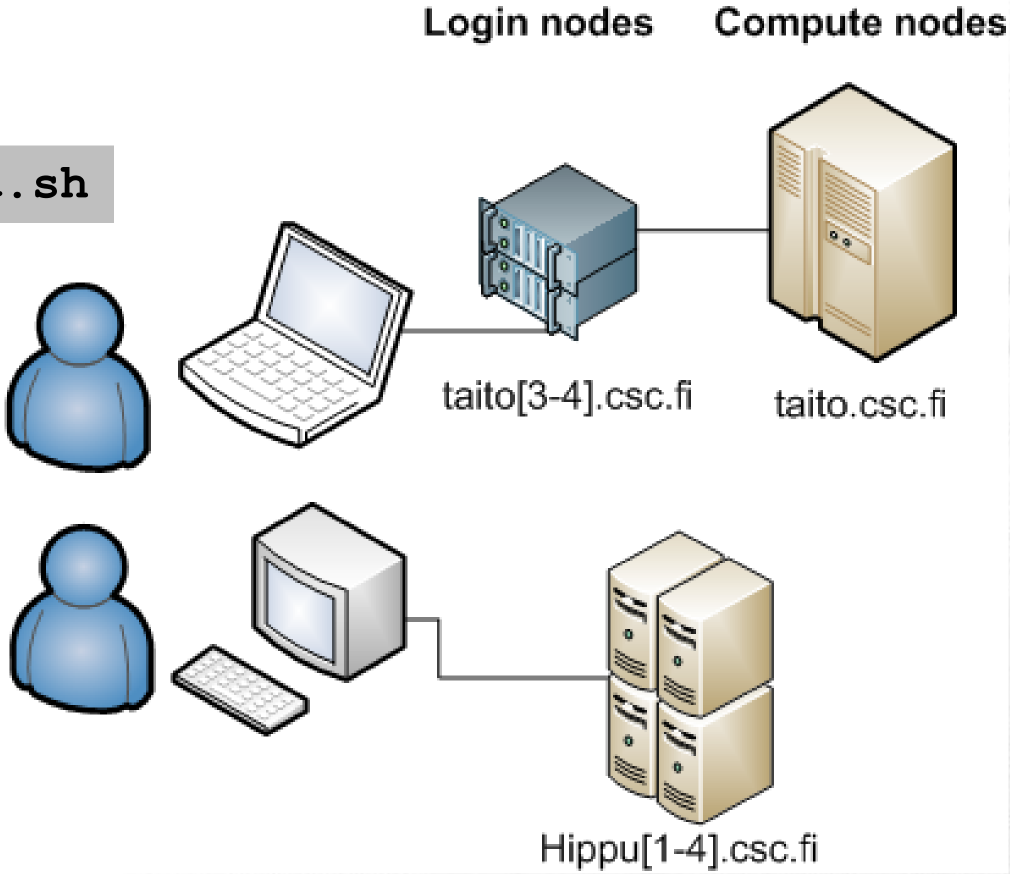
CSC Server Status

Target: Taito
Feature: load average
Period: last 7 days

Compute nodes are used via queuing system

```
sbatch job_script.sh
```

```
./my_prog &
```



Batch job overview

➢ Steps for running a batch job

1. Write a batch job script
   - Script details depend on server, check CSC Guide!
   - You can use the Batch Job Script Wizard in Scientist's User Interface:

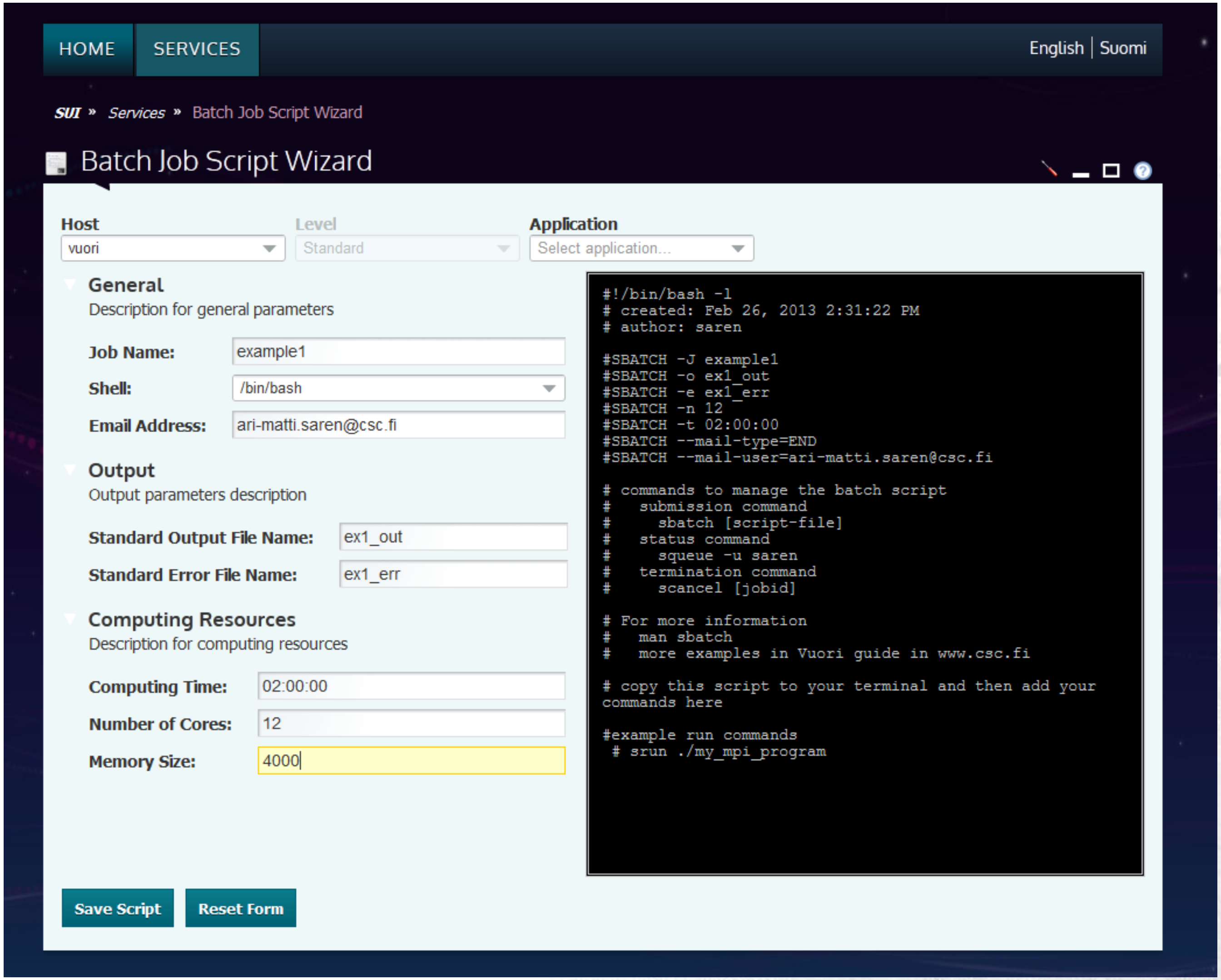
     https://sui.csc.fi/group/sui/batch-job-script-wizard

2. Make sure all the necessary files are in $WRKDIR
   - $HOME has limited space
   - Login $TMPDIR is not available on compute nodes

3. Submit your job

```
sbatch myscript
```

Batch Job Script wizard in Scientist’s User Interface



Batch Job Script Wizard

Host	Level	Application
vuori	Standard	Select application...

General

Description for general parameters

Job Name:	example1
Shell:	/bin/bash
Email Address:	ari-matti.saren@csc.fi

Output

Output parameters description

Standard Output File Name:	ex1_out
Standard Error File Name:	ex1_err

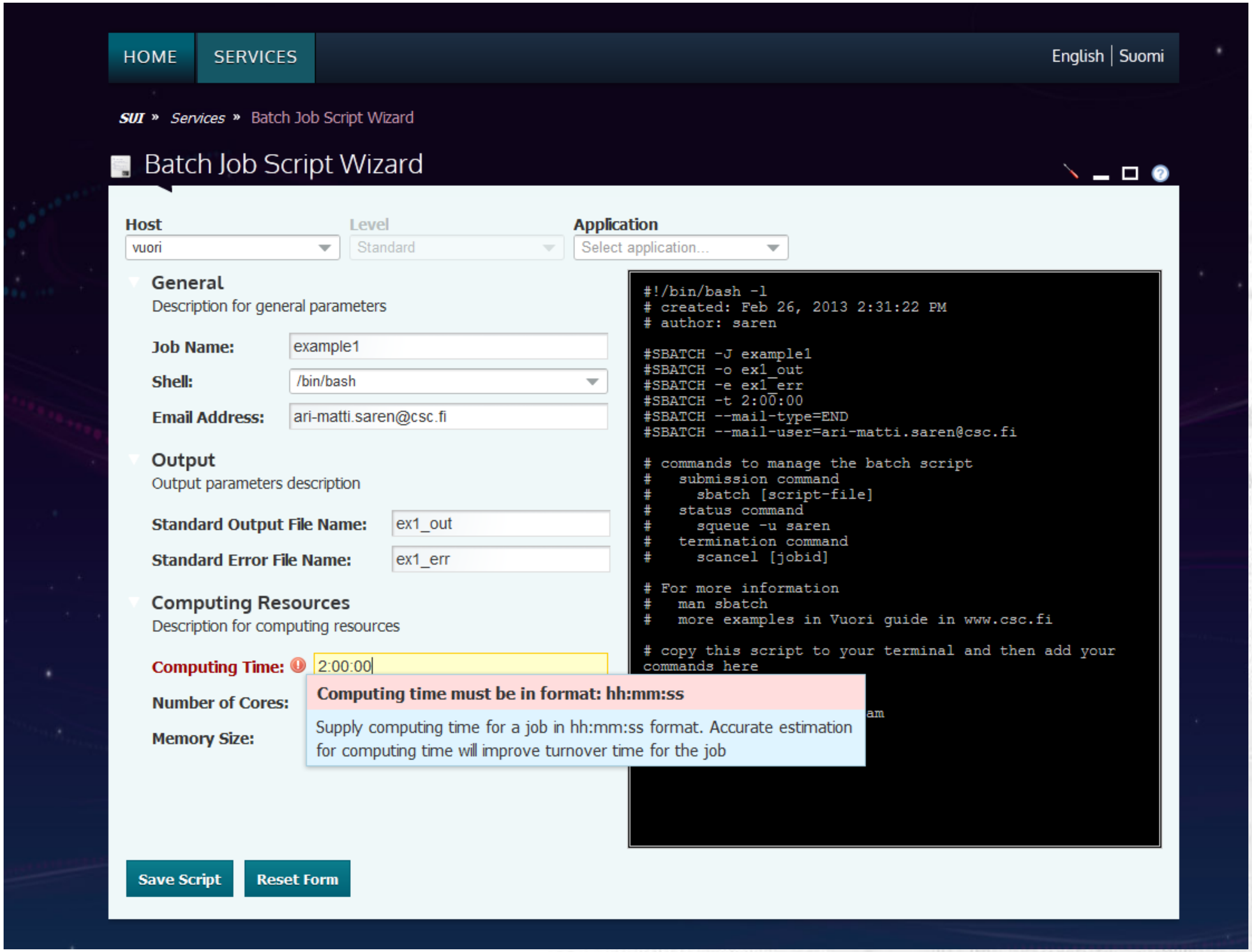
Computing Resources

Description for computing resources

Computing Time:	02:00:00
Number of Cores:	12
Memory Size:	4000

```
#!/bin/bash -l
# created: Feb 26, 2013 2:31:22 PM
# author: saren

#SBATCH -J example1
#SBATCH -o ex1_out
#SBATCH -e ex1_err
#SBATCH -n 12
#SBATCH -t 02:00:00
#SBATCH --mail-type=END
#SBATCH --mail-user=ari-matti.saren@csc.fi

# commands to manage the batch script
#   submission command
#     sbatch [script-file]
#   status command
#     squeue -u saren
#   termination command
#     scancel [jobid]

# For more information
#   man sbatch
#   more examples in Vuori guide in www.csc.fi

# copy this script to your terminal and then add your
commands here

#example run commands
 # srun ./my_mpi_program
```

Batch Job Script wizard in Scientist's User Interface



Batch Job Script Wizard

Host: vuori

Level: Standard

Application: Select application...

General

Description for general parameters

Job Name: example1

Shell: /bin/bash

Email Address: ari-matti.saren@csc.fi

Output

Output parameters description

Standard Output File Name: ex1_out

Standard Error File Name: ex1_err

Computing Resources

Description for computing resources

Computing Time: 2:00:00

Computing time must be in format: hh:mm:ss

Supply computing time for a job in hh:mm:ss format. Accurate estimation for computing time will improve turnover time for the job

Number of Cores:

Memory Size:

```
#!/bin/bash -l
# created: Feb 26, 2013 2:31:22 PM
# author: saren

#SBATCH -J example1
#SBATCH -o ex1_out
#SBATCH -e ex1_err
#SBATCH -t 2:00:00
#SBATCH --mail-type=END
#SBATCH --mail-user=ari-matti.saren@csc.fi

# commands to manage the batch script
#   submission command
#     sbatch [script-file]
#   status command
#     squeue -u saren
#   termination command
#     scancel [jobid]

# For more information
#   man sbatch
#   more examples in Vuori guide in www.csc.fi

# copy this script to your terminal and then add your
commands here


                         am
```

Batch jobs: what and why

- User has to specify necessary resources
  - Can be added to the batch job script or given as command line options for sbatch (or a combination of script and command line options)

- Resources need to be adequate for the job
  - Too small memory reservation will cause the job to fail
  - When the time reservation ends, the job will be terminated whether finished or not

- But: Requested resources can affect the time the job spends in the queue
  - Especially number of cores and memory reservation
  - Don’t request extra ”just in case” (time is less critical than memory wrt this)

- So: Realistic resource requests give best results
  - Not always easy to know beforehand
  - Usually best to try with smaller tasks first and check the used resources
  - You can check what was actually used with the `sacct` command

SLURM batch script contents

Example serial batch job script on Taito

```
#!/bin/bash -l
#SBATCH -J myjob
#SBATCH -e myjob_err_%j
#SBATCH -o myjob_output_%j
#SBATCH --mail-type=END
#SBATCH --mail-user=a.user@foo.net
#SBATCH --mem-per-cpu=4000
#SBATCH -t 02:00:00
#SBATCH -n 1
#SBATCH –p serial

module load myprog
srun myprog -option1 -option2
```

#!/bin/bash -l

- Tells the computer this is a script that should be run using bash shell
- Everything starting with "**#SBATCH**" is passed on to the batch job system (Slurm)
- Everything (else) starting with "**#** " is considered a comment
- Everything else is executed as a command

```
#!/bin/bash -l
#SBATCH -J myjob
#SBATCH -e myjob_err_%j
#SBATCH -o myjob_output_%j
#SBATCH --mail-type=END
#SBATCH --mail-user=a.user@foo.net
#SBATCH --mem-per-cpu=4000
#SBATCH -t 02:00:00
#SBATCH -n 1
#SBATCH -p serial

module load myprog
srun myprog -option1 -option2
```

#SBATCH -J myjob

- Sets the name of the job
- When listing jobs e.g. with **squeue**, only 8 first characters of job name are displayed.

```
#!/bin/bash -l
#SBATCH -J myjob
#SBATCH -e myjob_err_%j
#SBATCH -o myjob_output_%j
#SBATCH --mail-type=END
#SBATCH --mail-user=a.user@foo.net
#SBATCH --mem-per-cpu=4000
#SBATCH -t 02:00:00
#SBATCH -n 1
#SBATCH -p serial

module load myprog
srun myprog -option1 -option2
```

```
#SBATCH -e myjob_err_%j
#SBATCH -o myjob_output_%j
```

- Option **-e** sets the name of the file where possible error messages (stderr) are written
- Option **-o** sets the name of the file where the standard output (stdout) is written
- When running the program interactively these would be written to the command promt
- What gets written to stderr and stderr depends on the program. If you are unfamiliar with the program, it's always safest to capture both
- `%j` is replaced with the job id number in the actual file name

```
#!/bin/bash -l
#SBATCH -J myjob
#SBATCH -e myjob_err_%j
#SBATCH -o myjob_output_%j
#SBATCH --mail-type=END
#SBATCH --mail-user=a.user@foo.net
#SBATCH --mem-per-cpu=4000
#SBATCH -t 02:00:00
#SBATCH -n 1
#SBATCH -p serial

module load myprog
srun myprog -option1 -option2
```

```
#SBATCH --mail-type=END
#SBATCH --mail-user=a.user@foo.net
```

```
#!/bin/bash -l
#SBATCH -J myjob
#SBATCH -e myjob_err_%j
#SBATCH -o myjob_output_%j
#SBATCH --mail-type=END
#SBATCH --mail-user=a.user@foo.net
#SBATCH --mem-per-cpu=4000
#SBATCH -t 02:00:00
#SBATCH -n 1
#SBATCH -p serial

module load myprog
srun myprog -option1 -option2
```

- Option **`--mail-type=END`** = send email when the job finishes

- Option **`--mail-user`** = your email address.

- If these are selected you get a email message when the job is done. This message also has a resource usage summary that can help in setting batch script parameters in the future.

- To see actually used resources try also: **`sacct -l -j <jobid>`** (more on this later)

`#SBATCH -n 1`

- Number of cores to use

- It’s also possible to control on how many nodes you job is distributed. Normally, this is not needed. By default use all cores in allocated nodes:
  - **`--ntasks-per-node=16`**

- Check documentation: http://research.csc.fi/software
  - There’s a lot of software that can only be run in serial

- OpenMP applications can only use cores in one node

```
#!/bin/bash -l
#SBATCH -J myjob
#SBATCH -e myjob_err_%j
#SBATCH -o myjob_output_%j
#SBATCH --mail-type=END
#SBATCH --mail-user=a.user@foo.net
#SBATCH --mem-per-cpu=4000
#SBATCH -t 02:00:00
#SBATCH -n 1
#SBATCH -p serial

module load myprog
srun myprog -option1 -option2
```

#SBATCH --mem-per-cpu=4000

```
#!/bin/bash -l
#SBATCH -J myjob
#SBATCH -e myjob_err_%j
#SBATCH -o myjob_output_%j
#SBATCH --mail-type=END
#SBATCH --mail-user=a.user@foo.net
#SBATCH --mem-per-cpu=4000
#SBATCH -t 02:00:00
#SBATCH -n 1
#SBATCH -p serial

module load myprog
srun myprog -option1 -option2
```

- The amount of memory reserved for the job in MB
  - 1000 MB = 1 GB
- Memory is reserved on per-core basis even for shared memory (OpenMP) jobs
- Keep in mind the specifications for the nodes. Jobs with impossible requests are rejected (try **`squeue`** after submit)
- If you reserve too little memory the job will be killed (you will see a corresponding error in the output)
- If you reserve too much memory your job will spend much longer in queue and potentially waste resources (idle cores)

#SBATCH -t 02:00:00

TIP: If you're unsure of the syntax, use Batch job wizard in SUI

```
#!/bin/bash -l
#SBATCH -J myjob
#SBATCH -e myjob_err_%j
#SBATCH -o myjob_output_%j
#SBATCH --mail-type=END
#SBATCH --mail-user=a.user@foo.net
#SBATCH --mem-per-cpu=4000
#SBATCH -t 02:00:00
#SBATCH -n 1
#SBATCH -p serial

module load myprog
srun myprog -option1 -option2
```

- Time reserved for the job in hh:mm:ss
- When the time runs out the job will be terminated!
- With longer reservations the job queue longer
- Limit for normal serial jobs is 3d (72 h)
  - if you reserve longer time, the job will go to ”longrun” queue (limit 7d)
  - In the longrun queue you run at your own risk. If a batch job in that queue stops prematurely no compensation is given for lost cpu time!
  - In longrun you likely queue for a longer time: shorter jobs and restarts are better (safer, more efficient)
- Default job length is 5 minutes → need to be set by yourself.

`#SBATCH -p serial`

➢ The queue the job should be submitted to

➢ Queues are called ”partitions” in SLURM

➢ You can check the available queues with command

`sinfo -l`

```
#!/bin/bash -l
#SBATCH -J myjob
#SBATCH -e myjob_err_%j
#SBATCH -o myjob_output_%j
#SBATCH --mail-type=END
#SBATCH --mail-user=a.user@foo.net
#SBATCH --mem-per-cpu=4000
#SBATCH -t 02:00:00
#SBATCH -n 1
#SBATCH -p serial

module load myprog
srun myprog -option1 -option2
```

```
PARTITION AVAIL  TIMELIMIT   JOB_SIZE ROOT SHARE     GROUPS  NODES       STATE NODELIST
serial*      up 3-00:00:00          1   no YES:4        all    514       mixed c[5-274,276-453,455-473, …
serial*      up 3-00:00:00          1   no YES:4        all      3        idle c[275,454,474]
parallel     up 3-00:00:00       1-28   no    NO        all    514       mixed c[5-274,276-453,455-473, …
parallel     up 3-00:00:00       1-28   no    NO        all      3        idle c[275,454,474]
longrun      up 7-00:00:00          1   no YES:4        all    514       mixed c[5-274,276-453,455-473,…
longrun      up 7-00:00:00          1   no YES:4        all      3        idle c[275,454,474]
test         up      30:00        1-2   no YES:4        all      1     drained c4
test         up      30:00        1-2   no YES:4        all      3        idle c[1-3]
```

```
module load myprog
srun myprog -option1 -option2
```

```
#!/bin/bash -l
#SBATCH -J myjob
#SBATCH -e myjob_err_%j
#SBATCH -o myjob_output_%j
#SBATCH --mail-type=END
#SBATCH --mail-user=a.user@foo.net
#SBATCH --mem-per-cpu=4000
#SBATCH -t 02:00:00
#SBATCH -n 1
#SBATCH -p serial

module load myprog
srun myprog -option1 -option2
```

- Your commands
  - These define the actual job to performed: these commands are run on the compute node.
  - See application documentation for correct syntax
  - Some examples also from batch script wizard in SUI
- Remember to load modules if necessary
- By default the working directory is the directory where you submitted the job
  - If you include a **`cd`** command, make sure it points to correct directory
- Remember that input and output files should be in $WRKDIR (or in some case $TMPDIR)
- **`srun`** tells your program which cores to use. There are also exceptions…

Most commonly used sbatch options

Slurm option	**Description**
--begin=*time*	defer job until HH:MM MM/DD/YY
-c, --cpus-per-task=*ncpus*	number of cpus required per task
-d, --dependency=*type:jobid*	defer job until condition on jobid is satisfied
-e, --error=*err*	file for batch script's standard error
--ntasks-per-node=*n*	number of tasks per node
-J, --job-name=*jobname*	name of job
--mail-type=*type*	notify on state change: BEGIN, END, FAIL or ALL
--mail-user=*user*	who to send email notification for job state changes
-n, --ntasks=*ntasks*	number of tasks to run
-N, --nodes=*N*	number of nodes on which to run
-o, --output=*out*	file for batch script's standard output
-t, --time=*minutes*	time limit in format hh:mm:ss
--mem-per-cpu=<number in MB>	maximum amount of real memory per allocated cpu required by the job in megabytes
--mem=<number in MB>	maximum memory per node

SLURM:
Managing batch jobs in Taito

Submitting and cancelling jobs

- The script file is submitted with command

```
sbatch batch_job.file
```

  - *Optional:* sbatch option are usually listed in the batch job script, but they can also be specified on command line, e.g.

```
sbatch -J test2 -t 00:05:00 batch_job_file.sh
```

- Job can be deleted with command

```
scancel <jobid>
```

Queues

- The job can be followed with command `squeue`:

`squeue`	(shows all jobs in all queues)
`squeue -p <partition>`	(shows all jobs in single queue (partition))
`squeue -u <username>`	(shows all jobs for a single user)
`squeue -j <jobid> -l`	(status of a single job in long format)

- To estimate the start time of a job in queue

```
scontrol show job <jobid>
```

row "StartTime=..." gives an estimate on the job start-up time, e.g.

```
StartTime=2014-02-11T19:46:44 EndTime=Unknown
```

- `scontrol` will also show where your job is running
- If you add this to the end of your batch script, you'll get additional info to stdout about resource usage (works for jobs run with srun)
  - `used_slurm_resources.bash`

Job logs

TIP: Check MaxRSS to see how much memory you need and avoid overbooking

- Command `sacct` can be used to study past jobs
  - Usefull when deciding proper resource requests

`sacct`	Short format listing of jobs starting from midnight today
`sacct -l`	long format output
`sacct -j <jobid>`	information on single job
`sacct -S YY:MM:DD`	listing start date
`sacct -o`	list only named data fields, e.g.
`sacct -u <username>`	list only jobs submitted by username

```
sacct -o jobid,jobname,maxrss,state,elapsed -j <jobid>
```

Available nodes/queues

- You can check available nodes in each queue with command:

```
sjstat -c
```

```
Scheduling pool data:
------------------------------------------------------------
Pool        Memory  Cpus  Total Usable   Free  Other Traits
------------------------------------------------------------
serial*    64300Mb    16    501    501      5
serial*   258000Mb    16     16     16      0  bigmem
parallel   64300Mb    16    501    501      5
parallel  258000Mb    16     16     16      0  bigmem
longrun    64300Mb    16    501    501      5
longrun   258000Mb    16     16     16      0  bigmem
test       64300Mb    16      4      3      3
hugemem   1551000Mb   32      2      2      2  bigmem
```

Most frequently used SLURM commands

Command	**Description**
`srun`	Run a parallel job.
`salloc`	Allocate resources for interactive use .
`sbatch`	Submit a job script to a queue.
`scancel`	Cancel jobs or job steps.
`sinfo`	View information about SLURM nodes and partitions.
`squeue`	View information about jobs located in the SLURM scheduling queue
`smap`	Graphically view information about SLURM jobs, partitions, and set configurations parameters
`sjstat`	display statistics of jobs under control of SLURM (combines data from sinfo, squeue and scontrol)
`scontrol`	View SLURM configuration and state.
`sacct`	Displays accounting data for batch jobs.

Parallel jobs (1/2)

- Only applicable if your program supports parallel running

- Check application documentation on number of cores to use
  - Speed-up is often not linear (communication overhead)
  - Maximum number can be limited by the algorithms
  - Make sure (test) that using more cores speeds up calculation

- Mainly two types: MPI jobs and shared memory (OpenMP) jobs
  - OpenMP jobs can be run only inside one node
    - All cores access same memory space
  - MPI jobs can span several nodes
    - Each core has its own memory space

Parallel jobs (2/2)

- Memory is normally reserved per-core basis
  - For OpenMP jobs divide total memory by number of cores
  - Take care to only request possible configurations
  - If you reserve a complete node, you can also ask for all the memory

- Each server has different configuration so setting up parallel jobs in optimal way requires some thought

- See server guides for specifics: http://research.csc.fi/guides
  - Use Taito for large memory jobs
  - Sisu for massively parallel jobs
  - Check also the software specific pages for examples and detailed information: http://research.csc.fi/software

Array jobs (advanced usage)

- Best suited for running the same analysis for large number of files

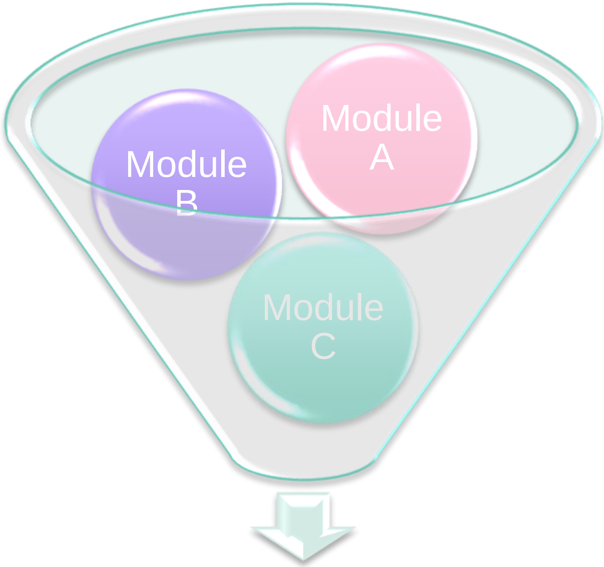
- #SBATCH --array=1-100
- Defines to run 100 jobs, where a variable `$SLURM_ARRAY_TASK_ID` gets each number (1,2,…100) in turn as its value. This is then used to launch the actual job (e.g. `srun myprog input_ $SLURM_ARRAY_TASK_ID > output_ $SLURM_ARRAY_TASK_ID`)
- Thus this would run 100 jobs:

```
srun myprog input_1 > output_1
srun myprog input_2 > output_2
…
srun myprog input_100 > output_100
```

- For more information
  - http://research.csc.fi/taito-array-jobs

Compiling your program

Why make?



Program

- program separated into several files
- multiple inter-dependant modules
- compilation and linking becomes easily a nightmare
  - especially when developing the program!

Why make?

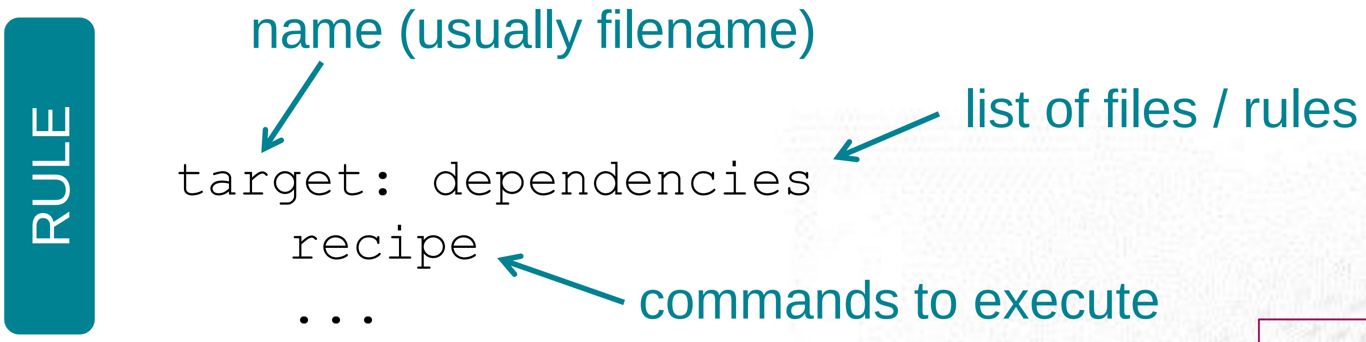
- when code has been modified, there are two approaches to compile the program:
  - re-compile everything → too slow
  - keep records and re-compile only what is needed → too much work

- make makes life easier by taking care of all the book keeping

Makefile

- defines:
  - work-flow(s) for producing target(s)
  - dependencies of each target
  - library paths, compiler flags etc.
- directives for conditional definitions etc.
- # starts a comment
- usually called `Makefile`
  - other choices: `makefile`, `GNUmakefile`

Basic syntax



RULE

name (usually filename)

list of files / rules

commands to execute

```
target: dependencies
    recipe
    ...
```

example:

```
foo.o: foo.c bar.h    # module foo
    cc -c foo.c

clean:                # remove all
    rm *.o
```

Note: use tabs instead of spaces to indent recipes!

Basic syntax

- *target*
  - usually the file that is produced by the recipe
  - name of an action also commonly used
    - for example: clean, distclean
- *dependencies*
  - a list of (source) files needed by the recipe
  - may also be other targets
- *recipe*
  - a list of commands to execute to make target

Logic of make

- read general macro definitions etc.
- call the rule for *target*
  - check when *dependencies* were changed
  - if any of the *dependencies* have changed, the *target* is re-built according to the *recipe*

- *dependencies* may also be *targets* for other rules
  - in that case, make calls those rules

Simple example

```
hello: main.o sub1.o sub2.o sub3.o
  f90 -o hello main.o sub1.o sub2.o sub3.o
main.o: main.f90
  f90 -c main.f90
sub1.o: sub1.f90
  f90 -c sub1.f90
sub2.o: sub2.f90
  f90 -c sub2.f90
sub3.o: sub3.f90
  f90 -c sub3.f90
clean:
  rm hello main.o sub1.o sub2.o sub3.o
```

Which target?

- by default, the first target is called
  - ’`hello`’ in the previous example
- target can be also specified when running `make`
  - `make target`
  - `make clean`
  - `make main.o`

Variables

- contain a string of text

```
variable = value
```

- substituted in-place when referenced

  $(variable) → value

- sometimes also called macros
- shell variables are also available in the makefile
  - $(HOME), $(USER), …

Two flavors of variables in GNU make

- recursive variables
  - defined as: `foo = bar`
  - expanded when referenced

```
foo = $(bar)
bar = $(ugh)
ugh = Huh?

$(foo) → Huh?
```

- simple / constant variables
  - defined as: `foo := bar`
  - expanded when defined

```
x := foo
y := $(x) bar
x = later

$(x) → later
$(y) → foo bar
```

Variables

- by convention variables are name in ALL-CAPS

- in the previous example we could have used a variable to store the names of all objects
  - `OBJ = main.o sub1.o sub2.o sub3.o`

Simple example revisited

```
OBJ = main.o sub1.o sub2.o sub3.o
hello: $(OBJ)
  f90 -o hello $(OBJ)
main.o: main.f90
  f90 -c main.f90
sub1.o: sub1.f90
  f90 -c sub1.f90
sub2.o: sub2.f90
  f90 -c sub2.f90
sub3.o: sub3.f90
  f90 -c sub3.f90
clean:
  rm hello $(OBJ)
```

Common variables

- some common variables
  - CC
  - CFLAGS
  - FC
  - FCFLAGS
  - LDFLAGS
  - OBJ
  - SRC

Special variables

- $@
  - name of the target

```
client: client.c
        $(CC) client.c -o $@
```

- $<
  - name of the first dependency

```
client: client.c
        $(CC) $< -o $@
```

Special variables

- $+
  - list of all dependencies
- $^
  - list of all dependencies (duplicates removed)
- $?
  - list of dependencies more recent than target

```
client: client.c
        $(CC) $+ -o $@
```

Special variables

- $*
  - common prefix shared by the target and the dependencies

```
client: client.c
        $(CC) -c -o $*.o $*.c
```

Special characters

- / continues a line
- # starts a comment
- @ executes a command quietly
  - by default, make echos all commands executed
  - this can be prevented by using @-sign at the beginning of the command

```
@echo ”quiet echo”

→ quiet echo
```

```
echo ”normal echo”

→ echo ”normal echo”
  normal echo
```

Special characters

- if there is an error executing a command, make stops
  - this can be prevented by using a – sign at the beginning of a command

```
clean:
        -rm hello
        -rm $(OBJ)
```

Implicit rules

- one can use special characters to define an implicit rule
- e.g. quite often target and dependencies share the name (different extensions)
  - define an implicit rule compiling an object file from a Fortran 90 source code file

```
%.o: %.f90
	$(F90) $(FFLAGS) -c -o $@ $<
```

Example revisited again

```
OBJ = main.o sub1.o sub2.o sub3.o

# implicit rule for compiling f90 files
%.o: %.f90
  f90 -c -o $@ $<

hello: $(OBJ)
  f90 -o hello $(OBJ)

clean:
  rm hello $(OBJ)
```

Built-in functions

- GNU make has also built-in functions
  - for a complete list see:
    - `www.gnu.org/software/make/manual/make.html#Functions`
- strip, patsubst, sort, …
- dir, suffix, basename, wildcard, …
- general syntax
  - `$(function arguments)`

Command line options

- `-j` parallel execution
- `-n` dry-run
  - shows the command, but does not execute them
- `-p` print defaults
  - shows default rules and values for variables before execution
- `-s` silent-run
  - do not print commands as they are executed

Command line options

- variables can also be defined from the command line
  - `make CC=gcc ”CFLAGS=-O3 -g” foobar`

Complete example

```
SRC = main.f90 sub1.f90 sub2.f90 sub3.f90
OBJ = $(patsubst %.f90, %.o, $(SRC))
F90 = gfortran
FFLAGS =
DEST = bin

# implicit rule for compiling f90 files
%.o: %.f90
   $(F90) $(FFLAGS) -c -o $@ $<

hello: $(DEST)/hello

$(DEST)/hello: $(OBJ)
   $(F90) $(FFLAGS) -o $@ $(OBJ)

clean:
   -rm $(OBJ)
   -rm $(DEST)/hello

# extra dependencies
sub2.o: modules.o
```

Science services at CSC: a short introduction

Software and databases at CSC

Software selection at CSC:

- http://research.csc.fi/software

Science discipline specific pages:

- http://research.csc.fi/biosciences
- http://research.csc.fi/chemistry

Chipster data analysis environment:

- http://chipster.csc.fi

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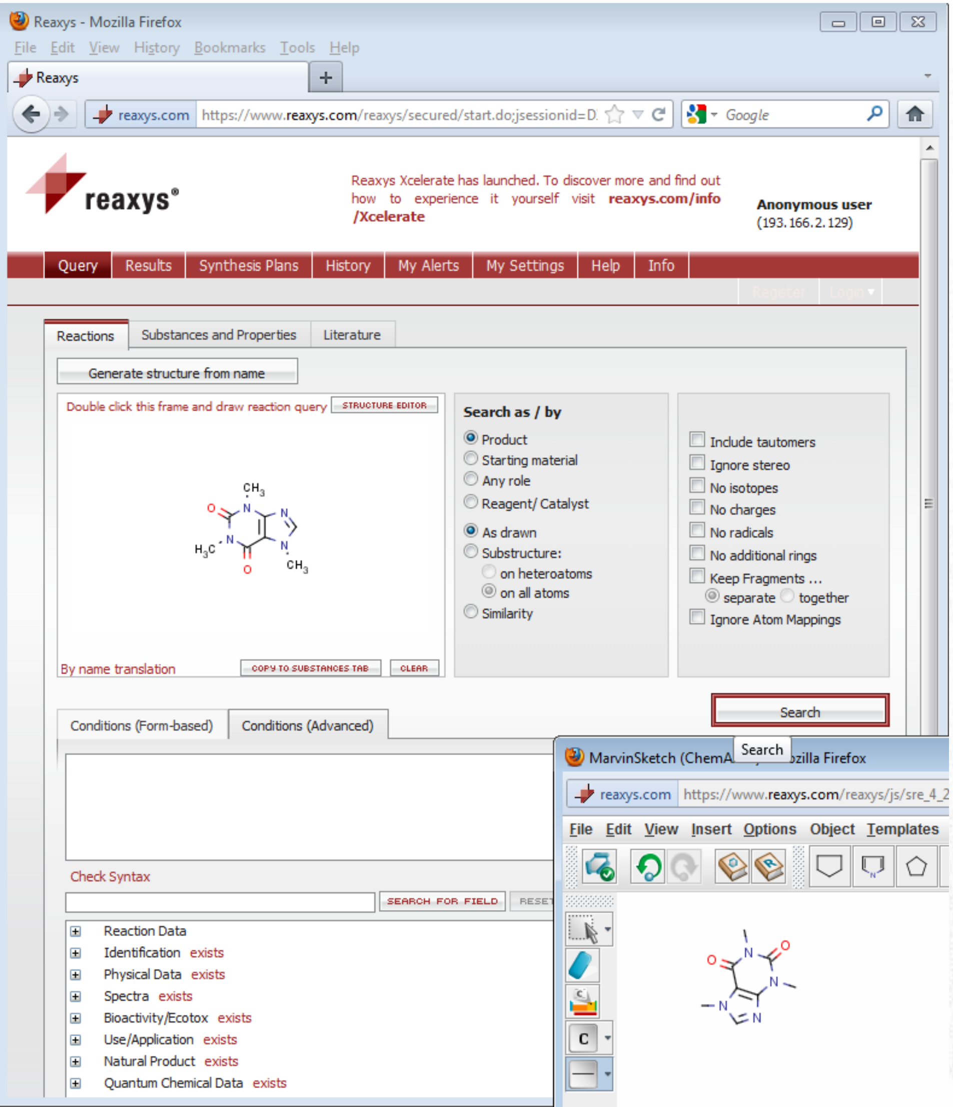
Innovation from CrossFire Beilstein


Reaxys - Mozilla Firefox
File Edit View History Bookmarks Tools Help
Reaxys
reaxys.com https://www.reaxys.com/reaxys/secured/start.do;jsessionid=D
Google
Query Results Synthesis Plans History My Alerts My Settings Help Info
Reactions Substances and Properties Literature
Generate structure from name
STRUCTURE EDITOR
COPY TO SUBSTANCES TAB CLEAR
Search
Conditions (Form-based) Conditions (Advanced)
SEARCH FOR FIELD RESET
MarvinSketch (ChemA... Mozilla Firefox
reaxys.com https://www.reaxys.com/reaxys/js/sre_4_2
File Edit View Insert Options Object Templates

Reaxys Xcelerate has launched. To discover more and find out how to experience it yourself visit reaxys.com/info/Xcelerate

Anonymous user (193.166.2.129)

Double click this frame and draw reaction query

By name translation

Search as / by

● Product
○ Starting material
○ Any role
○ Reagent/ Catalyst

● As drawn
○ Substructure:
○ on heteroatoms
● on all atoms
○ Similarity

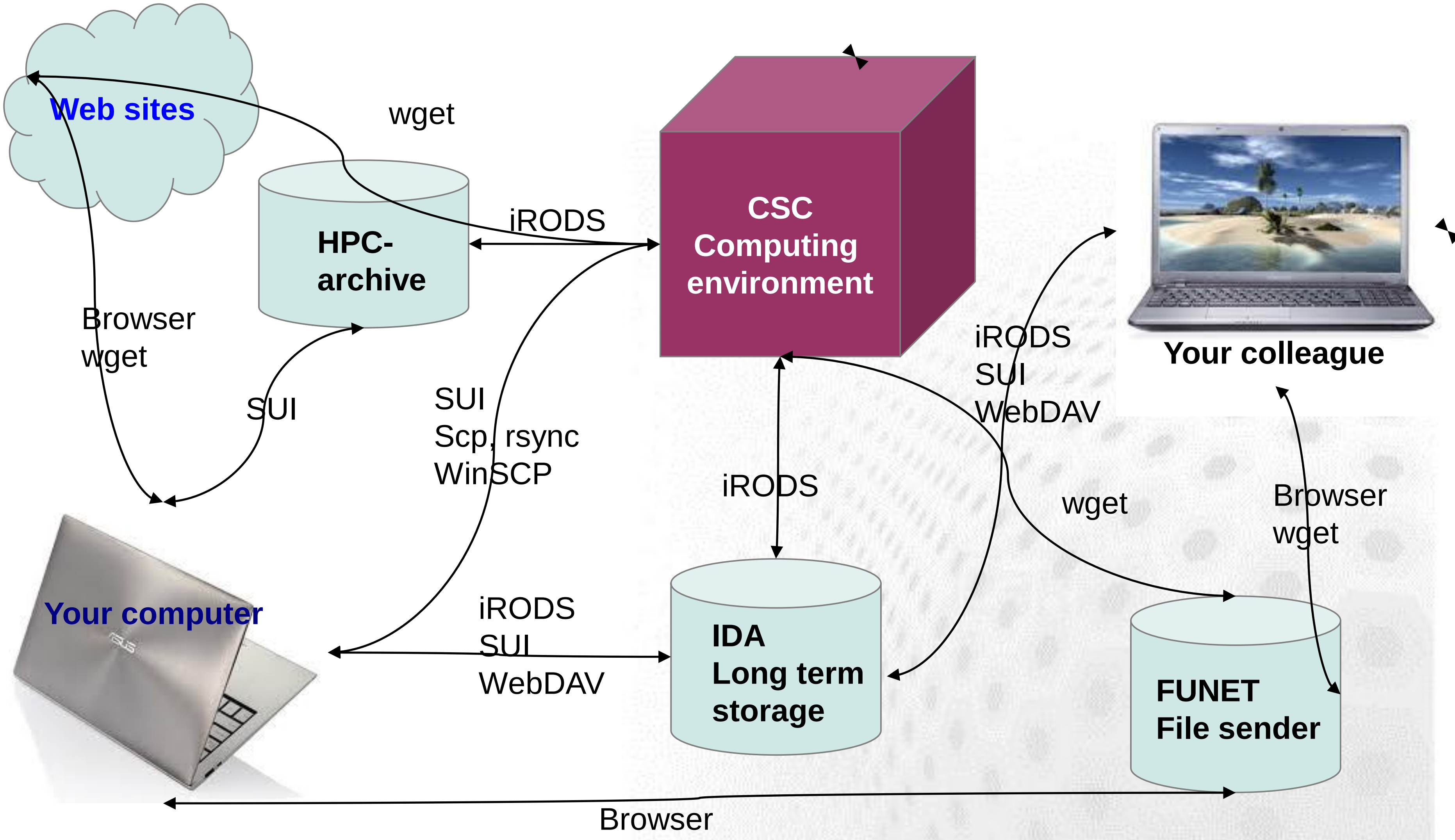
□ Include tautomers
□ Ignore stereo
□ No isotopes
□ No charges
□ No radicals
□ No additional rings
□ Keep Fragments ...
● separate ○ together
□ Ignore Atom Mappings

Check Syntax

- Reaction Data
- Identification exists
- Physical Data exists
- Spectra exists
- Bioactivity/Ecotox exists
- Use/Application exists
- Natural Product exists
- Quantum Chemical Data exists

- Use: www.reaxys.com
- No installations needed
- Properties, reactions, references of molecules and substances
- Consortium based
  - Aalto, Helsinki, Jyväskylä Universities and Technical Universities of Tampere and Lappeenranta
  - Costs often shared by many groups/libraries
- Current consortium agreement until end of 2014
- http://research.csc.fi/-/reaxys

Moving data to and from CSC



HPC Archive and IDA

- **IDA**

- Storage service for research data
- quotas are grated by the Universities and Academy of Finland
- several different interfaces
- accessible through normal network connections
- part of the Tutkimuksen tietoaineistot (www.tdata.fi)

- **HPC Archive**
  - Intended for CSC users
  - 2TB / user
  - Replaces the $ARCHIVE
  - Only command line interface to the CSC servers

IDA storage service

- iRODS based storage system for storing, archiving and sharing data
- The service was launched 2012
- Usage through personal accounts and projects
- Each project has a shared directory too
- Speed: about 10 GB/min at the servers of CSC
- CSC host's the service

Three interfaces:

- WWW interface in Scientists' User Interface
- network directory interface for Linux, Mac (and Windows XP)
- command line tools (i-commands installed at the servers of CSC)

Troubleshooter: Interactive session to deal with open questions and specific problems