



May 20th, 2016

Lecturers:
Luis Alves
Johan Guldmyr
Tomasz Malkiewicz
Kimmo Mattila
Ulf Tigerstedt (remotely)



## **Program**



| 09:30 - 10:00 | Morning coffee & registration   |
|---------------|---|
| 10:00 – 10:15 | Introduction: grid computing vs. local clusters, batch queue systems and cloud        |
| 10:15 - 11:00 | Introduction to grids   |
| 11:00 - 11:30 | Obtaining personal certificates hands-on  |
| 11:30 - 12:00 | NorduGrid ARC middleware hands-on   |
| 12:00-12:45   | Lunch (on own expense)  |
| 12:45 - 13:30 | Writing job description files hands-on  |
| 13:30 - 14:00 | Submitting and monitoring jobs hands-on   |
| 14:00-14:15   | Coffee  |
| 14:15 - 14:45 | Arcrunner grid job manager and MPI jobs on the grid hands-on                          |
| 14:45 - 15:00 | Wrap-up   |
| 15:00 - 15:30 | Troubleshooter: Interactive session to deal with open questions and specific problems |

## **Practicalities**



- Keep the name tag visible
- 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



#### CSC?

- Non-profit company owned by Ministry of education and culture
- Services mainly free for researchers
- Applications, computational capacity, user support, FUNET, information management services, data services
- Participating in 15 EU projects



#### Round robin



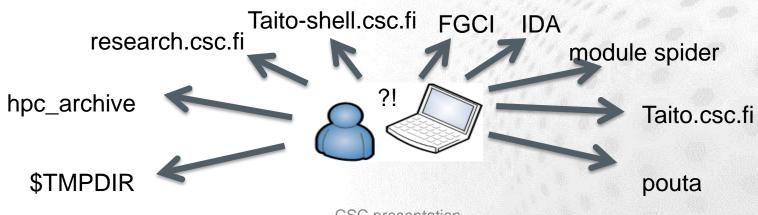
- Clément Fiere
- Matthew Hudson
- Khalid Latif
- Sofia Khan
- Pär Håkansson
- Trung Hieu Nguyen
- Markus Rauhalahti
- Eelis Solala





## **Learning target**

Know how to choose right server (resource)





#### Clusters

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





#### Finnish Grid Infrastructure - FGCI

- Distributed computing capacity
- 12 universities/research institutes + CSC
- Requires a certificate
- Preinstalled software
- ARC –middleware
- From your own computer or Taito

```
Oulu

Kuopio

Joensuu

Jyväskylä

Tampere

Lappeenunta

Turku

Espoo

Abo

Helsinki
```

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

FGCI guide



## Server use profiles



- FGCI (Dell/HP)
- Serial and parallel (12/16/24 cores)
- cPouta (HP) Cloud
- Serial and parallel (16 cores)
- Taito-shell (HP)
- Interactive jobs
- Very long jobs
- Auto queue, shared resources

- Sisu (Cray XE40)
- Parallel from 72 up to thousands of cores
- Scaling tests 1008+
- Taito (HP)
- Serial and parallel upto 448/672 cores
- Huge memory jobs
- Lots of preinstalled software

## Main Computing capacity: Sisu, Taito, FGCI

|              | Sisu<br>(Phase 2) | Taito<br>(Phase 2)                                     | FGCI<br>prerelease   |
|--------------|-------------------|--|--|
| Availability | 2014-             | 2015-  | 2016-  |
| СРИ          | x 12 and 2 x 8    | d Sandy Bridge, 2<br>cores, 2.6 GHz,<br>v3 and E5-2670 | Intel Xeon, 2 x 6 cores,<br>2.7 GHZ, X5650 and 4x12<br>Intel Xeon CPU E7-4830v3<br>@2.1GHz |
| Interconnect | Aries             | FDR IB   | QDR IB   |
| Cores        | 40512             | 9768+9216  | 7308+3600  |
| RAM/node     | 64 GB             | 64/128/256/<br>1536 GB                                 | 128/256/512 GB   |
| Tflops       | 1688              | 515  | 218  |
| GPU nodes    | -                 | 50   | ?  |
| Disc space   | 4 PB              | 4 PB   | 1+ PB  |



## Cloud computing: three service models

- Software as a Service (SaaS)
  - e.g. Chipster
- Platform as a Service (PaaS)
- Infrastructure as a Service (laaS)
  - e.g. Pouta



## cPouta – computing in the Cloud

- cPouta
  - Virtual machines on demand
  - Taito hardware
  - Dedicated resources (HPC focus)
- More freedom and flexibility
- More responsibility

#### cPouta's use cases



- Enhanced security isolated virtual machines
- Advanced users able to manage servers
- Difficult workflows can't run on Taito
- Complex software stacks
- Ready made virtual machine images
- Deploying tools with web interfaces
- "We need root access"

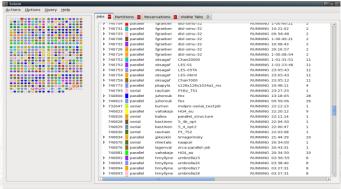
If you can run on Taito – run on Taito
If not – Pouta might be for you

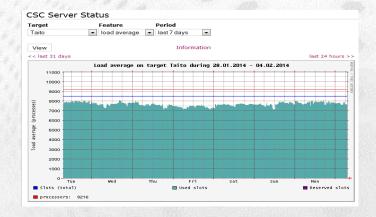
Pouta user guide: <a href="https://research.cisc.fi/pouta-user-guide">https://research.cisc.fi/pouta-user-guide</a>

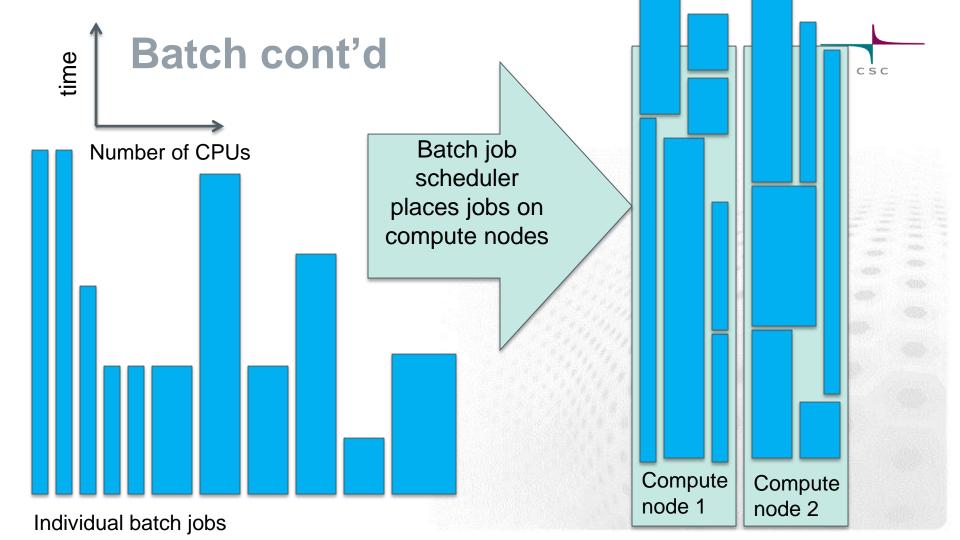


What is a batch system?

- 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)

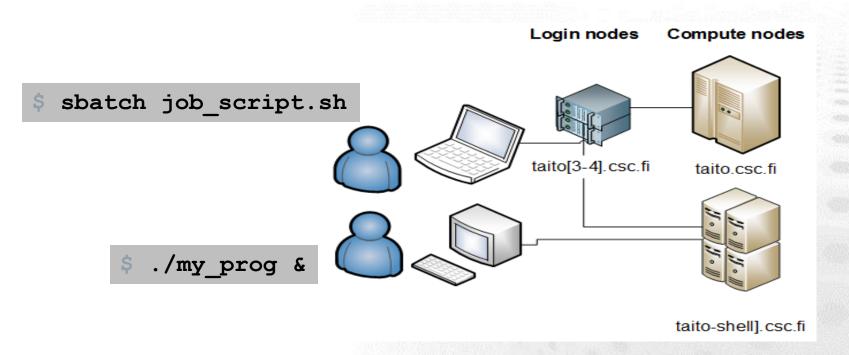








# Compute nodes are used via queuing system



## **Using grid**



- The jobs are submitted using the ARC middleware (http://www.nordugrid.org/arc/)
  - Using ARC resembles submitting batch jobs in Taito or Sisu
- ARC is installed Taito, but in many cases you can install it to your local machine too.

#### Sample ARC job description file



```
&
(executable=runbwa.sh)
(jobname=bwa 1)
(stdout=std.out)
(stderr=std.err)
(gmlog=gridlog 1)
(walltime=24h)
(memory=8000)
(disk=4000)
(runtimeenvironment>="APPS/BIO/BWA 0.6.1")
(inputfiles=
( "query.fastq" "query.fastq" )
( "genome.fa" "genome.fa" )
(outputfiles=
 ( "output.sam" "output.sam" )
```



## **Example serial batch job script on Taito**

```
#!/bin/bash -1
#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
#SBATCH --constraint=snb
```