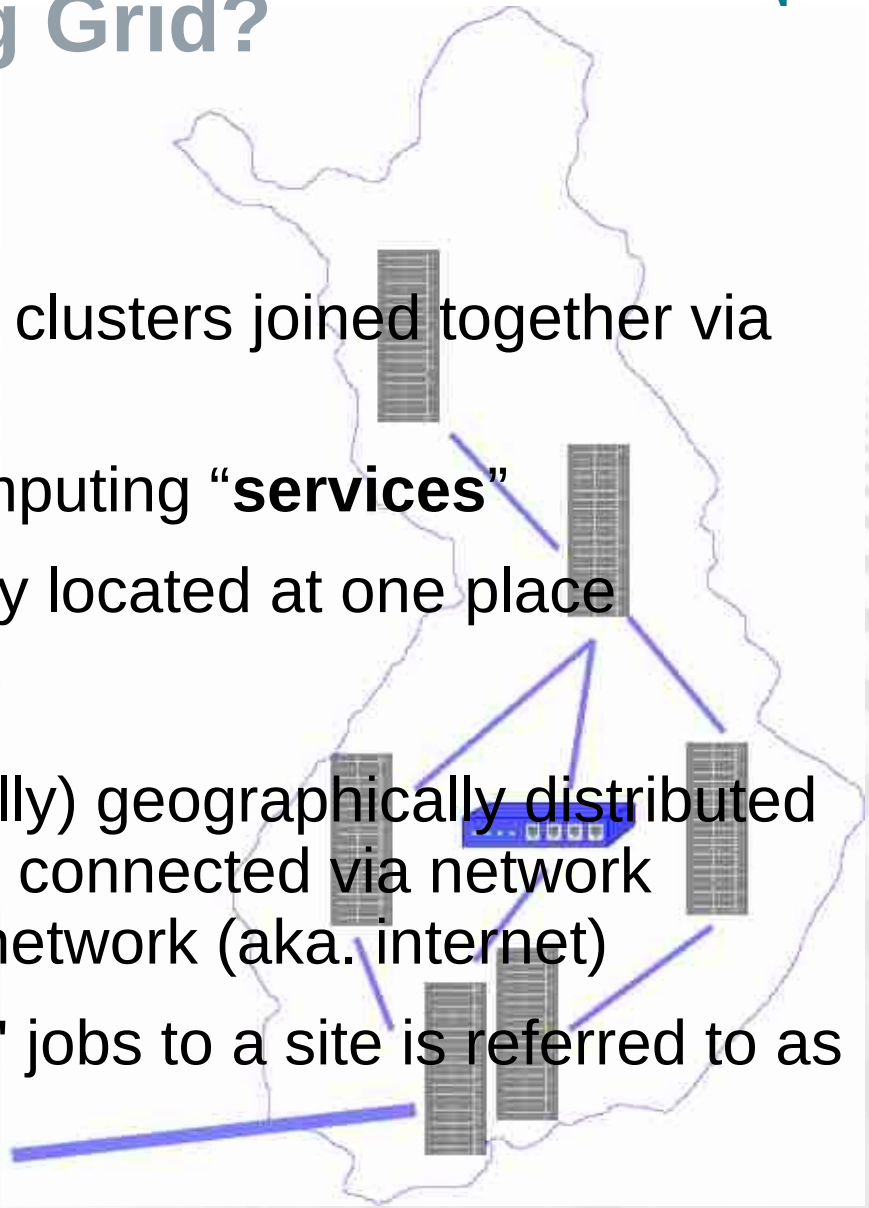
A National Computing Grid: FGI

Ulf Tigerstedt, Kimmo Mattila, Luis Alves

What is a computing Grid?

- **Site:**
  - One or more computing clusters joined together via network interfaces
  - Can also host other computing "**services**"
  - Generally geographically located at one place
- **Computing GRID:**
  - A number of sites (usually) geographically distributed where the frontends are connected via network interfaces to the GRID network (aka. internet)
  - Software to direct users' jobs to a site is referred to as **Grid Middleware**

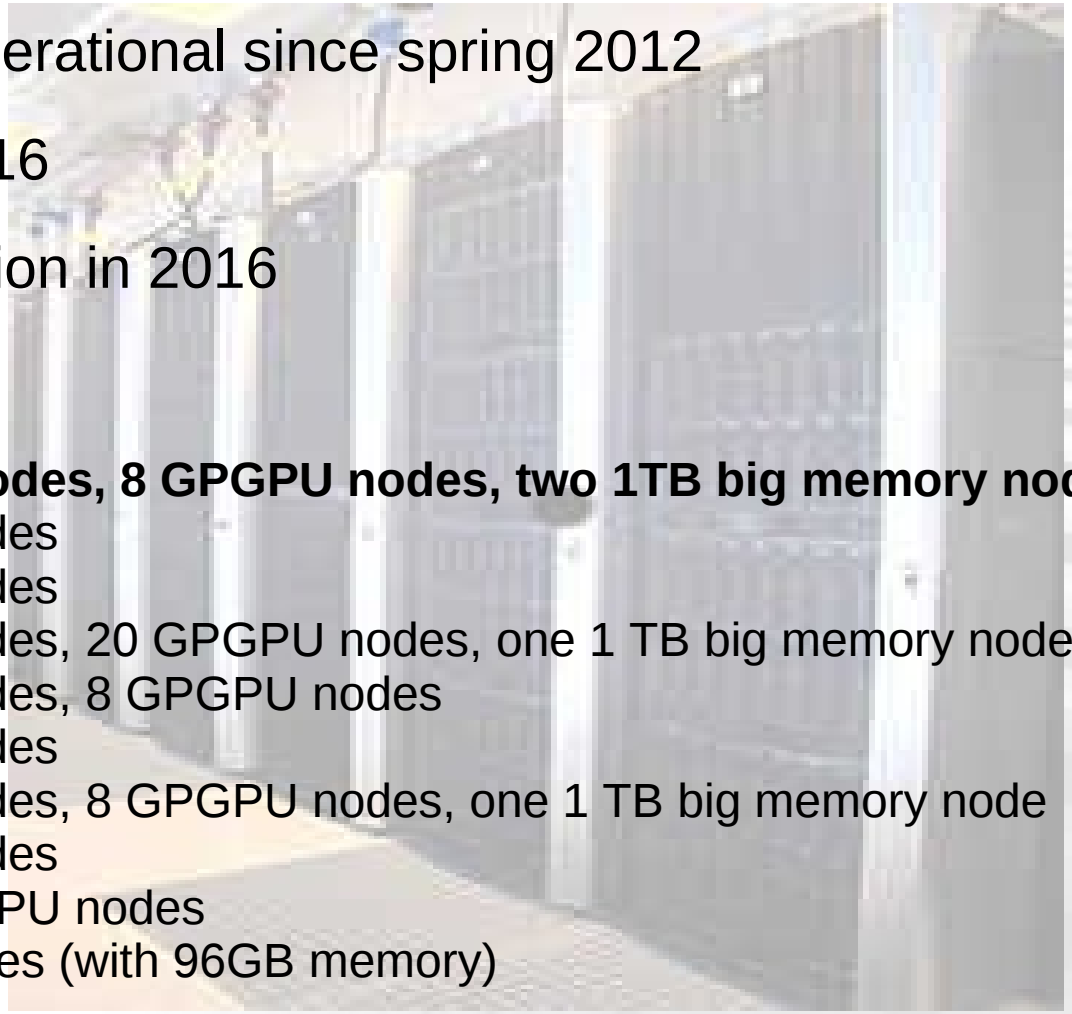


- **Virtual Organisation (VO):**
  - A community which has a common research or software requirement
    - Not geographically bound
    - Existing VOs can be easily joined
    - New VOs can be easily created

    (more on VOs further on)

FGCI - Backgroud

- FGI has been fully operational since spring 2012
- **Upgrade** to FGCI 2016
- New FCGI in production in 2016



Old setup

Aalto:	**112 nodes, 8 GPGPU nodes, two 1TB big memory nodes**
Lappeenranta:	16 nodes
Eastern Finland:	64 nodes
Helsinki:	49 nodes, 20 GPGPU nodes, one 1 TB big memory node
Jyväskylä:	48 nodes, 8 GPGPU nodes
Oulu:	30 nodes
Tampere (TUT):	37 nodes, 8 GPGPU nodes, one 1 TB big memory node
Turku:	20 nodes
Åbo Akademi:	8 GPGPU nodes
CSC:	24 nodes (with 96GB memory)

FGCI - Background

- Local use is open at all sites
- Sites maintain their own clusters:
  - Site administrators are encouraged to collaborate and communicate
    - Weekly meetings
    - Providing grid software support for users
    - Becoming part of the FGCI community
- Small team from CSC manage the general administration

Makeing Grid available for users

- CSC manages the FGCI grid environment
- CSC represents Finland as the National Grid Provider in EGI (European Grid Infrastructure)
  - FGCI is connected to EGI through common tools, protocols and agreements
- FGCI uses the ARC middleware
  - Developed by NorduGrid, part of the European Middleware Initiative (EMI)
- Grid functionality is fully operational across all sites.

What FGCI can offer you:

- Hardware resources
  - More resources than a single University can offer
  - Distributed nature means better availability even when the local cluster is full
  - Local account is not required!
- Software
  - There are a number of software packages already available for use via the grid
    - Runtime environments list is available at

https://confluence.csc.fi/display/fgi/Grid+Runtime+Environments

- Support
  - CSC provides GRID administrative support, software AND user support

send an email to : helpdesk@csc.fi

What do you need to get started?

1. Apply for a grid certificate from GEANT/digicert (a kind of grid passport)
2. Join the FGI VO (Access to the resources)
3. Install the certificate to Scientists' User Interface and Taito
(4. Install ARC client to your local Mac or Linux machine for local use)

Instructions:
http://research.csc.fi/fgci-user-guide

Please ask help to get started!
servicedesk@csc.fi

What do you need?

- Certificate
- VO membership
- The ARC client tools
  - Installable on
    - most Linux versions
    - MAC OSX
  - ARC is available at CSC in Taito.csc.fi
    - Also available on your local cluster login node

Certificates and Virtual Organizations

User accounts in grids - Certificates

- Grids do not use usernames and passwords
- Users are authenticated using x509 certificates
- If your home university is compatible with GÉANT network you can get a certificate from DigiCert

  https://www.digicert.com/sso

  – Certificate type: **Grid premium**
- Other option: Nordugrid certificate through CSC

User accounts in grids - Certificates

- Certificate is valid for one year
- Digicert installs the new certificate to your browser –> **Use your personal computer for obtaining the certificate!**
- Certificate must be transported to a machine where ARC middleware is used. ARC default:
  - `userkey.pem` and `usercert.pem` in `$HOME/.globus`

User accounts in grids - Certificates

- You can use the **My Certificates** repository for storing, transporting and converting your certificate:

  https://sui.csc.fi/group/sui/my-certificates

User accounts in grids – Virtual Organizations

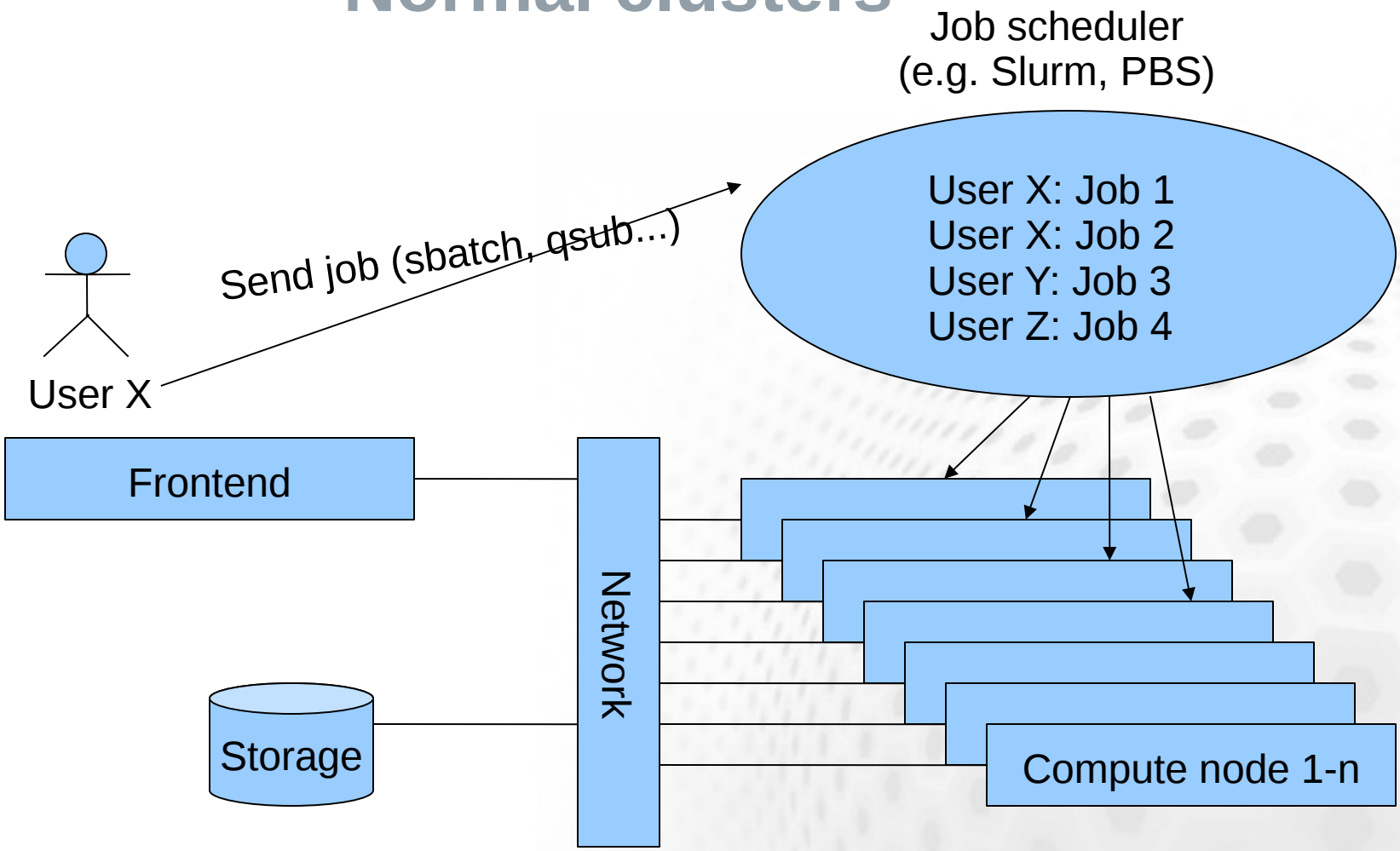
- FGCI Users must join **fgi.csc.fi VO**
  - Resources are given VOs, VOs give the resource to users.
  - To join fgi.csc.fi VO, **u**se the browser that has your certificate and go to:

    https://voms.fgi.csc.fi:8443/voms/fgi.csc.fi

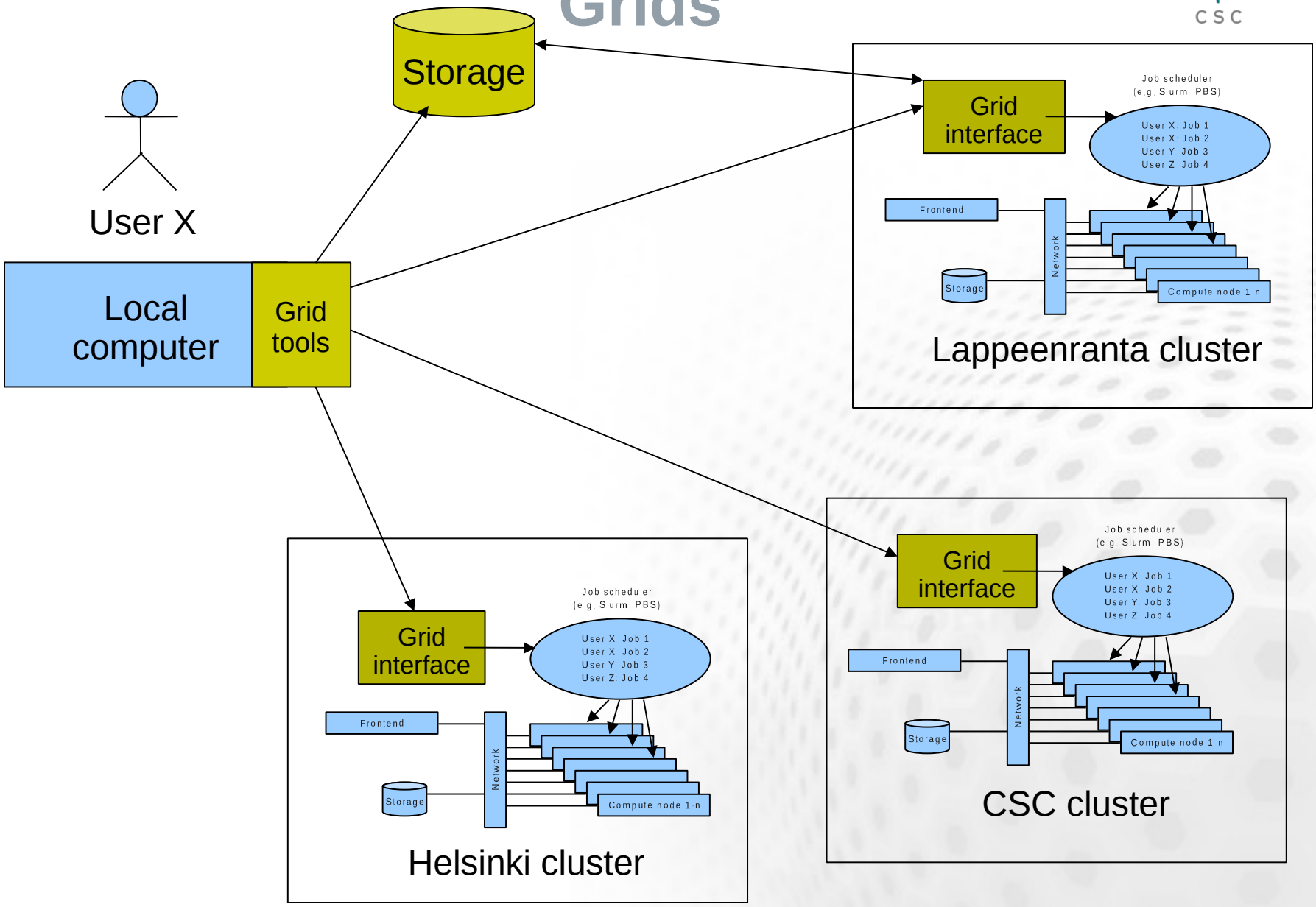
  - Membership is valid for one year
  - Many other VO:s exist for grid and Cloud computing
  - You can use same certificate in all VO:s

Grid Technologies: The ARC middleware

Normal clusters



Grids


Storage
User X
Local computer
Grid tools
Grid interface
Job scheduler (e.g. Slurm, PBS)
User X: Job 1
User X: Job 2
User Y: Job 3
User Z: Job 4
Frontend
Network
Storage
Compute node 1..n
Lappeenranta cluster
Grid interface
Job scheduler (e.g. Slurm, PBS)
User X: Job 1
User X: Job 2
User Y: Job 3
User Z: Job 4
Frontend
Network
Storage
Compute node 1..n
Helsinki cluster
Grid interface
Job scheduler (e.g. Slurm, PBS)
User X: Job 1
User X: Job 2
User Y: Job 3
User Z: Job 4
Frontend
Network
Storage
Compute node 1..n
CSC cluster

Grids and ARC

- The ARC middleware is used in FGCI
  - Server side
  - Client tools
- Also other grid middleware used in Europe
  - gLite
  - Unicore
  - condor

Using Grid

The jobs are submitted using the ARC middleware (http://www.nordugrid.org/arc/)

- Using ARC resembles submitting batch jobs in Taito
- ARC is installed inTaito, but you can install it to your local machine too.

Basic ARC commands:

`arcproxy -S fgi.csc.fi`	(Set up grid proxy certificate for 12 h)
`arcsub` ***`job.xrsl`***	(Submit job described in file job.xrsl)
`arcstat -a` or ***`job_id`***	(Show the status of all grid jobs)
`arcget` ***`job_id`***	(Retrieve the results of a grid job)
`arckill -a` or ***`job_id`***	(kill the given grid job)
`arcclean -a` or ***`job_id`***	(remove job related data from the grid)

ARC job

An ARC grid conputing task is defined with two files

1. Command file

A linux command script containing the commands to be executed

2. Job descriotion file

xrsl formatted text file defining the required resources (time, memory, CPUs etc) and files (command scripts, input files, output)

Sample ARC job script (runbwa.sh)

```
#!/bin/sh
echo "Hello BWA!"
bwa index genome.fasta
bwa aln -t $BWA_NUM_CPUS genome.fasta query.fastq > out.sai
bwa samse genome.fasta out.sai query.fastq > output.sam
echo "Bye BWA!"
exit
```

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)
(count=1)
(runtimeenvironment>="APPS/BIO/BWA_0.6.1")
(inputfiles=
( "query.fastq" "query.fastq" )
( "genome.fa" "genome.fa" )
)
(outputfiles=
  ( "output.sam" "output.sam" )
)
```

Input and output in job description files

Copy *datasetXYZ.dat* to the execution cluster as a file called *input.txt.*

```
(inputfiles=
( "input.txt" "datasetXYZ.dat" )
)
```

Copy *datasetXYZ.dat* to the execution cluster. Use the same name:

```
(inputfiles=
( "datasetXYZ.dat" "" )
)
```

Make `arcget` to retrieve all the files from the remote execution directory:

```
(outputfiles=("/" "" ))
```

Using Grid

- Run Time Environment (RTE): Definition file to use a software installed on a grid linked cluster (analogous to the “module load” command in the servers of CSC)

Bioscience related Run Time Environments in FGI:

- https://confluence.csc.fi/display/fgi/Grid+Runtime+Environments

  - **AMBER 12**
  - **AutoDock**
  - **BLAST**
  - **BOWTIE (0.12.7 and 2.0.0)**
  - **BWA**
  - **Cufflinks**
  - **EMBOSS**
  - **Exonerate**
  - **Freesurfer**
  - **FSL**
  - **GROMACS**
  - **GSNAP**
  - **GSNAP**
  - **HMMER**
  - **InterProscan**
  - **Matlab compile runtime**
  - **MISO**
  - **MrBayes**
  - **NAMD**
  - **R/Bioconductor**
  - **SAMtools**
  - **SHRiMP**
  - **TopHat**

Software in FGI

- Some scientific software is pre-installed
  - Primarily open source software
- Runtime environment defines a software setup

(analogous to *environment modules* in clusters)

https://confluence.csc.fi/display/fgi/Runtime+Environments

- You can also run your own programs in FGI
- If you have suggestions, contact us

Other ways to use the FGI

- Arcrunner: automatic job submission tool for large grid-job sets
- Automatic command line interfaces for: AutoDock, BLAST, BWA, BOWTIE2, InterPro, SHRIMP and Exonerate
- Matlab Compiler Runtime
- batch script wizard on SUI!

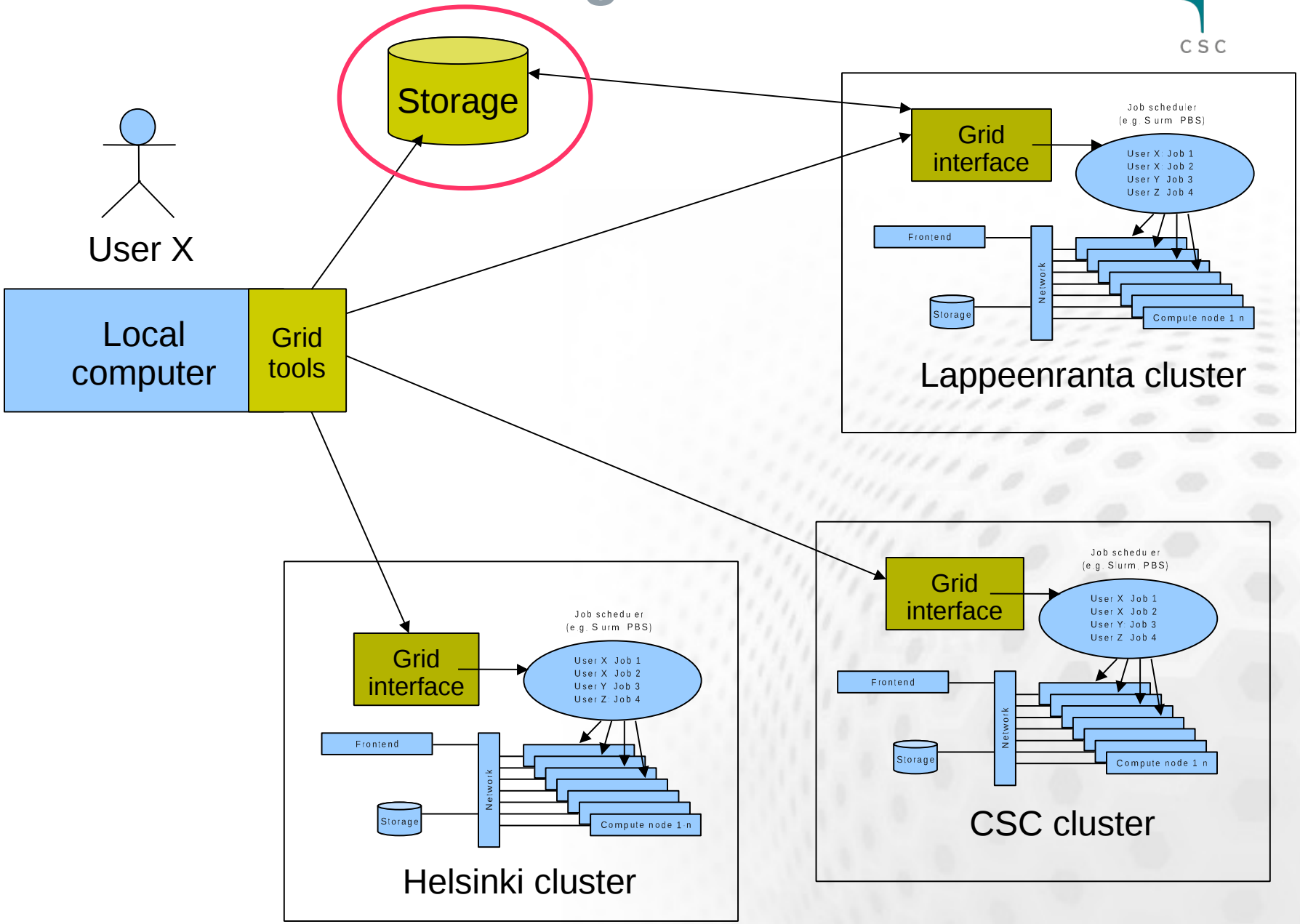
Arcrunner

- automatic job submission tool for large grid-job sets

```
arcrunner –xrsl my_job.xrsl
```

- Arcrunner work logic:
    1. Search for the given xrsl file in all subdirectories,
    2. if the file is found submit it to FGCI
    2. Monitor the status of subimitted jobs.
    3. If job finishes, retrieve the results
    4. If job fails, resubmit it to another cluster
- Available in Taito but can be installed locally too
- Error tolerant: you can continue interrupted arcrunner task by re-executing the command

Storage elemet



Storage element

- A storage site between you and grid clusters
- Linked to a cache propetry in the computing sites → middleware don't need to copy frequently used files for each grid job
- Wery useful with big datasets that will be used in several jobs
  - srm://bombay.csc.fi/fgi/userdirs
- Publicly visible
- Create your own directory under userdirs

Storage element - Usage

Copy data to storage element:

```
arccp bidgb.txt srm://bombay.csc.fi/fgi/userdirs/my_username/bigdb.txt
```

- Directories are automatically created

List data in the storage element

```
arcls -l srm://bombay.csc.fi/fgi/userdirs/my_username
```

Remove data in the storage element

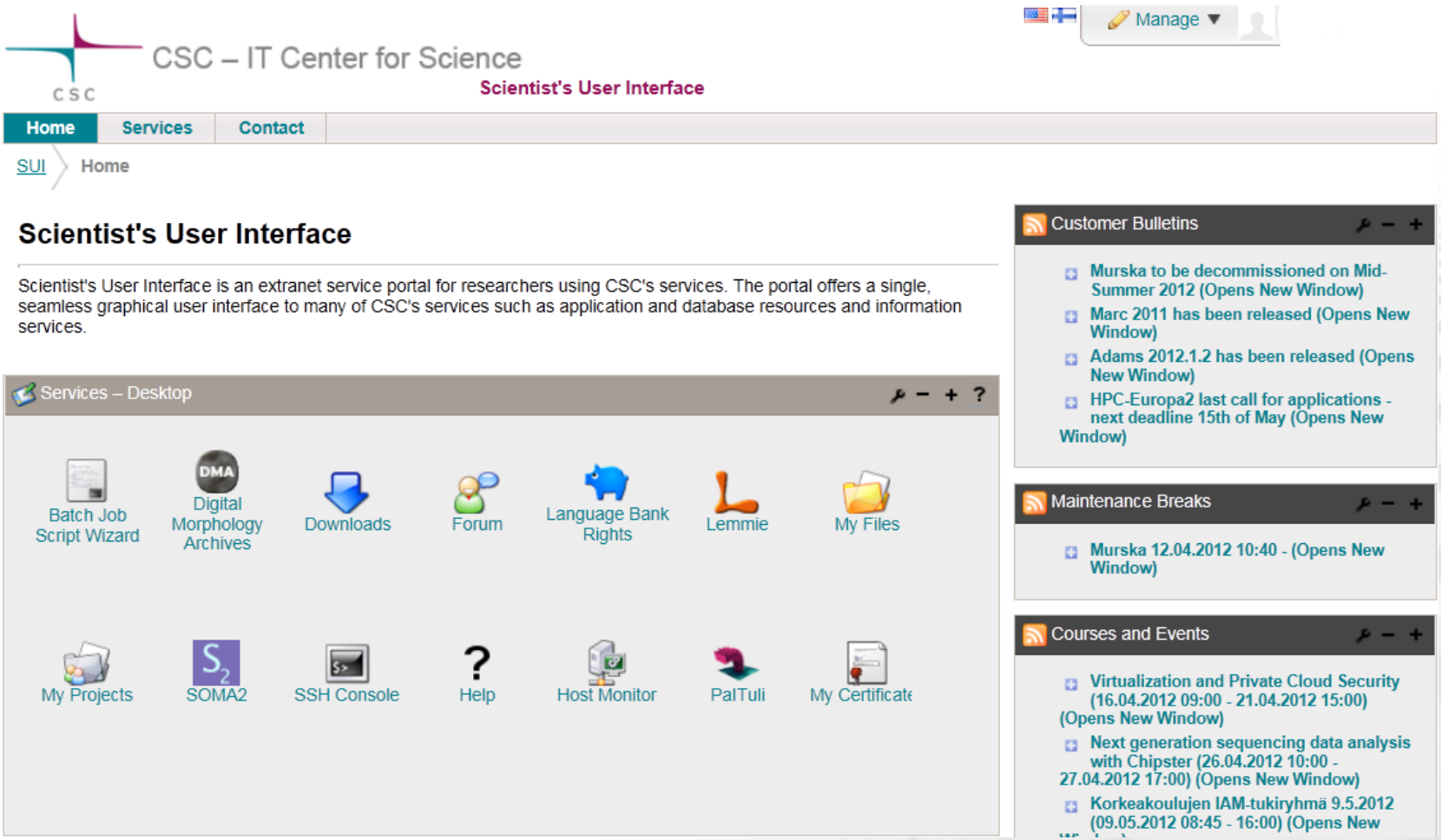
```
arcrm srm://bombay.csc.fi/fgi/userdirs/my_username
```

Using data in the grid job:

```
(inputfiles=
  ( “bigdb.txt” “srm://bombay.csc.fi/fgi/userdirs/my_username/bigdb.txt”)
)
```

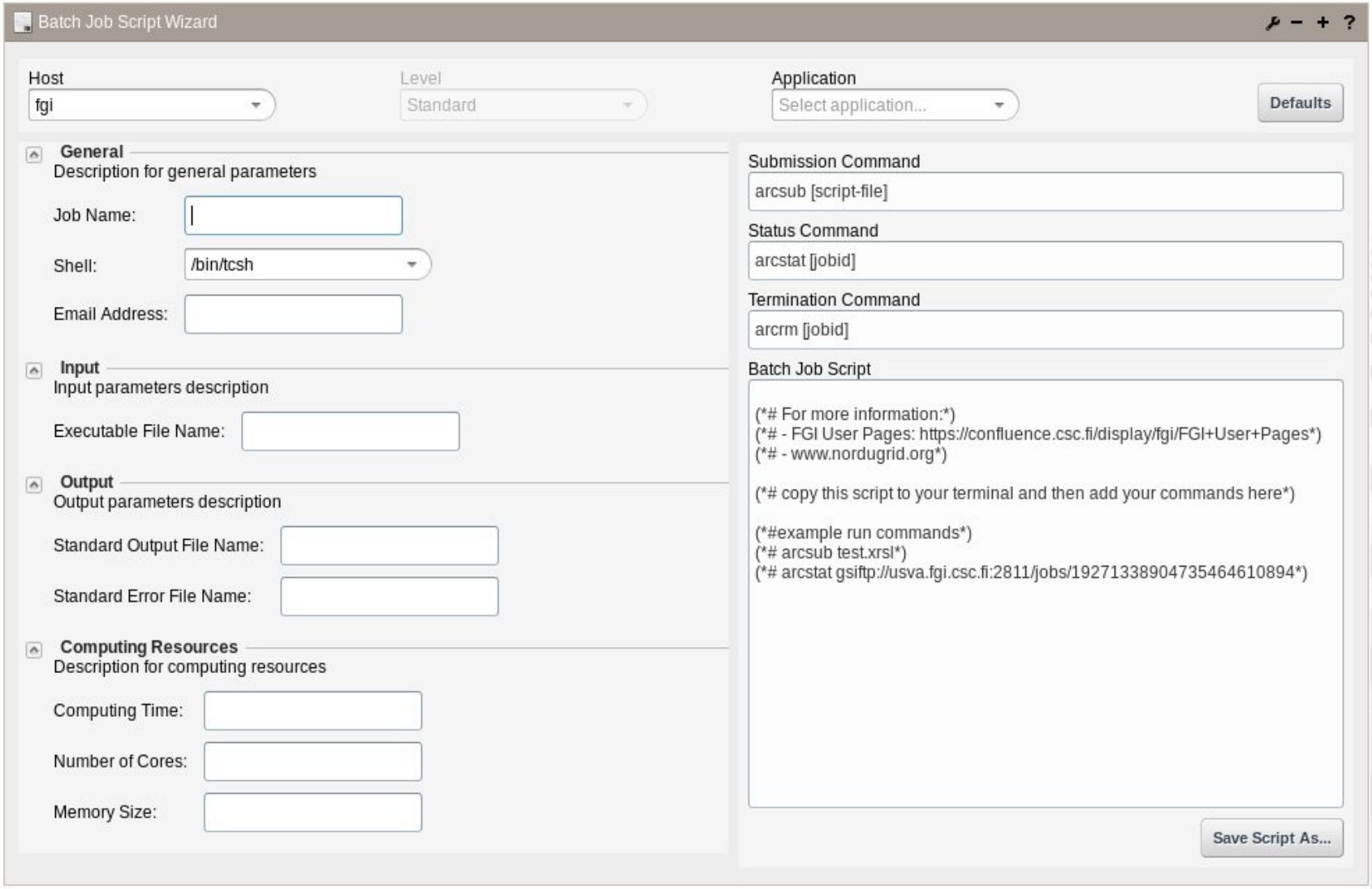
Scientist's User Interface: SUI

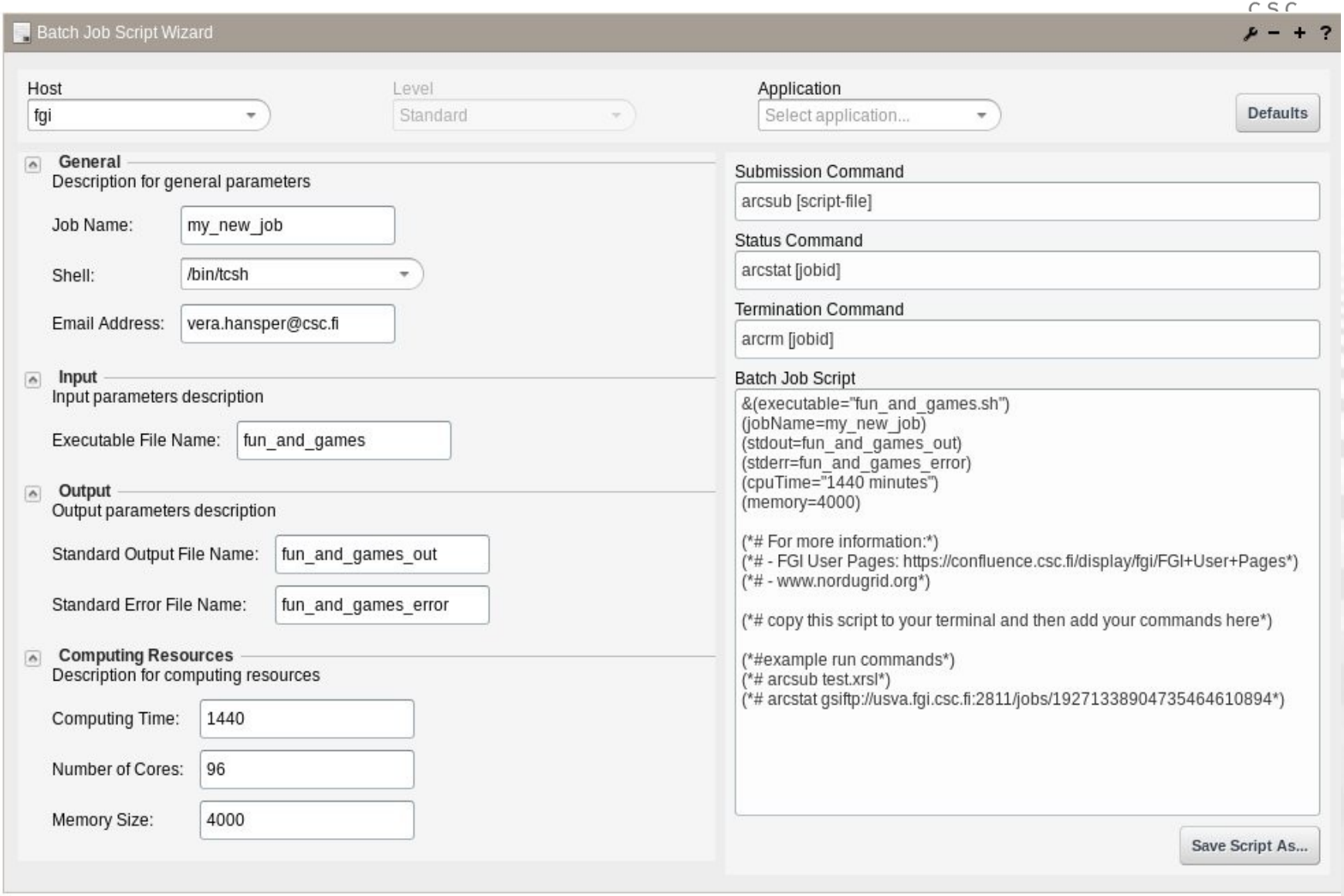
http://sui.csc.fi



More info at: http://www.csc.fi/english/research/SUI_presentation/download

Batch job wizard




Batch Job Script Wizard
Host
fgi
Level
Standard
Application
Select application...
Defaults
General
Description for general parameters
Job Name:
my_new_job
Shell:
/bin/tcsh
Email Address:
vera.hansper@csc.fi
Input
Input parameters description
Executable File Name:
fun_and_games
Output
Output parameters description
Standard Output File Name:
fun_and_games_out
Standard Error File Name:
fun_and_games_error
Computing Resources
Description for computing resources
Computing Time:
1440
Number of Cores:
96
Memory Size:
4000
Submission Command
arcsub [script-file]
Status Command
arcstat [jobid]
Termination Command
arcrm [jobid]
Batch Job Script
&(executable="fun_and_games.sh")
(jobName=my_new_job)
(stdout=fun_and_games_out)
(stderr=fun_and_games_error)
(cpuTime="1440 minutes")
(memory=4000)
(*# For more information:*)
(*# - FGI User Pages: https://confluence.csc.fi/display/fgi/FGI+User+Pages*)
(*# - www.nordugrid.org*)
(*# copy this script to your terminal and then add your commands here*)
(*#example run commands*)
(*# arcsub test.xrsl*)
(*# arcstat gsiftp://usva.fgi.csc.fi:2811/jobs/19271338904735464610894*)
Save Script As...


FGI
FINNISH GRID
INFRASTRUCTURE
A NEW FINNISH NATIONAL GRID
Tartun yliopisto
University of Tartu
egi
www.csc.fi