



Scientist User Interface

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CSC – IT Center for Science Ltd.

Scientist Interface



- WWW interface for CSC
- Still in development
- You can influence the contents

Scientist interface

- monitoring and managing your user account at CSC
- managing files in the servers of CSC
 - at the moment files in Hippu, Vuori and Murska
- Launch SSH console sessions

Scientist interface



- Use the Soma2 drug discovery environment
- Download software and data sets provided by CSC.
- Create batch job scripts for Louhi and Murska servers

Main page



CSC – IT Center for Science

Scientist's User Interface - BETA



Scientist's User Interface

Home

Services

Contact

Scientist's User Interface

Scientist's User Interface is an extranet service portal for researchers using CSC's services. The portal offers a single, seamless graphical user interface to many of CSC's services such as application and database resources and information services.

Services — Desktop

Batch Job Script Wizard

SSH Console

Forum

Downloads

My Files

DMA
Digital Morphology Archives

S₂
SOMA2

My Projects

Customer Bulletins

- [GOLD Suite v.5.0 installed in Murska](#)
- [New Maestro version 9.1 installed](#)
- [HPC-Europa2 call for applications - next deadline 15.9.](#)
- [Recent B3LYP calculations with CASTEP have errors](#)

Maintenance Breaks

- [Tutkijan käyttöliittymä / The Scientist's interface 13.09.2010 10:00 - 14:00](#)
- [Louhi 08.09.2010 06:00 - 16:00](#)

Courses and Events

- [Introduction to R programming \(06.09.2010 09:00 - 07.09.2010 16:00\)](#)
- [CSC Supercomputing Environment \(14.09.2010 09:00 - 16:00\)](#)
- [High-performance computing](#)

My files



The screenshot shows a Mozilla Firefox browser window displaying the 'My Files' page of CSC. The browser's address bar shows the URL `https://sui.csc.fi/group/sui/my-files`. The page header includes the CSC logo and the text 'CSC – IT Center for Science' and 'Scientist's User Interface - BETA'. A navigation menu has 'Home', 'Services', and 'Contact' tabs. The main content area is titled 'My Files' and shows a search bar with the text 'hippu'. Below the search bar is a table with columns for FILENAME, SIZE, OWNER, GROUP, PERMISSIONS, and LAST MODIFIED. The table lists three files: \$HOME, \$METAWRK, and \$WRKDIR, all owned by 'bergman' and belonging to the 'csc' group. A sidebar on the left shows 'MY PLACES' with a tree view including 'hippu', '\$HOME (Same for all hosts)', '\$METAWRK (Same for all hosts)', '\$WRKDIR', 'murska', and 'vuori'. The browser's status bar at the bottom shows 'Done' and the system tray includes 'FoxyProxy - Default' and several application windows like 'login', 'burden table...', 'The GIMP', and 'Layers, Ch...'. The system clock in the top right corner of the browser window shows 12:54.

FILENAME	SIZE	OWNER	GROUP	PERMISSIONS	LAST MODIFIED
\$HOME		bergman	csc	rwX-----	Sep 6, 2010 9:23 AM
\$METAWRK		bergman	csc	rwX-----	Aug 29, 2010 9:13
\$WRKDIR		bergman	csc	rwX-----	Aug 29, 2010 9:13

Batch job creator



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Home Services Contact

Batch Job Script Wizard

Host: Level: Application:

General
Description for general parameters

Job name:

Shell:

E-mail address:

Output
Standard output/error file definitions

Standard output file name:

Standard error file name:

Computing resources
Description for computing resources

Computing time:

Number of cores:

Cores/Node:

Memory size:

Submission Command:

Status Command:

Termination Command:

Batch Job Script:

Downloads



- Datasets provided by CSC
- Program manuals

The screenshot shows the CSC website's 'Downloads' page. The header includes the CSC logo, the text 'CSC – IT Center for Science', and 'Scientist's User Interface - BETA'. A navigation bar contains 'Home', 'Services', and 'Contact'. The main content area is titled 'Downloads' and includes a search bar and a table of folders. The table lists four folders: 'Contracts and Agreements', 'Course Material', 'Manuals', and 'Software', each with a link to subfolders and counts for folders and documents. Below the table, it says 'Showing 4 results.' and another section for 'Showing 0 results.' is partially visible.

Folder	# of Folders	# of Documents
Contracts and Agreements Contracts and Agreements related to software usage Subfolders: Accelrys , LMS International NV , Schrödinger , SIMULIA	9	9
Course Material Material categorized by event Subfolders: Crossfire Commander Webinar , Gaussian Workshop 09 , Reaxys Webinar	3	3
Manuals Manuals categorized by vendor Subfolders: CSD System , SIMULIA	3	12
Software Software packages categorized by vendor Subfolders: Accelrys , LMS International NV , Schrödinger , SIMULIA	30	65

Forum



CSC – IT Center for Science

Scientist's User Interface - BETA



Scientist's User Interface

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My Posts

My Subscriptions

Recent Posts

Statistics

Search

Search Categories

Category

Categories

Threads

Posts

[1. News and Announcements](#)

[Scientist's User Interface related news and announcements](#)

0

4

4

Actions

[2. Services Discussion](#)

[Discussion on services in Scientist's User Interface](#)

[Subcategories: Batch Job Script Wizard, Downloads, My Account, My Files, My Projects, More »](#)

6

12

24

Actions

[3. General Discussion](#)

[Any Scientist's Interface related discussion](#)

0

1

2

Actions

Showing 3 results.

My Projects



CSC – IT Center for Science

Scientist's User Interface - BETA



Scientist's User Interface



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PROJECT NAME	PROJECT MANAGER	CPU QUOTA REMAINING
CSC user's maintenance	Jari Rajala	714,073.393
	Jussi Heikonen	93,811.442

CPU Usage



Interval Begin Date: Interval End Date:

1/10



9/10



HOST	USER	CPU SECONDS	BILLING UNIT
murska		9,210.43	2.558

Project Information



Project Name:

Project Identifier:

Project Manager: Jussi Heikonen

Field of Science: Ympäristötieteet

Date of Issue: Aug 8, 2005 12:00:00 AM

Date of Expiry: Aug 8, 2011 12:00:00 AM

Project Description: [Show](#)

Last Updated: Aug 8, 2005 12:00:00 AM

CPU Quota



Quota: 93,814

Quota Used: 2.558

SSH console



The screenshot shows a Mozilla Firefox browser window displaying the SSH Console Application at `https://sui.csc.fi/sshconsole/view.jsp`. The terminal output includes:

```
Q-[Docs]-----Q
! User's guide available at http://www.csc.fi/english/pages/louhi_guide/
!
Q-[Directories]-----Q
! -> On Louhi $HOME, $METAWRK, and $ARCHIVE are mounted only on login nodes.
!   Files older than 90 days are automatically deleted from $WRKDIR
! -> Available modules can be listed with command: module avail
!
Q-[Queues]-----Q
! -> Available queues :
!   * parallel (default)
!     - jobs from 8-2048 cores up to 3 day walltime
!     - default walltime is 4 hours
!     - small jobs (8-32 cores) with up to 1 h walltime will run faster
!   * test
!     - 0-128 cores up to 15 min walltime, default walltime 1 min
!
! Queues are noninteractive!
!
! If you don't want your jobs to be rerun from the very beginning after a
! temporary unavailability of the execution host, specify "-r n" for "qsub"
! or "#PBS -r n" in a batch job script. The default is "-r y".
Q-[News]-----Q
! 2010-08-24: xt-asyncnpe 4.2 and xtpe-barcelona loaded as default.
!
Q-----Q
louhi-login3 ~> exit
logout
```

Two dialog boxes are overlaid on the browser window:

- Select Authentication Method(s)**: A dialog box with a lock icon and a question mark, asking to select an authentication method. The list includes `publickey` (selected), `password`, and `keyboard-interactive`. Buttons for `Cancel` and `Proceed` are at the bottom.
- Warning**: A dialog box with a question mark icon, displaying the message: "93.166.7.76' is unknown. The host key fingerprint is 1f 5a dd 50 a ea 82 c2 81 ab db c'." Below the message are buttons for `No`, `Yes`, and `Always`.

The browser's status bar at the bottom shows "Disconnected" and "FoxyProxy: Default".



Compiling programs

Compilers

- Multiple compiler environments available
 - PGI - Portland group Inc(default)
 - Pathscale
 - GNU
 - INTEL
- Change using modules
 - module switch PrgEnv-pgi PrgEnv-gnu

Compiling



- Same wrapper for all compiler suites
- MPI refers to Message passing interface

Language	Compiler (Vuori, Murska)	Compiler (Louhi)	Compiler (Hippu)	File Suffix
Fortran 90/95	mpif90	ftn	f90	.f .F .f90 .F90 .f95 .F95
Fortran 77	mpif77	f77	f77	.f .F
C	mpicc	cc	cc	.c .i
C++	mpiCC	CC	CC	.C .cc .ii

Compiler man pages

- Environment dependent manual information available:
 - man [pgcc | pgCC | pgf95]
 - man [craycc | crayCC | crayftn]
 - man [gcc | g++ | gfortran]
 - man [icc | icpc | ifort]

Compiling

- You should always use the wrappers
 - compiling (not pgf90 etc.)
 - linking (not ld)
- Wrappers will include most of the relevant libraries

Simple compiling example



- `(mpi)f90 -o hello.x hello.f90`
- `(mpi)cc -o helloc.x hello.c`

```
bergman@hippu1:~/scienv_comp>  
bergman@hippu1:~/scienv_comp> f90 -o hello.x hello.f90  
bergman@hippu1:~/scienv_comp> ./hello.x  
Hello World  
bergman@hippu1:~/scienv_comp> cc -o helloc.x hello.c  
bergman@hippu1:~/scienv_comp> ./helloc.x  
Hello World  
bergman@hippu1:~/scienv_comp> □
```

Compiling optimizations

- Compiler switch `-O<n>` controls compilation optimization
 - `n` is 1,2,3 or 4
 - 3 or 4 should be used with caution, because they may change results
- Example
 - f90 `-O2` -o hello.x hello.f90

Compiler switches

- c Compiles only, produces unlinked object filename.o
- o filename assigns the name filename to the executable. Default: a.out
- g Produces symbolic debug information
- Olevel Specifies whether to optimize or not and at which level

Using Libraries

- `mpif90 -L~/lib -llibname`
 - uses library `libname` and adds `~/lib` to library search path
- `mpicc -lm`
 - math library `math.h`
- **Compiler switches for libraries**
 - `-Idirname` Searches directory `dirname` for include files or module files
 - `-Ldirname` Searches directory `dirname` for for library files specified by `-l`
 - `-llibname` Searches the specified library file with the name `liblibname.a`

Libraries cont'd

- Common libraries included with simple module load
 - ACML
 - AMD Core Math Library
 - -lacml
 - IMSL
 - international Mathematics and Statistics Library

Machine Guides

- Murska

http://www.csc.fi/english/pages/murska_guide/index_html

- Louhi

http://www.csc.fi/english/pages/louhi_guide/index_html

- Vuori

http://www.csc.fi/english/pages/vuori_guide/index_html

- Hippu

http://www.csc.fi/english/pages/hippu_guide/index_html

Other interesting material



- Data services guide

<http://www.csc.fi/english/pages/data-services>

- Linux Basics

http://www.csc.fi/english/pages/data-services/linux_basics

- Software and databases

http://www.csc.fi/english/research/software/index_html