Risorse CINECA per il calcolo scientifico @polimi

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CINECA - HPC and Innovation Unit
Italy

5 e 11 novembre 2013
Politecnico di Milano

www.cineca.it

Agenda

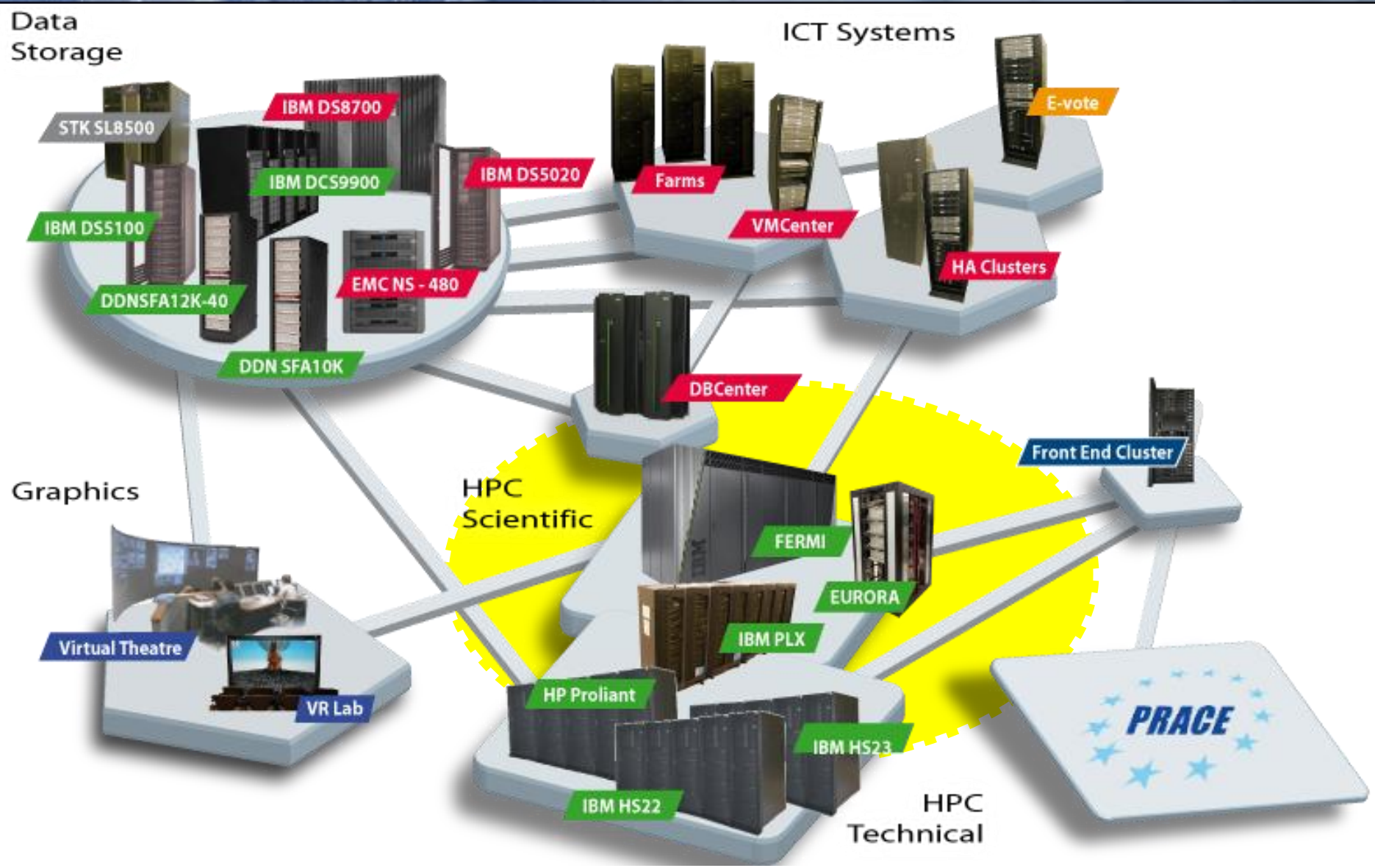
- CINECA 2.0
- Accesso alle risorse di calcolo HPC
- Convenzione di Ateneo POLIMI
- Accesso alle risorse: dettagli
- Esempio di utilizzo di applicativi ed ambienti presenti
- Domande aperte

CINECA 2.0

CINECA
è un Consorzio non profit costituito da 69 università italiane, l'Istituto Nazionale di Oceanografia e di Geofisica Sperimentale (OGS), il Consiglio Nazionale delle Ricerche (CNR) e il Ministero dell'Istruzione, dell'Università e della Ricerca (MIUR).

CINECA è il maggior centro di calcolo in Italia, uno dei più importanti nel mondo.
Il Dipartimento SuperCalcolo, Applicazioni e Innovazione (SCAI):

- gestisce *l'infrastruttura* HPC,
- fornisce supporto e risorse alla ricerca italiana e europea,
- **promuove iniziative di trasferimento tecnologico per l'industria**.


Data Storage
STK SL8500
IBM DS8700
IBM DCS9900
IBM DS5020
IBM DS5100
EMC NS - 480
DDNSFA12K-40
DDN SFA10K
ICT Systems
Farms
VMCenter
E-vote
HA Clusters
DBCenter
Front End Cluster
Graphics
Virtual Theatre
VR Lab
HPC Scientific
FERMI
EURORA
IBM PLX
HP Proliant
IBM HS23
IBM HS22
HPC Technical
PRACE

FERMI

Name: Fermi
Architecture: BlueGene/Q (10 racks)
Processor type: IBM PowerA2 @1.6 GHz
Computing Nodes: 10.240
Each node: 16 cores and 16GB of RAM
Computing Cores: 163.840
RAM: 1GByte / core (163 TByte total)
Internal Network: 5D Torus
Disk Space: 2PByte of scratch space
Peak Performance: 2PFlop/s

N. 12 in Top 500 rank (June 2013)

National and PRACE Tier-0 calls

EURORA

Architecture: Hybrid cluster by EUROTECH
Processor type: Intel Xeon E5-2687W Sandy Bridge-EP 3.1GHz
Computing Nodes: 64
Each node: 16 cores, 16GB/32 of RAM + 2 acceler
Computing Cores: 1.024
RAM:
Accelerators: 64 NVIDIA Tesla K20 +
64 Intel Xeon-Phi 5120D (MIC)
Internal Network: Infiniband & Custom
Peak performance: 110 TFlops

N. 1 in Green 500 rank (June 2013)

National and PRACE PrepAccess calls

PLX

Name: PLX
Architecture: IBM Hybrid Cluster
Processor type: Intel Xeon (Exa-Core Westmere) X 5645 @ 2.4 GHz
Computing Nodes: 274
Each node: 12 cores, 48GB of RAM, 2 GPUs
Computing Cores: 3.288
RAM: 14TByte
Internal Network: Infiniband 4xQDR switches (40 Gb/s)
Accelerators: 548 GPUs:
Peak Performance: 32 TFlops
565 TFlops SP GPUs
283 TFlops DP GPUs

National and PRACE Tier-1 calls

Accessi HPC

- Piattaforme con selezione:
  - Regionali
  - Nazionali
  - Europee
- Piattaforme senza selezione:
  - Convenzione d'Ateneo 2013

Piattaforme con Selezione

LISA	ISCRA	PRACE
Bando co-finanziato con Regione Lombardia Ricercatori Lombardi	Italian SuperComputing Resource Allocation Ricercatori Italiani	Ricercatori Europeo

- **LISA:** http://www.hpc.cineca.it/services/lisa
- **ISCRA:** http://www.hpc.cineca.it/services/iscra
- **PRACE:** http://www.prace-ri.eu/Call-Announcements?lang=en

Piattaforma senza selezione

Convenzione d'Ateneo 2013:

- Monte ore: 600 k ore su Eurora/PLX + 6.000 k ore su Fermi
- Scadenza: giugno 2014
- Servizi inclusi: user support

Per accedere POLIMI ha stabilito di identificare dei referenti Dipartimentali a cui vengono accreditati dei monte-ore associati a macro-*progetti. I referenti inseriscono le persone all'interno del loro* monte-ore come collaboratori.

Referenti di Ateneo

Dipartimento	Referente	FERMI (Kh)	EURORA (Kh)	Attivato
ENERGIA	D'ANGELO GIOVANNI	500	50	SI
TECNOLOGIE AEROSPAZIALI	MANTEGAZZA PAOLO	500	50	SI
INGEGNERIA CIVILE	GHISI ALDO FRANCESCO	500	50	SI
MECCANICA	MICCOLI STEFANO	500	50	SI
MATEMATICA	PAGLIERI LUCA	500	50	SI
INGEGNERIA GESTIONALE	MOSCONI ROCCO ROBERTO	500	50	NO
ELETTRONICA	BREVEGLIERI LUCA	500	50	SI
CHIMICA	CAVALLOTTI CARLO ALESSANDRO	500	50	SI

Tot assegnate: 4.0 mln -- 400 k

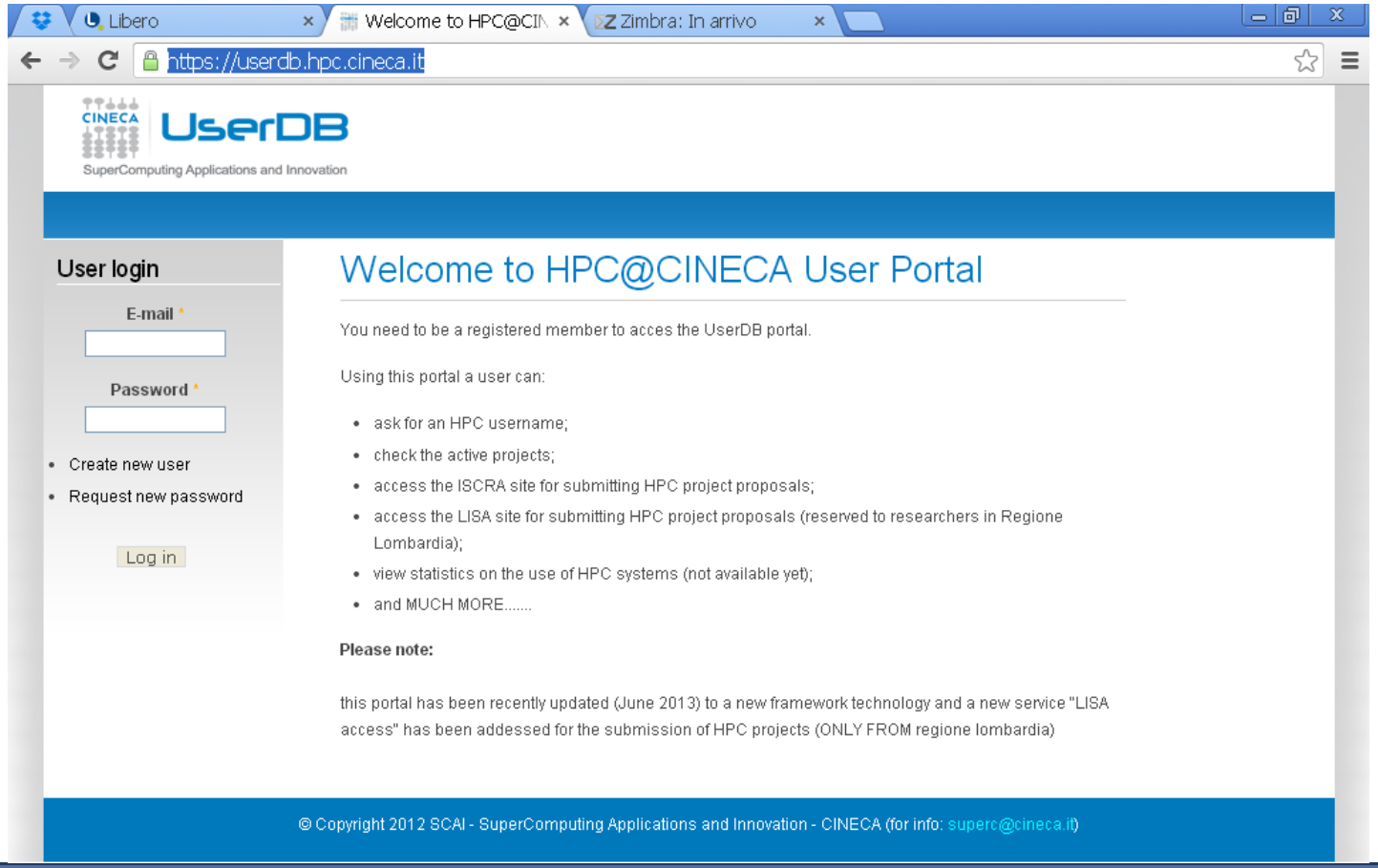
Da assegnare: 2.0 mln -- 200 k

Accesso alla convenzione

1. Iscrizione User DB CINECA (https://userdb.hpc.cineca.it/)
   - https://userdb.hpc.cineca.it/hpc-access (elenco azioni da completare)
2. Contattare referente di Dipartimento POLIMI chiedendo di essere inserito come collaboratore nel progetto di interesse
   - Referente si connette allo userDB sotto myprojects ed edita il nuovo collaboratore (edit/save)
3. Accesso alla piattaforma
4. Job submission

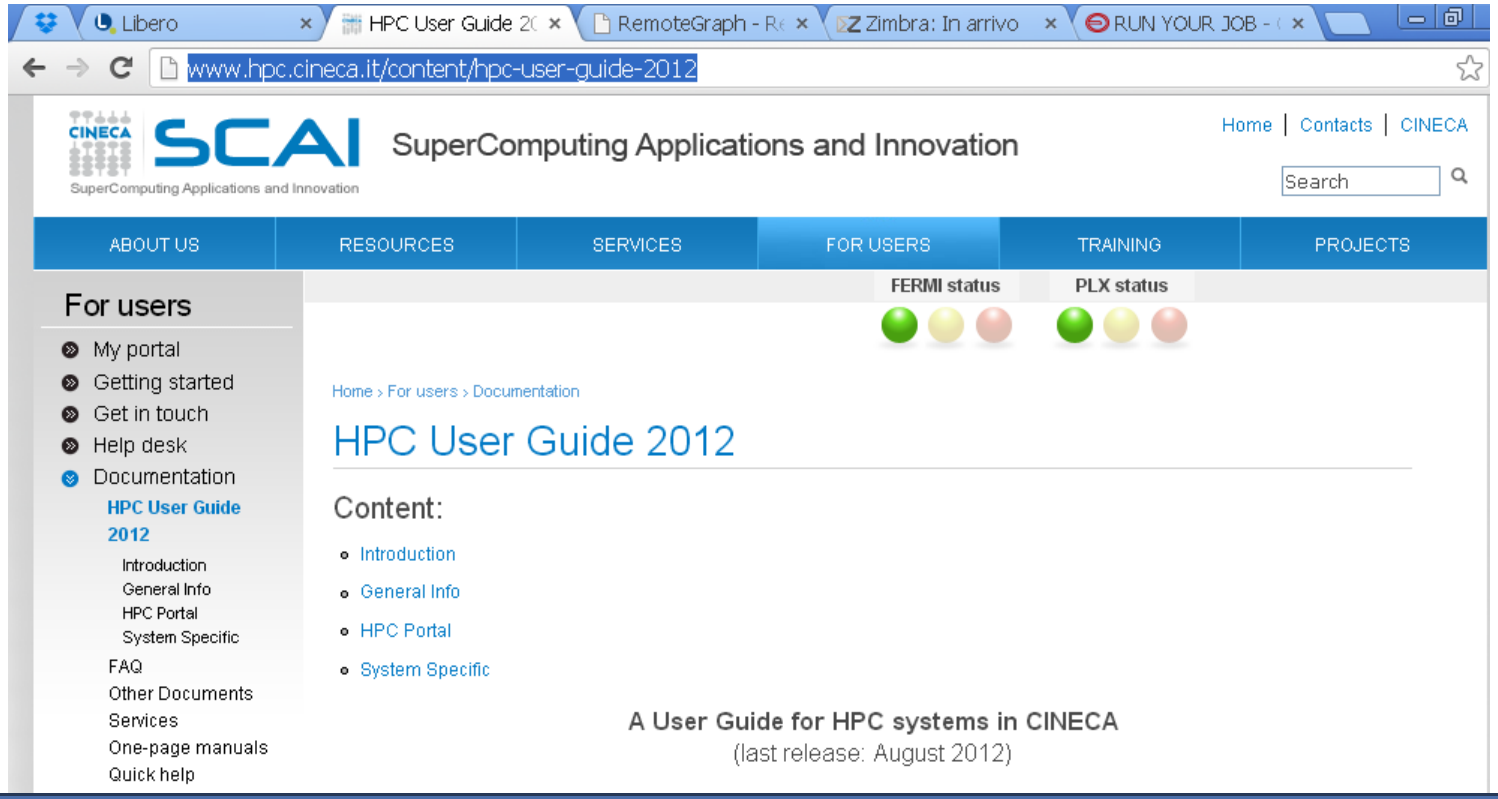
Iscrizione userDB CINECA

https://userdb.hpc.cineca.it/



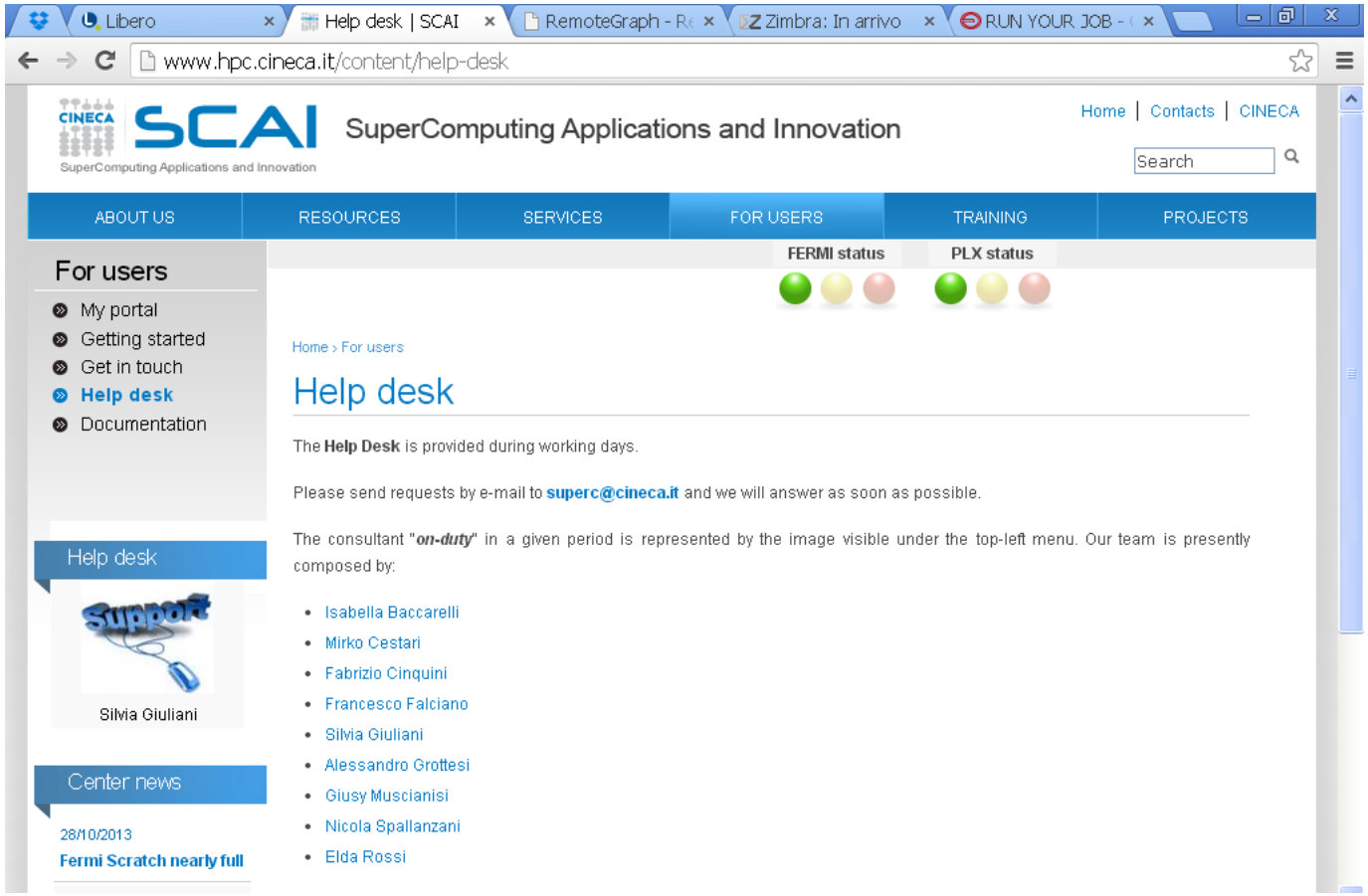
Informazioni generali

http://www.hpc.cineca.it
http://www.hpc.cineca.it/content/hpc-user-guide-2012



Helpdesk

http://www.hpc.cineca.it/content/help-desk



Get in touch

CINECA SCAI SuperComputing Applications and Innovation

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ABOUT US | RESOURCES | SERVICES | FOR USERS | TRAINING | PROJECTS

FERMI status PLX status

For users
- My portal
- Getting started
- Get in touch
- Help desk
- Documentation

Help desk

Alessandro Grottesi

Center news

30/10/2013
Crush of some running jobs on FERMI

28/10/2013
Fermi Scratch nearly full

23/10/2013
Fermi back to production

23/10/2013
Fermi temporarly unavailable

» more Center News

Home › For users

Get in touch

How to get Center's announcements (HPC-news)

We manage a mailing list (**HPC-news**) for posting announcements, scheduled downs, software updates, any problems and so on, about our HPC computing resources. It is advisable for HPC users to be included in that list!

You can subscribe (or unsubscribe) to HPC-news by sending an email from the address you want to subscribe. You can consult the archive browsing the archive web site.

To subscribe to HPC-new:

send a mail to listserv@list.cineca.it
in the body --> "subscribe hpc-news"
in the subject --> any string...

To unsubscribe to HPC-new:

send a mail to listserv@list.cineca.it
in the body --> "unsubscribe hpc-news"
in the subject --> any string...

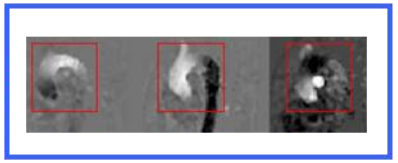
To consult the archive:
for the recent archive go to → Center News
for the full archive go to → http://list.cineca.it/archives/hpc-news.html

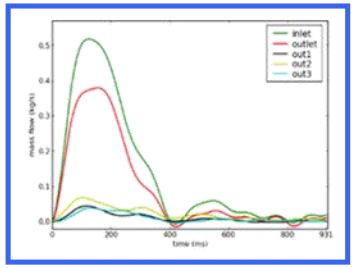
Premessa workflow CAE

PRE-PROCESSING → COMPUTATION → POST PROCESSING

COMPUTATIONAL

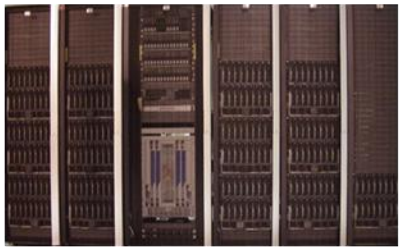
PHYSICS





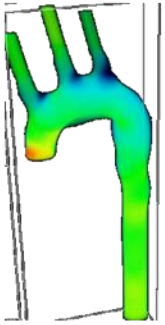
MODEL

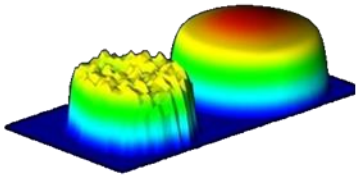
SOLVING



HPC ENVIRONMENT

VISUALIZATION





RESULTS

Pre/computing/post

Computing:
Non richiede interazione, BATCH processing.

Pre/Post possono richiedere interazione (GUI):
-RCM (Remote Connection Manager)
-Webcompute (su framework engineframe)

Applicativi disponibili

- Solutori
- Pre-processing (meshatori)
- Post-processing (visualizzazione)

Solutori

PLX/ EURORA

FERMI

- OpenFoam
  - Partial Diff Eq
  - OpenSource (per tutti)
- Ansys (CFD/mechanical/ …)
  - General sw for mech and CFD
  - 1 Licenza accademica contemporanea fino a 64 cores
  - Priorità utenti LISA (fare richiesta a superc)
- Abaqus
  - Finite Element Analyzer
  - licenza accademica
  - Priorità utenti LISA (fare richiesta a superc)
- StarCCM+
  - CFD (anche pre e post-processing)
  - 16 licenze accademiche fino a 128 cores
  - Priorità utenti LISA (fare richiesta a superc)
- Elmer
  - Finite element Sw for multiPhys
  - Open Source (per tutti)

Pre-processing

PLX/
EURORA

- Pointwise
  - Mesh Generation Software for CFD
  - Due licenze (una con priorità calcolo industriale)
  - Priorità utenti LISA (fare richiesta a superc)
  - Utilizzabile via webcompute e RCM (interfaccia grafica) o tramite script

Post-processing

PLX/
EURORA

- Paraview
  - Open Source Scientific Visualisation
  - Utilizzabile via webcompute e RCM
  - OpenSource (per tutti)
- Tecplot 360
  - CFD Visualization software
  - Due licenze accademiche (fare richiesta a superc)
  - Utilizzabile via RCM

Computing: Accesso alle macchine

Modalità di accesso previste:

1. ssh client
2. sftp client
3. Web-based via Engineframe (Nice Tech.)
4. Grafica (GUI):
   - RCM
   - webcompute

Ssh (Secure Clients)

Shell per utenti Linux (scp, ssh)

per utenti windows:

- Putty (ssh)
- TECTIA client (ssh)
- Winscp per utenti windows (sftp)

Esempio utilizzo

- Moduli e loro caricamento
- Utilizzo openfoam batch
- Utilizzo Ansys/Fluent batch
- Utilizzo paraview con GUI

PLX login: *ssh login.plx.cineca.it*

```
Last login: Wed Oct 30 08:35:17 2013 from 131.175.80.185
*****************************************************************************
*                                                                           *
*  Welcome to PLX DataPlex Cluster @ CINECA  -  RedHat EL 5.6!              *
*                                                                           *
*  Qlogic QDR (40Gb/s) Infiniband high-performance network                  *
*                                                                           *
*  274 Compute node                                                         *
*  - 2 esa-core Intel(R) Xeon(R) CPU E5645 @2.40GHz per Compute node        *
*  - 48 GB RAM per Compute node                                             *
*  - 2 Nvidia Tesla M2070 GPU per Compute node                              *
*  8 Fat node                                                               *
*  - 2 quad-core Intel(R) Xeon(R) CPU X5570 @2.93GHz per Fat node           *
*  - 128 GB RAM per Fat node                                                *
*  3352 Total cores                                                         *
*                                                                           *
*  6 Remote Visualization Login                                             *
*  2 Nvidia QuadroPlex 2200 S4                                              *
*                                                                           *
*  PBSpro 10.4 batch scheduler                                              *
*                                                                           *
*  http://www.hpc.cineca.it/content/ibm-plx-gpu-user-guide-0                *
*  for a guide on PLX                                                       *
*                                                                           *
*  mailto: superc@cineca.it  for support                                    *
*                                                                           *
*****************************************************************************
[rponzini@node342 ~]$
```

Moduli disponibili: *module avail*

```
[rponzini@node342 ~]$ module avail
------------ /cineca/prod/modulefiles/profiles ------------
profile/advanced      profile/base(default) profile/engineering
```

module load profile/engineering

```
$ module load profile/engineering
$ module available

------------ /cineca/prod/modulefiles/profiles -----------------------
profile/advanced      profile/engineering   profile/base(default)

……

------------ /cineca/prod/modulefiles/engineering/tools --------------
paraview/4.0.1--gnu--4.5.2 tecplot/2012R1  python/2.7.3--gnu--4.5.2

-------- /cineca/prod/modulefiles/engineering/applications ----------
abaqus/6.12-1      elmer/2011                pointwise/17.0_R1
ansys/145          openfoam/2.2.1-gnu-4.7.2  starccm+/8.04.010/Acd
```

module help

```
$ module help abaqus

abaqus-6.12-1
The Abaqus Unified FEA product suite offers powerful and complete solutions for both routine and
    sophisticated engineering problems covering a vast spectrum of industrial applications.
-------------------------------------------------------------------------------
Example of a batch job for running on 4 nodes 8 procs for node (cpus=32) using the input my_data

#!/bin/bash
#PBS -N abq_parallel
#PBS -j oe
#PBS -l walltime=0:10:00
#PBS -l select=4:ncpus=8:mpiprocs=8
#PBS -A <Account_number>
#PBS -q parallel
cd $PBS_O_WORKDIR
module load autoload abaqus
cp $ABAQUS_HOME/Documentation/example_cineca/my_data.inp .
cp $ABAQUS_HOME/Documentation/example_cineca/my_data.f .
echo "Running on " `hostname`
echo "Working dir is $PBS_O_WORKDIR"
echo "Job started at " `date`
abaqus job=my_data user=my_data cpus=32 interactive
echo "Job finished at " `date`
-----------------------------------
```

```
This application is restricted access. To be enabled please
contact superc@cineca.it.
To check license server status:
abaqus licensing lmstat -a -c 7400@license02-a.cineca.it
```

module load & show

```
$ module load abaqus
WARNING: abaqus/6.12-1 cannot be loaded due to missing prereq.
HINT: the following modules must be loaded first: intel/11.1—binary

$  module load autoload abaqus
### auto-loading modules intel/11.1--binary
### auto-loading modules openmpi/1.4.5--intel--11.1--binary
$
$ module show abaqus
-------------------------------------------------------------------
/cineca/prod/modulefiles/engineering/applications/abaqus/6.12-1:

module-whatis   The Abaqus Unified FEA product suite offers …
conflict        abaqus
setenv          ABAQUS_HOME /cineca/prod/applications/abaqus/6.12-1/binary
prepend-path    PATH    /cineca/prod/applications/abaqus/6.12-1/binary/Commands :
prepend-path    LIBPATH /cineca/prod/…/6.12-1/code/lib  :
prepend-path    LD_LIBRARY_PATH /cineca/prod/…/6.12-1/code/lib  :
prepend-path    MANPATH /cineca/prod/…/6.12-1/binary/Documentation/docs/v6.12/pdf_boo
-------------------------------------------------------------------
```

[rponzini@node342 rponzini]$ more carica220

module purge
module load profile/engineering
module load autoload openfoam

[rponzini@node342 rponzini]$ more carica-ansys145

module purge
module load profile/engineering
module load autoload ansys/145

Caricamento ambiente CFD

Fluent (Ansys)

[rponzini@node342 rponzini]$ source carica-ansys145

[rponzini@node342 rponzini]$ which fluent

/cineca/prod/applications/ansys/145/intel--12.1--binary/v145/fluent/bin/fluent

OpenFoam

[rponzini@node342 rponzini]$ source carica220

[rponzini@node342 rponzini]$ which pisoFoam

/cineca/prod/applications/openfoam/2.2.0-gnu-4.7.2/openmpi--1.6.3--gnu--4.7.2/OpenFOAM-2.2.0/platforms/linux64GccDPOpt/bin/pisoFoam

Job interattivi

```
[rponzini@node342 rponzini]$ qsub -I
qsub: ERROR: Account number None is not valid for user rponzini

[rponzini@node342 rponzini]$ qsub -I -A cin_staff
qsub: waiting for job 1344006.node351.plx.cineca.it to start
qsub: job 1344006.node351.plx.cineca.it ready
```

Job list

```
[rponzini@node004 ~]$ qstat -n -u $USER

node351.plx.cineca.it:
                                                          Req'd  Req'd   Elap
Job ID          Username Queue    Jobname    SessID NDS TSK Memory Time  S Time
--------------- -------- -------- ---------- ------ --- --- ------ ----- - -----
1343893.node351 rponzini visual   rponzini-p   7087   1   1    --  12:00 R 01:09
   node097ib0/1
1344001.node351 rponzini dcv_visu XTerm       14722   1   1    --  06:00 R 00:08
   node098ib0/1
1344003.node351 rponzini dcv_visu ParaView    16633   1   1    --  06:00 R 00:06
   node098ib0/2
1344004.node351 rponzini dcv_visu ParaView    22661   1   1    --  06:00 R 00:02
   node098ib0/3
1344006.node351 rponzini debug    STDIN       27624   1   1    4gb 00:30 R 00:00
   node004ib0/3
1344007.node351 rponzini privatel HL_18kt     30341  10 120  470gb 48:00 R 00:00
   node196ib0/0*12+node197ib0/0*12+node198ib0/0*12+node199ib0/0*12
   +node201ib0/0*12+node202ib0/0*12+node205ib0/0*12+node206ib0/0*12
   +node207ib0/0*12+node208ib0/0*12
```

Fluent Job submission

```
#!/bin/sh
#PBS -N test32
#PBS -j oe
#PBS -q parallel
#PBS -l select=4:ncpus=12:mpiprocs=8
#PBS -l walltime=24:0:0
#PBS -A cin_staff
#PBS -V

cd $PBS_O_WORKDIR
module load profile/engineering
module load autoload ansys
NPROCS=`wc -l < $PBS_NODEFILE`
echo "Job started at `date` on nodes: `cat $PBS_NODEFILE` "

EXEC=`which fluent`

time $EXEC  3ddp -i journal.jou -t$NPROCS -g -ssh -pinfiniband.ofed -mpi=intel >& myout4x8.out -
    cnf=${PBS_NODEFILE}
wait
echo "Job finished at `date` "
```

OpenFoam Job submission

```
#!/bin/sh
#PBS -j oe
#PBS -m abe
#PBS -M r.ponzini@cineca.it
#PBS -l select=6:ncpus=12:mpiprocs=6:mem=10gb
#PBS -A cin_staff
#PBS -V

cd $PBS_O_WORKDIR
module load profile/advanced
module load autoload openfoam

NPROCS=`wc -l < $PBS_NODEFILE`

echo "Job started at `date` on nodes: `cat $PBS_NODEFILE` "
decomposePar
EXEC=`which multiphaseEulerFoam`

time mpirun -machinefile $PBS_NODEFILE -np $NPROCS $EXEC -parallel >& out-36-
   simple_spare_lowU.log

echo "Job finished at `date` "
```

Pre/computing/post

Computing:
Non richiede interazione, BATCH processing.

Pre/Post possono richiedere interazione (GUI):
-RCM (Remote Connection Manager)
-Webcompute (su framework engineframe)

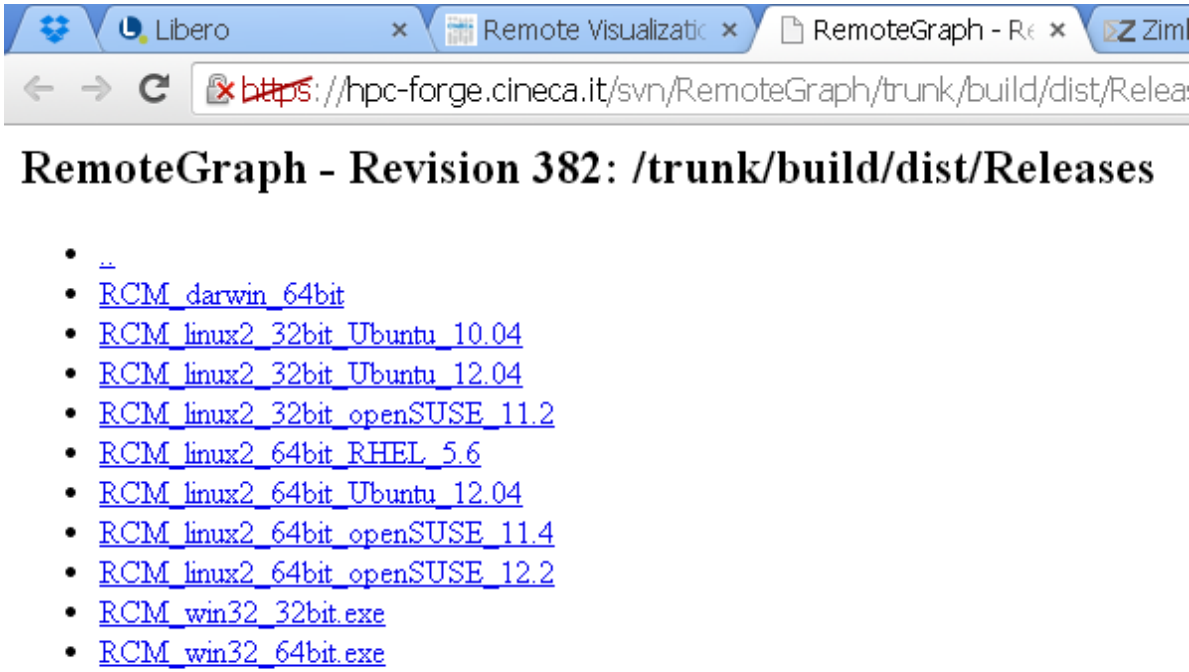
Applicativi con GUI e visualizzazione remota

- Due differenti strumenti, entrambi utilizzano gli acceleratori grafici su PLX/EURORA, entrambi si basano su grafica “remota”
  - **RCM: Remote Connection Manager**
  - ***Webcompute***
- *Utili per pre e post-processing*

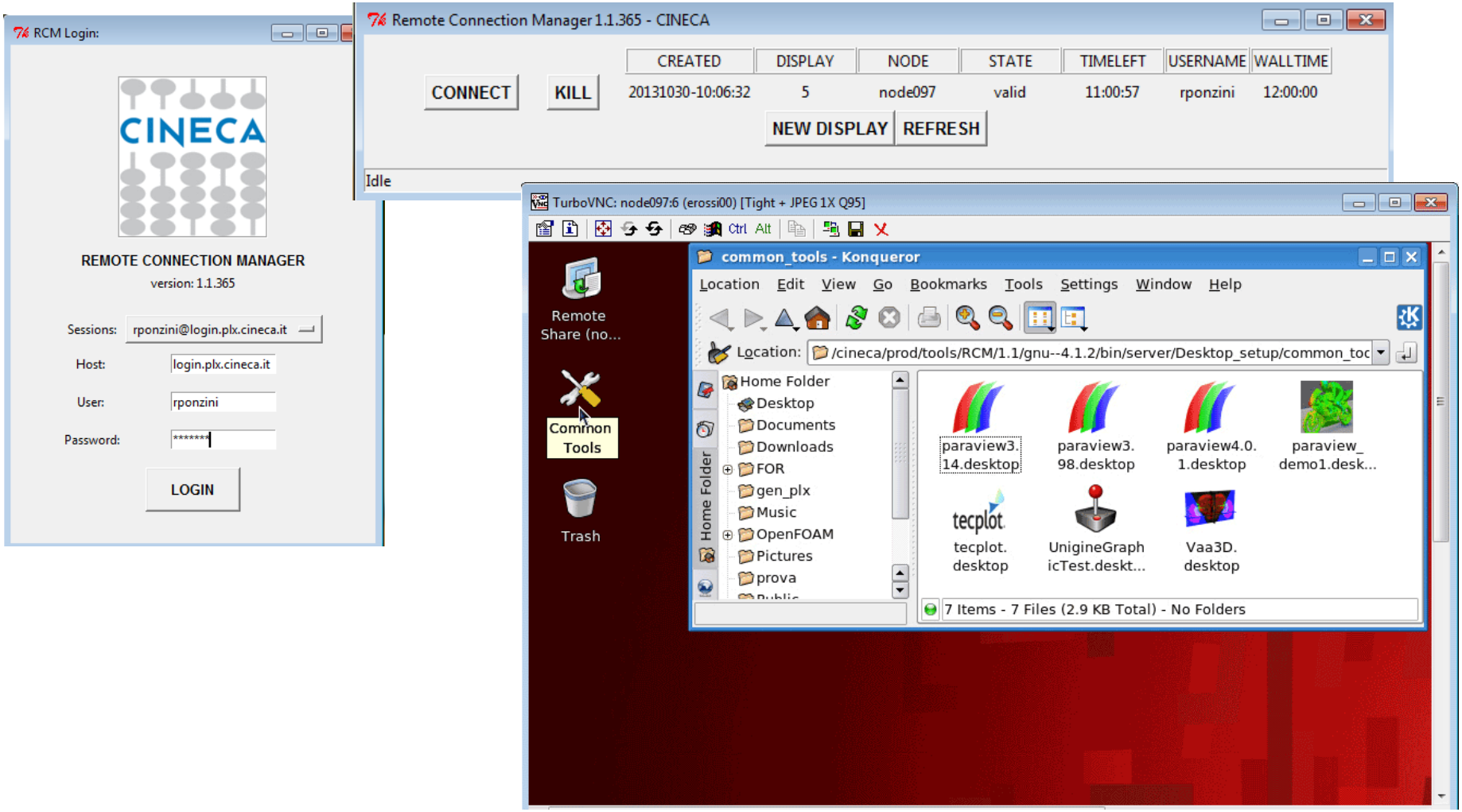
RCM: Remote Connection Manager

http://www.hpc.cineca.it/content/remote-visualization

- Sito di dipartimento *www.hpc.cineca.it*
- Seguire il link services → RemoteVisualiz → download
- Scaricare il client corretto per la propria workstation
- eseguirlo

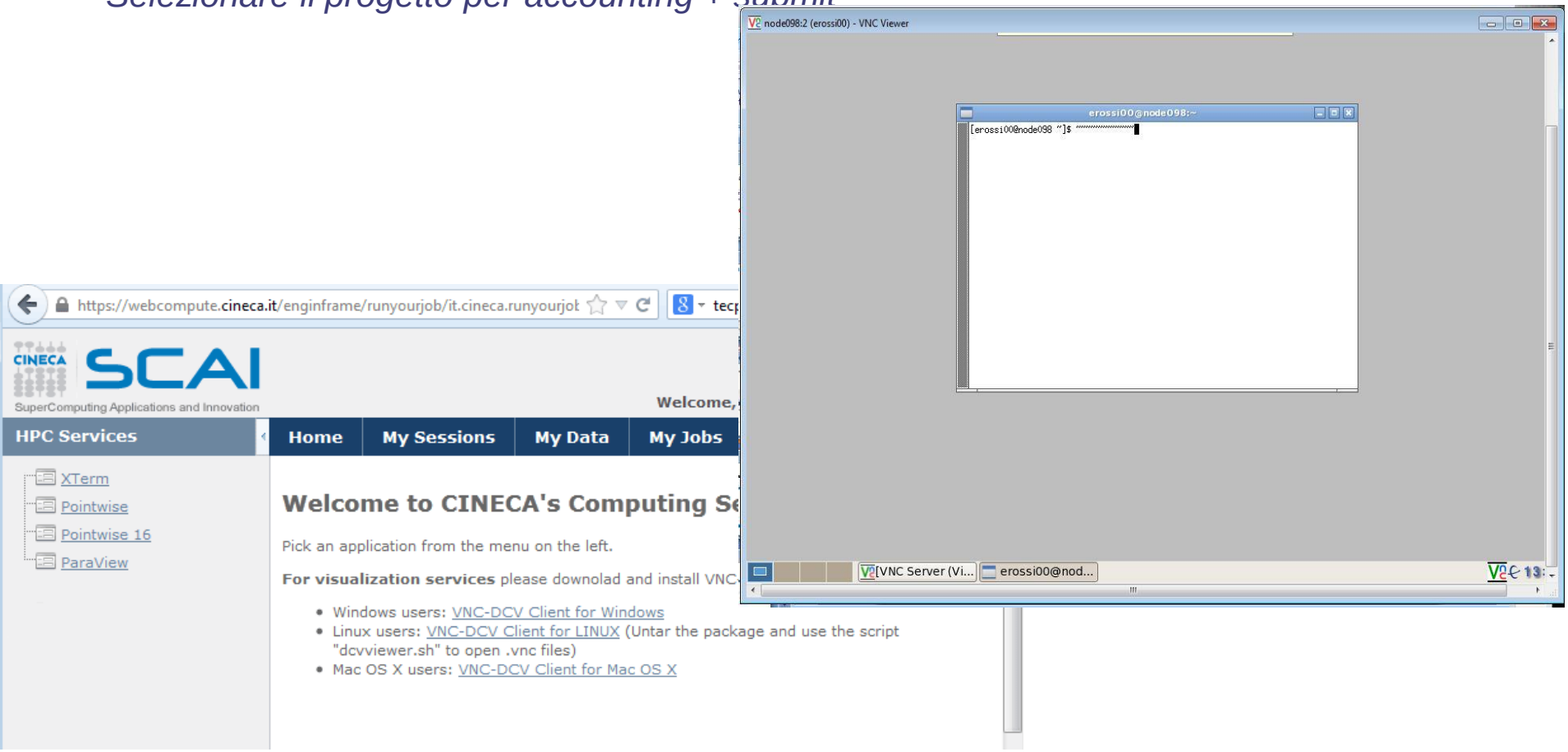


RCM: Remote Connection Manager



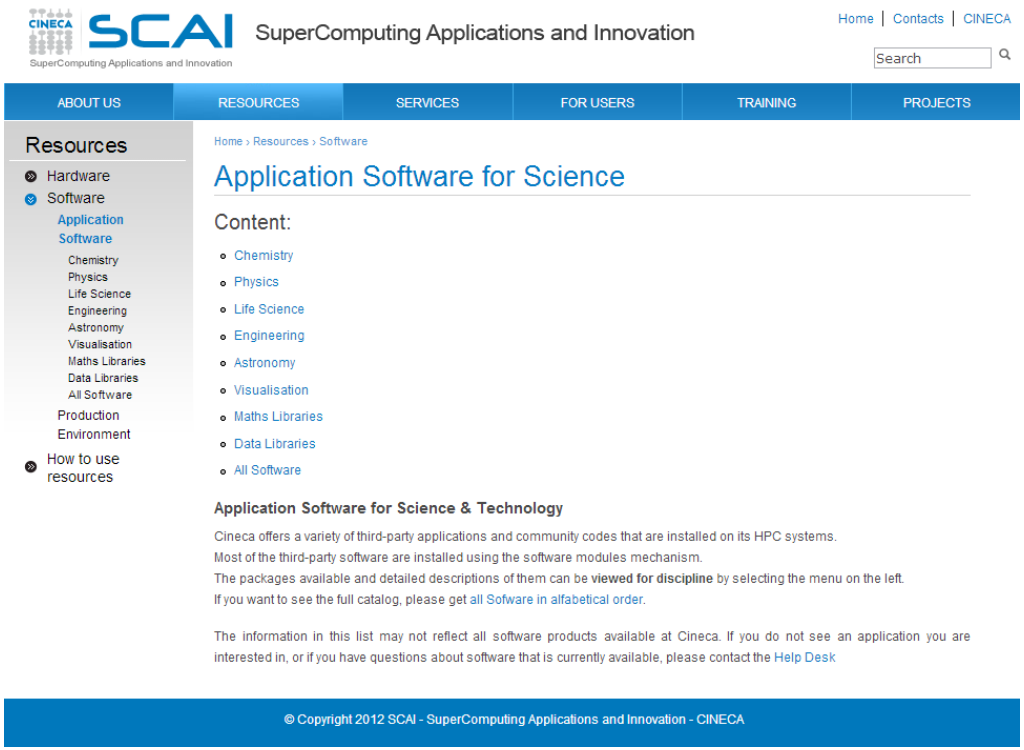
webcompute

- Sito `webcompute.cineca.it`
- Scaricare il client corretto per la propria workstation (solo al prima volta)
- *Selezionare il servizio di interesse (Xterm o applicativo)*
- *Selezionare il progetto per accounting + submit*



Domande aperte

http://www.hpc.cineca.it/content/application-software-science



Sw engineering

Resources
- Hardware
- Software
  - Application Software
    - Chemistry
    - Physics
    - Life Science
    - Engineering
    - Astronomy
    - Visualisation
    - Maths Libraries
    - Data Libraries
    - All Software
  - Production Environment
- How to use resources

Home › Resources › Software › Application Software › Resources software - Engineering

Resources software - Engineering

Name	Version	Description	Topic	Availability	Target user
Abaqus	6.12-1	Finite Element Analyzer	Engineering	EURORA, IBM PLX	academic
ANSYS	12.0, 12.1, 13.0, 13.4, 14.0, 14.5	General purpose software for mechanical engineering	Engineering	IBM PLX	restricted
ELMER	2011	Open Source Finite Element Software for Multiphysical Problems	Engineering, Physics	IBM PLX	all
OpenFOAM	2.1.1	The OpenFOAM® (Open Field Operation and Manipulation) CFD Toolbox can simulate anything from complex fluid flows involving chemical reactions, turbulence and heat transfer, to soliddynamics, electromagnetics and the pricing of financial options.	Engineering, Physics	IBM BG/Q FERMI, IBM PLX	all
parFE - parallel mu-FE	0.2	A fully-parallel mu-FE code	Engineering, Maths Libraries	IBM PLX	all
R - statistical computing and graphics	3.0.2, 2.15.1	Statistical computing and graphics	Engineering, Life Science	EURORA, IBM PLX	all
stata-statistics	10.0.0	Fast, powerful statistical package designed for researchers of all disciplines.	Engineering, Life Science, Physics	IBM PLX	all