Risorse CINECA per il calcolo scientifico @UniBG

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CINECA - HPC and Innovation Unit
Italy

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Università degli Studi di Bergamo

www.cineca.it

Agenda

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

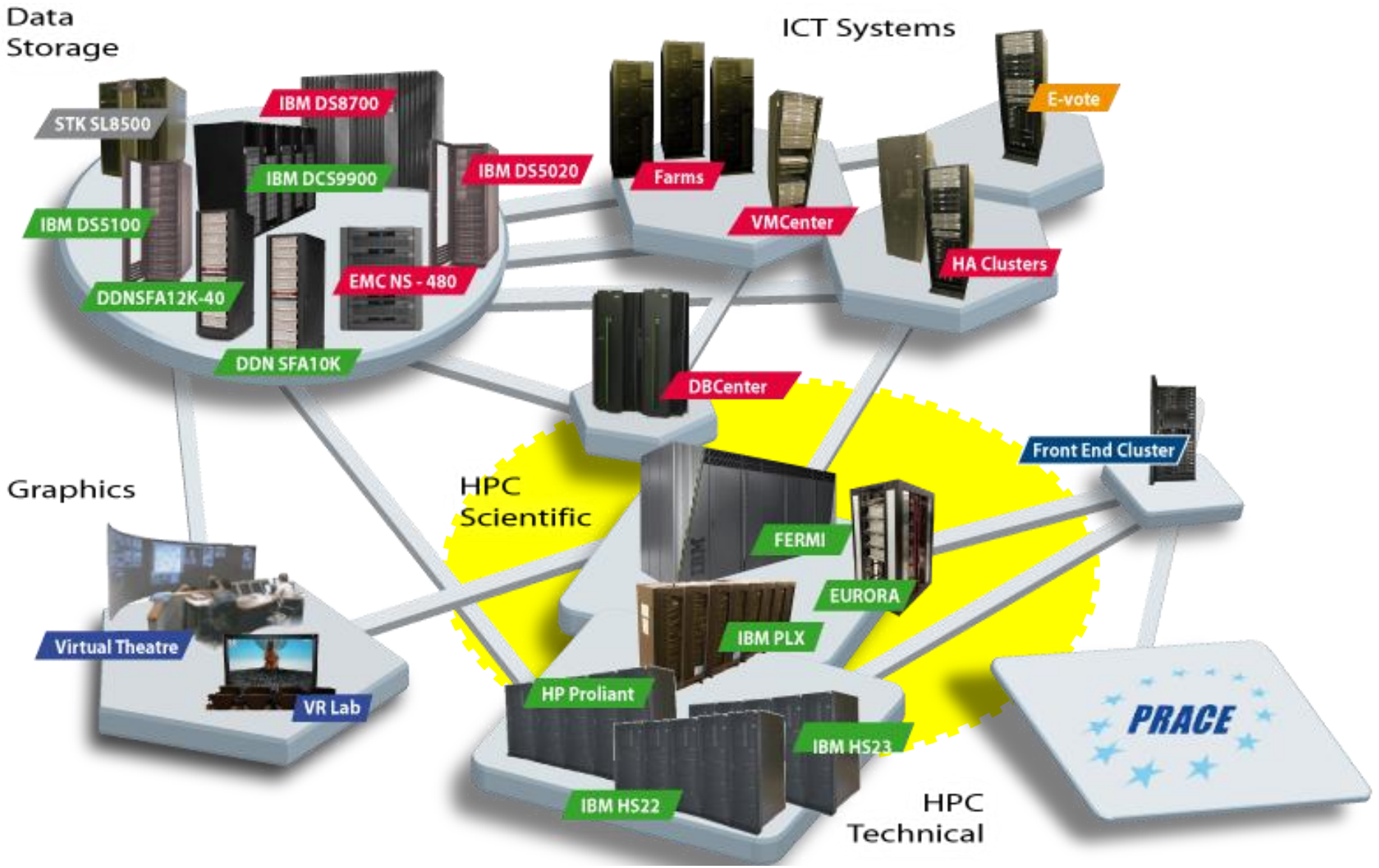
CINECA 2.0

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).

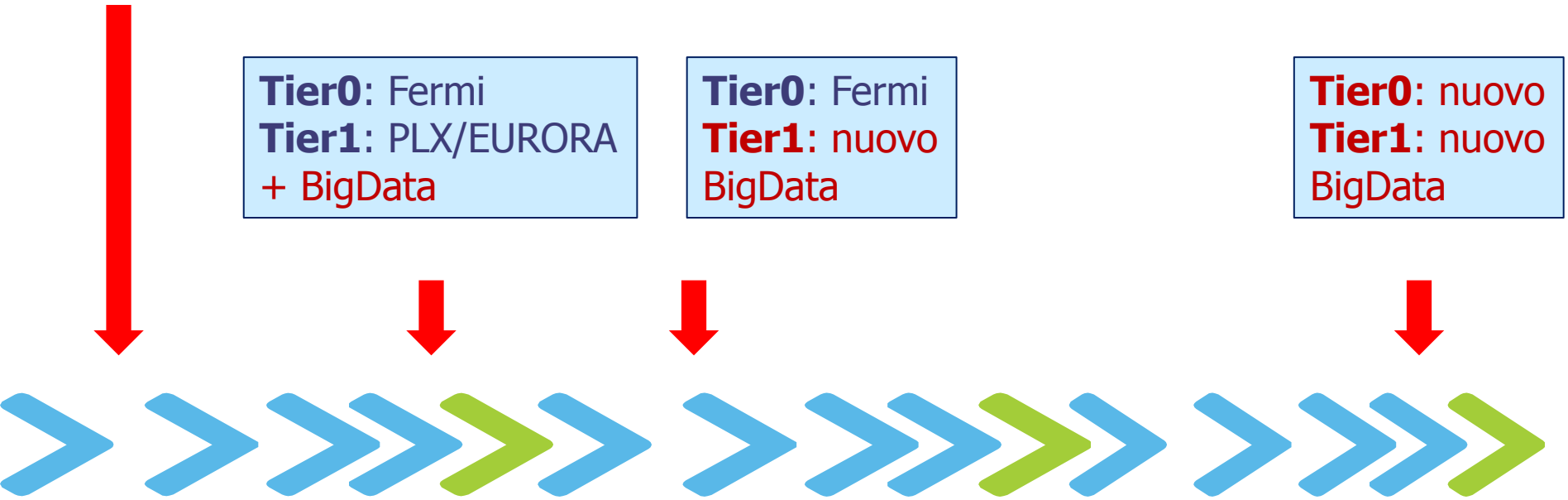
CINECA è il maggior centro di calcolo in Italia, uno dei più importanti nel mondo.
Il Dipartimento SuperCalcolo, Applicazioni e Innovazione (SCAI):

- 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
HPC
Scientific
FERMI
EURORA
IBM PLX
Virtual Theatre
VR Lab
HP Proliant
IBM HS23
IBM HS22
HPC
Technical
PRACE

L'infrastruttura di calcolo

Tier0: Fermi
Tier1: PLX/EURORA



FERMI

Sistema di punta, solo per applicativi estremamente scalabili

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
Power Consumption: 820 kWatts

N. 12 in Top 500 rank (June 2013)

National and PRACE Tier-0 calls

EURORA

Sistema sperimentale, dotato di acceleratori di ultima generazione

Architecture: Hybrid cluster by EUROTECH
Processor type: Intel Xeon Sandy Bridge 3.1GHz
Computing Nodes: 64
Each node: 16 cores, 16GB/32 of RAM + 2 acceler
Computing Cores: 1.024
RAM: 1GB/core
Accelerators: 64 NVIDIA Tesla K20 +
64 Intel Xeon-Phi 5120D (MIC)
Internal Network: Infiniband & Custom
Peak performance: 110 TFlops
Power consumption: 30 kWatts

N. 1 in Green 500 rank (June 2013)

National and PRACE PrepAccess calls

PLX

Sistema classico, produzione codici più tradizionali

Name: PLX
Architecture: IBM Hybrid Cluster
Processor type: Intel Xeon Westmere @ 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

Next BigData (1Q 2014)

- finalizzare l'installazione nel primo semestre del 2014
- cluster di piccole – medie dimensioni (ordine 64 nodi) per analisi/storage dati di grandi dimensioni e hosting applicativi per il post-processing (anche web-based)
- circa 5PB di storage on-line e 5PB di archive (TAPE).

Next Tier1 system (Mid 2014)

Name: ???

Architecture: Hybrid Cluster

Processor type: Intel Xeon Ivy Bridge (2.4 – 3GHz)

Computing Nodes: 500

Computing Cores/cpu: 8 - 12

RAM/core: 1GB (partizione con più RAM)

Internal Network: Infiniband QDR (o FDR)

Accelerators: >500 GPUs Nvidia K40:

Peak Performance: 1PFlops (300TF solo cpu)

Cooling: liquid/ free cooling

Energy consuming: < 400KW

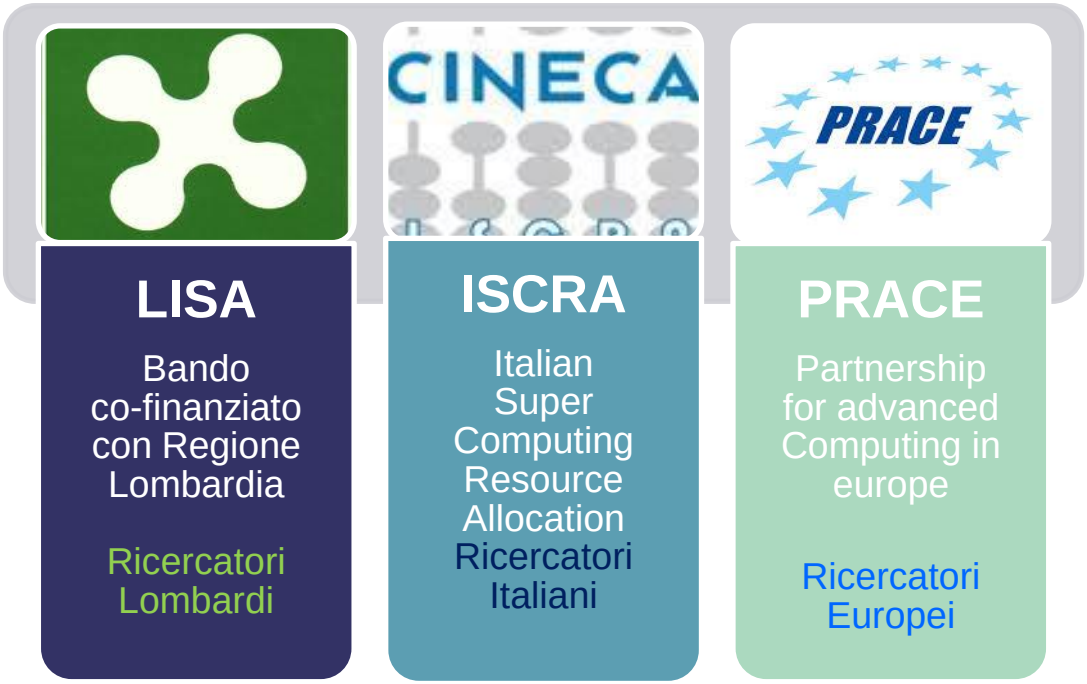
Next Tier0 system (Late 2015)

- Fermi, attuale sistema di punta – tier0 – giunge a naturale scadenza
- Sarà sostituito con altro sistema di analoga potenza per rispettare gli impegni italiani ed europei (ordine di 50PFlops -or- 50M€)
- *L'architettura BG/Q non verrà ulteriormente sviluppata da IBM , la* scelta terrà conto della tecnologia più aggiornata

Accessi HPC

- Modalità con selezione:
  - Regionali (Lombardia)
  - Nazionali
  - Europee
- Modalità senza selezione:
  - Convenzione d'Ateneo 2013

Piattaforme con Selezione



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

Piattaforma senza selezione

Convenzione d'Ateneo 2013:

- Monte ore: 93 k ore su Eurora/PLX + 1.000 k ore su Fermi
- Scadenza: maggio 2014
- Servizi inclusi: user support

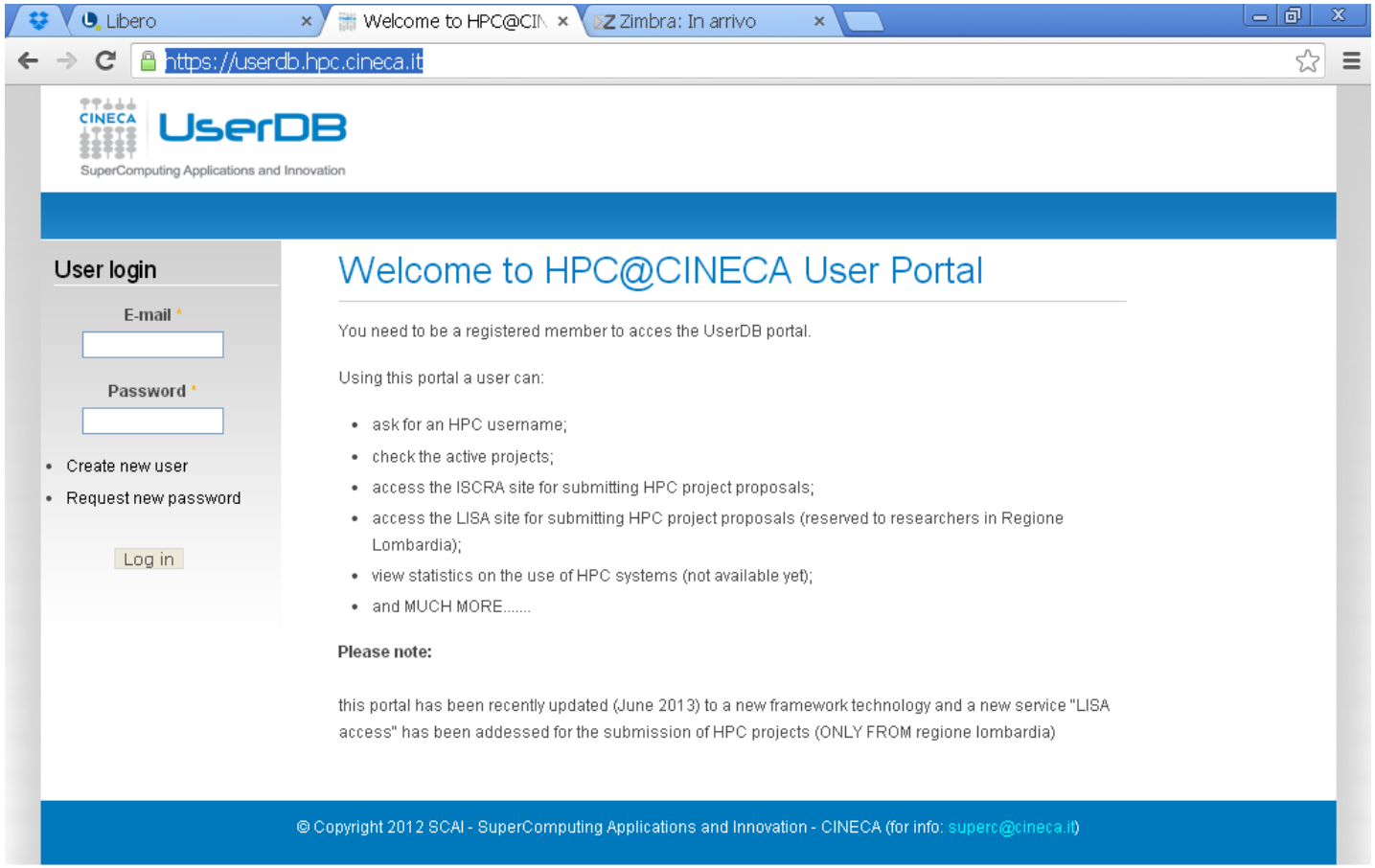
Il referente per la distribuzione del monte ore è il prof. Enrico Cavalli.

Al momento sono state assegnate 10 + 2 k ore su Eurora/PLX

Accesso alla convenzione

1. Iscrizione UserDB CINECA (https://userdb.hpc.cineca.it/)
   - (… solo se non si possiede già uno username)
   - Registrazione
2. *Ottenere l'assegnazione ad un progetto*
   - Chiedere al referente della convenzione (**E.Cavalli**) di attivare un progetto a proprio nome
   - Chiedere al PI di un progetto già attivato di essere nominato collaboratore
3. Richiesta accesso HPC (da UserDB)
   - (… solo se non si possiede già lo username)
   - Link "HPC access" (elenco azioni da completare)
   - Una mail automatica comunica coordinate per l'accesso (il gg dopo)
4. I referenti (PI) dei progetti che hanno ottenuto del monte ore possono aggiungere autonomamente i propri collaboratori
   - PI si connette allo UserDB sotto myprojects ed aggiunge il nuovo collaboratore (edit/save)
5. Accesso alla piattaforma (ssh o web interface)
6. Job submission

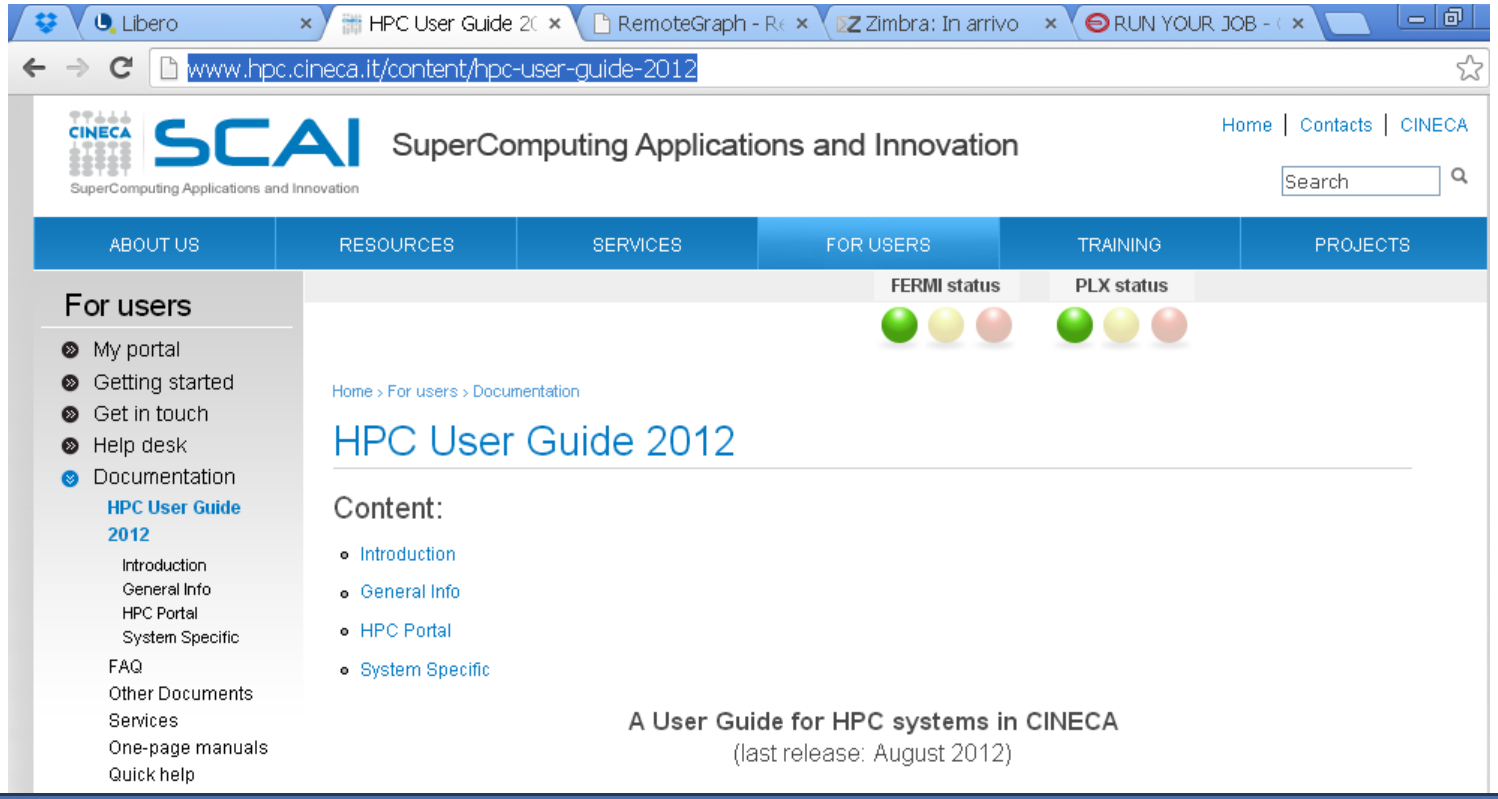
Iscrizione userDB CINECA



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

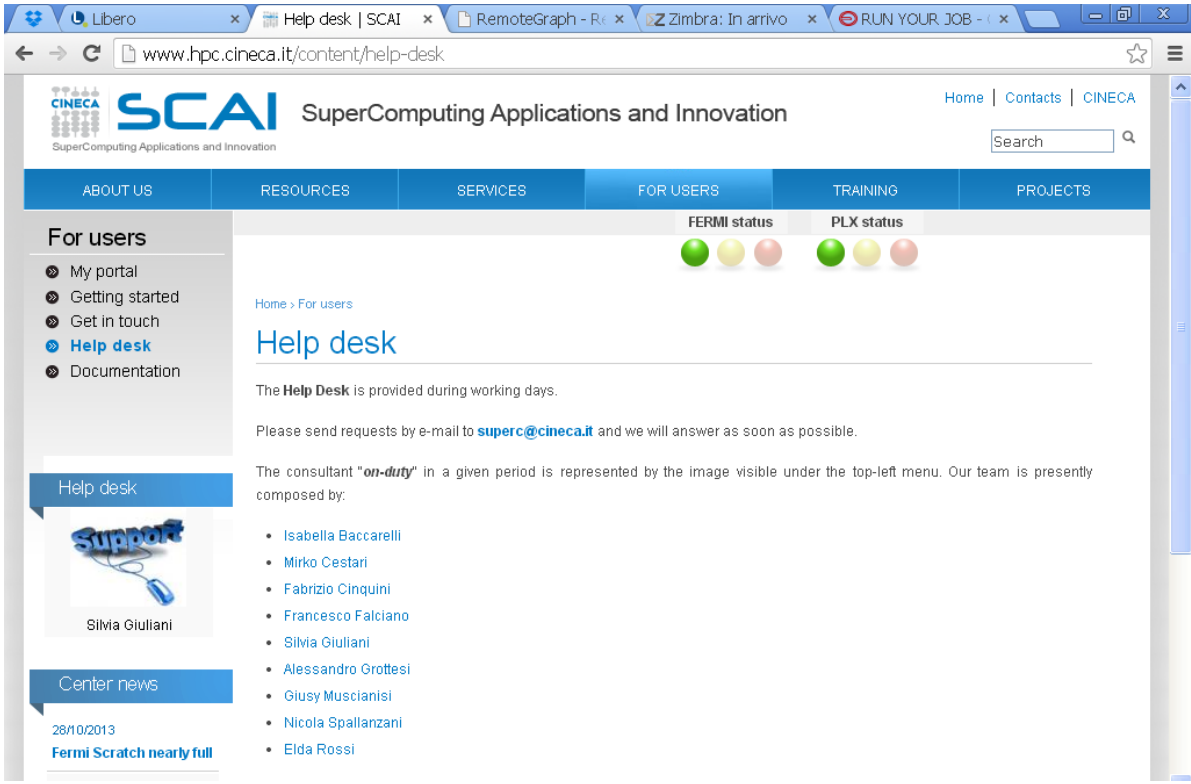
Informazioni generali documentazione

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

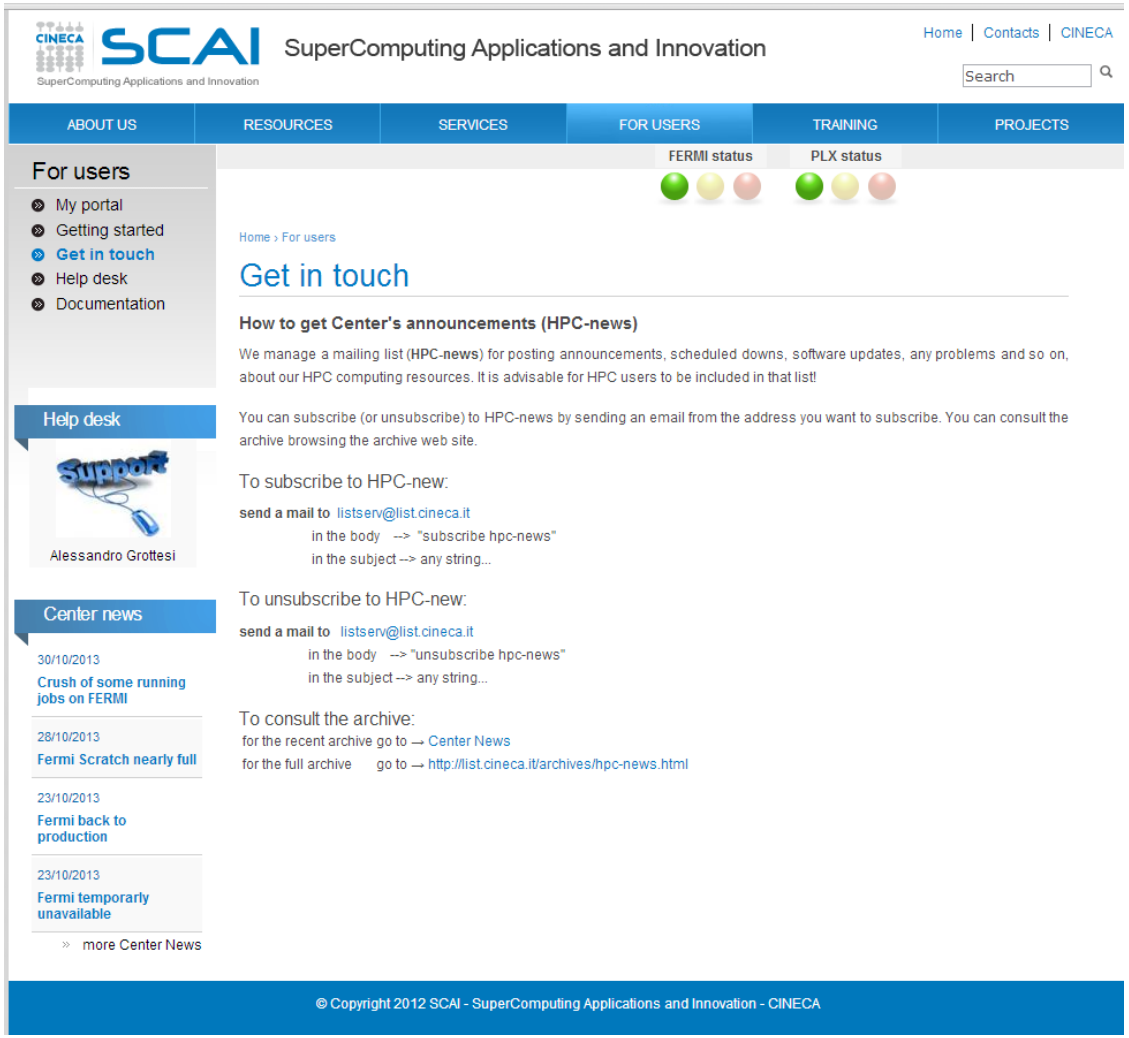


HelpDesk

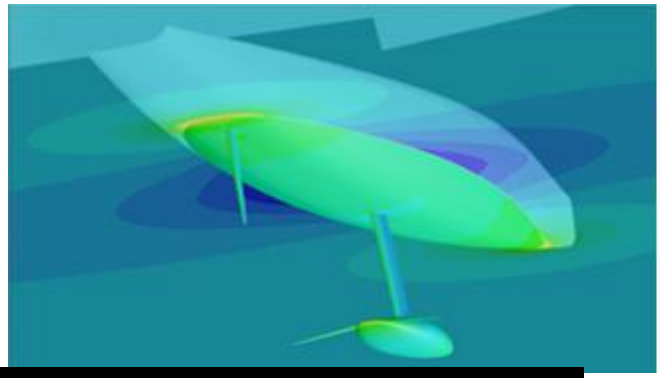
- Tramite mail a superc@cineca.it
  - Sistema di ticketing
  - Sempre un consulente in orario lavorativo
  - Possibilità di consulenza specialistica

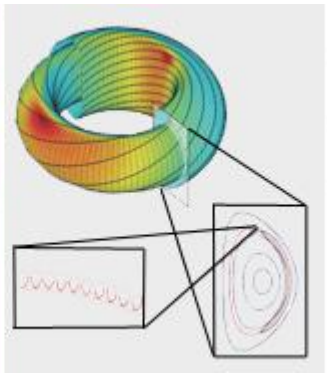


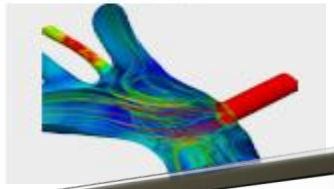
Get in touch: HPCnews



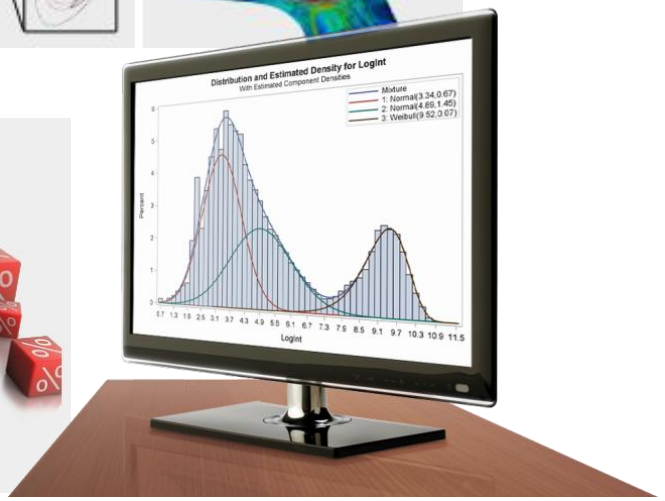
Cosa può fare CINECA per I suoi utenti







engineering



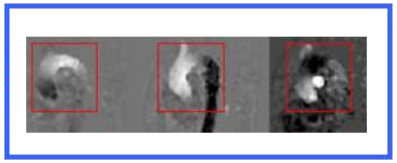
others

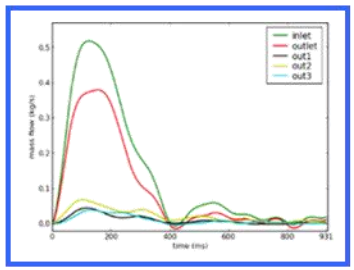
Premessa workflow CAE

PRE-PROCESSING → COMPUTATION → POST PROCESSING

COMPUTATIONAL

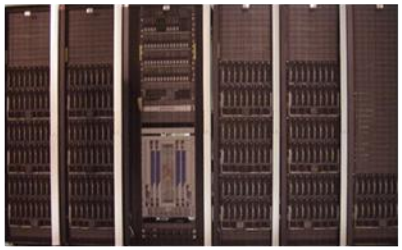
PHYSICS





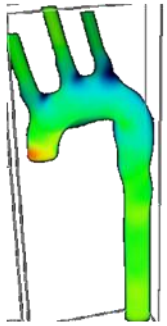
MODEL

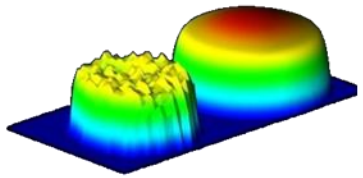
SOLVING



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

FERMI

- OpenFoam
  - Partial Diff Eq
  - OpenSource (per tutti)
- Ansys (CFD/mechanical)
  - General sw for Mech (Ansys) and CFD (Fluent, CFX)
  - 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/Code_Saturne/ …
  - Finite element Sw for multiPhys
  - Open Source (per tutti)

Pre-processing

PLX

- 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

- 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. Accesso interattivo: ssh client
2. Accesso tramite interfaccia:
   - Web-based via WebCompute
   - RCM: remote connection manager
3. Trasferimento dati: sftp client

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/base)*

```
$ module available

------------ /cineca/prod/modulefiles/profiles ----------------------
profile/advanced      profile/base(default)       profile/engineering
……
------------ /cineca/prod/modulefiles/base/libraries --------PETSc/3.0.0--openmpi--1.3.3--
gnu--4.1.2
PETSc/3.0.0--openmpi--1.3.3--intel--11.1--binary(default)

------------ /cineca/prod/modulefiles/base/compilers ------------
IntelMPI/4.0—binary          gnu/4.1.2(default)
gnu/4.5.2                    intel/11.1--binary(default)
openmpi/1.3.3--gnu--4.1.2    openmpi/1.3.3--intel--11.1—binary

------------ /cineca/prod/modulefiles/base/applications ------------
R/2.10.1                       gromacs/4.6.1
abinit/6.12.3                  meep/1.1.1(default)
adf/2010.02b(default)          molcas/7.6
amber/11(default)              mopac/2009(default)
amber/12                       namd/2.8(default)
cp2k/2.3(default)              pyfrag/2007.02(default)
desmond/3.0.3                  stata/10
….
```

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

Esecuzione degli applicativi

- La produzione si svolge normalmente *“in batch”*
  - Un file contiene lo script completo del lavoro
  - Il file viene “sottomesso” ad uno schedulatore che allocherà le risorse richieste appena disponibili
  - FERMI: LoadLeveler; PLX/EURORA: PBS
- *E’* possibile prenotare tramite lo schedulatore anche sessioni *“*interattive*”*
- Lavorando con le interfacce, la modalità batch e gli schedulatori sono *“*mascherati*”*
- Per lavorare in batch (per la produzione) è necessario avere anche un progetto valido con budget (account_no)

Username <-> account_no

- Username
  - Personale (erossi00, rponzini, mcremone)
  - Permette l'accesso e l'utilizzo interattivo
  - viene chiuso dopo un anno senza progetti
- Account_no
  - Budget per l'utilizzo batch
  - Periodo di validità, budget, hosts, PI, collaboratori
  - "saldo –b" fornisce info aggiornate

```
$ saldo -b
-------------------------------------------------------------------------------------------------------
account       start     end       total        localCluster   totConsumed    totConsumed
                                 (local h)   Consumed(local h)    (local h)             %
-------------------------------------------------------------------------------------------------------
try11_test    20110301  20111201  10000            2000            5000           50.0
cin_staff     20110323  20200323  200000000      479621          8933910           4.5

$ saldo -ba try11_test
erossi00 ffalcian mcestari fvitale0 sgiulian
-------------------------------------------------------------------------------------------------------
account     start      end       total        localCluster   totConsumed     totConsumed
                                (local h)   Consumed(local h)    (local h)             %
-------------------------------------------------------------------------------------------------------
try11_test  20110301   20111201   10000            2000            5000           50.0
```

Job batch (PLX)

```
$ cat job
#!/bin/bash
#PBS -l select=1:ncpus=4
#PBS -l walltime=20:00
#PBS -e myJob.err
#PBS -o myJob.out
#PBS -A cin_staff

cd $PBS_O_WORKDIR
module load g09
export GAUSS_SCRDIR=$CINECA_SCRATCH/g09/tmp
….
g09 < test000.com  > test000.out
```

```
$ qsub job
1485921.node351.plx.cineca.it
```

```
$ qstat
```

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)**

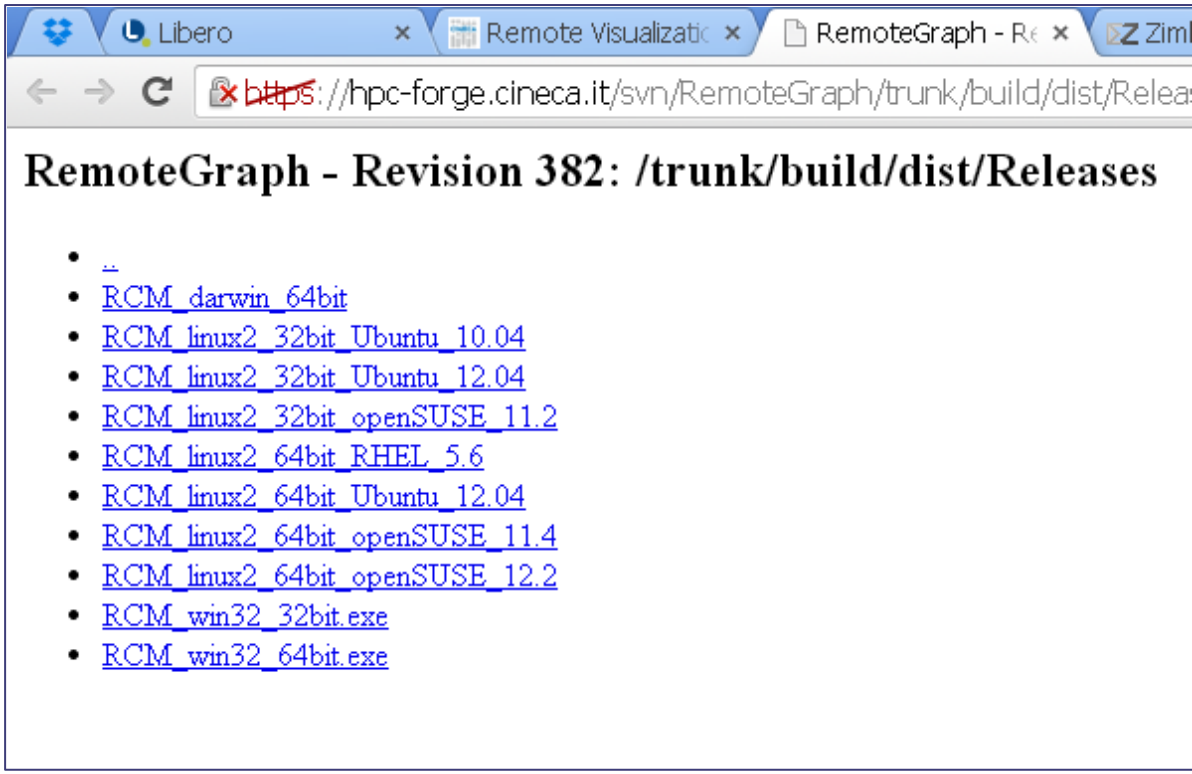
Applicativi con GUI e visualizzazione remota

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

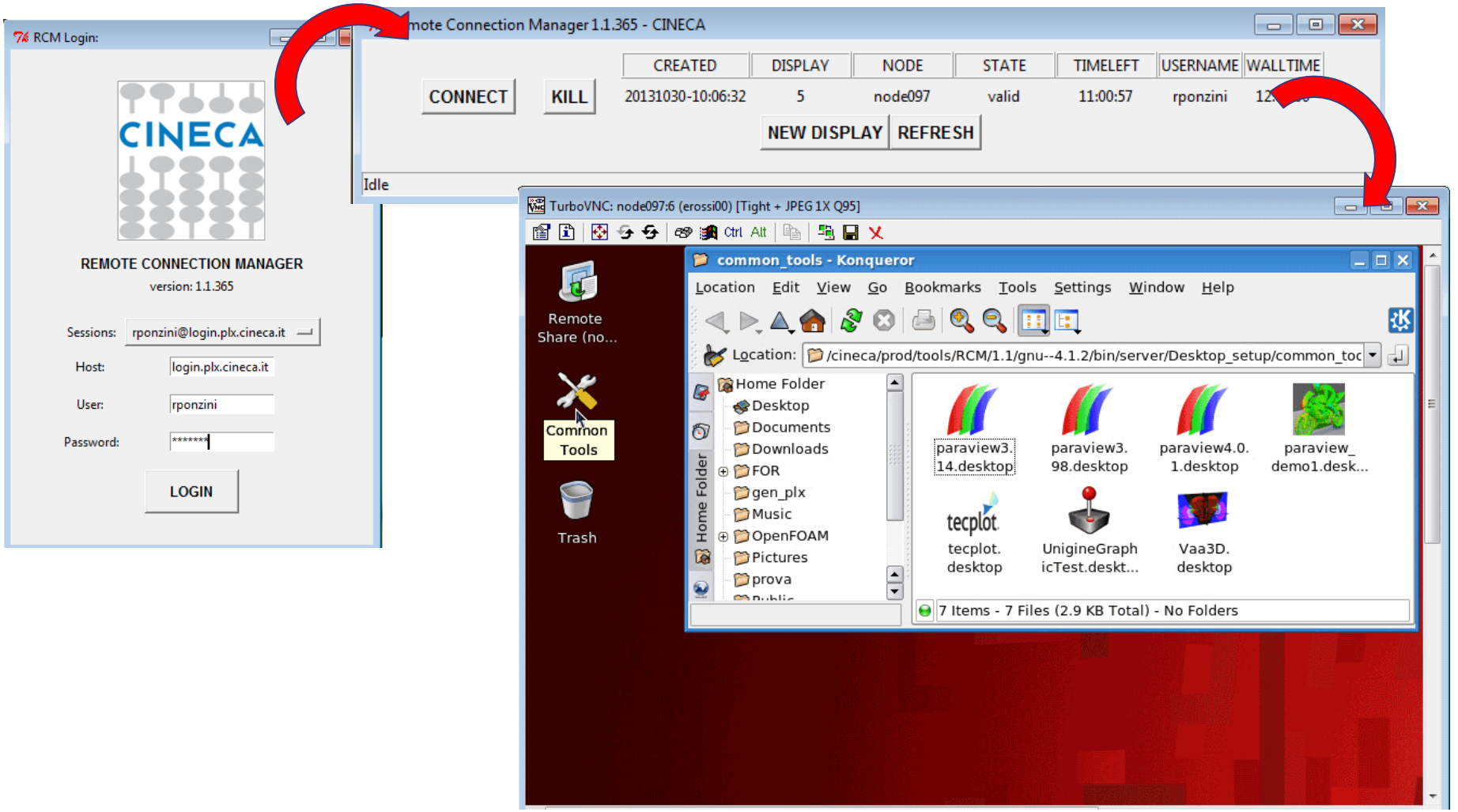
RCM: Remote Connection Manager

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

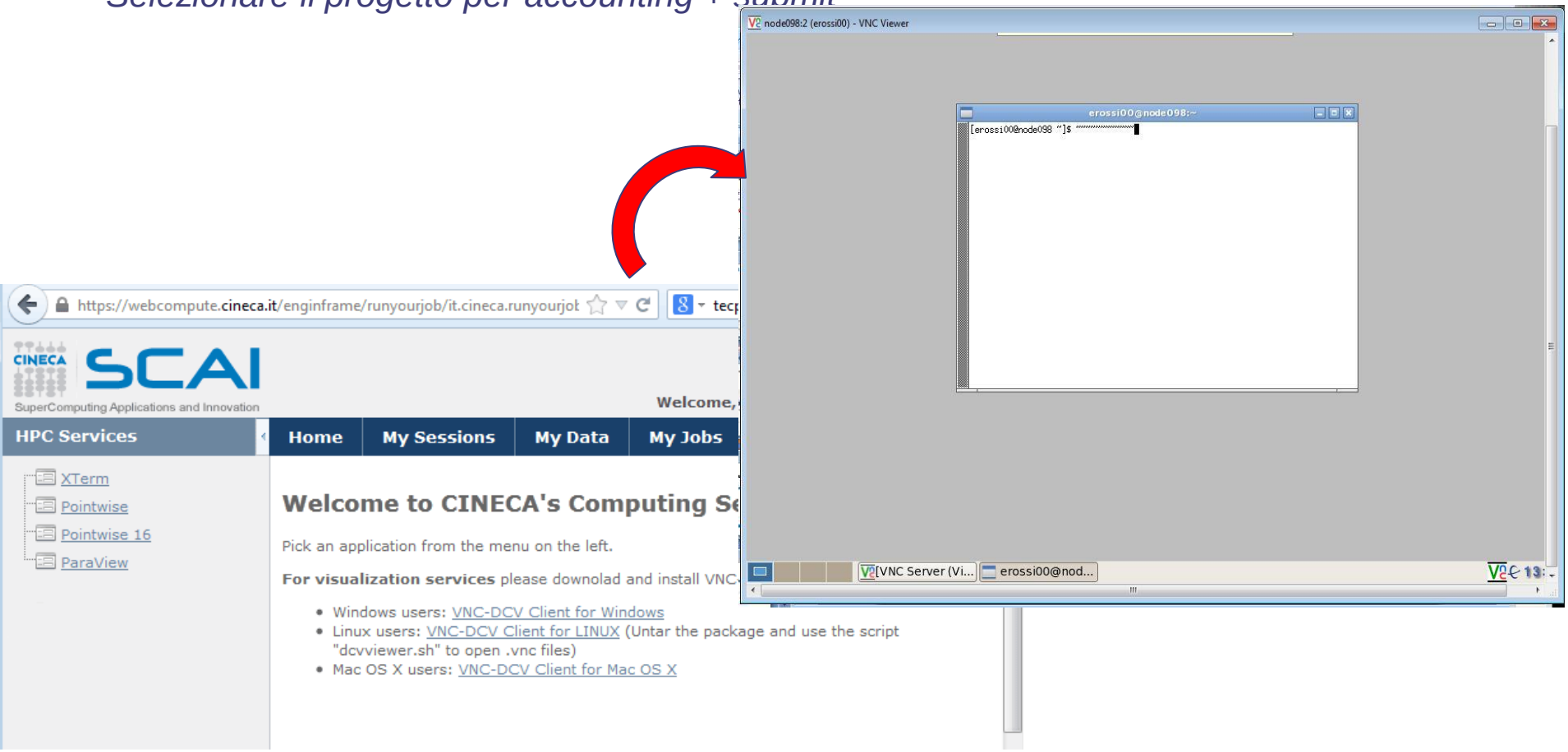


Remote Connection Manager



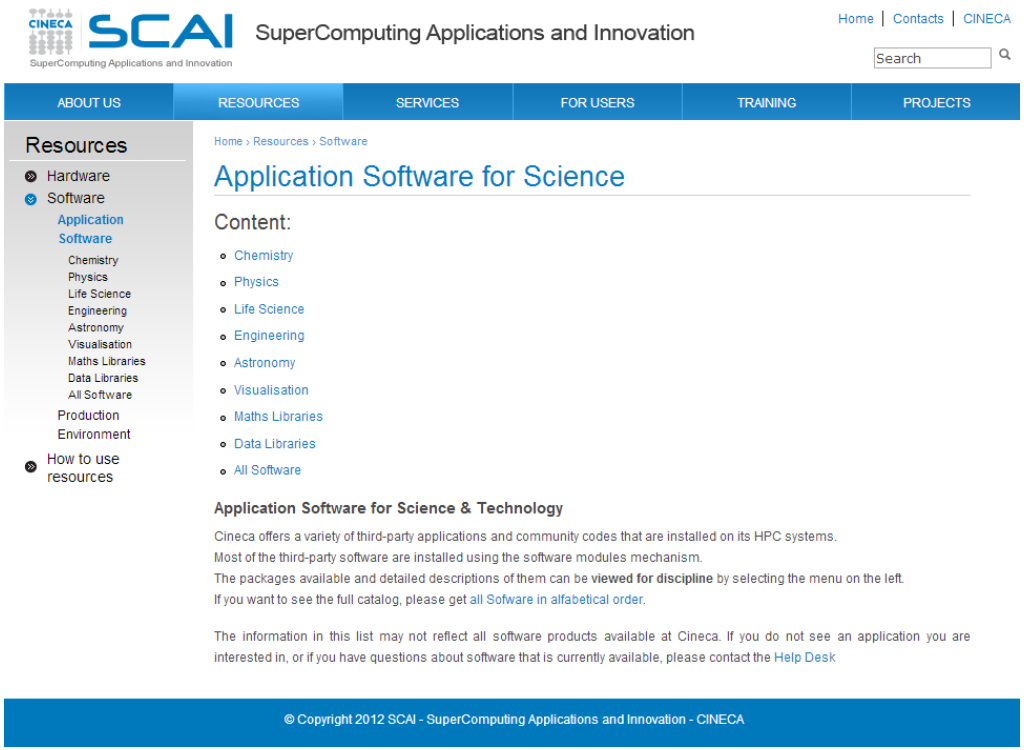
webcompute

- 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*

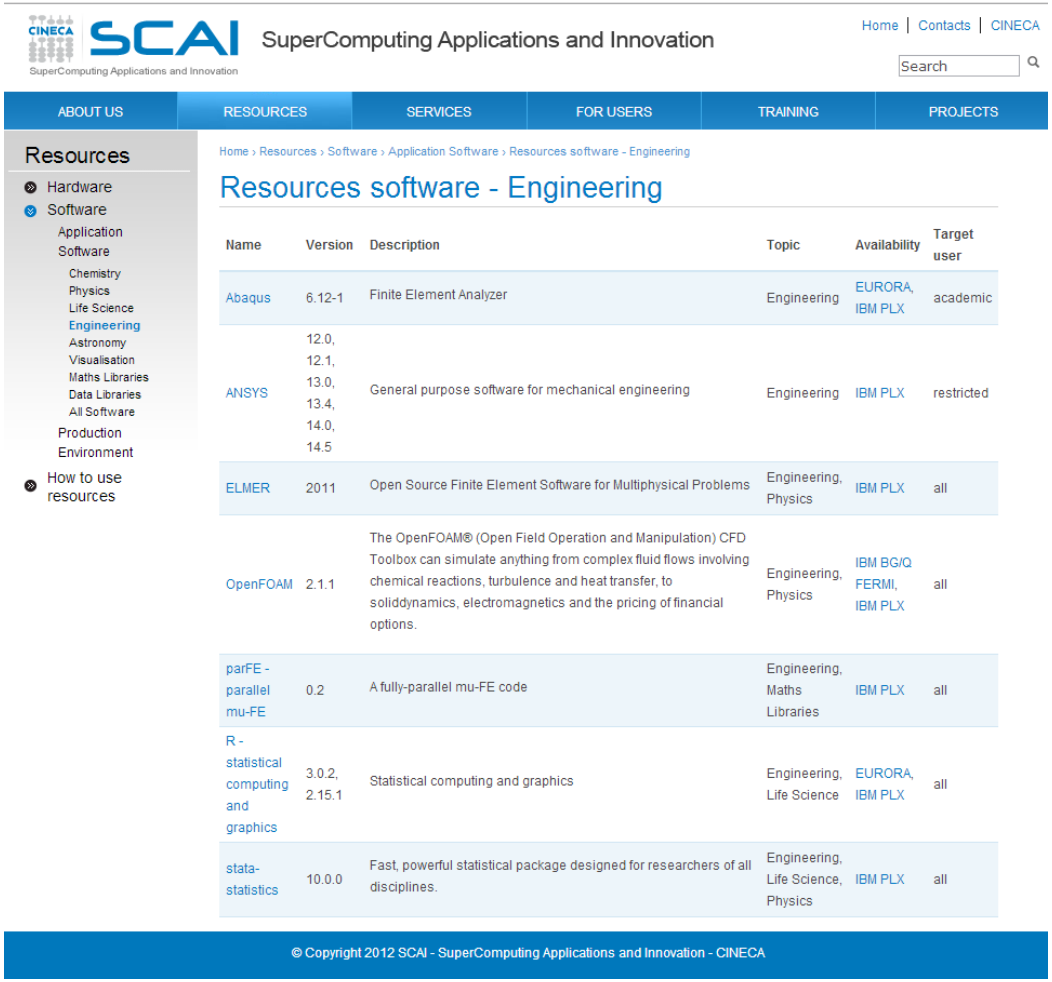


Applicativi pre-istallati

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



Sw engineering



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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


WHAT
WHO
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WHY