



Italian National Agency for New Technologies,
Energy and Sustainable Economic Development

ENEAGRID/CRESCO6

High Performance Computing Infrastructure

*Data bases, modelling and High Performance Computing for Perovskite PV
Webinar 8th February 2022*

Simone Giusepponi / TERIN-ICT-HPC



```
1101 0110 1100  
0101 0010 1101  
0001 0110 1110  
1101 0010 1101  
1111 1010 0000
```



ENEAGRID/CRESCO6 HPC Infrastructure

All computing facilities in ENEA are integrated within ENEAGRID that is characterized by solid structural components integrated in a user-friendly environment. The ENEA main computing facility is CRESCO6 that is an HPC system consisting of 434 nodes/20832 cores with a peak of 1.4 PFlops. The webinar describes how to operate in the ENEAGRID framework to use CRESCO6 HPC cluster and can be summarized in three main points:

- 1. How to get a user account in ENEAGRID.**
- 2. How to access to computing facilities.**
 - a. SSH at the front-end nodes.
 - b. ThinLinc Graphical User Interface.
 - I. ThinLinc client on PC.
 - II. dedicated webpage: <https://cresco-in-gui.portici.enea.it/main/>;

Using ThinLinc it is possible to select the CMAST (Computational Materials Science and Technology) profile
- 3. How to open issues in ENEAGRID.**

ENEAGRID/CRESCO Clusters

www.cresco.enea.it

Computational RESearch Centre on COmplex systems

CRESCO6 (1400 Tflops, 20832 cores)

- 434 nodes 2x24 cores Intel Xeon Platinum 8160 @2.1 GHz;
192 GB RAM, 500GB SATA II disk, Intel Omni-Path 100 GB/s.

CRESCO4 (40 Tflops, 2048 cores)

- 128 nodes 2x8 cores Intel E5-2670 @2.6 GHz;
64 GB RAM, 500GB SATA II disk, IB QDR 40 GB/s.

CRESCO4SM (60 cores)

- 5 nodes 2x6 cores Intel E5-2643 v2 @3.5 GHz;
768 GB RAM, 1TB SATA II disk, IB QDR 40 GB/s.

CRESCO4F (20 Tflops, 1024 cores)

- 64 nodes 2x8 cores Intel E5-2670 @2.6 GHz;
64 GB RAM, 500GB SATA II disk, IB QDR 40 GB/s.

CRESCO4C (10 Tflops, 512 cores)

- 32 nodes 2x8 cores Intel E5-2670 @2.6 GHz;
64 GB RAM, 500GB SATA II disk, IB QDR 40 GB/s.

NEW FORTHCOMING CRESCO CLUSTERS IN 2022

CRESCO7 (1400Tflops)

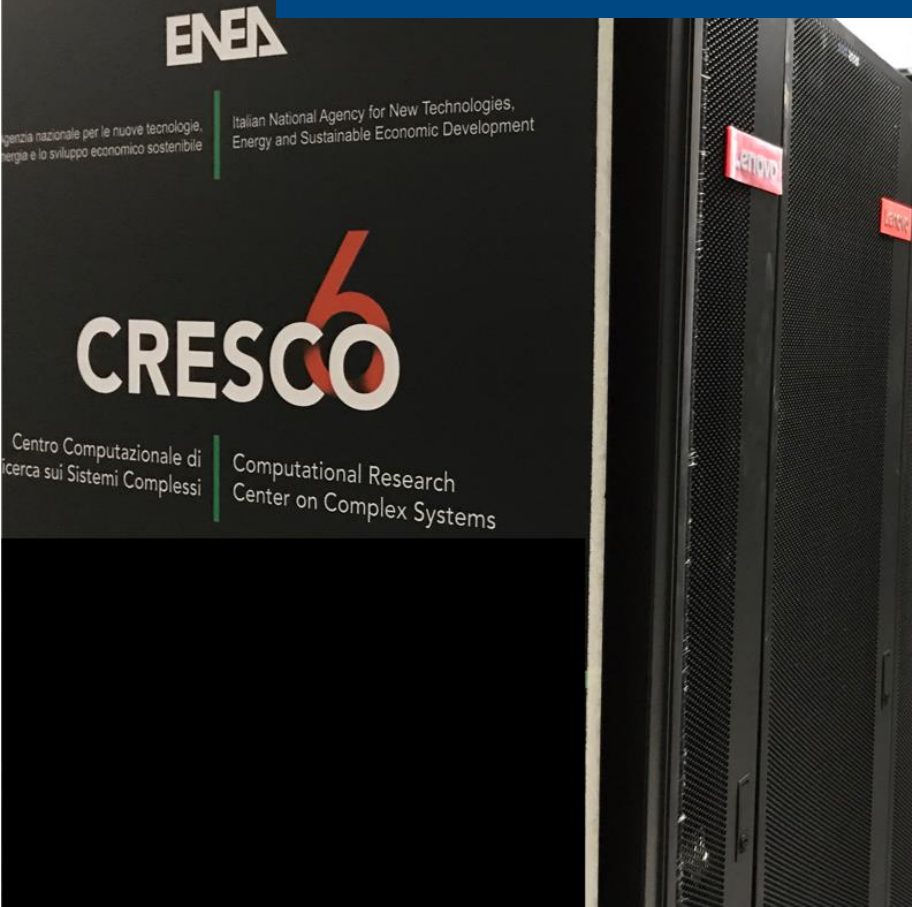
- 100 nodes dual socket Sapphire 54 + 10 nodes single socket Sapphire 54, 2 GPU NVIDIA A100;

CRESCO7F

- 8 nodes dual socket AMD, 1 GPU NVIDIA A100 + 8 nodes dual socket IBM PPC 8, 4 GPU NVIDIA P100;

ENEAGRID/CRESCO Clusters

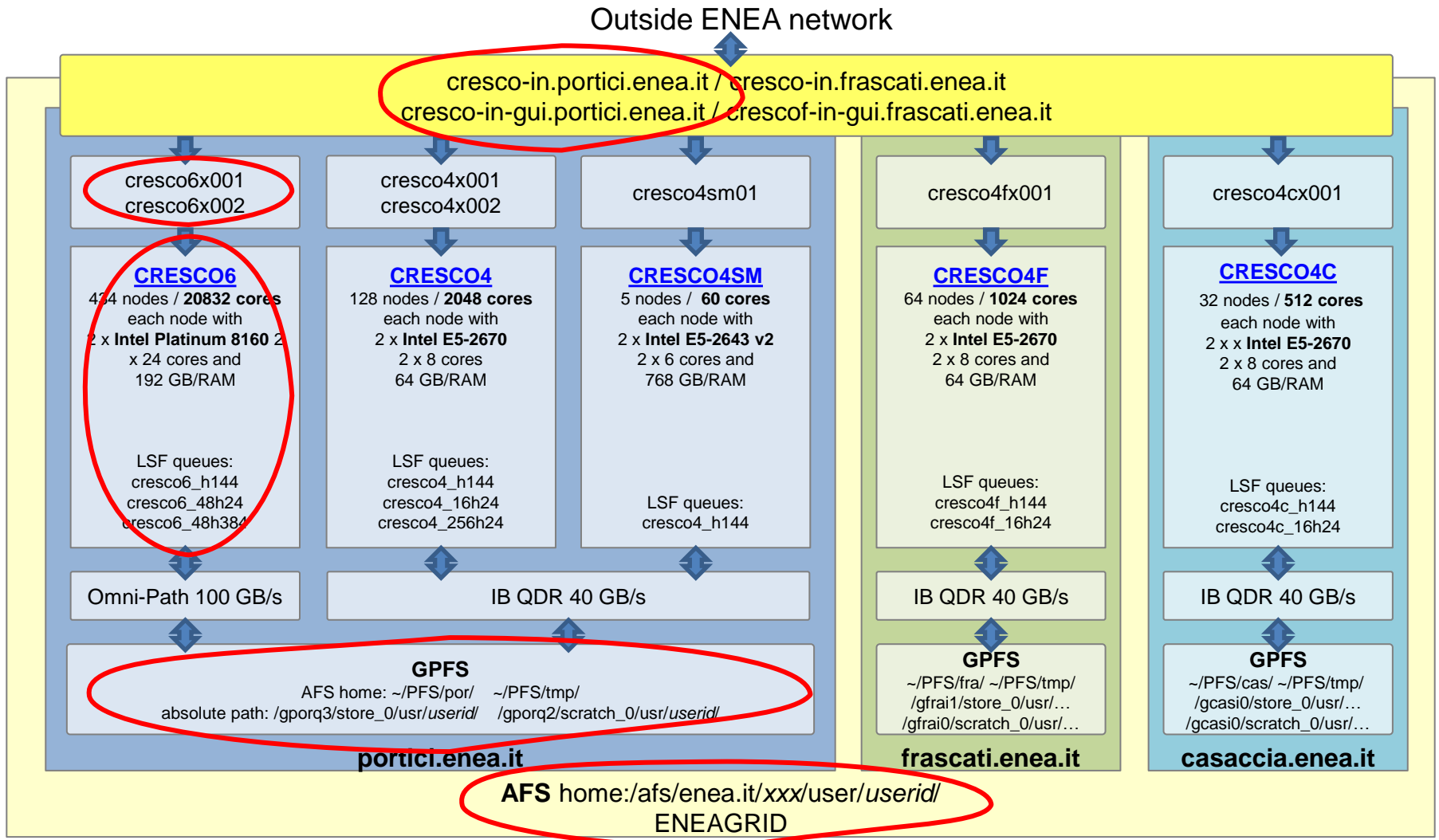
ENEAGRID/CRESCO an integrated computational infrastructure



Provides a unified user environment and a homogeneous access method for all users irrespective of their location

- Authentication via Kerberos 5
- Filesystems:
 - Geographic filesystem AFS/OpenAFS
 - Parallel filesystem IBM/GPFS
- Resource manager IBM/LSF
- User web interface:
 - THINLINC
 - Jobrama: job status & Accounting

ENEAGRID/CRESCO Clusters



How to get a user account in ENEAGRID

To get access to the ENEAGRID infrastructure look at ENEA CRESCO PORTAL
www.eneagrid.enea.it/CRESCOportal/

Home TERIN TERIN-ICT TERIN-ICT-HPC Account Manager Ticket System Jobrama FRA-POR

CINECA progetto Tedat UNIONE EUROPEA PON Ricerca e Competitività 2007-2013 Ministero dell'Istruzione, dell'Università e della Ricerca Ministero dello Sviluppo Economico ENEA Agenzia nazionale per le nuove tecnologie, l'energia e lo sviluppo economico sostenibile

HPC User Notices
HPC News
HPC Webinars
CRESCO Seminars
Usage Rules Acknowledgements

TOP500 HPCG

VIRTUAL LABS
ENEAGRID TERIN-ICT-HPC
EoCoE2 - EXTREME

CRESCO HPC Reports
ENEAGRID Primer
ENEAGRID AFSDataSpace
3D GraphLab
Ateco HPC
Ateco 3D
ENEAGRID New Techs

CRESCO: Computational RESearch Centre on COmplex systems

Access to CRESCO via FARO application

Web access to ENEAGRID uses ThinLinc technology on cresco-in-gui.portici.enea.it

ENEAGRID - CRESCO clusters Docs - ENEAGRID Primer

News
2021/12/03 Environment: ENEA online platform on air quality in Italy

HPC User notices
2021/12/23: Presidio ridotto CRESCO dal 24/12/2021 al 09/1/2022 // CRESC...

>>> MAPPE Covid19 da ENEA <<<

CRESCO4 CLUSTER TEDAT PROJECT - PON 2007-2013
WEBPAGE OF THE CRESCO PON 2002-2006 PROJECT, TENDER 1575

- ENEAGRID/CRESCO
- Account Request
- How to get to Portici
- Contacts
- ENEAGRID Phone directory

TOOLS AND SERVICES

- ENEAGRID TicketSystem
- Job Monitor~Jobrama
- Password verify/change
- ENEAGRID Software
- ENEAGRID AFSbox
- ENEABOX
- WARC (intranet)
- System Management
- CRESCO Connect Room
- HPC Connect Room
- ICT Connect Room
- AI Connect Room
- Patrimonio Culturale Room
- Eufusgw Connect Room
- ENEAGRID PhoneConference

ENEAGRID

new account change password check password reset password account policy

new account

Name and surname
Phone number
Mail

request motivations

ENEAGRID Employee ENEA - Fellow Educational External

ENEAGRID contact (if available)

Name and surname
Phone number
Mail

Captcha

I have read, understood, and accepted the terms of service

for more information read the privacy policy

send

and fill the form at <https://gridaccount.enea.it/>

How to get a user account in ENEAGRID

The screenshot shows the ENEAGRID registration interface. At the top, there are links for 'new account', 'change password', 'check password', and 'reset password'. Below these is an 'accept policy' link. The main section is titled 'new account' and contains several input fields: 'Name and surname', 'Phone number', and 'Mail'. There is a 'request motivations' text area. Below this are radio buttons for user categories: 'ENEA Employee', 'ENEA - Fellow', 'Educational', and 'External'. Another section, 'ENEA contact (if available)', has similar input fields. A captcha with the number '2865800' is present. A checkbox labeled 'I have read, understood, and accepted' is followed by a red circle around the text 'Terms of service'. At the bottom, there is a green 'send' button and a link to 'for more information read the privacy policy'.

User account => *userid* + *password*

These rules are summarized as follows:

- i) the use of the available scheduling system (LSF) for the proper use of computational resources and the prevention of front-end systems overload;
- ii) the appropriate use of the on-line data space, subject to ENEA/ICT quota policies (e.g. contents must be coherent within the declared activity and activities should not regularly overload storage systems);
- iii) the proper use of the identification and authorization systems (e.g.: registered users cannot lend their credentials to unregistered third party subjects, nor use other people's credentials; the user must provide an E-mail address and a telephone number and must keep these contact data updated at any time).

Within these general terms, the generation of an **account for external users of ENEAGRID/CRESCO requires the presentation of a document, written on the institution's letterhead, signed by the responsible officer of the home institution and addressed to:**

AI Responsabile di ICT,
ENEA
Lungotevere Thaon di Revel, 76
00196 Rome - ITALY

The document must be provided in pdf format and must be sent as an attachment to an E-mail to hpc-account-request@enea.it.

The document must specify clearly:

1. the motivation for the interest in the use of ENEAGRID/CRESCO HPC systems;
2. the willingness to comply with conditions i), ii) and iii) of the present document;
3. a short description of the research activity, its objectives and its timetable;
4. the indication of the approximate size of the required computational resources (number of computing cores, total CPU time, amount of data space);
5. a statement declaring if the computing activity is funded within the framework of national or international projects; in the latter case, access to the resources will be subjected to the stipulation of a specific agreement, involving either an appropriate fee for the use of the ENEAGRID/CRESCO resources, or a form of participation of ENEA/ICT to the project;
6. the willingness to express the scientific acknowledgement of the utilization of ENEAGRID/CRESCO systems in the case of publications, whose form and extent (thanks, co-signatures, etc.) shall be determined case by case depending on the amount of computing time utilized by the user and to what extent the collaboration and support provided by ENEA/ICT staff has been instrumental for the work being published;
7. the commitment to add acknowledgements for the utilization of the ENEAGRID/CRESCO computing infrastructure in any paper referring the obtained results and notify ENEA/ICT as soon as the publication is submitted/accepted. The publication must be notified to ICT by the submission of a specific ticket "Publication Notification" in the ticketing system <https://gridticket.enea.it>.

How to access the computing facilities

There are two modalities of access:

a. **SSH** at the front-end node **cresco-in.portici.enea.it**

b. **ThinLinc** Graphical User Interface

i. ThinLinc client on PC.

ii. dedicated webpage: <https://cresco-in-gui.portici.enea.it/main/>

How to access the computing facilities

SSH at the front-end node `cresco-in.portici.enea.it`

Mobaxterm

<https://mobaxterm.mobatek.net/>

```
giuseps@cresco-in.portici.enea.it
[2022-02-02 17:51:48]
[Simone.Desktop-Simone] ssh -X giuseps@cresco-in.portici.enea.it
Warning: Permanently added 'cresco-in.portici.enea.it' (RSA) to the list of known hosts.
giuseps@cresco-in.portici.enea.it:~$
Last login: Thu Dec 23 13:54:45 2021 from host-87-1-187-112.retail.telecomitalia.it
===== Front-end Menu =====
Host cresco-in2.portici.enea.it on Med Feb 02 17:52:21 CET 2022
Local tty /dev/pts/4 connected from remote host desktop-simone.dhcpnet.casaccia

Welcome to user giuseps on ENEAGRID/CRESCO Clusters

For general information see:
http://www.eneagrid.enea.it
http://www.cresco.enea.it

This host is a ssh gateway to CRESCO front-ends for users connecting from NON ENEA networks.
This host MUST NOT be used neither as Front-end nor for Data Transfer by sftp/scp.
When connecting from ENEA networks, please access directly the Front-end by ssh.
For scp/sftp from NON ENEA networks please use cresco-scp.portici.enea.it.

You are connected to cresco-in2.portici.enea.it.
Please select a Front-end in the following list
*** Site-----Host-----
1) Portici: cresco4x001
2) Portici: cresco4x002 (also for interactive jobs)
3) Portici: cresco6x001
4) Portici: cresco6x002 (also for interactive jobs)
5) Portici: cresco4sm01 (node with 768 GB RAM, also for interactive jobs)
6) Casaccia: cresco4cx001
7) Frascati: cresco4fx001
8) Frascati: xcrescox044 (only for development and test)
9) Brindisi: crescob-nv11 (only for AI projects)
*** Select the frontend or (0)exit and logout >
```

```
giuseps@cresco-in.portici.enea.it
Please select a Front-end in the following list
*** Site-----Host-----
1) Portici: cresco4x001
2) Portici: cresco4x002 (also for interactive jobs)
3) Portici: cresco6x001
4) Portici: cresco6x002 (also for interactive jobs)
5) Portici: cresco4sm01 (node with 768 GB RAM, also for interactive jobs)
6) Casaccia: cresco4cx001
7) Frascati: cresco4fx001
8) Frascati: xcrescox044 (only for development and test)
9) Brindisi: crescob-nv11 (only for AI projects)
*** Select the frontend or (0)exit and logout > 3
*** selected frontend is: cresco6x001.portici.enea.it
ssh -X giuseps@cresco6x001.portici.enea.it
Last login: Mon Jan 31 15:27:28 2022 from cresco4-fg2.portici.enea.it

Welcome to ENEAGRID/CRESCO!

=====
ENEAGRID/CRESCO is the infrastructure of the computational resources of ENEA TERIN-ICT Division
[Dipartimento Tecnologie energetiche e Fonti Rinnovabili (TERIN)/Divisione per lo sviluppo Sistemi per l'Informatica e l'I
CT]
http://www.ict.enea.it
Information about ENEAGRID/CRESCO can be found at the page: http://www.eneagrid.enea.it
The main computational resources are CRESCO HPC systems: http://www.cresco.enea.it
located in Portici (main site),Frascati,Casaccia,Brindisi,Bologna

A primer for ENEAGRID/CRESCO can be found at: http://www.eneagrid.enea.it/ENEAGRID_info.html
User support is provided at http://gridticket.enea.it.

Access conditions & Citation/Acknowledgement rules for ENEA employees:
http://www.eneagrid.enea.it/rules/CondizionidIUtilizzoUtenzaENEA.html

Access conditions & Citation/Acknowledgement rules for non ENEA users:
http://www.eneagrid.enea.it/rules/CondizionidIUtilizzoEN.html

Your username is:
giuseps
Your contact data are:
Mail:simone.giuseppi@enea.it Phone:-----
You are an external user. ENEA contact Mail:
*** Please check these data and submit a ticket via ENEA-GRID ticketing
system (https://gridticket.enea.it) if they are not up to date

UNREGISTERED VERSION - Please support the development by subscribing to the professional edition here: http://mobaxterm.mobatek.net
```

`ssh userid@cresco-in.portici.enea.it`

How to access the computing facilities

ThinLinc Graphical User Interface - Client on PC

www.cendio.com

The image shows two overlapping screenshots of the ThinLinc website. The top screenshot shows the main navigation menu with the 'Download' link circled in red. The bottom screenshot shows the 'ThinLinc downloads' page, also with the 'Download' link in the navigation menu circled in red. The main content of the bottom screenshot is a table of download options for ThinLinc Clients.

ThinLinc downloads			
For users - ThinLinc Clients			
Windows	32-bit/64-bit	-	-
macOS	-	64-bit	-
Linux RPM	32-bit	64-bit	ARMv7 hard-float
Linux DEB	32-bit	64-bit	ARMv7 hard-float
Linux tar.gz	32-bit	64-bit	ARMv7 hard-float

For Administrators - **ThinLinc Server (Linux only)**

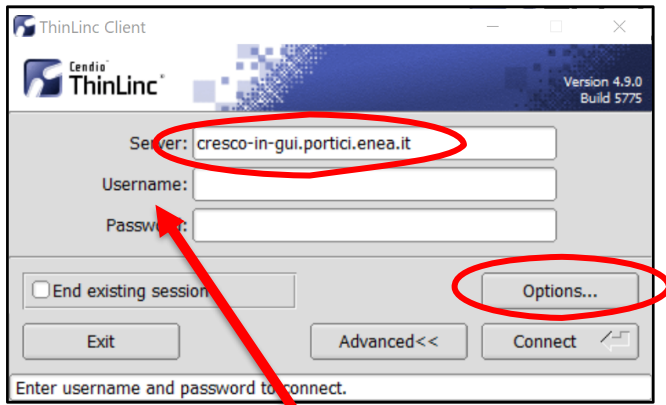
Cendio offers these downloads primarily for evaluation and testing purposes. For large organizations, multiple testing licenses and technical support are provided during the evaluation upon request. This download is also available for small user groups and home users for free, with a maximum of 5 concurrent users, for more details see the FAQ.

[Download ThinLinc Server bundle](#) [FAQ](#) [Share your ThinLinc use case](#)

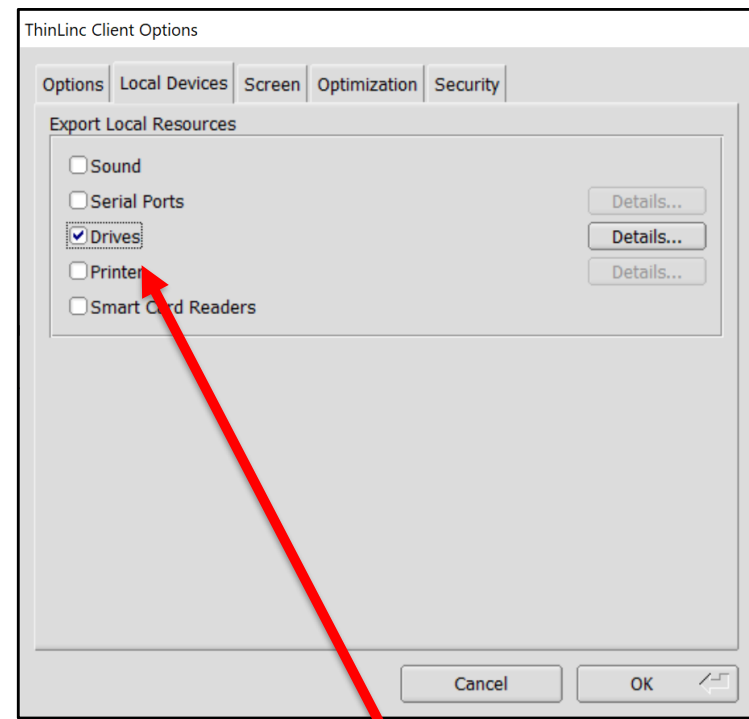
Other ThinLinc Client versions

How to access the computing facilities

ThinLinc Graphical User Interface Client on PC



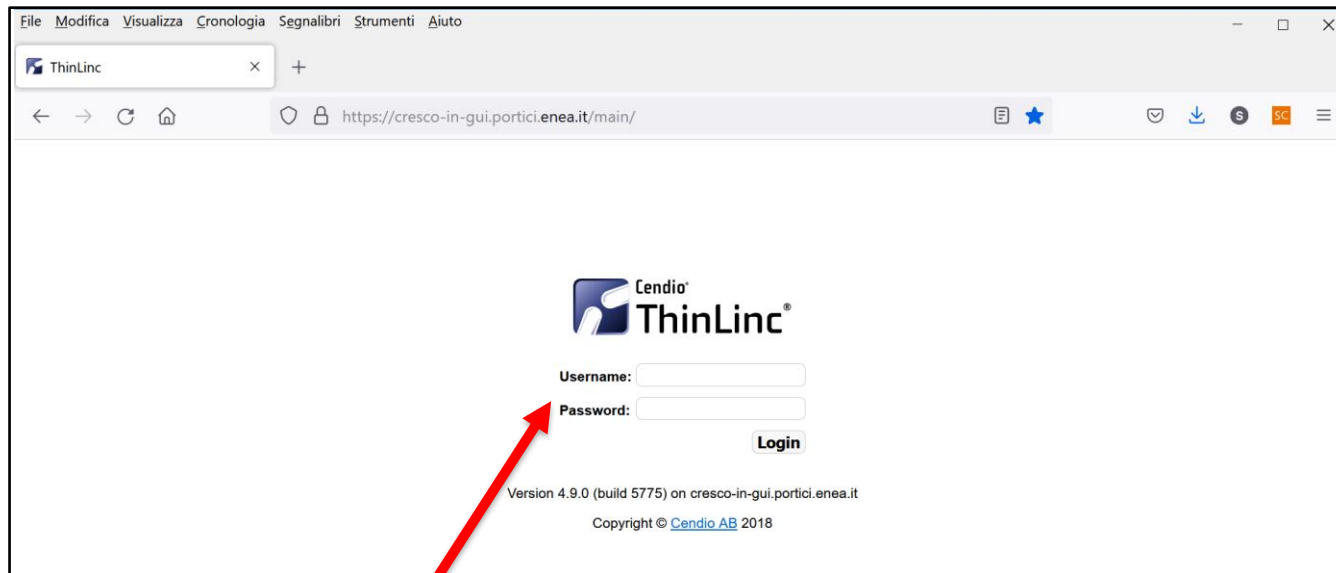
ENEAGRID *userid* and *password*



For example the hard disk of the PC

How to access the computing facilities

ThinLinc Graphical User Interface - dedicated webpage
<https://cresco-in-gui.portici.enea.it/main/>



ENEAGRID *userid* and *password*

How to access the computing facilities

ThinLinc Graphical User Interface CMAST profile

The image displays three sequential screenshots of the ThinLinc graphical user interface. The first screenshot shows the 'Welcome to ENEAGRID Web Interface' page with a 'Forward' button circled in red. The second screenshot shows the 'ThinLinc Profile Chooser' dialog box, where the 'CMAst Virtual Lab' profile is selected and the 'OK' button is circled in red. The third screenshot shows the CMAST virtual lab desktop environment, featuring a 'Graphics' application icon and other desktop icons like 'xmgrace', 'XCRYSDEN', 'VMD', and 'VESTA'.

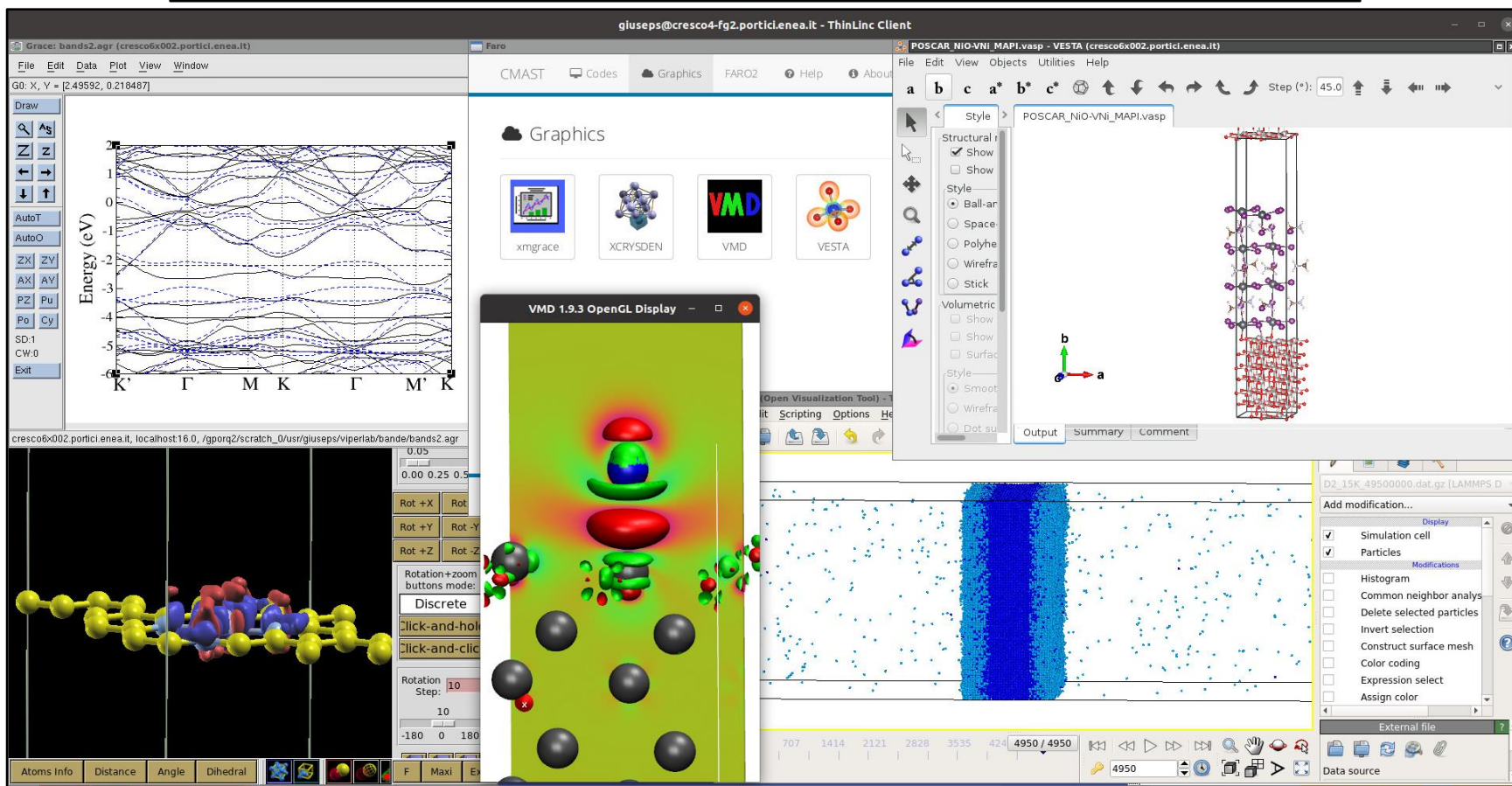
CMAST virtual lab

Computational MAterials Science and Technology

<http://www.afs.enea.it/project/cmast>

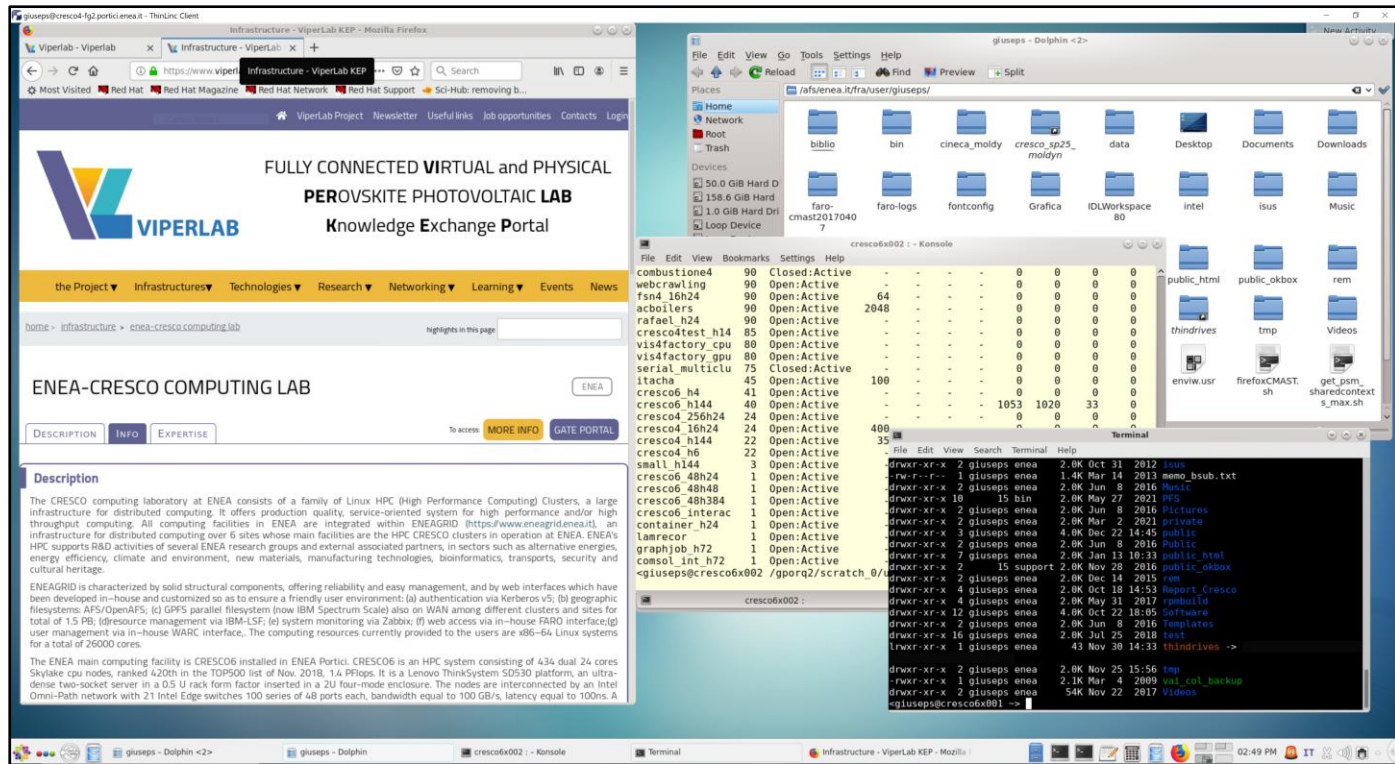
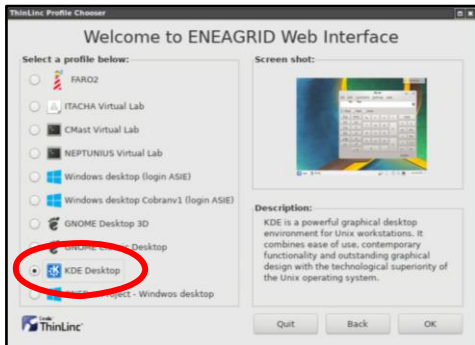
How to access the computing facilities

ThinLinc Graphical User Interface CMAST profile



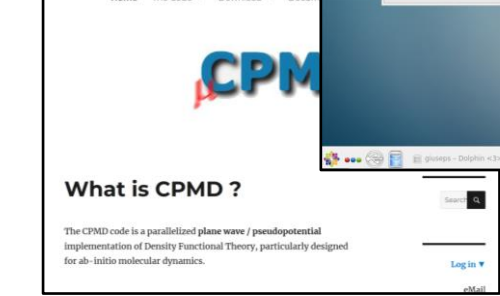
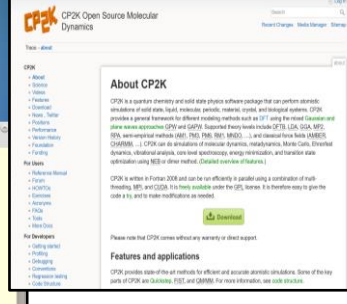
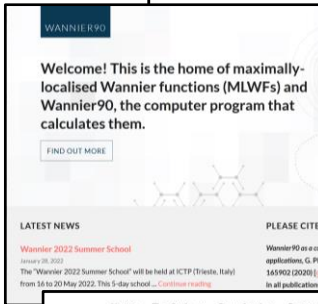
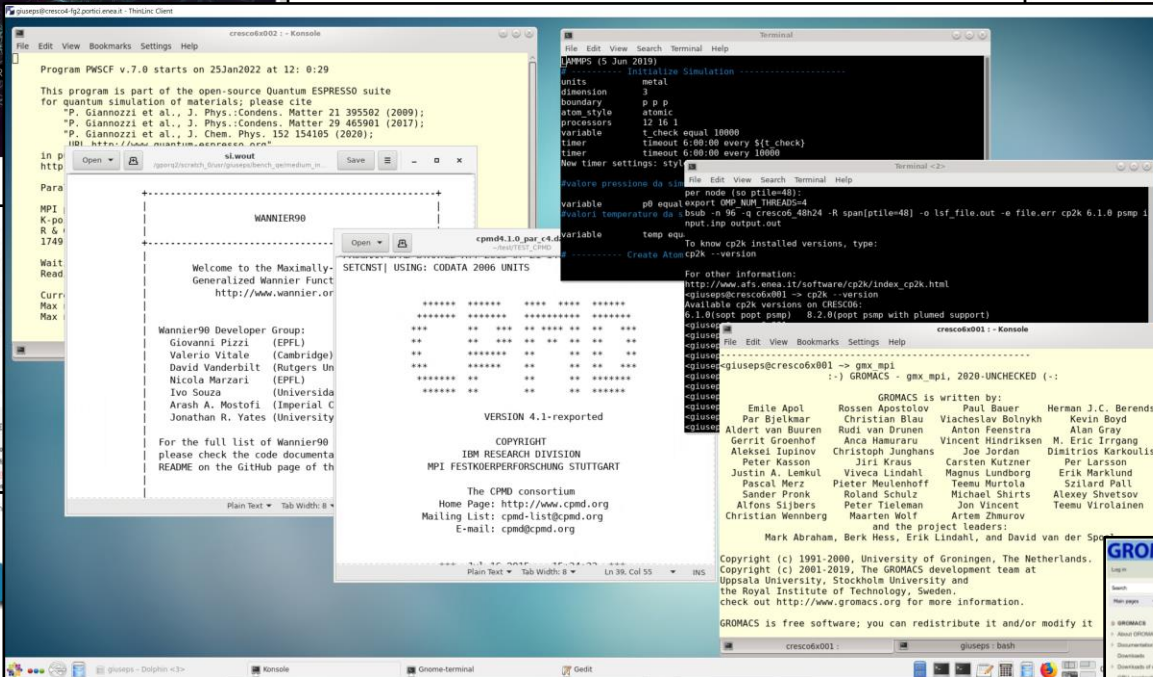
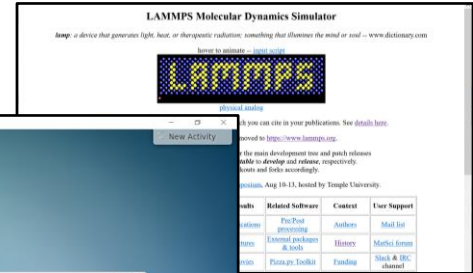
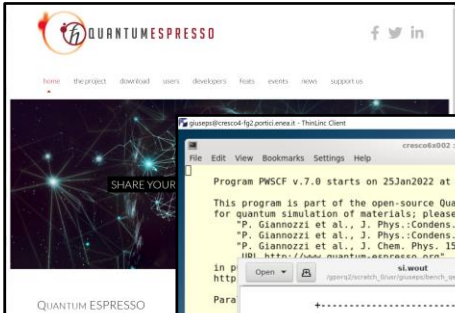
How to access the computing facilities

ThinLinc Graphical User Interface KDE desktop profile



How to access the computing facilities

ThinLinc Graphical User Interface CMAST Lab



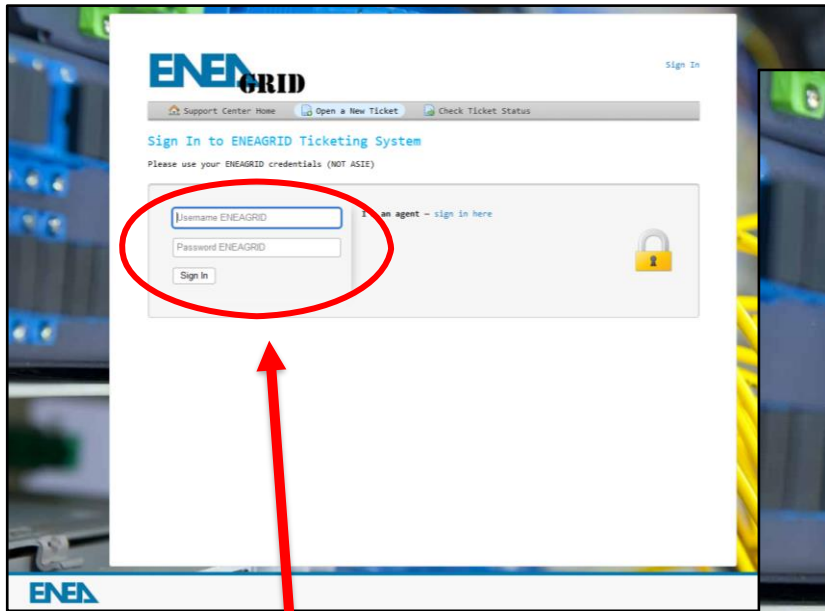
How to open issues in ENEAGRID

To open an issues in ENEAGRID go at www.eneagrid.enea.it/CRESCOportal/

The image shows a screenshot of the ENEAGRID website. The top navigation bar includes links for Home, TERIN, TERIN-ICT, TERIN-ICT-HPC, Account Manager, Ticket System (circled in red), and FRA-POR. Below the navigation bar is a banner with logos for CINECA, CRESO6, progetto Tedat, and ENEA. The main content area features a sidebar with links for HPC User Notices, HPC News, HPC Webinars, CRESO Seminars, Usage Rules, and Acknowledgements. The main content area displays the CRESO logo and a section titled "Access to CRESO via FARO application" with a link to "cresco-in-gui.portici.enea.it". Below this is a section for "ENEAGRID - CRESO clusters Docs - ENEAGRID Primer" and a "News" section with a link to "2021/12/23: Presidio ridotto CRESO dal 24/12/2021 al 09/1/2022 // CRESO...". The right sidebar contains a list of links for ENEAGRID services. The bottom right corner shows a "Ticket System" interface with a "Sign In" button and a "Support Center Home" button. The "Open a New Ticket" button is circled in red.

or directly at <https://gridticket.enea.it/>

How to open issues in ENEAGRID



ENEAGRID *userid* and *password*





Thanks for your attention

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simone.giusepponi@enea.it

