



Enabling Grids for
E-science in Europe

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Compchem VO's user support

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University of Perugia

What do we expect from the Grid?

- Access to a world-wide virtual computing laboratory with almost infinite resources
- Transparent access to distributed data and
- Easy workload management
- Application interfaces easy to use



The Molecular Science community and the EGEE project



- The EGEE Grid environment represents for this community the high valued infrastructure able to supply
 - the necessary **computational power**
 - A suitable **middleware** able to let people collaborate together and access the common resources in a secure way.
- The **CompChem VO** has been created to support such computational needs and pivoting the access to the EGEE Grid facilities.

- CompChem VO is running in the EGEE production Grid from the end of 2004 to support **Computational Chemistry** applications (<http://compchem.unipg.it>)
- The VO has 21 users
- Several EGEE sites are supporting the VO
 - the Italian EGEE sites, CESGA (Spain), IN2P3 (France), Trinity College of Dublin (Ireland), CYFRONET and POZNAN Supercomputing Center (Poland), Hellas Grid and GRNET (Greece), University of Cyprus (Cyprus).

The CompChem users

Organization	User	Contact email
University of Barcelona	Margarita Alberti	maw <at> qf.ub.es
University of the Basque Country (Spain)	Ernesto Garcia	qfpgapae <at> vc.ehu.es
University of Perugia (Italy)	Dimitris Skouteris, Leonardo Arteconi, Alessandro Costantini, Max Porrini	{dimitris, bodynet, alex, max} <at> dyn.unipg.it
Cyfronet (Poland)	Mariusz Sterzel	m.sterzel <at> cyfronet.pl
IMIP- Italian National Research Council (Italy)	Domenico Bruno	d.bruno <at> area.ba.cnr.it
CESGA (Spain)	Javier Lopez	jlopez <at> cesga.es
University of Vienna (Austria)	Hans Lischka	hans.lischka <at> univie.ac.at
University of Cyprus (Cyprus)	Constantinos Zeinalipour-Yazdi	zeinalip <at> ucy.ac.cy
ENEA (Italy)	Carlo Scio	scio <at> Frascati.enea.it
Vilnius University (Lithuania)	Gintaras Urbelis	gintaras.urbelis <at> chf.vu.lt
Center for Parallel Computers (Sweden)	Olav Vahtras	vahtras <at> pdc.kth.se
University of Crete and FORTH (Greece)	Stavros C Farantos	farantos <at> iesl.forth.gr

COST in Chemistry D37 action: GridChem

- Most of the CompChem users started the collaboration in the COST in Chemistry D23 Action, called *Metachem*
- COST is one of the longest-running instruments supporting co-operation among scientists and researchers across Europe with **35 member countries**.
- In the COST in Chemistry program has been recently activated the Action D37, called *GridChem*
 - devoted to deploy the most important **computational chemistry codes** in the Grid and the existing e-infrastructures
- EGEE and CompChem VO **will support** the activities of the Action and new users are expected to join the VO.

Main characteristics of CompChem applications

- Both **CPU-bound** and **data intensive** jobs are present
 - Massive submission of sequential jobs running on different input datasets
- **Parallel jobs**: some programs have been structured to run in parallel.
 - Contribution of compchem to MPI international workshop, Dublin, Dec 11-12th, 2006.
- **Interactive jobs**: GEMS (Grid Enabled Molecular simulator)
- We are implementing Grid Services
 - to access the standard functionalities of the programs
 - to create visualization and Web3D interfaces in order to visualize the simulations coming from the calculations

Software management

- Programs ported in the Grid environment (ABCtraj, Venus, DI_Poly, Rwavepr, Chimere, etc)
- To optimise the use of the packages and facilitate the users we are planning to

maintain the software from a central location

This permit to the user

- Compile each program on the target architecture
 - Solve the most frequent **dependencies** of used programs (F90 compiler, mpi library, etc)
- User support and trouble ticketing system are available on compchem webpage.

<http://compchem.unipg.it>



[EGEE Home](#) | [Technical Pages Home](#) | [Calendar](#) | [Agenda](#) | [Glossary](#)



CompChem Virtual Organization



[CompChem Info Sheet](#) | [CompChem FAQ](#) | [Report a problem on CompChem to the EGEE Support Team \(GGUS\)](#)

The CompChem Virtual Organization has been established in the [EGEE](#) Production Grid environment to support the Computational Chemistry applications. The collaboration has been defined in a **Memorandum of Understanding**. The text of the MoU is available [here](#).

To be enabled to EGEE Grid you need a valid X.509 Certificate. If do not have it, you must request it to the Certification Authority that serves your Institution or your Country. If in trouble check the [LCG User registration](#) guide to find the most suitable Certification Authority for your needs.

To join CompChem VO, please connect with a web browser equipped with your personal X.509 certificate to the following URL:
<https://voms.cnaf.infn.it:8443/voms/compchem/webui/request/user/create>.

A short description of the operations to be performed to start using CompChem VO is available [here](#).

If you are an administrator of an EGEE Grid production site, please follow the [following instructions](#) to support the CompChem VO applications in your site.

[The CompChem VO Manager](#)

What the users do

- They **don't use** any kind of ticketing system
- They use a more direct (but often not more easy and quick) way to solve their problems inside the Grid
 - Mailing (and/or calling) directly the site administrator

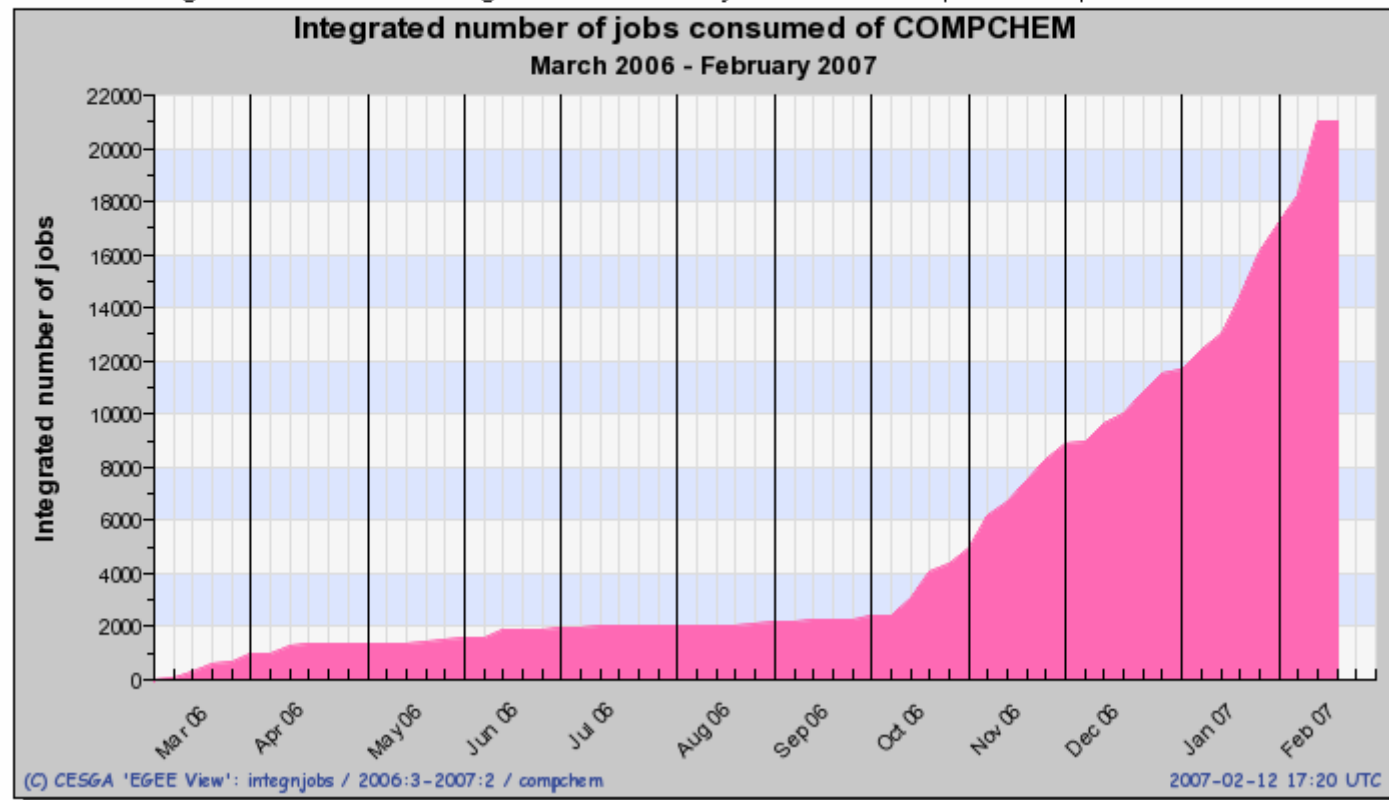
What the site administrator(s) do

- Use Italian INFNGrid ticketing system (**EGEE SA1 ITALY**) for any problem regarding the Grid status
 - 90% of the problems have been resolved
 - The solution of some problems is still in progress
- Don't use directly GGUS
- Use GGUS via EGEE SA1 ITALY
- Propose the use of both compchem FAQ and ticketing systems

Some statistics

EGEE Integrated number of jobs consumed per VO. March 2006 - February 2007.

The following chart shows the integrated number of jobs consumed per week per each selected VO.

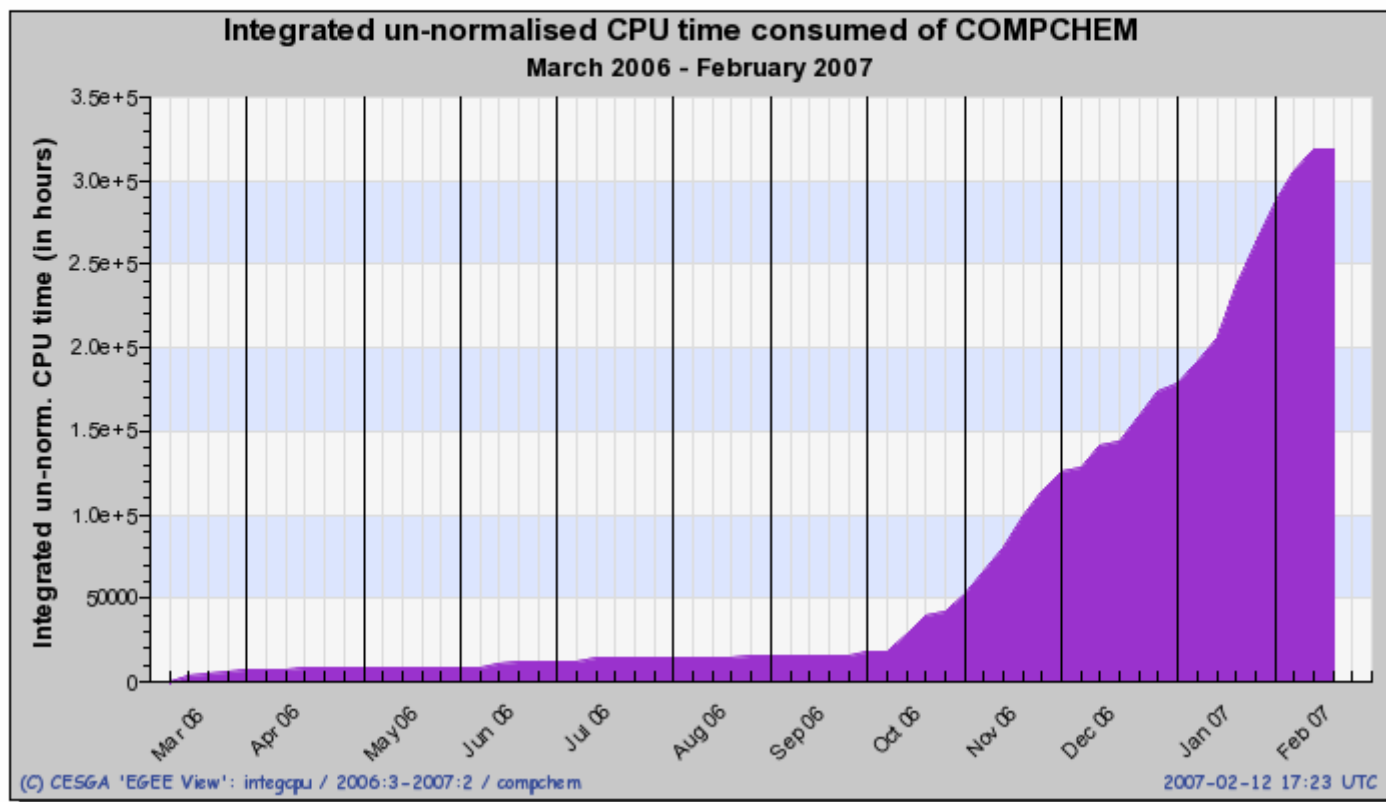


Hours of CPU per week

EGEE Integrated un-normalised CPU time consumed per VO.

March 2006 - February 2007.

The following chart shows the integrated un-normalised CPU time consumed per week per each selected VO.

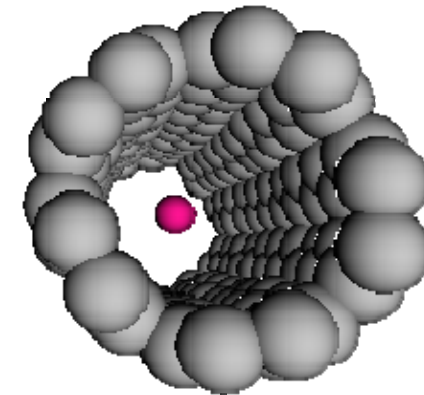


Some results

Temperature / K	Density / Kg m ⁻³	Pressure / bar	Simulation time / ns
200 ± 3	613.4 ± 4.4	1.714 ± 28	0.1
205 ± 4	607.5 ± 5.6	1.731 ± 27	0.1
210 ± 3	602.5 ± 5.3	1.853 ± 28	0.1
215 ± 4	596.6 ± 5.4	1.862 ± 26	0.1
220 ± 4	591.2 ± 6.6	1.934 ± 28	0.1
225 ± 4	585.8 ± 5.7	1.902 ± 29	0.1
230 ± 4	583.7 ± 5.9	1.723 ± 28	0.1

Density value of Propane in liquid phase 582 Kg m⁻³ at T=230 K at P=1.013 bar

Calculated thermodynamics properties of propane bulk system with 288 molecules of Propane



Ion in a Carbon NanoTube