The Molecular Science challenges in EGEE

Osvaldo Gervasi[1], Antonio Laganà[2], Leonardo Arteconi[2], Cristian Dittamo[1]

[1]Dept. of Math and Comp Sci, University of Perugia

[2]Dept. of Chemistry, University of Perugia

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Information Society and Media

Outline

- **The Molecular Science community**
- **CompChem VO**
  - Management and support
  - Current status
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- **Type of applications**
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- **Some results**
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The Molecular Science community

- **The understanding of the behavior of molecular systems is of great importance for the progress of**
  - the life sciences
  - several industrial applications.
- **The Molecular Science community performs the study of molecular systems by using simulations that require an heavy demand of computational resources.**
- **It is mandatory to put together the competencies of various laboratories to achieve ambitious results:**
  - active collaboration between people with complementary expertise
  - interaction between various computational approaches

The Molecular Science community

- **The EGEE Grid environment represents for this community the high valued infrastructure able to supply**
  - the necessary computational power
  - the proper 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.**
- **Several EGEE sites are supporting the VO, in particular the Italian EGEE sites, CESGA (Spain), CYFRONET and POZNAN Supercomputing Center (Poland), Hellas Grid and GRNET (Greece), University of Cyprus (Cyprus).**

The management of CompChem VO

- **The management of the VO is based on the collaboration between two Departments of Perugia University**
- **Chair: Prof. Antonio Laganà, Dept. of Chemistry**
- **VO manager: Dr. Osvaldo Gervasi, Dept of Mathematics and Computer Science**
- **Support team:**
  - Dr. Cristian Dittamo
  - Dr. Francesca Gentili
  - Dr. Matteo Diarena

CompSci

  - Dr. Leonardo Pacifici
  - Dr. Leonardo Arteconi
  - Dr. Massimiliano Porrini

Chemistry

How to join CompChem VO

- **A Consortium agreement has to be signed by the partner laboratory**
- **Each partner may be involved at different levels:**
  - User: implementation on the Grid of a suite of codes of exclusive interest for the implementing laboratory
  - Code offer: the laboratory confers to the VO a stable suite of codes
  - Service offer: the laboratory participates to the management of the Grid infrastructure (manpower, hardware, service brokering and monitoring, etc), the development of joint projects etc.

The CompChem users

Organization	Actor	Contact email
University of Barcelona	Margarita Alberti	maw at qf.ub.es
University of the Basque Country	Ernesto Garcia	qfpgapae at vc.ehu.es
University of Perugia	Dimitris Skouteris	dimitris at dyn.unipg.it
University of Geneva	Laura Gagliardi	laura.gagliardi at unipa.it
IMIP- Italian National Research Council	Mario Capitelli	m.capitelli at area.ba.cnr.it
University of Goteborg	Gunnar Nyman	nyman at phc.gu.se
University of Crete	Stavros C Farantos	farantos at iesl.forth.gr
University of Vienna	Hans Lischka	hans.lischka at univie.ac.at
Swiss Federal Institute of Technology (ETH)	Hans Peter Luethi	hans.luethi at sl.ethz.ch

The Grid added value

- **Software integration into distributed workflows**
  - to assemble applications out of various (different or complementary) distributed competences coordinated via the Grid: electronic structure, elementary dynamics, statistical averaging, interfacing the experiment.
- **Computational Campaigns**
  - to evaluate properties depending on the fate of few out of millions, billions or even more events by distributing the execution of the computations on the Grid
- **Collaborative Engineering of knowledge**
  - to handle chemical information and knowledge including training and production of new knowledge
- **Security Infrastructure**
  - The state-of-the-art tools to share computational resources and to share computational codes among institutions in a secure fashion.

Type of applications

- **Quasiclassical (production)**
  - ABCtraj
  - Venus
  - DL-POLY
- **Quantum Time Dependent (production)**
  - RWAVEP
- **Quantum Time Independent (test)**
  - APH3D
- **Electronic structure (in test on a vanilla Globus environment)**
  - MOLPRO
  - GAMESS, GAMESS-UK
  - Columbus (test phase will start soon)

CompChem Requirements

- **Dynamic extension of the proxy in the VOMS authentication system.**
- **We are mainly interested in using homogeneous clusters to control**
  - **Performance** (estimated duration of the job)
  - **Numerical precision** of the calculations
- **Several applications take advantage from the use of the Intel Fortran Compiler, available for free. The availability of IFC is important to improve the performance of the applications in the local environment of a given site.**
- **The inbound/outbound connectivity of the working nodes is required in order to guarantee the communication with GEMS portal**

CompChem issues

- **Licensed software (Gamess, Molpro, Venus, etc) should be declared by the enabled CEs and requested by the jobs in the Requirements field of the JDL, so that the licensed software could be used where the software licence will be available.**
- **Cal Loomis has activated the MPI working group, that is a subgroup of the EGEE TCG, devoted to optimise the G-lite support of MPI (and MPICH-G2). The optimisation and the wide availability of the support of parallel jobs is an important issue of CompChem VO. In particular we are interested in:**
  - LAM/MPI: to execute the various packages in parallel
  - MPICH-G2 to allow the scheduling among the nodes of different CEs
  - The scheduling of parallel jobs should not penalize requests for a large number of nodes
- **Recently the execution of job experience problems with some sites (job aborted) for unknown reasons.**

Some results

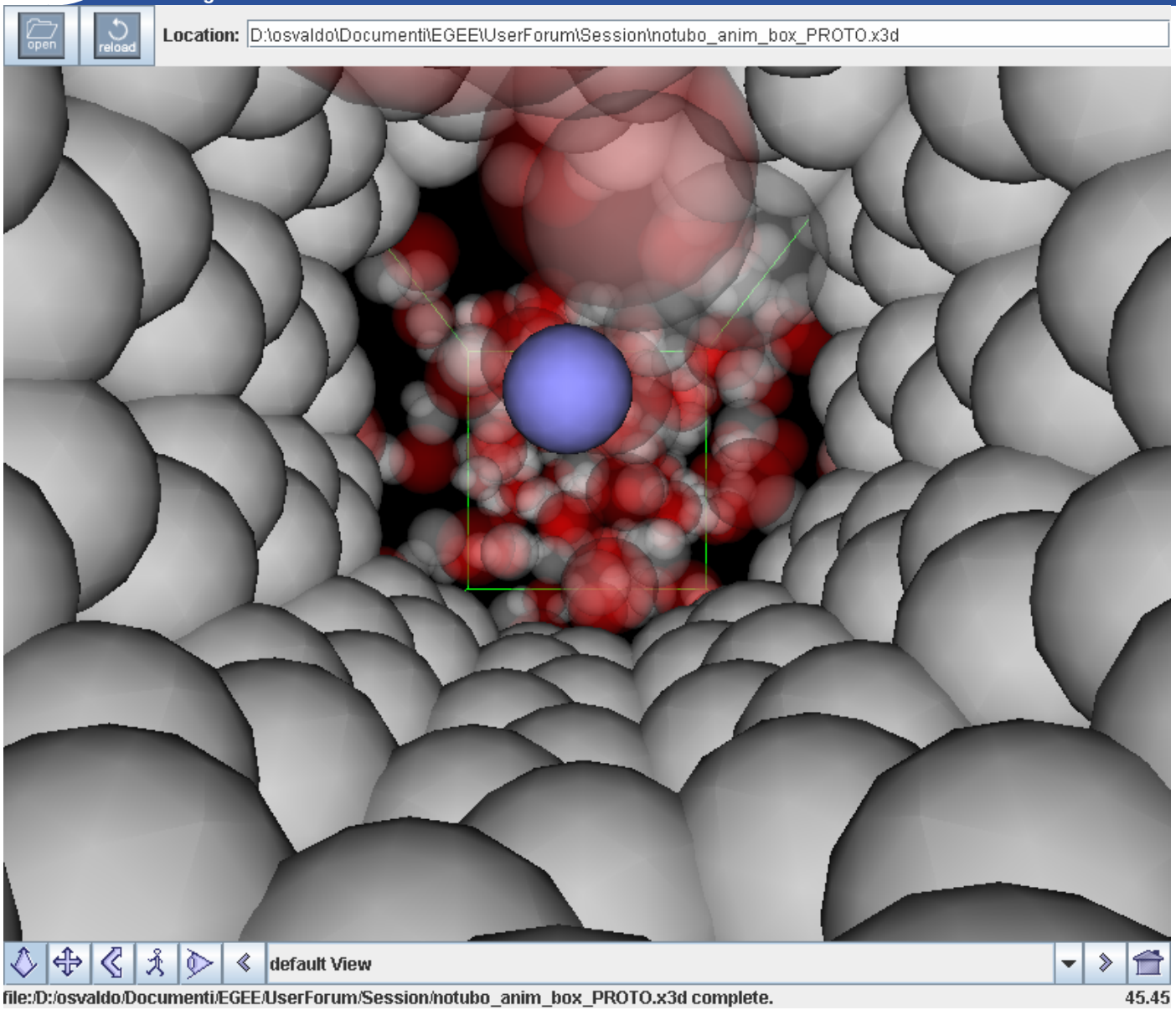
- **Study of the quasiclassical properties of polyatomic systems (intensive campaign using Venus code)**
  - Low atmosphere molecular systems
  - Astrochemistry
  - Spacecraft reentering
  - Environmental Chemistry
- **Ionic permeability on molecular structures (using DL-POLY).**
  - Ion transportation through molecular pores for biological modeling
  - Carbon nanotubes (CNT) modeling
  - Conduction and semi-conduction
  - Molecular devices

Some results (i)

- **Quantum treatment of molecular processes.**
  - Reactive scattering of small molecules
  - Wave packet approaches to molecular processes
  - Non-adiabatic transitions
  - Tunnelling
  - Resonance's
  - Alignment and orientation effects
  - Ion conductivity in CNT

Some results (i)

The ions forced to flow into the nanotube by the applied potential difference along z-axis are counted



Conclusions

- **The difficulties of operating under the unfounded status**
- **Heavy manpower demand for routinary Grid operations**
- **High request for supporting end-user applications**
  - Nanotubes
  - Life sciences
  - Statistical Thermodynamics
  - Molecular Virtual Reality
- **Standard environments and training to get started**
- **Sustainability of the cooperation**
- **gLite migration**