Enabling Grids for E-science in Europe

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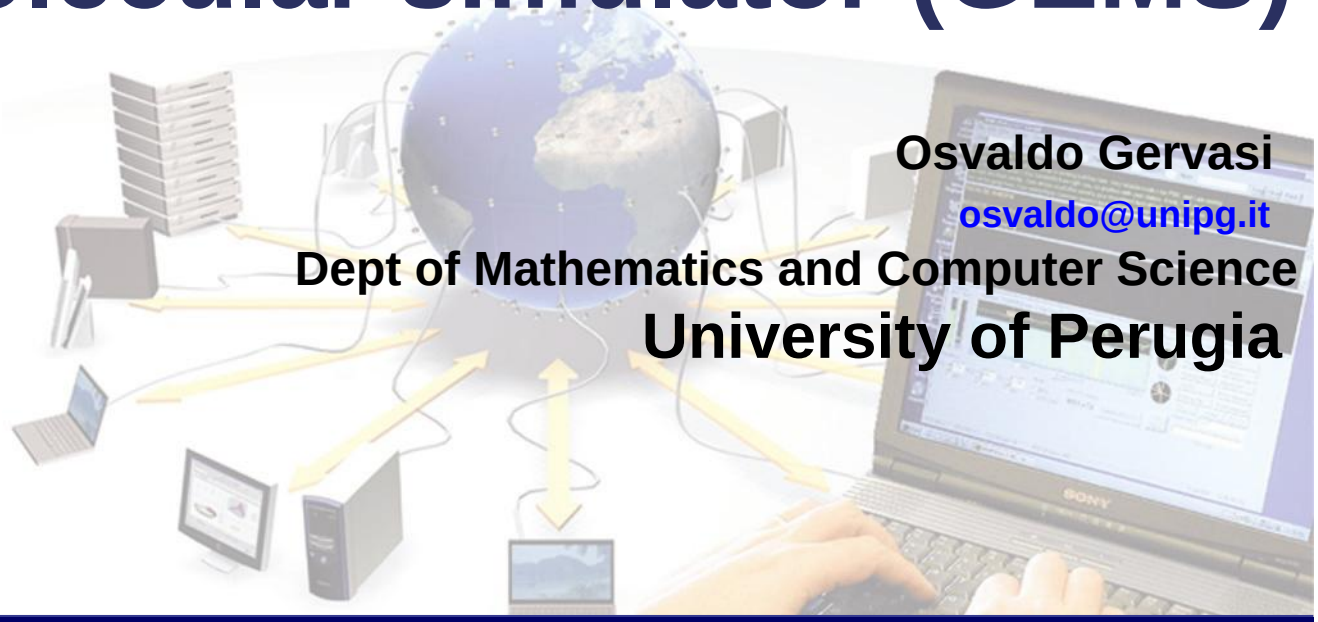
Advances in the Grid enabled molecular simulator (GEMS)



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Introduction

- CompChem VO is running in the EGEE production Grid from the end of 2004.
- A MoU has been signed between EGEE and the CompChem Virtual Community.
- The Grid Enabled Molecular Simulator (GEMS) is the product to be deployed during the collaboration. Our efforts are presently focused on:
  - Porting new computational chemistry programs in the EGEE Grid
  - Developing the workflow environment interfaced with the programs
- As CompChem VO we have ported in the EGEE Grid a new application, Chimere, external to the molecular simulator.

CompChem VO

- CompChem VO has been established to support Computational Chemistry applications (see the web site: http://compchem.unipg.it).
- It is presently a small VO. We are promoting in several ways the VO among the Computational Chemistry community ad new users are expected.
- We have activated all instruments EGEE has made available for the user support and for the trouble ticketing system. This makes our life easier.
- To optimise the usage of the involved packages and facilitate the users we are installing the VO packages in the various sites that are supporting CompChem.
  - Each program will be compiled on the target architecture
  - We will be able to solve the dependencies of the VO programs (F90 compiler, mpich, etc)

COST in Chemistry D37 action: *GridChem*

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- COST is one of the longest-running instruments supporting co-operation among scientists and researchers across Europe. COST now has 35 member countries.
- The COST in Chemistry program has been recently activated the Action D37, called *GridChem*
- The Action is 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.

COST in Chemistry D37 action: *GridChem*

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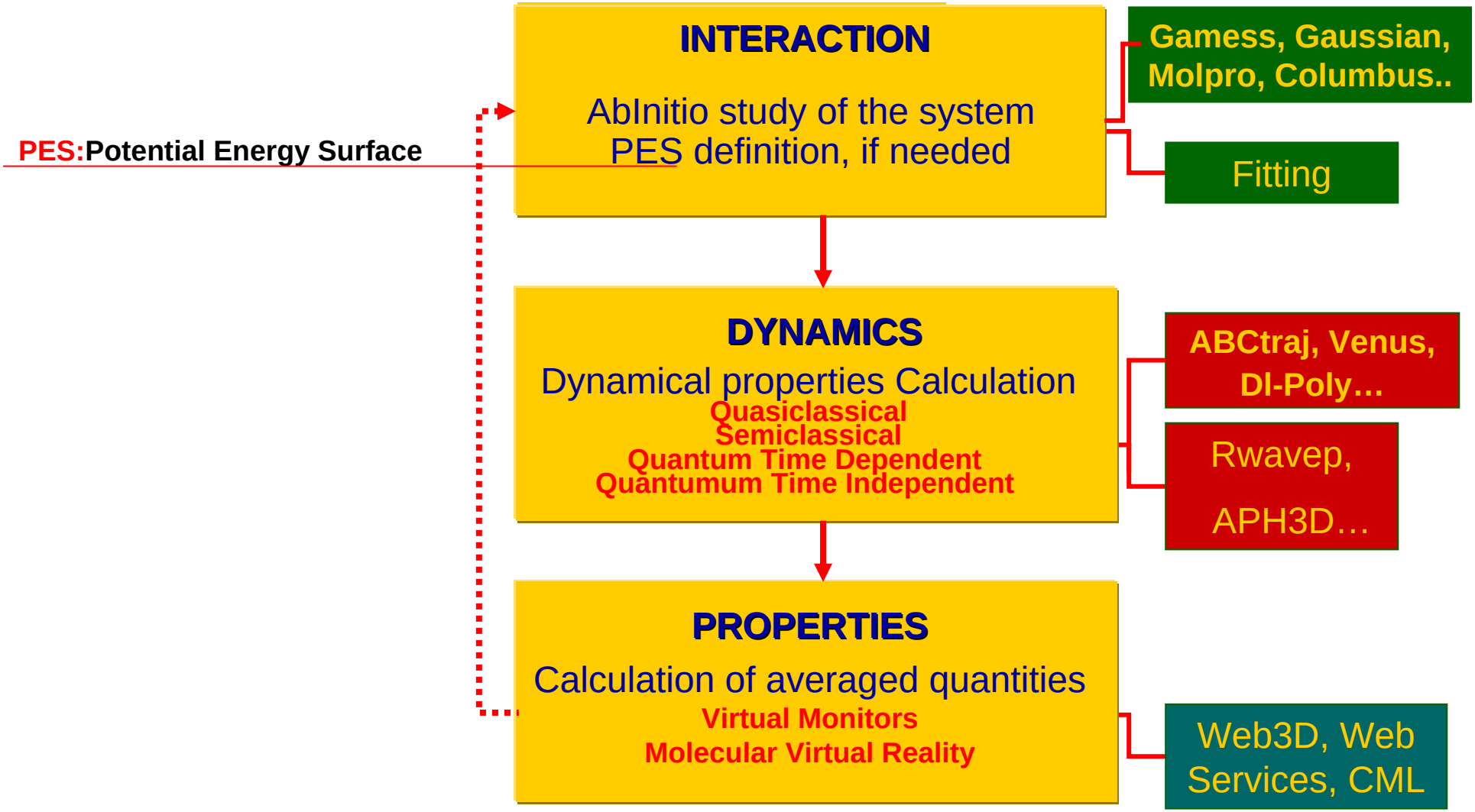
- Four working group have been activated in GridChem Action:
  - Photodyn (Photochemical and photobiological dynamics simulations)
  - Qdyn (Quantum Dynamical simulations)
  - Elams (Web3D technologies, Visualization, Grid Services for computational chemistry programs)
  - DeciQ (data interoperability among computational chemistry programs and common representation of the information)
- Two other working groups (one that will group all the owners of the main computational chemistry programs, the other related to workflows for computational chemistry) is waiting for the formal approval.

GEMS workflow



The Interaction module

- The module related to the ab initio study of the molecular systems is still a prototype. In the near future we plan to make available to the users the following programs:
  - GAMESS
  - COLUMBUS
- Several activities planned in the COST Action GridChem are a matter of this module.
- Regarding the popular commercial programs Gaussian and Molpro we will collaborate with the Gaussian VO.

The Fitting module

- The Ab initio study of the system produces a grid of values that need to be interpolated (best fitting process) in order to produce a functional form of the Potential Energy Surface (PES)
- Some constraints must be reproduced by the functional form (i.e.: spectroscopic and experimental information).
- The functional form have to satisfy some mathematical constraints of the application used to perform the dynamical study of the system (i.e.: the function must be derivable)
- Several types of functional forms are used. They have different properties and degree of accuracy (LEPS, Bond Order, Rotating Bond Order, etc).

The Dynamics module

- In the Dynamics modules we consider all programs that perform the dynamical simulations, using (if required by the method) a given functional representation of the Potential Energy Surface and providing the estimate of the reaction observables.
- The following programs have been implemented :
  - Quasiclassical approach
    - ABCtraj (atom + diatom)
    - Venus (many atoms)
    - DL-Poly (complex and biological systems)
  - Quantum approach
    - Rwavepr (time dependent approach)

The Dynamics module: some results

- The group of the University of the Basque Country carried out a computational campaign to study the properties of the reaction

$$OH+CO \rightarrow H+CO_2$$

- The results of such a campaign contributed to the understanding of this important system for the combustion of hydrocarbons with air. In the next months the same system will be studied using the Rwavepr program, based on a more accurate Quantum Time Dependent method.
- In the Dept. of Chemistry of Perugia the behaviour of Ions moving through a Carbon Nano Tube has been studied. At room temperature the ion is trapped in the CNT and oscillates at the TeraHertz frequency. This behaviour may be interesting for several industrial applications.

The Observable module: Web3D and Grid Services

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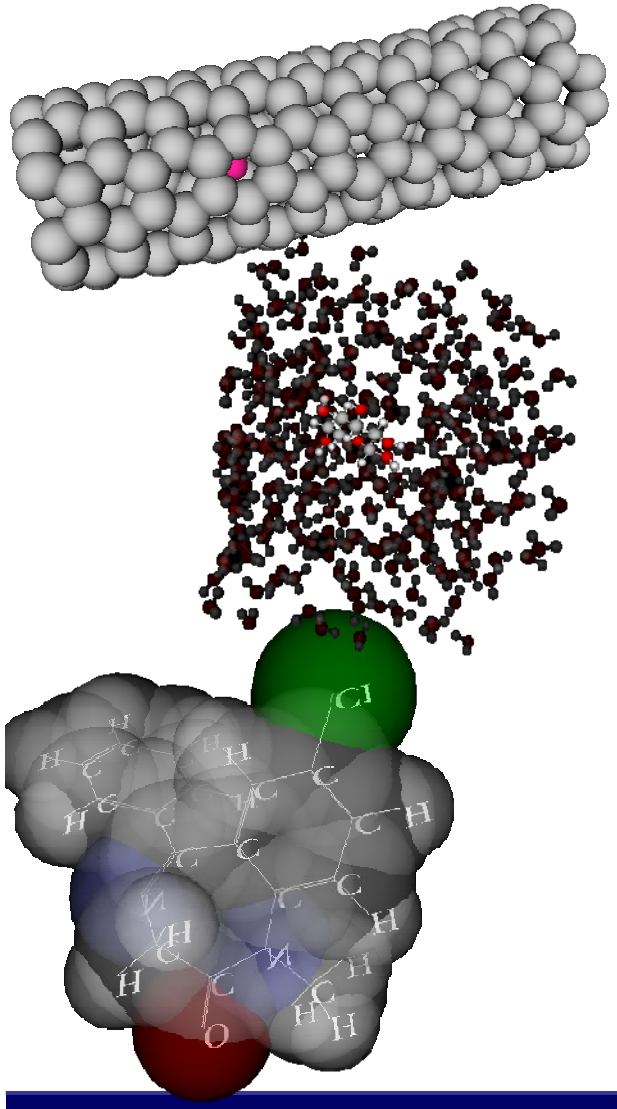
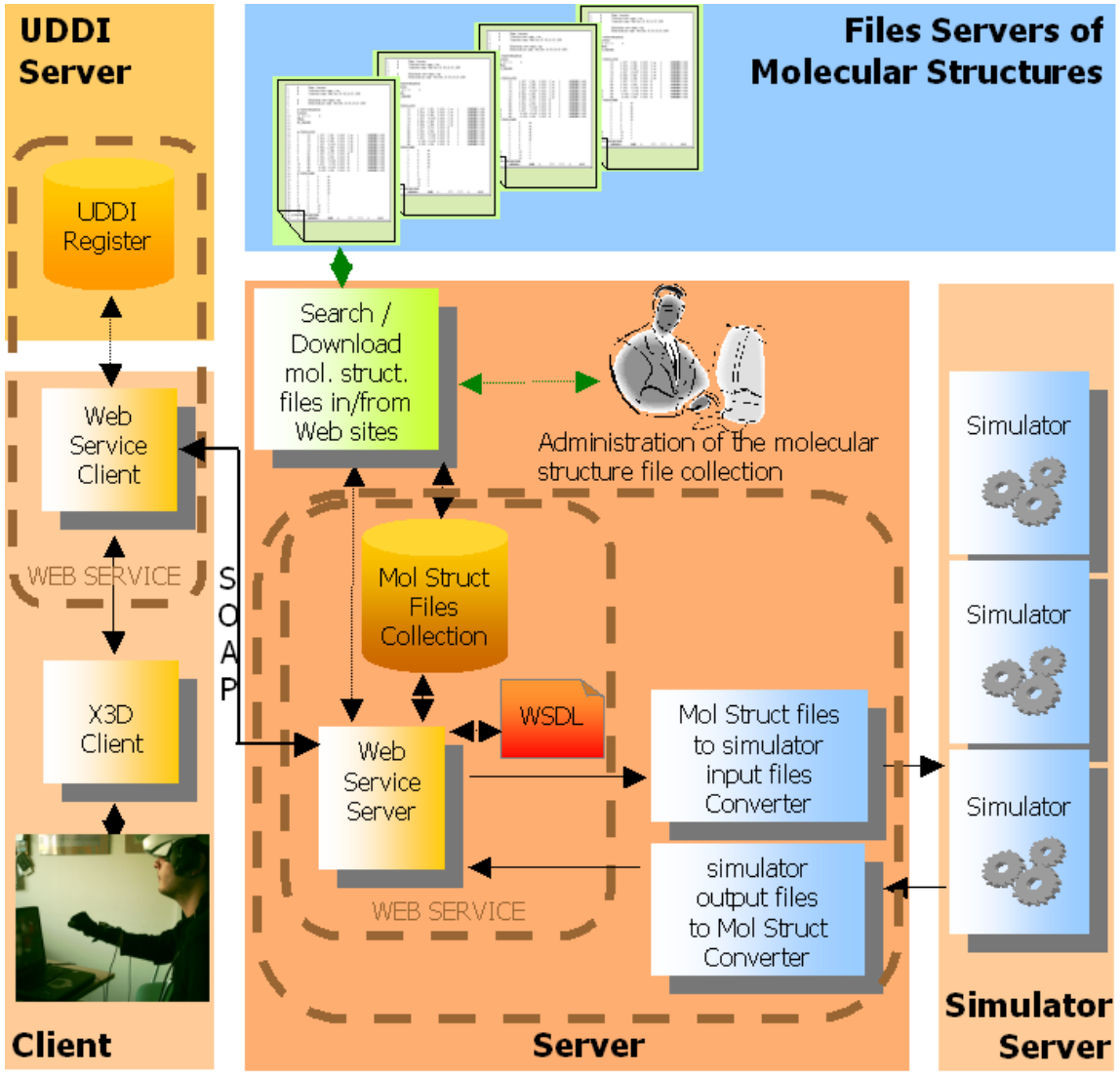


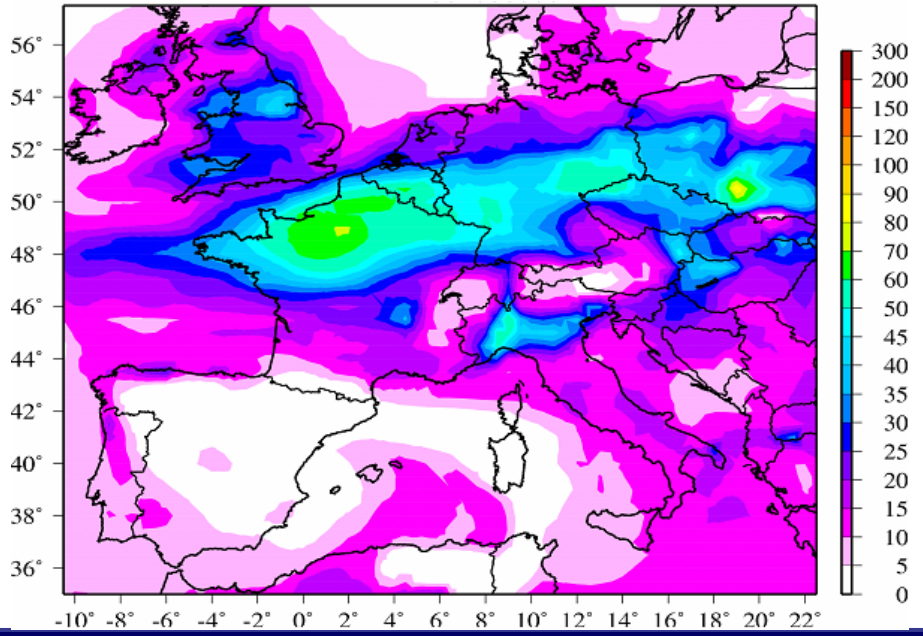


New applications: Chimere

- Chimere implements a chemistry transport model to provide daily forecasts of ozone, aereosol and other polluttants
- It offers the option to include several gas phase chemical mechanisms
- More than 300 chemistry and photo chemistry reactions of 80 gaseous species

Requirements:

- Fortran 90 compiler
- MPICH



Sample output of Chimere: simulation of Surface PM10 concentrations

Conclusions

- GEMS is moving from the status of prototype to an environment suitable for production runs.
- Venus and Dl-Poly are used in the EGEE Grid environment to perform massive computational campaigns.
- Rwavep (quantum time-dependent approach) is also used this way.
- Some programs will be included in GEMS, thanks to the collaboration established in the COST D37 Action, GridChem
- We will enhance the available instruments for the researcher, based on visualization and Web3D technologies, to facilitate its analysis of the simulation results.
- We are looking for new collaborations in the Computational Chemistry community