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Socially impacting grid services from the Chemistry heavy user community

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Conclusions

The porting of key ab initio approaches to molecular simulations onto the grid using tools developed by other communities and developing new tools ad hoc designed for the Chemistry and molecular science one has shown to be highly effective not only for further development of grid technologies and related chemical applications but also for paving the way for developing higher education virtual campus technologies, governing emergencies, designing innovative processes and materials for the quality of life, energetic problems and environmental issues of high social impact.

Overview

The work of the community of computational chemists and molecular scientists is at the core of several innovation and technological advances of the modern society. To this end we have joined our efforts (carried out within the COMPCHEM VO) with those of some members of the GAUSSIAN (CYFRONET) one belonging to the same Computational Chemistry area to prepare the ground for joining other communities like MoSGrid (UCO) and ENEA-GRID (ENEA) in building a Heavy User Community (HUC). Our effort has focused on adopting (with appropriate adaptations) some basic Grid tools, including those designed and implemented by other HUCs to support their users, by assembling suitable workflows for chemistry and molecular science applications, by manag-ing repositories related repositories and proposing appropriate mechanisms to foster the formation of collaborative research within the community.

Impact

The impact of our work has materialized into the offer to the members of our community of GEMS, a prototype simulator able to start from first principles and end up, in a complete a priori fashion, by evaluating the signal of crossed beam experiments and the values of reactive cross sections and rate coefficients. The tools used for that purpose (the KEPLER workflow, the data models of Q5cost and D5cost, the grid framework of GriF) drive the user through the massive calculations needed by the above mentioned packages to allow a realistic modeling based on a complex combination of building blocks in which ab initio treatments, dynamics, kinetics, fluid dynamics, statistical sampling can be combined together with statistical treatments and rendering techniques to build versatile user centric instruments.
Examples of the application of this approach have been worked out of software devoted to the con-struction of scenarios for the production of secondary pollutants, to the labeling of chemical products and to the assemblage of distributed repositories for learning objects. The development of grid im-plemented versions of this software that is being taken care of in our laboratory is aimed at making sustainable, within the chemistry community, the development of grid tools and applications and at producing as well a high social and economic fall out by tackling area of applications relevant to envi-ronmental, health and educational aspects

The improvement and further development on the distributed platform of EGI of the molecular level components of those software is, in fact, a clear citizens-oriented target that impacts not only the work of chemists, materials technologists, engineers, biologists etc. working on the development of faster and more efficient modelling of complex systems starting from the microscopic level but also (and even more) the every day activities of students and generic citizens.

Description of the work

The work focused on the design and development of ab initio grid empowered molecular simulators of complex physical phenomena and technologies to the end of assembling study cases for building grid services of social relevance.

Among the software tools and computer applications considered for this purpose are:

- Middleware, workflows and frameworks: this is a set of tools like FARO, KEPLER and GriF that are being analysed and compared with other products already implemented in EGI. The first of them is targeted to foster the communication between the EGI grid and other platforms (like that of ENEA). The second of them is a workflow used for the assemblage of the grid empowered molecular simula-tors. The third one is a framework based on a JAVA Service Oriented Architecture (SOA) designed to facilitate the use of the Grid by non specialists by properly selecting the user interface, the computing element and the storage element.
- Electronic structure: this is a layer of application software made of highly successful quantum Chemistry packages (like GAMESS, GAUSSIAN, MOLPRO, DALTON, MOLCAS, NWCHEM, TURBOMOLE, etc.), which are at present solid foundations of any determination of molecular struc-tures and properties.
- Dynamics: this is a layer of Molecular dynamics codes like either VENUS, DL_POLY, GRO-MACS, CPMD, CP2K, NAMD, etc. treating molecular systems as an ensemble of particles or RWAVEPR, MCTDH, FLUSS, ABC, etc. treating molecular systems as quantum waves and there-fore requiring a larger size of node memory.
- Multiscale and statistical treatments: this is a set of services based on grid simulations of natural structures and processes based on multi-scale and multi-physics approaches starting from the nanoscale level and including when appropriate fluid dynamics, randomization, virtual reality, data mining, etc..

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