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Towards a Material and Molecular Science Research Community

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Leveraging on a grid and cloud based synergistic use of the Molecular and Materials Sciences research skills of its members, the Chemistry, Molecular & Materials Science and Technology (CMMST) community has developed on the European Grid Infrastructure (EGI) a set of activities, softwares and human services aimed at supporting Computational Chemistry applications.
In this endeavour, fundamental is the synergy established between the MOSGrid and ScalaLife projects and the COMPCHEM, GAUSSIAN, IBERGRID Virtual Organizations (VO) of EGI aimed at formulating a proposal for the setup a specific Virtual Research Community (VRC) in EGI. The proposal has been formulated as a deliverable of the EGI-InSPIRE Virtual Team (VT) project "Towards a CMMST VRC"promoted by the members of the COMPCHEM VO.
Central aspects of the document are the assemblage of a live library of interoperable codes, the implementation of a set of tools facilitating the selection of appropriate computing elements among the available HTC and HPC platforms, the design of a credit system rewarding the work done on behalf of the community and the adoption of de facto standards for quantum chemistry and molecular dynamics data formats.

Wider impact and conclusions

The adopted synergistic computing model meets the dreams of the most recent generations of computational scientists and allows CMMST members to run highly complex applications not only by having flat access to the hybrid grid platform but also, for example, by exploiting the advanced features of some workflow structured computing procedures used and assembled to carry out even virtual experiments. This approach and the related activities have led to the heavy engagements of the resources of the various National Grid Initiatives (NGI)s of EGI such as France, Greece, Spain, Italy, Poland and United Kingdom. This European cluster has represented the solid platform for proposing collaborative developments of CMMST computations in OSG groundent the interaction with the US project XSEDE. Efforts are undergoing also to open similar collaboration perspectives in Asia.

Description of work

Presently, Molecular Simulations have taken the lead in the investigation of structure, dynamics, surface properties and thermodynamics of inorganic, biological and polymeric systems because they can provide a high level of detail in the description of processes at sub nanometer scale. This has been made possible by the use of concurrent computing and by the synergism achievable on grid and cloud platforms. To this end, an EGI-InSPIRE Virtual Team project has been established among the CMMST community members with the purpose of assembling a VRC out of the above mentioned COMPCHEM, GAUSSIAN and IBERGRID VOs.
The synergistic nature of the proposed community model became of crucial importance for those theoretical and computational chemists who carry out multi-scale simulations of realistic systems in order to reproduce their observable physical properties by starting from first principles and composing different expertise. This has fostered the a la carte use of appropriate Grid tools (portals, workflows, frameworks, etc.) and chained modules of applications made available to the members of the community by EGI, CMMST and other providers.
The already established level of synergy has allowed the investigation of different CMMST themes like: Energy storage devices: Gas hydrates formation, Membrane micropores: ion channel simulation, Aerothermodynamics effects in spacecraft reentry: heat transfer evaluation from molecular dynamics, Virtual crossed beam experiments: estimating the efficiency of elementary reactive processes intervening in combustion. Central to this effort has been the assemblage of the Grid Empowered Molecular Simulator (GEMS) in which electronic structure, nuclei dynamics and statistical treatments are chained together in a suitable workflows to the end of computing observable properties of realistic systems with atomistic granularity.

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