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A priori modeling of chemical reactions on a grid-based virtual laboratory: towards standard representations of data for molecular chemistry

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We have assembled on the COMPCHEM segment of the EGEE Grid Infrastructure the core of the Grid Empowered Molecular Simulator (GEMS) queueing in a common workflow a suite of - adequately "gridified" - codes for the a priori modeling of elementary chemical processes. The communication between applications from different scientific domains is fostered by the use of common data formats. A test calculation is shown for the benchmark H + H2 reaction.

Detailed analysis

GEMS is a grid-based molecular simulator that can act as a molecular science computational engine in complex multiscale chemical contexts. The general procedure for the modeling of chemical reactions is articulated as follows:

A) evaluate the potential energy between the atoms involved at a set of geometries concurrently;
B) get an analytical representation of the Potential Energy Surface (PES) by fitting the obtained values;
C) run the dynamics on the resulting PES at several initial conditions concurrently and extract the reactive properties.

The intermediate B) step is a single, fast task. On the contrary, the A) and C) steps are extremely Grid-empowerable. In fact, in line with the grid philosophy, larger sets of geometries (or of initials conditions) can be dealt with at the time of a single geometry (initial condition) calculation just adding more computer power to the Grid.

We confine our attention here to the simple gas-phase prototype exchange reaction A + BC (v,j) -> AB (v',j') + c. This is the simplest model of a chemical reaction were a bond is broken and a new one is formed and can be treated at the highest level of theory.

Conclusions and Future Work

Due to the use of common data formats, we have been able to assemble the core of GEMS for a grid execution aimed at accurately modeling chemical reactions. The complete workflow has been executed for the benchmark H + H2. Grid performances are highlighted and results compared to previous calculations.

We are currently working at enlarging the sets of codes integrated, further improve their interoperability, and extend the treatment to the more complex cases to which the three-step procedure sketched in a previous section applies. For instance, in the near future, to the four-atom problem.

Impact

Progress in the capability to simulate chemical processes at the molecular level is an important component of the advance in modeling natural phenomena, designing new materials and products, mastering new technologies and carrying out innovative experiments. This progress requires assembling various pieces of software,

convergence of the competences of different experts, concurrence of the elaboration on several processors. The difficulty of gathering in the same place all the necessary hardware, software and human resources, makes computational grid platforms the ideal environment for the exploitation of collaborative computing and interoperability.

The past few years have seen significant progress in the grid-porting of scientific applications by the COMPCHEM Virtual Organization on the EGEE grid. Moreover, the problem of interoperability among a large class of codes pertaining to the Quantum Chemistry domain singled out the need for the definition of common data formats, such as the Q5Cost standard.

This work treasures the efforts made in both directions and represents a solid ground for future advances towards a universal molecular simulator.

Keywords

elementary reactions, virtual laboratory, grid-workflow, interoperability

URL for further information

http://www.hpc.unipg.it/srampino/urgems.html

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