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A Grid execution model for Computational Chemistry Applications using GC3Pie and AppPot

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Description of the Work

The applications chosen to be implemented in the GC3Pie workflow are:
- GFIT3C, a routine performing the global fitting of the potential energy surfaces in triatomic systems.
- ABC, a quantum mechanical atom-diatom reactive scattering program aimed at carrying out accurate calculations of the quantum S matrix elements to the end of evaluating reaction probabilities and state-to-state integral and differential cross sections. The above mentioned applications have been individually ported into the Grid environment thanks to a collaboration between the COMPCHEM VO and the User Support Unit of the Italian Grid Initiative (IGI). These applications belong to the set of computational applications in which GEMS, the Grid Empowered Molecular Simulator of COMPCHEM VO, is articulated.

In a typical usecase the user provides the ab-initio points of the potential energy surface that need to be fitted by the GFIT3C application. The output provided by the application (fitting file) is then used when compiling the ABC source code and running it on the grid infrastructure.
Out of the different usecases considered during the porting procedure, various factors had to be taken into account like the dependencies from the libraries and compilers used. For this reason, we chose a cloud-like approach in which both the compilation of the application binaries and the parameter study execution are framed within virtual machines that do provide a homogeneous and uniform environment.

Conclusions

The porting of legacy computational chemistry applications onto the Grid infrastructure, together with the development of the related workflows and visualization tools, is being carried out as part of a more general effort to build a solid platform for assembling accurate multi scale realistic simulations and for establishing an advanced molecular and material science research environment.

Impact

The building of a library of molecular dynamics codes to be offered to the users of the COMPCHEM virtual organization, assembled out of a group of molecular and material sciences laboratories committed to implement related computer codes on the EGI production Grid infrastructure, is changing the research environment of molecular scientists. Such library of molecular dynamics codes is going to be offered to users as a service including both the concurrent production of numerical results and related graphical rendering. On this ground the adoption of the framework GC3Pie allowed us to define event-related dependencies between different applications and execute them simultaneously on a large scale distributed computing infrastructure.
The main difference with other popular workflow systems is the programmatic creation of workflows. There is no fixed and pre-defined structure of the workflows: the entire execution schema is assembled at runtime

and steps can be added and removed dynamically as the program progresses, adapting to the outcome of individual computations.
The implemented case study demonstrates the validity of this approach and makes available a reusable example for other groups which are interested in porting their applications to production Grid systems.

Overview (For the conference guide)

The increasing availability of computer power on Grid platforms has prompted the implementation of complex computational chemistry suites of codes on distributed systems and, at the same time, the development of appropriate frameworks allowing to define event-related dependencies between applications (which may involve different computer environments) in a workflow-like fashion. The work carried out to implement complex computational chemistry usecases on distributed systems making use of the high throughput execution framework GC3Pie and the AppPot cloud/grid virtual machines (both developed by GC3, University of Zurich) is here presented and discussed. The work has been carried out in collaboration with the User Support Unit of the Italian Grid Initiative (IGI) which tackled the part related to the porting of the single applications.

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