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Computational chemistry experiments over a web service-oriented grid

We will describe the implementation of effective numerical differentiation techniques aimed to obtaining different energy derivatives of quantum chemical energies and properties on a service-oriented grid where the computational workflow is spawned over multiple, geographically distributed, sites. The application porting over the grid and its extension as a web service over local and wide area networks is fully outlined.
A description of the procedures developed for these experiments is given in full detail and the applicability of the methodology to similar problems pointed out.

Detailed analysis

The application is composed of three layers each performing a given task: (1) a pre-processing tier; (2) a task execution tier and, finally (3) a data collector
tier for the post-processing phase.
The first step of the pre-processing is implemented via a proper web
interface where a WS interacts with the end-user for the authentication, data input and job configuration.
In a second step the pre-processing WS builds up an execution table containing all the input files that are generated taking into account the user data of the first step. The domain of this phase is the http server running the WS and all the data are locally stored and managed.
The second tier of the application is a java class responsible for the
task generation for each of the input files created by the pre-processing WS. The java class, dispatches over the grid nodes the scripts for
the execution of the QM code. While the load balancing algorithm
is able to cope with various execution queues to obtain the maximum node loads, QM jobs depend also on the specific input data.
The post-processing stage is the most customizable one depending on the specific results to be extracted from QM outputs.

Conclusions and Future Work

We have presented an innovative solution
to the execution of top class applications such those currently
in use in QM calculations.We have
setup a grid environment and developed the necessary
code sections to port largely used QM packages
over a distributed, wide area network grid. This
computational experiment has proven to provide a
stable environment when built up with advanced
technologies such as service-oriented grid architectures
and web services.
The computational benefits of this solution have been
proven to be even better than locally executed parallel applications

Impact

Computational chemistry requires huge computing resources in order to
solve quantum mechanical (QM) Hamiltonians describing the properties of molecular species by means of variational and/or perturbative many-body approaches.
As a consequence, several studies are in progress with the aim of setting up innovative strategies able to deal in an effective way with the increasing
complexity of the molecular systems of current interest, which are still in the domain of classical simulations.
However, in the foreseeable future software developments will not change the general situation that leading calculations using quantum chemistry methods
require a huge computing power either in terms is of CPUand/or I/O resources and top-level computer architectures are often used. Those computing machines are often built on top of commodity components and this trend seems well consolidated even for the upcoming parallel architectures.
As an alternative we propose a new Web Service which has several new appealing features, i.e. (1) it is architecture independent,(2) it is modular, that is, configurable for user or site requirements,(3) it is dynamical, that is,
executable on available nodes.

Keywords

Computational chemistry, energy and property derivatives, Web Service

URL for further information

http://idea.sns.it

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