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The CompChem VO and a Grid application for spacecraft reenty simulations

Friday 11 May 2007 09:00 (20 minutes)

Describe the scientific/technical community and the scientific/technical activity using (planning to use) the EGEE infrastructure. A high-level description is needed (neither a detailed specialist report nor a list of references).

The Compchem VO users perform the study of the properties of
molecular systems on the
EGEE Grid production environment performing massive computational
campaigns. We are
developing some tools and Web Services based on Web3D and
visualization technologies
to interact with the simulators running on the Grid. This enables
the researchers to
interact with the Grid during the simulation and to represent the
outcomes of the
simulation in an effective and more productive way.

Report on the experience (or the proposed activity). It would be very important to mention key services which are essential for the success of your activity on the EGEE infrastructure.

In collaboration with the COST Action D37, called GridChem, we
are developing some
visualization tools and Web3D based Web Services to strengthen
the user interaction
with the Grid, where the Simulators are running. In this way the
user is enabled to
interact with the Simulator as far as the simulation progresses
instead of waiting
for its end. This facility increases the interest of the
researcher in the Grid
approach and in some circumstances avoid her/him exhausting
waiting times due to
wrong operating conditions or closed paths. The Grid environment
is becoming a rich
environment where sophisticated and complex simulation
environments could be
implemented combining various simulation environments and open
services. Furthermore
the graphic, multimedia or virtual reality based interaction
with the Grid
environment and will reinforce the user's experience of the
computational
power of the Grid.

With a forward look to future evolution, discuss the issues you have encountered (or that you expect) in using the EGEE infrastructure. Wherever possi-

ble, point out the experience limitations (both in terms of existing services or missing functionality)

The COST Action GridChem will develop the visualization and Web3D
Services in the
EGEE Grid environment. Most of the partners of the six Working
Groups of the Action
are joining Compchem VO and a significant increase of the number
of users and of the
available simulation codes is expected in the next couple of
years. We are confident
that the collaboration of Compchem users in the dissemination of
computer codes and
visualization web Services will be of great importance for the
EGEE community.

Describe the added value of the Grid for the scientific/technical activity you (plan to) do on the Grid. This should include the scale of the activity and of the potential user community and the relevance for other scientific or business applications

Our activity is based on EGEE infrastructure and services for
making efficient
simulations in the shortest time. To this end the tuning made in
EGEE to support
efficiently user applications requiring various types of MPI APIs
is really
important. In fact, most of the applications we use for making
simulations of
molecular systems, Carbon Nano Tubes and biological systems are
structured in
parallel and require an efficient parallel environment to reduce
the wall clock time
required for a simulation. The EGEE Grid environment represents
for our community the
most suitable environment to share competencies and resources in
a secure way and the
most powerful environment to perform massive computational
campaigns to determine the
properties of molecular systems in a fastest way. The
availability of large
computational facility scattered on the most powerful and
reliable research centers
is of invaluable importance for our community of users.

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