

Leiden Grid Infrastructure for Computational Chemistry

Observed trends in computational chemistry:

- Computers are becoming cheaper and more diverse.
- Computing resources are decentralized and often not owned solely by a single group.
- Chemistry software becomes increasingly harder to compile, install and setup.
- Average group only uses 'at most' five applications.
- Most computational work focuses on results and hardly any time or interest is left to learn about high performance computing.

- Computer resources of NCF and individual groups should be bundled into a Grid so they can be shared.

- Need to have an easy to user-interface for each application.
- Applications should be setup by knowledgeable person on the relevant machines for the group.

LGI is a middle-ware that allows for:

- Easy setup on computers of NCF and your group.
- Easy setup for (chemical) applications.
- Easy to administer for standard UNIX administrators.
- Ease of use and takes care of security.
- Ease of adaptation to various application specific user interfaces.

VASP

Gaussian

ADF

SPO-DVR

SA-DVR

Classical

Huygens
LISA

Laptop
FWNC7003
BOINC
Nocona
Woodcrest
Harpertown

