egee

Enabling Grids for E-sciencE

Computational Chemistry

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www.eu-egee.org

Information Society
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Enabling Grids for E-sciencE

- **Members:**
  - ACC Cyfronet AGH   42 PM
  - University of Perugia   18 PM
  - CESNET   6 PM
  - Royal Institute of Technology (SE-VR)   6 PM
  - University of Insbruck   6 PM

- **Total 78 PM**

Enabling Grids for E-sciencE

- **Provide stable, reliable and easy to use web portal for chemists with plug-ins to chemical software packages**
  - to easy grid usage
  - to attract non experienced users accustomed to GUIs
- **Further extend application portfolio**
  - parallel version of software packages which are ported already
  - new software packages
  - better software integration
- **Develop Grid license models**
- **Integrate the chemical community and start/extend cooperation with other communities**

Enabling Grids for E-sciencE

- **Documentation**
  - which software we have, where is installed, how to use is, who's responsible, etc.
  - use cases concerning license models
    - what to do in order to port commercial application
    - how to fulfill all the license requirements when software is in production
- **First line support for users**
- **Chemical software packages**
- **Visualization and tools**
  - ECCE

Enabling Grids for E-sciencE

- **Users newly coming to the Grid**
  - who would like to using the software installed on it

- **Members of our community, looking for**
  - access to specified software or specified computational chemistry method(s)
  - help in order to bring their own software to the Grid

- **Members of other communities**
  - looking for access to chemical software
  - who would like to start a cooperation in order to gain access to some data generated by chemical computations

Enabling Grids for E-sciencE

- **ACC Cyfronet**
  - Cluster coordination
  - development of web portal with software plug-ins
  - chemical software porting
- **Perugia University**
  - coordination and integration of Compchem VO
  - plug-ins for Columbus, DL-POLY
  - software porting
- **CESNET**
  - further development of Charon
  - software porting for VOCE VO
- **University of Insbruck**
  - continuation of Wien2k portal development
  - optimization of Wien2k workflow
- **KTH**
  - further development of ECCE/gLite port
- **Every centre**
  - documentation and reporting
  - first line support
  - development of grid license models
  - community integration

Enabling Grids for E-sciencE

- **Applications (number, type, number of users using it, etc.)**
- **?**

Enabling Grids for E-sciencE

- **The hardest part…**
  - lack of discipline among partners
- **Workshops and phone conferences to bring the community together**
- **Communication inside partners - via email**
  - in difficult cases phone calls (use to work in the past)
- **Try to convince users that GGUS is not evil**
  - to avoid direct contact with VO software manager