Chemistry Packages on the Grid
State of the Art and Future Prospects

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user & application support
CESNET
• **Computational chemistry**
  – Aim, means and methods

• **Current grid approaches**
  – Application porting
  – Virtual organizations
  – High-level frameworks
  – Customized solutions

• **EGI / SSC era**
  – CCMST establishment
• Summary of algorithms and their implementations used to solve real chemical problems
• Allows prediction and subsequent confirmation of experimental data
• Collaboration with experimentalists is essential
• Validation by experiments
Computational chemistry aims

• **Utilization of computational methods for prediction of**
  - dynamic properties of (bio)-molecular systems
  - reaction mechanisms
  - structure

• **Development of new computational methods for**
  - faster obtaining of results
  - more accurate results
  - results unavailable by common methods
Computational chemistry methods

- Quantum Mechanics (QM)
- Molecular Mechanics (MM)
- Hybrid approach (QM/MM)

- Molecular Dynamics (MD)
Quantum Mechanics

- Based on basic physical laws (Schrödinger equation)
- Accurate X extremely computationally demanding
- Applicable for small systems (~150 atoms)
- Currently non-applicable for biomolecules and systems in explicit solvent
- Use
  - systems optimization
  - evaluation of systems stability
  - proposal of reaction mechanisms
  - molecular properties (vibrational and absorption spectra, and many others)
Molecular Mechanics

• Based on Newton’s physics
• Molecular properties approximated as model of mass points interconnected by springs
• Force field model
• Results comparable with QM, can be better (validation by experiment)

• Use
  – applicable for biomacromolecules
  – simulation of systems in explicit solvents
  – systems up to size of ~100 000 atoms
  – can not decribe cleavage and creation of chemical bond
  – can not be used to study reaction mechanisms
• Hybrid Quantum Mechanics / Molecular Mechanics
• Applicable for large systems (biopolymers, proteiny, nucleic acids, …)
• Description of reaction mechanisms
  – area where reaction proceeds is described by QM
  – the rest of the system plus solvent is described by MM
Molecular Dynamics

- Description of system as dependence on time
- Integration of Newton’s motion equations

\[ F_i = m_i a_i \]

- Length of current simulations
  - in orders of tens of ns (MM)
  - hundreds of ps (QM)
• **QM**  Gaussian, Turbomole, Gamess US/UK, …
• **MM**  Amber, Charmm, Gromacs, Tinker, …
• **MD**  Amber, Gromacs, Gromos, NAMD, …
<table>
<thead>
<tr>
<th>ID</th>
<th>Name</th>
<th>Application Name</th>
<th>Discipline</th>
<th>Sub-Discipline</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>70</td>
<td>SFS</td>
<td>Supramolecular Functional Systems, Rotaxanes and Catenanes, Loading Cytochrome d</td>
<td>Computational Chemistry</td>
<td>Molecular biochemistry</td>
<td>Computational modelling and simulation studies of switching and shuttling processes at the molecular level are expected to provide valuable information for further miniaturization of electronic and nanoelectro-optic devices. The knowledge will be increased for the molecular recognition between molecules that participate as components of molecular devices and machine, as well as for the nature of the chiral effect in organic systems. Insights will be gained on the role of chiral effects in inorganic...</td>
</tr>
<tr>
<td>91</td>
<td>ABC</td>
<td>ABC</td>
<td>Computational Chemistry</td>
<td>Quantum physics</td>
<td>The ABC program uses a coupled-channel hyperspherical coordinate method to solve the Schrödinger equation for the motion of the three nuclei (A, B, and C) on a single Born-Oppenheimer potential energy surface. The coupled-channel method used involves a simultaneous separation of the wave function in the hyperspherical coordinates of all three chemical arrangements (ABC, ABC, CBA). The quantum reactive scattering boundary conditions are applied exactly, without the...</td>
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<tr>
<td>92</td>
<td>WCTDH</td>
<td>Multi-Configurational Time-Dependent Hartree</td>
<td>Computational Chemistry</td>
<td>Other</td>
<td>The multi-configurational time-dependent Hartree (MCTDH) method is nowadays considered as one of the most powerful tools for the quantum dynamics simulation of multidimensional systems. Unlike conventional wave packet methods, the MCTDH approach the wave function is expressed on a basis of time-dependent functions, which evolve along with the system. The use of this time dependent basis sets turns up into a much smaller basis dimension than a...</td>
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</tbody>
</table>
• Computational chemistry EGEE virtual organizations
  – COMPCHEM
    http://compchem.unipg.it/
  – VOCE
  – Gaussian VO
    http://egee.grid.cyfronet.pl/Applications/gaussian-vo
  – Turbomole VO
    http://egee.grid.cyfronet.pl/Applications/turbomole-vo
### Virtual organizations

#### iSoftrepo - Interactive Software Repository

<table>
<thead>
<tr>
<th>Site Info</th>
<th>CEL - Charon Extension Layer</th>
</tr>
</thead>
<tbody>
<tr>
<td>sites / voce</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Categories</th>
<th>Categories (versions)</th>
<th>List of realizations</th>
<th>Tree of realizations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular Mechanics and Dynamics</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>* autodock</td>
<td>* gromacs</td>
<td>* solvate</td>
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<tr>
<td>Quantum Mechanics and Dynamics</td>
<td></td>
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</tr>
<tr>
<td>* abinit</td>
<td>* dalton</td>
<td>* pcgamess</td>
<td>* uspp</td>
</tr>
<tr>
<td>Conversion and Analysis</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>* babel</td>
<td>* octave</td>
<td>* cpmd2cube</td>
<td>* kbps</td>
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<tr>
<td>* hml</td>
<td>* rthml</td>
<td>* openbabel</td>
<td>* pdb2pqr</td>
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<td>Visualization</td>
<td></td>
<td></td>
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<tr>
<td>* gnuplot</td>
<td>* grace</td>
<td>* ligplot</td>
<td>* molscript</td>
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<td>* povray</td>
<td>* raster3d</td>
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<td>Nuclear Magnetic Resonance</td>
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<td>* getdp</td>
<td>* mpb</td>
<td>* octave</td>
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<td>* glibc</td>
<td>* hwtoken</td>
<td>* u-voce</td>
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<td>* voce</td>
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CharonGUI interface

CharonGUI interface showing the CharonGUI window with the following details:

- Projects: Molecular dynamics, AMBER package testing, Free enzyme dynamics, Quantum mechanics, Single point energy, Docking studies.
- Jobs: AMBER package testing
- Description: The computational study of lectin-saccharide interactions employs methods of molecular docking and molecular dynamics. The aim of the project is a development of a reliable in silico based method of precognition of defined mutants of the important proteins.
- Status: idle
- Job submission:
  - psubmit: long plsek
  - File Name:
    - plsek: 90 jul 9, 2008
    - pokus.com: 98 jul 9, 2008
Multiple ligand trajectory docking
• Domain-specific Specialized Support Centre (SSC)
• Computational Chemistry and Material Science and Technology SSC (CCMST)
  – Support the members of the CCMST community in structuring and running their applications for a grid environment of shared hardware and software resources
  – Adoption and increase of popularity models and standards for molecular and material knowledge allowing a reuse of quantum chemistry data and codes for an easy connection of different packages and grid interoperability
  – Implementation on the grid libraries of codes relevant to the CCMST community as web services
  – Design and development of tools for the evaluation of quality of services (QoS) and users (QoU) to be used to build a grid economy based on a credit system for collaborative work within CCMST