Session Program

1-5 Oct 2007

EGEE'07

GEMS: Grid Empowered Molecular Simulators and CompChem Tools

Europe Congress Center
Budapest Hungary

Monday 1 October

14:00

GEMS: Grid Empowered Molecular Simulators and CompChem Tools
Session | **Location:** Europe Congress Center, REGE I, Budapest Hungary

14:00–14:30

About handling on the Grid quantum molecular knowledge related to molecular simulators

14:30–15:00

Ab initio photodynamics calculations on the Grid: approaches and applications

15:00–15:30   **Activities of the COST D37 Computational Chemistry Workflow Group**

15:30

16:00

GEMS: Grid Empowered Molecular Simulators and CompChem Tools
Session | **Location:** Europe Congress Center, REGE I, Budapest Hungary

16:00–16:20   **The CompChem Virtual Organization**

16:20–16:40   **Adaptation of chemical dynamics codes to the GRID**

16:40–17:05   **Chemistry visualization tools in an integrated discovery cycle**

17:05–17:30

A proposal for a data format to help program interchange in the Quantum Chemistry domain

17:30