

## **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**

15:30

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

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