

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

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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