



# EGEE'07

## Monday 01 October 2007

### GEMS: Grid Empowered Molecular Simulators and CompChem Tools - REGE I (14:00-15:30)

time	[id] title	presenter
14:00	[218] About handling on the Grid quantum molecular knowledge related to molecular simulators	
14:30	[202] Ab initio photodynamics calculations on the Grid: approaches and applications	
15:00	[219] Activities of the COST D37 Computational Chemistry Workflow Group	

### GEMS: Grid Empowered Molecular Simulators and CompChem Tools - REGE I (16:00-17:30)

time	[id] title	presenter
16:00	[220] The CompChem Virtual Organization	
16:20	[360] Adaptation of chemical dynamics codes to the GRID	
16:40	[222] Chemistry visualization tools in an integrated discovery cycle	
17:05	[221] A proposal for a data format to help program interchange in the Quantum Chemistry domain	