Session Program

12–16 Apr 2010

5th EGEE User Forum

Computational Chemistry

Uppsala University

Tuesday 13 April

11:00

Computational Chemistry

Session | **Location:** Uppsala University, Room IV

11:00–11:20

Porting of Computational Chemistry legacy applications on the EGEE Grid platform: computational aspects and visualization tools

Speaker
Dr Alessandro Costantini

11:20–11:40

Ab initio grid chemical software ports – transferring knowledge from EGEE to Polish NGI

Speaker
Dr Mariusz Sterzel

11:40–12:00

A priori modeling of chemical reactions on a grid-based virtual laboratory: towards standard representations of data for molecular chemistry

Speaker
Dr Sergio Rampino

12:00–12:20

Molecular and material science innovative applications on the grid

Speaker
Dr Stefano Cozzini

12:30

14:00

Computational Chemistry

Session | **Location:** Uppsala University, Room IV

14:00–14:20

pKa Calculations of Key Ionizable Protein Residues in Acetylcholinesterase

Speaker
Mr Jiri Wiesner

Location
Uppsala University, Room IV

14:20–14:40

Protein Molecular Dynamics and Free Energy Calculations on the EGEE Production Grid

Speaker
Stavros Farantos

Location
Uppsala University, Room IV

14:40–15:00

A multiconfiguration time-dependent Hartree algorithm for non-Born-Oppenheimer calculations

Speaker
Dr Dimitrios Skouteris

Location
Uppsala University, Room IV

15:00–15:20

MCTDH Quantum Dynamics in EGEE: Advances Made and Improvements needed

Speaker
Dr Fermin Huarte

Location
Uppsala University, Room IV

15:30