

1st Daresbury-Jülich Workshop on HPC Applications in Fluid and Molecular Dynamics

7th-8th May 2013

Place: Rotunda (Building.16.4, 1st floor, Room-Nr. 301)

Agenda Tuesday 7th May

12.30 **Reception and buffet lunch**

13.30 Norbert Attig: *Welcome*

13:50 Paul Gibbon: *Simulation Labs at JSC*

14:10 Paul Sherwood: *The Scientific Computing Department and the Hartree Centre at STFC*

14:40 Lukas Arnold: *Fire simulations in civil engineering*

15:20 Matthias Meinke: *Simulation of flows with immersed moving boundaries*

16:00 **COFFEE**

16:30 Godehard Sutmann: *Particle-based hydrodynamics and applications*

17:10 David Emerson: *An overview of computational engineering at Daresbury*

17:50 Mike Nicolai: *Simulation and optimisation of biomedical devices*

18.30 Transfer to Jülich Hotel Kaiserhof

19.00 **Joint dinner at Restaurant Rossini, Jülich**

Wednesday 8th May

08:30	Transfer to FZJ
09:00	Paolo Crosetto: <i>Fluid-structure interaction and CFD benchmarking</i>
09:40	Charles Moulinec : <i>Code_Saturne and the Telemac system</i>
10:20	COFFEE
10:40	Michael Schlottke: <i>Parallel Mesh Generation for Hierarchical Cartesian Grid Methods</i>
11:20	Ivo Kabadshow: <i>FMM and Gromacs</i>
12:00	Ilian Todorov: <i>Molecular Simulation Software (DL-POLY etc)</i>
12:40	LUNCH
13:40	Thomas Müller: <i>Conceptual aspects of parallel electronic structure codes</i>
14:20	Tom Keal: <i>Task-farming parallelism in ChemShell</i>
15:00	Viorel Chihaiia: <i>Performance optimisation of coarse-graining MD codes IBISCO and OCCAM</i>
15:40	Wrap up and discussion for further workshop(s)
16:00	Transfer to Düsseldorf airport

Participants Daresbury:	Participants JSC/AiA:
Paul Sherwood	Paul Gibbon
David Emerson	Godehard Sutmann
Charles Moulinec	Lukas Arnold
Ilian Todorov	Mike Nicolai
Tom Keal	Paolo Crosetto
	Thomas Müller
Participants AiA, RWTH Aachen:	Viorel Chihaiia
Matthias Meinke	Ivo Kabadshow
Michael Schlottke	Norbert Attig

Hotel Kaiserhof (A) – Restaurant Rossini (B)

