Jülich CECAM School 2015
Computational Trends in Solvation and Transport in Liquids

	Monday 23 March	Tuesday 24 March	Wednesday 25 March	Thursday 26 March	Friday 27 March
9:00-10:00	9:45-10:00 Opening	*Gerald Mathias* QM/MM-MD	*Christian Holm* Transport in Electrolyte Solutions	*Rodolphe Vuilleumier* Ab initio Molecular Dynamics Approach to Solvation and Chemical Reactions	*Dmitri Fedosov* Smooth Dissipative Particle Dynamics for Complex Flow
10:00-11:00	*Kurt Kremer* Adaptive Resolution MD	*Robert Franke* Continuum Solvation Modeling of Solute/Solvent Interactions	*Rebecca Wade* Brownian Dynamics for Biomolecular Recognition	*Daniel Potts* Advances in Parallel (N)FFT for Fast Molecular Simulations	*Matthias Heyden* Biomolecular Solvation
11:00-11:30	**Coffee Break**				
11:30-12:30	*Daniel Borgis* Classical Density Functional Theory for Complex Solutions	*Marisol Ripoll* Multi-Particle Collision Dynamics: Methods and Applications	*Andrij Kovalenko* RISM-3D Integral Equation Theory Combined with MD for Molecular Solvation	*Roland Netz* Simulation Techniques for Solvation-Induced Surface-Interactions at Prescribed Water Chemical Potential	*Michele Ceriotti* Path Integral MD for Quantum Solvents
12:30-14:00	**Lunch Break**				
14:00-15:00	*Dominik Horinek* Force Field Molecular Dynamics for Solvation	*Jens Harting* Lattice Boltzmann: Colloids at Interfaces	*Thorsten Hater / Peter Philippen* Introduction to GPU Programming	*Stefan Kast* Solvation from Liquid-State Integral Equation Theory	
15:00-16:00	*Wim Briels* Responsive Particle Dynamics	*Lars Schäfer* Coarse-Grain Water and Solutions: Hybrid AA/CG with MARTINI	Practical Session GPU	*Jörg Behler* High-Dimensional Neural Network Potentials as a Tool to Study Solvation	
16:00-16:30	**Coffee Break**				
16:30-17:30	*Maxim Fedorov* Advanced Atomistic Methods for Molecular Solvation	*Dirk Pleiter* Modern Trends in Hardware Developments Especially GPU	Practical Session GPU	*Christos Likos* Phenomenological Coarse-Grained Potentials for Soft Matter Systems	
Evening	**Reception and Get-Together**	**Poster-Session I**	**Poster-Session II**	**Excusion and Conference Dinner**	