IAS Winter School and CECAM Tutorial 2012
Hierarchical Methods for Dynamics in Complex Molecular Systems

	Monday **5 March** **Materials Sciences**	**Tuesday** **6 March** **Biosystems**	**Wednesday** **7 March** **Advanced Methods**	**Thursday** **8 March** **Flow Simulations**	**Friday** **9 March** **Numerics & Parallel Computing**
9:00-10:00	9:45-10:00 Opening	*Mark E. Tuckerman* Exploration of Multi-Dimensional Free Energy Landscapes in Molecular Dynamics	*Alessandro Curioni* Fast Algorithms for QM on Modern HPC	*Luigi Delle Site* Adaptive Resolution Molecular Dynamics: Extension to Quantum Problems	*Danny Perez* Accelerated Molecular Dynamics Methods
10:00-11:00	*Doros N. Theodorou* Tracking the Dynamics of Systems Evolving through Infrequent Transitions in a Network of Discrete States	*Ivano Tavernelli* Methods on TDDFT-Based Nonadiabatic Dynamics with Applications	*Gerhard Hummer* Non-Equilibrium Molecular Dynamics for Biomolecular Systems Using Fluctuation Theorems	*Burkhard Dünweg* Coupling Molecular Dynamics and Lattice Boltzmann to Simulate Brownian Motion	*Peter Bastian* Simulating Multiphase Flow in Porous Media Using DUNE
11:00-11:30	**Coffee Break**				
11:30-12:30	*Paolo Carloni* Hybrid Car-Parrinello MD / MM Simulations: A Powerful Tool for the Investigation of Biological Systems	*Nikos L. Doltsinis* Simulating Light-Induced Phenomena in Soft Matter	*Teodoro Laino* Multigrid QM/MM Approaches in ab initio Molecular Dynamics	*Roland G. Winkler* Flow Simulations with Multiparticle Collision Dynamics	*Ulrich Rüde* Multigrid on Parallel Computers
12:30-14:30	**Lunch Break**				
14:30-15:30	*Christoph Dellago* Transition Path Sampling for Materials - Hard and Soft	*Frauke Gräter* Simulation Techniques for Studying the Impact of Force on (Bio)Chemical Processes	*Bernd Mohr* Introduction to Parallel Computing	*Pep Español* Dissipative Particle Dynamics	
15:30-16:30	*Jörg Behler* Neural Network Potentials for Efficient Large-Scale Molecular Dynamics	*Christine Peter* Coarse Grained Models for Multiscale Simulations of Biomolecular Systems	Practical Session	*Simone Melchionna* Large-Scale Simulations of Blood Flow with Coarse-Grained Cells	
16:30-17:00	**Coffee Break**				
17:00-18:00	*Alexander Hartmaier* Large-Scale Molecular Dynamics Studies of Dislocation Dynamics, Plasticity and Fracture of Materials	*Volkhard Helms* Particle-Based Dynamics Simulations of Multi-Protein Systems and Cellular Compartments	Practical Session	*Dmitry A. Fedosov* Simulations of Blood Flow on the Cell Scale	
Evening	**Reception and Get-Together**	**Poster-Session I**	**Poster-Session II**	**Conference Dinner**	