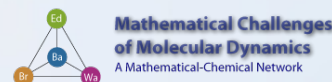


EPSRC NETWORK MATHEMATICAL CHALLENGES OF MOLECULAR DYNAMICS



Third Annual Conference

Monday 7th - Wednesday 9th March 2011



Organisers: Ben Goddard (IC Chem. Eng.), Serafim Kalliadasis (IC Chem. Eng.), Greg Pavliotis (IC Maths)

PROGRAMME

All talks will take place in the Council Room, 170 Queen's Gate

MONDAY 7TH MARCH 2011

- 09:30-09:50 **Registration and Tea/Coffee**
09:50-10:00 **Opening Remarks**
10:00-10:45 **Richard Catlow** (UCL) *TBC*
10:45-11:00 **Tea/Coffee**
11:00-11:45 **Julia Yeomans** (Oxford) *Continuum Modelling of Complex Fluids*
11:45-12:30 **Doros Theodorou** (Athens) *Molecular dynamics-based investigations of the energy hypersurface of glass-forming materials*
12:30-13:00 **Mike Payne** (Cambridge) *Novel methods for exploiting quantum mechanics in atomistic simulations*
13:00-14:00 **Lunch**
14:00-14:45 **Marcus Müller** (Göttingen) *Soft coarse-grained models for multi-component polymer melts and lipid membranes*
14:45-15:30 **George Jackson** (Imperial) *Fluctuations in nanoscale liquid drops and the consequent inadequacies of a mechanical (pressure tensor) route to the surface tension*
15:30-15:45 **Tea/Coffee**
15:45-16:15 **Davide Marenduzzo** (Edinburgh) *Computer simulations of active matter: dynamics and pattern formation in bacterial suspensions*
16:15-16:45 **Dean Sayle** (Cranfield) *Mapping Nanostructure: A Systematic Enumeration of Nanomaterials by Assembling Nanobuilding Blocks at Crystallographic Positions*
16:45-17:15 **Lev Sarkisov** (Edinburgh) *Interactions of Phospholipid Bilayers with Several Classes of Amphiphilic α -Helical Peptides: Insights from Coarse-Grained Molecular Dynamics Simulations*
17:15-17:45 **Ilian Todorov** (Daresbury) *TBC*

TUESDAY 8TH MARCH 2011

- 09:30-10:00 **Tea/Coffee**
10:00-10:45 **Gero Friesecke** (TU Munich) *TBC*
10:45-11:00 **Tea/Coffee**
11:00-11:45 **Mark Peletier** (Eindhoven/Bath) *Understanding the origins of the Wasserstein gradient flows*
11:45-12:30 **Andrew Stuart** (Warwick) *Gradient Flow, Hamiltonian Dynamics and Sampling*
12:30-13:00 **Florian Theil** (Warwick) *Gamma limit for transition paths*
13:00-14:00 **Lunch**
14:00-14:45 **Frédéric Hérau** (Nantes) *Tunnel effect for the Fokker-Planck equation*
14:45-15:30 **Ben Leimkuhler** (Edinburgh) *Two Ideas for Molecular Thermodynamics: Efficient Thermostats and Stochastically Driven Force Perturbation*
15:30-15:45 **Tea/Coffee**
15:45-16:15 **Michael Herrmann** (Saarbruecken) *Waves and Oscillations in Hamiltonian Lattices*
16:15-16:45 **Carsten Hartmann** (FU Berlin) *Low-rank approximation of bilinear systems with applications to control of open quantum systems and single-molecule pulling*
16:45-17:15 **Giacomo Mazzi** (Leuven) *Multiscale study of chemical reactions with lateral interactions*
Dinner Details TBA

WEDNESDAY 9TH MARCH 2011

- 09:30-10:00 **Tea/Coffee**
10:00-10:45 **Martin Hairer** (Warwick) *A toy model of extreme non-equilibrium*
10:45-11:30 **Frank Noé** (FU Berlin) *Modeling conformational dynamics of macromolecules from simulations and experiments*
11:30-12:00 **Ruslan Davidchack** (Leicester) *Cleaving method for determining solid-liquid interfacial free energy in molecular systems: Results for simple models of water*
12:00-12:30 **Adrian Mulholland** (Bristol) *Protein dynamics and enzyme catalysis: insights from simulations*
12:30-14:00 **Closing Remarks and Lunch**