Warwick
Mathematics Research Centre

Warwick EPSRC Symposium 2008/09
Challenges in Scientific Computing
Organiser: Andrew Stuart

Monday 1 – Friday 5 June 2009

Workshop on Molecular Dynamics

Organisers: Michael Allen (Warwick), Mark Rodger (Warwick),
Ben Leimkuhler (Edinburgh), Giovanni Ciccotti (Rome)

All talks will be in Lecture Room MS.05 in the Zeeman Building

Monday 1 June 2009

09:00–09:45 **Registration** in B1.37
09:45–10:30 **Peter T. Cummings** (Vanderbilt) *Direct simulation-based evidence for fluid-solid transition in nanoconfined non-polar fluids*
10:30–11:00 Coffee in the Mathematics Common Room
11:00–11:45 **Gabor Csanyi** (Cambridge) *Full sampling of atomic configurational spaces*
11:45–12:30 **Mikko Karttunen** (Western Ontario) *Multiscale modeling of lipid and surfactant systems*
12:30–14:00 Lunch
14:00–14:45 **Debra Searles** (Griffith) *The dissipation function and the properties of highly non-equilibrium systems*
14:45–15:30 **William Hoover** (Ruby Valley) *Shockwave simulation using molecular dynamics*
15:30–16:00 Tea in the Mathematics Common Room
16:00–16:45 **Matej Praprotnik** (ETH Zürich) *Adaptive resolution molecular dynamics simulation*
16:45–17:30 **Karl Travis** (Sheffield University) *A study of radiation-induced disorder in Pu-doped ceramics using molecular dynamics and topological analysis*
17:30 Drinks and snacks in the Mathematics Common Room

Tuesday 2 June 2009

09:00–09:45 **Eric Vanden-Eijnden** (New York) *Theory and modeling of reactive events*
09:45–10:30 **Sara Bonella** (Rome 1) *Free energy barriers for local hydrogen diffusion in sodium alanates*
10:30–11:00 Coffee in the Mathematics Common Room
11:00–11:45 **Weiqing Ren** (New York) *A seamless multiscale method and its application to complex fluids*
11:45–12:30 **Robert D. Skeel** (Purdue) *Maximum flux transition paths of conformational change*
12:30–14:00 Lunch in the Mathematics Common Room
14:00–14:45 **David Coker** (Boston) *Mixed quantum-classical methods for treating coherent quantum dynamics in model multichromophore light harvesting systems*
14:45–15:30 **Ron Elber** (Texas) *Milestoning*
15:30–16:00 Tea in the Mathematics Common Room
16:00–16:45 **Frank Pinski** (Cincinnati) *Transition paths for molecular motion: What are the characteristics of the most probable paths?*
16:45–17:30 **Massimo Noro** (Unilever Discover Port Sunlight) *Modelling (skin) lipid bilayers*

please turn over

Wednesday 3 June 2009

09:00–09:45 **Peter Bolhuis** (Amsterdam) *Efficient sampling of molecular dynamics trajectories connecting arbitrary metastable states*

09:45–10:30 **Christof Schütte** (Free University Berlin) *Markov state models: Theory and applications*

10:30–11:00 Coffee in the Mathematics Common Room

11:00–11:45 **Stephen Bond** (Illinois) *Measuring and correcting algorithmic bias in molecular dynamics averages*

11:45–12:30 **Christopher Sweet** (Notre Dame) *Simulation of long timescale dynamics of proteins using normal-mode Langevin*

12:30–14:00 Lunch in the Mathematics Common Room

14:00 Coach depart from the rear of the Mathematics Institute for a trip to Stratford-upon-Avon and Theatre

Thursday 4 June 2009

09:00–09:45 **Florian Müller-Plathe** (Darmstadt) *Trends in materials simulation - a molecular dynamics miscellany*

09:45–10:30 **Karl Kirschner** (Fraunhofer Institute SCAI, St Augustin) *Connecting quantum mechanics to coarse-grained simulations: the role of force field development*

10:30–11:00 Coffee in the Mathematics Common Room

11:00–11:45 **Glenn Martyna** (Watson Research Centre, IBM) *Treating manybody polarization and manybody dispersion in complex systems: The quantum Drude oscillator formalism*

11:45–12:30 **David Manolopoulos** (Oxford) *Competing quantum effects in the dynamics of a flexible water model*

12:30–14:00 Lunch

14:00–14:45 **David Wales** (Cambridge) *Energy landscapes and dynamics: from clusters to biomolecules*

14:45–15:30 **Adrian Mulholland** (Bristol) *Protein dynamics and enzyme catalysis: insights from simulations*

15:30–16:00 Tea in the Mathematics Common Room

16:00 **Poster Session** with snacks and soft drinks

19:30 **Dinner** at Loch Fyne in Kenilworth

Friday 5 June 2009

09:00–09:45 **Rodolphe Vuilleumier** (Pierre et Marie Curie, Paris) *Microscopic flow around a diffusing particle*

09:45–10:05 **Jiri Vanicek** (EPFL Lausanne) *Efficient evaluation of accuracy of quantum molecular dynamics using dephasing representation*

10:05–10:25 **Rebecca Notman** (Warwick) *Molecular dynamics simulations of peptides interacting with quartz surfaces*

10:25–11:00 Coffee in the Mathematics Common Room

11:00–11:45 **Mark Tuckerman** (New York University) *Developments in conformational sampling using molecular dynamics*

11:45–12:30 **David Quigley** (Warwick) *Simulating orientational specificity in the growth of calcite on self-assembled monolayers*

12:30–14:00 Lunch in the Mathematics Common Room

14:00–14:45 **Mitchell Luskin** (Minnesota) *Non-ergodicity of Nosé-Hoover dynamics*

14:45–15:30 **Steven Kenny** (Loughborough) *Atomistic modelling of problems in materials science*

15:30–16:00 Tea in the Mathematics Common Room

If you have any questions during the workshop please see either Hazel Higgens or Yvonne Collins in Room B1.37 which is opposite the Common Room

For further information on these and other events see:
go.warwick.ac.uk/mathsevents
or contact the
Mathematics Research Centre • Zeeman Building • University of Warwick • Coventry • CV4 7AL • UK
Email: mrc@maths.warwick.ac.uk • Phone: +44 (0)24 7652 8317 • Fax: +44 (0)24 7652 3548

THE UNIVERSITY OF WARWICK