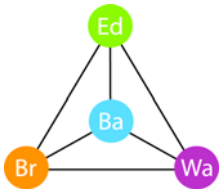

Mathematical Challenges of Molecular Dynamics
A Mathematical-Chemical Network

WARWICK MATHEMATICS RESEARCH CENTRE

EPSRC Network Mathematical Challenges of Molecular Dynamics

First Annual Conference

Monday 14th – Wednesday 16th July 2008

Organisers: M Allen (Warwick), G Friesecke (Warwick/TU Munich), S Islam (Bath), B Leimkuhler (Edinburgh), S Wiggins (Bristol), J Zimmer (Bath)

Local Organiser: G. Friesecke

The network is a joint initiative of the Universities of Bath, Bristol, Edinburgh and Warwick, funded by EPSRC since April 1, 2008. It is devoted to covering all mathematics-related aspects of molecular dynamics, and the full spectrum of scales, from electronic to atomistic, conformational, mesoscopic and macroscopic.

Conference website: http://www2.warwick.ac.uk/fac/sci/maths/research/events/2007_2008/
Network website: http://www.bath.ac.uk/math-sci/md-net/

PROGRAMME

All talks will be in Lecture Room B3.02 in the Zeeman Building

Monday 14th July 2008

Chair: Mike Allen, Gero Friesecke

10:00-11:00 **Registration** in Room B1.37 the MRC and **Coffee** in the Mathematics Institute Common
11:00-11:10 **Opening remarks** by the network coordinators
11:10-11:55 **Adrian Sutton** (Imperial) *Orderly and disorderly behaviour at interfaces*
12:00-12:45 **Luigi Delle Site** (MPI for Polymer Research, Mainz) *The adaptive resolution simulation scheme (AdResS): Basic principles and applications*
12:45-14:00 Buffet Lunch in the Mathematics Institute Common Room
14:00-14:45 **Ben Leimkuhler** (Edinburgh) *Gentle ergodic thermostats*
14:50-15:35 **Peter Haynes** (Imperial) *ONETEP: linear-scaling density-functional theory with local orbitals and plane waves*
15:35-16:15 Tea in the Mathematics Institute Common Room
16:15-16:40 **Andrew Stuart** (Warwick) *Transition paths in molecules: gradient descent in pathspace*
16:45-17:10 **Greg Pavliotis** (Imperial) *Parameter estimation for multiscale diffusions*
17:15-17:40 **Pooja Panchmatia** (Bath) *Ion diffusion in complex silicate materials*
17:45-18:30 **POSTER SESSION** Room B1.01
19:30 Workshop Dinner, The Cross at Kenilworth, New Street, Kenilworth

Tuesday 15th July 2008

Chair: Saiful Islam, Ben Leimkuhler

09:30-10:15 **Giovanni Ciccotti** (Rome) *Some challenges confronting MD*
10:15-11:00 Coffee in the Mathematics Institute Common Room
11:00-11:45 **Eric Vanden Eijnden** (Courant) *Transition pathways of rare reactive events in molecular simulations*
11:50-12:35 **Mark Rodger** (Warwick) *Finding infrequent events with MD: methods for studying crystal nucleation*
12:35-14:00 – lunch break –
14:00-14:45 **Oliver Junge** (TU Munich) *On a sparse discretization of transfer operators and an application to conformation dynamics of molecules*
14:50-15:15 **Mike Allen** (Warwick) *Thermostats for soft matter simulations*
15:20-15:45 **Johannes Zimmer** (Bath) *Computing classical trajectories: stationary action revisited*
15:45-16:15 Tea in the Mathematics Institute Common Room
16:15-16:40 **Emad Noorizadeh** (Edinburgh) *Hypoelliptic thermostatting methods*
16:45-17:10 **Volker Betz** (Warwick) *Breaking the chain*
17:15-17:40 **Hartmut Schwetlick** (Bath) *From lattice models to macroscopic dissipation*
17:45-18:10 **Karsten Matthies** (Bath) *Derivation of kinetic descriptions from atomistic dynamics*
19:00 Buffet Dinner in the Mathematics Institute Common Room
[21:00 Steering Committee Meeting]

Wednesday 16th July 2008

Chair: Johannes Zimmer

09:30-10:15 **Steve Wiggins** (Bristol) *Recent advances in the high dimensional Hamiltonian dynamics and geometry of reaction dynamics*
10:15-11:00 Coffee in the Mathematics Institute Common Room
11:00-11:45 **Murthy Guddati** (North Carolina State) *Coupling molecular dynamics with continuum models through perfectly matched discrete layers*
11:50-12:15 **Gero Friesecke** (Warwick/TU Munich) *Quantum versus classical MD in the presence of electrostatic singularities and eigenvalue crossings*
12:20-12:45 **Guido Germano** (Marburg) *Computer simulation of liquid crystals and other complex systems*
12:50-13:15 **Alexei Likhtman** (Reading) *Molecular dynamics of generic entangled polymers and multiscale approach*
13:15 Closing remarks by the organizers

If you have any questions during the Workshop please go to the MRC in Room B1.37 opposite the Common Room




For further information on these and other events see:
www2.warwick.ac.uk/fac/sci/maths/research/events/2007_2008/
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