

EPSRC NETWORK MATHEMATICAL CHALLENGES OF MOLECULAR DYNAMICS
Second Annual Conference – Monday 13 - Wednesday 15 July 2009



**Mathematical Challenges
of Molecular Dynamics**
A Mathematical-Chemical Network



THE UNIVERSITY OF
WARWICK



PROGRAMME

ALL TALKS WILL TAKE PLACE IN 8W2.5, IN THE BUILDING OF THE SCHOOL OF MANAGEMENT

MONDAY 13TH JULY 2009

Chair: Johannes Zimmer

10:00-11:00 Registration in foyer outside room 8W2.5. **Tea/Coffee** in room 8W2.23

11:00-11:10 Opening remarks by the network coordinators

11:10-11:55 Michel Peyrard (Lyon) *Adding a Dimension to DNA Melting Curves*

12:00-12:45 David Manolopoulos (Oxford) *Speeding Up Path Integral Simulations*

12:45-14:00 Lunch in Wessex Restaurant (in Wessex House Building)

Chair: Saiful Islam

14:00-14:45 Richard James (Minnesota) *Objective Molecular Dynamics*

14:50-15:35 Bill Smith (Daresbury) *Grand Scale Molecular Dynamics*

15:35-16:15 Tea/Coffee in 8W2.23

16:15-16:40 Benjamin Goddard (Warwick) *Superadiabatic Transition Histories in Quantum MD*

16:45-17:10 Dmitry Nerukh (Cambridge) *Phase Space Diffusion in Molecular Liquids: Non-stationary Random Walk Model*

17:15-17:40 Johannes Giannoulis (München) *On the Analytical Justification of the Passage from Quantum to Classical MD*

17:45-20:00 Poster Session in the Foyer of the School of Management, building 8W

TUESDAY 14TH JULY 2009

Chair: Gero Friesecke

9:30-10:15 Frédéric Legoll (Paris) *Effective Dynamics for Reaction Coordinates*

10:15-11:00 Tea/Coffee in 8W2.23

11:00-11:45 Graeme Ackland (Edinburgh) *Phase Transitions in Martensites*

11:50-12:35 Weiqing Ren (New York) *A Seamless Multiscale Method and its Application to Complex Fluids*

12:35-14:00 Lunch in Wessex Restaurant (in Wessex House Building)

Chair: Graeme Ackland

14:00-14:45 Glenn Martyna (IBM) *Simulating Materials with Atomic Detail at IBM: From Biophysics to High-tech Applications*

14:50-15:15 Carsten Hartmann (Berlin) *Systematic Coarse-graining Strategies for Linear Systems*

15:20-15:45 Robert Jack (Bath) *Dynamical Large Deviations in Glass-forming Liquids*

15:45-16:15 Tea/Coffee in 8W2.23

16:15-16:40 Ruslan Davidchack (Leicester) *Discretisation Errors in MD Simulations with Thermostats*

16:45-17:10 Sara Fortuna (Warwick) *Agent Based Algorithm for Molecular Self-organisation*

17:15-17:40 Hartmut Schwetlick (Bath) *A Convergent Approximation of Long-time Hamiltonian Trajectories in MD*

17:45-18:10 Martin Uhrin (Edinburgh) *A Novel Application of MD: Coagulating Semi-rigid Dust Grains in Protoplanetary Disks*

WEDNESDAY 15TH JULY 2009

Chair: Florian Theil

9:30-10:15 Paul Tupper (Montréal) *Shadowing the Trajectories of Molecular Dynamics*

10:15-11:00 Tea/Coffee in 8W2.23

11:00-11:45 John Maddocks (Lausanne) *Coarse Graining Large Scale MD Simulations of DNA*

11:50-12:15 Natalia Marsinovich (Warwick) *Modelling the Self-assembly of Polycarboxylic Acids*

12:20-12:45 Robert MacKay (Warwick) *Isomerisation of Retinal*

12:50-13:15 Steve Parker (Bath) *Application of Molecular Dynamics to Mineral-Water interfaces*

13:15 Closing remarks