Challenges in statistical mechanics: from mathematics to molecular dynamics to technological applications

Monday 7th – Thursday 10th December 2105

Organisers: Ben Goddard (Edinburgh), Serafim Kalliadasis (Imperial), Michela Ottobre (Heriot-Watt), Grigorios A. Pavliotis (Imperial), Johannes Zimmer (Bath).

Programme

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

Monday 7th December 2015

09:30–09:50 **Registration**
09:50–10:00 **Opening Remarks**
10:00–11:00 **Mark Peletier** (Eindhoven) *Open problems in the upscaling of dislocations*
11:00–11:30 **Tea/Coffee**
11:30–11:50 **Miguel Duran Olivencia** (Imperial) *Dynamical Density Functional Theory for Systems of Orientational Colloids Including Inertia and Hydrodynamic Interactions*
11:50–12:35 **Jens Marklof** (Bristol) *Generalized linear Boltzmann equations for particle transport in polycrystals*
12:35–14:00 **Lunch**
14:00–14:45 **Rob Jack** (Bath) *Protein (mis)folding and glass transitions*
14:45–15:30 **Matthew Borg** (Edinburgh) *TBA*
15:30–16:00 **Tea/Coffee**
16:00–16:45 **Doros Theodorou** (Athens) *Multiscale Molecular Simulations of Polymer Matrix Nanocomposites*
17:00– **Discussion**

Tuesday 8th December 2015

09:30–10:30 **Julia Yeomans** (Oxford) *Droplets bouncing on superhydrophobic surfaces*
10:30–11:00 **Tea/Coffee**
11:00–11:45 **Peter Coveney** (UCL) *Combining Dynamical Models on Several Scales: Multiscale Modelling of Polymer-Clay Nanocomposites*
11:45–12:30 **Celia Reina** (Pennsylvania) *Geometry of dissipative evolution equations*
12:30–14:00 **Lunch**
14:00–14:45 **Arnaud Ducet** (Oxford) *Gibbs flow for approximate transport with applications to Bayesian computation*
14:45–15:30 **Rosemary Harris** (Queen Mary) *Random walkers with extreme value memory: modelling the peak-end rule*
15:30–16:00 **Tea/Coffee**
16:00–16:45 **Ben Leimkuhler** (Edinburgh) *The state of the art of the timestep: enhanced sampling of molecular systems using extended dynamics*
17:00– **Discussion**
19:00 **Dinner** *Olives Restaurant, 140 Gloucester Rd, SW7 4QH*

Wednesday 9th December 2015

09:30–10:30 **Gero Friesecke** (Munich) *Pair densities in density functional theory: cross-over from strict correlations to mean field behaviour*
10:30–11:00 **Tea/Coffee**
11:00–11:45 **Carsten Hartmann** (Berlin) *Probing the properties of soft matter: optimal design of single molecule experiments*
11:45–12:30 **Gabriel Stoltz** (Cermics) *Error estimates for transport coefficients in molecular dynamics*
12:30–14:00 **Lunch**
14:00–14:20 **Urbain Vaes** (Imperial) *Hermite spectral method for multiscale SDEs*
14:20–14:40 **Andreas Nold** (Imperial) *From the nano to the macroscale - Bridging scales for the moving contact line problem*
14:40–15:10 **Tea/Coffee**
15:10–15:55 **Marc Pradas** (Open) *Noise-Induced critical transitions in multiscale systems*
15:55–16:40 **Joel De Coninck** (de Mons) *Wetting dynamics: a case study*
16:40– **Discussion**

Thursday 10th December 2015

09:30–10:15 **Angelos Michaelidis** (UCL) *Structure and dynamics of water at interfaces: Surfing water droplets and ice formation*

10:15–10:35 **Yulong Lu** (Warwick) *Understanding transition paths using Gamma convergence*

10:35–11:05 **Tea/Coffee**

11:05–11:25 **Andrew Duncan** (Imperial) *Improving the performance of Langevin samplers by breaking detailed balance*

11:25–12:25 **Yannis Kevrekidis** (Princeton) **Closing the Workshop** *On the interplay of data miing with atomistic simulations: algorithms and issues from using diffusion map coordinates*

12:25–14:00 **Lunch**

14:00– **Discussion**