

Non-equilibrium molecular dynamics school: Tuesday, July, 12th

Speaker setup: 9:00 - 9:25 AM

09:25 - 09:30				Welcome
09:30 - 10:15	Peter	Daivis	RMIT University	Non-equilibrium thermodynamics - basics
10:15 - 11:00	Peter	Daivis	RMIT University	Non-equilibrium thermodynamics - extensions

Morning Tea: 11:00 - 11:30 AM

11:30 - 12:15	Billy	Todd	Swinburne University	Homogeneous atomistic systems
12:15 - 13:00	Billy	Todd	Swinburne University	Inhomogeneous systems

Lunch: 13:00 - 14:00

14:00 - 15:30				Software setup & Tutorial 1
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Afternoon Tea: 15:30 - 16:00

16:00 - 17:00				Tutorial 2
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Advanced scattering and microscopy school: Wednesday, July, 13th

Speaker setup: 9:00 - 9:25 AM

Session 1				
09:25 - 09:30				Welcome
09:30 - 10:15	David	Paganin	Monash University	Ghost-imaging using x rays and neutrons
10:15 - 11:00	Alison	Funston	Monash University	Scanning near-field optical microscopy (title TBC)

Morning Tea: 11:00 - 11:30 AM

Speaker setup

Session 2				
11:30 - 12:15	Susie	Seibt	Australian Synchrotron, ANSTO	Anything goes: SAXS/WAXS at the Australian Synchrotron
12:15 - 13:00	Andrew	Clulow	Australian Synchrotron, ANSTO	Small Angle Scattering from Solutions

Lunch: 13:00 - 14:00

Speaker setup

Session 3				
14:00 - 14:45	Andrew	Martin	RMIT	Introduction to fluctuation scattering: a new way to probe disordered 3D structure at advanced x-ray light sources.
14:45 - 15:30	Rico/Leonie	Tabor/V'ant Hag	Monash University	SANS and USANS

Afternoon Tea: 15:30 - 16:00

Speaker setup

Session 4				
16:00 - 16:45	Timothy	Petersen	Monash University	Hybrid reverse Monte Carlo modelling
16:45 - 17:00				Wrap-up remarks/closing

Meeting Day 1: Thursday, July, 14th

Speaker setup: 8:30 - 9:00 AM

Session 1: Colloids

Chair: Peter Daivis

09:00 - 09:10				Welcome
09:10 - 09:40	Asaph	Widmer-Cooper	University of Sydney	The Thermodynamic Origins of Chiral Twist in Monolayer Assemblies of Rod-like Colloids
09:40 - 10:10	Amelia	Liu	Monash University	Local stability and local structure of colloidal glasses
10:10 - 10:40	Gerd	Schroeder-Turk	Murdoch University	Microscopy analysis of bicontinuous phases in plant plastid membranes

Morning Tea: 10:40 - 11:10 AM

Speaker setup

Session 2: Scattering

Chair: Billy Todd

11:10 - 11:40	David	Paganin	Monash University	Fokker-Planck equation for optical beams
11:40 - 12:10	Jing	Fu	Monash University	Recent advances in nanoscale tomography of soft matters
12:10 - 12:40	Andrew	Martin	RMIT University	Introducing the Pair-Angle Distribution Function: measuring multi-atom statistics of disordered materials

Lunch: 12:40 - 14:00

Speaker setup

Session 3 A: Simulations - Principles

Chair: Debra Bernhardt

14:00 - 14:30	Ellie	Hajizadeh	University of Melbourne	ML-based optimisation for accelerated and targeted multiscale soft matter design
14:30 - 15:00	David	Huang	University of Adelaide	Systematic coarse-graining of molecular simulation models with anisotropic particles
15:00 - 15:30	Luca	Maffioli	Swinburne University of Technology	Measuring the response of highly confined fluids in a Couette flow: the TTCF formalism

Afternoon Tea: 15:30 - 16:00

Speaker setup

Session 3 B: Simulations - Principles

Chair: David Huang

16:00 -16:30	Stephen	Sanderson	University of Queensland	Machine learning a Time-Local Fluctuation Theorem for non-equilibrium steady-states
16:30 - 17:00	Tim	Duignan	University of Queensland	Accurate first principles simulation of salt water using deep learning.
17:00 - 17:20	Mikhail	Suyetin	Karlsruhe Institute of Technology	Proof of concept: Molecular Dynamics study of memory nanodevice based on Zn-MOF-74.

Informal Dinner

Meeting Day 2: Friday, July, 15th

Speaker setup: 8:30 - 9:00 AM

Session 5: Active Matter

Chair: Asaph Widmer-Cooper

09:00 - 09:30	Prabhakar	Ranganathan	Monash University	Cluster and conquer: invasion of a soft substrate by colonies of rod-shaped cells
09:30 - 10:00	Rahil	Valani	University of Adelaide	Generating active matter from strange attractors
10:00 - 10:30	Shibu	Saw	Roskilde University	Role of the configurational temperature in active-matter models

Morning Tea: 10:30 - 11:00

Speaker setup

Session 6 A: Simulations - Applications

Chair: Nathan Clisby

11:00 - 11:30	Shern	Tee	University of Queensland	When Is A Supercapacitor Like A Protein?
12:30 - 12:00	Dominic	Robe	Monash University	Linear viscoelasticity of associating star polymers
12:00 - 12:20	Isaac	Pincus	Monash University	Modelling dilute solutions of semiflexible polymers with excluded-volume and hydrodynamic interactions

Lunch: 12:20 - 13:40

Speaker setup

Session 6 B: Simulations - Applications

Chair: Rahil Valani

13:40 - 14:00	Patrick	Adams	RMIT University	Using the pair-angle distribution function to analyse protein structure.
14:00 - 14:20	Silpa	Mariya	Monash University	Are soft dendrimers dynamically equivalent to hard spheres?
14:20 - 14:40	Michael	Rinaudo	University of Sydney	Simulating nanoparticle superlattices with Molecular Dynamics
14:40 - 15:00	Sobin	Alosious	Swinburne University of Technology	The effect of electrostatic interactions on Kapitza resistance in nano-confined water.

Afternoon Tea: 15:00 - 15:30

Speaker setup

Session 6 C: Simulations - Applications

Chair: Dominic Robe

15:30 - 15:50	Christian	Zuluaga-Bedoya	University of Queensland	Entry resistance in flexible zeolitic nanosheets
15:50 - 16:10	Kyle	Stevens	University of Newcastle	Lennard-Jones potential and continuum modelling for heterogeneous molecules
16:10 - 16:30	Marltan	Wilson	University of Adelaide	General high-dimensional neural networks for anisotropic coarse-grained molecular simulation models
16:30 - 16:50	Sleebe	Varghese	Swinburne University of Technology	Improved methodology to compute the intrinsic friction coefficient at solid-liquid interfaces
16:50 - 17:00				Close