Workshop III: Surrogate Models and Coarsening Techniques

Monday October 30, 2017

8:00–8:55 *Check-In/Light Breakfast (Hosted by IPAM)*

8:55–9:00 *Welcome and Opening Remarks*

9:00–9:40 **Gregory Voth** (University of Chicago)
Ultra-Coarse-Graining and Its Applications

10:00–10:15 *Break*

10:15–10:55 **Gabor Csányi** (University of Cambridge)
How do we build good databases for machine learning of force fields?

11:15–11:30 *Break*

11:30–12:10 **Harald Oberhofer** (Technical University Munich (TUM))
Embedding Quantum Regions into Classical Environments

12:30–2:30 *Lunch (on your own)*

2:30–3:10 **Nuria Plattner** (Freie Universität Berlin)
Markov modeling of protein-protein interactions and their effects on protein conformational dynamics

3:30–4:00 *Break*

4:00–4:40 **Imre Risi Kondor** (University of Chicago)
Covariant neural networks for learning graphs and atomic potentials

Tuesday October 31, 2017

8:00–9:00 *Continental Breakfast*

9:00–9:40 **Frank Noe** (Freie Universität Berlin)
Beyond the second timescale in all-atom MD: shallow and deep kinetic models for biomolecules

10:00–10:15 *Break*

10:15–10:55 **Christine Shoemaker** (National University of Singapore)
General-purpose Surrogate Methods for Global Optimization and Uncertainty Quantification of Computationally Expensive Nonconvex Models with Some Environmental Applications

11:15–11:30 *Break*

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11:30–12:10 **Zachary Ulissi** (Carnegie-Mellon University)
Addressing Complexity with Surrogate Models in Computational Catalyst Design for Energy Applications

12:30–2:30 *Lunch (on your own)*

2:30–3:10 **Alexander Shapeev** (Skolkovo Institute of Science and Technology)
Simultaneous Learning and Exploring Atomistic Potential Surfaces: Current Progress and Mathematical Challenges

3:30–4:00 *Break*

4:00–4:40 *Lightning Poster Presentations*

5:00–6:30 *Poster Session & Reception (Hosted by IPAM)*

Wednesday November 1, 2017

8:00–9:00 *Continental Breakfast*

9:00–9:40 **Aaron Dinner** (University of Chicago)
A unified framework for umbrella sampling in reversible and irreversible systems

10:00–10:15 *Break*

10:15–10:55 **Albert Bartok-Partay** (Science and Technology Facilities Council)
Learning interactions from microscopic observables

11:15–11:30 *Break*

11:30–12:10 **Bettina Keller** (Freie Universität Berlin)
Girsanov reweighting for path ensembles and Markov state models

12:30–2:30 *Lunch (on your own)*

2:30–3:10 **Christine Peter** (Universität Konstanz)
Coarse grained simulation models and the challenge of representing conformational states, transitions, and responses

3:30–4:00 *Break*

4:00–4:40 **David Bindel** (Cornell University)
Scalable algorithms for kernel-based surrogates in prediction and optimization

Thursday November 2, 2017

8:00–9:00 *Continental Breakfast*

9:00–9:40 **Mark Tuckerman** (New York University)
Exploration and learning of energy and free energy landscapes

10:00–10:15 *Break*

10:15–10:55 **Steve Brunton** (University of Washington)
Data-driven characterization and control of complex systems

11:15–11:30 *Break*

11:30–12:10 **Olexandr Isayev** (University of North Carolina)
Towards Universal ML Potential for Organic Molecules

12:30–2:30 *Lunch (on your own)*

2:30–3:10 **Gus Hart** (Brigham Young University)
Extending the SOAP descriptor to make alloy GAP potentials

3:30–4:00 *Break*

4:00–4:40 **Gareth Conduit** (University of Cambridge)
Who needs atoms to design materials?

Friday November 3, 2017

8:00–9:00 *Continental Breakfast*

9:00–9:40 **Kurt Kremer** (Max Planck Institute for Polymer Research)
Open Systems Simulations of Macromolecular Solutes through Adaptive Resolutions Simulations (AdResS)

10:00–10:15 *Break*

10:15–10:55 **Cecilia Clementi** (Rice University)
Incorporating Experimental Data in Long Timescales Macromolecular Simulations

11:15–11:30 *Break*

11:30–12:10 **Thomas Miller** (California Institute of Technology)
Development of a coarse-grained model for co-translational membrane protein folding

12:30–2:30 *Lunch (on your own)*

2:30–3:10 **Richard Hennig** (University of Florida)
Machine-learning of crystal structure energy landscapes

3:30–4:00 *Break*

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4:00–4:40
TBA

IPAM strives to provide an inclusive environment free of harassment. IPAM does not tolerate sexual harassment, other forms of harassment, or sexual assault. Please familiarize yourself with our community agreement which includes instructions on reporting incidents by using the QR code to the right.