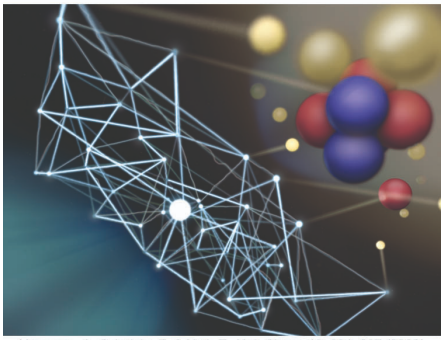
institute for pure & applied mathematics

Learning and Emergence in Molecular Systems

January 23 - 27, 2023



Hermann, J., Schätzle, Z. & Noé, F., Nat. Chem. 12, 891–897 (2020)

Scientific Overview

For molecular systems we know the laws of physics to extreme precision. Yet, our ability to compute properties of these systems to numerical precision is very limited. This is mainly due to two sources of computational intractability: quantum mechanics and chaos. Some aspects of these systems remain predictable at a macroscopic scale, but they require completely different variables, such as pressure, temperature and entropy. We call this emergent theory thermodynamics.

In the completely different discipline of machine learning, a fairly similar phenomenon takes place. The microscopic variables of an image are given by its constituent pixel values. We understand the world at the "emergent" level of objects and their relations, not at the level of pixels and edges. In deep learning (DL) emergence happens automatically through learning and some inductive biases such as symmetries.

A major question we want to address in this workshop is whether we can apply the same learning paradigm to the field of molecular science to learn the correct emergent variables and dynamics.

This workshop will include a poster session; a request for posters will be sent to registered participants in advance of the workshop.

This is a Julian Schwinger Workshop on Multiscale Physics, made possible by a gift from the Julian Schwinger Foundation for Physics Research (JSF).

Participation

Additional information about this workshop including links to register and to apply for funding, can be found on the webpage listed below. Encouraging the careers of women and minority mathematicians and scientists is an important component of IPAM's mission, and we welcome their applications.

Organizers

Xavier Bresson (National University of Singapore), **Cecilia Clementi** (FU Berlin), **Klaus-Robert Müller** (TU Berlin), **Patrick Riley** (Relay Therapeutics), **Max Welling** (Microsoft Research)

Speakers

Mohammed AlQuraishi (Harvard Medical School)
Xavier Bresson (National University of Singapore)
Steve Brunton (University of Washington)
Cecilia Clementi (FU Berlin)
Ron Dror (Stanford)
Rafael Gomez-Bombarelli (MIT)
Klaus-Robert Müller (TU Berlin)
Frank Noe (FU Berlin)
Kristin Persson (UC Berkeley)
Patrick Riley (Relay Therapeutics)
Jutta Rogal (NYU)
Tess Smidt (MIT)
Alexandre Tkatchenko (University of Luxembourg)
Anatole von Lilienfeld (University of Basel) and
Max Welling (Microsoft Research)

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For more information, visit the program webpage:
www.ipam.ucla.edu/EMS2023