MM 13: Invited Talk: Sinclair

Time: Tuesday 9:30–10:00 Location: SCH A 251

Invited Talk MM 13.1 Tue 9:30 SCH A 251

Exploring the Slow Dynamics of Interfaces and Glasses via Markov State Models — Siavash Soltani[1], Joerg Rottler[2,3], and •Chad Sinclair[1] — [1]Department of Materials Engineering, The University of British Columbia, Vancouver, BC, Canada V6T 1Z4 — [2]Department of Physics and Astronomy, The University of British Columbia, Vancouver, BC, Canada V6T 1Z1 — [3]Stewart Blusson Quantum Matter Institute, The University of British Columbia, Vancouver, BC, Canada V6T 1Z4

A persistent challenge for molecular simulations is to assess slow processes efficiently from short trajectories. Important examples of slow phenomena in materials are the motion of interfaces in alloy crystals or the structural relaxation in glass forming liquids. Markov State Models (MSM) are an attractive tool to unveil the slowest processes of a complex atomistic system in a low dimensional space of feature variables. This talk describes the predictions and insights gained from such MSMs constructed using machine learning techniques. For grain boundaries, the model learns a hierarchy of timescales associated with transformations between geometrically distinct motifs. When applied to a binary glass former, our model finds a transition timescale between states that is larger than the conventional structural alpha-relaxation time. In both systems, the MSMs are able to access kinetics at temperatures where brute force calculations become computationally expensive or impossible.