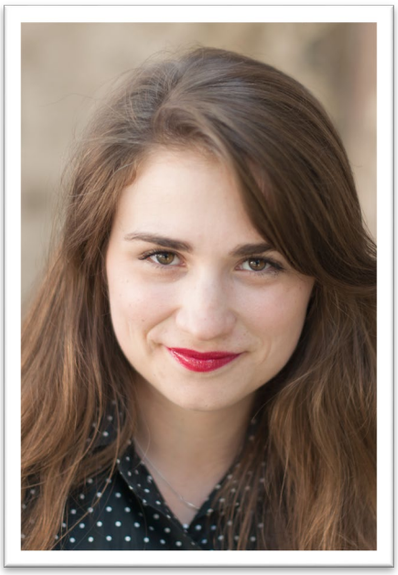
PHYSICAL MATH Seminar

Optimizing non-equilibrium processes using differentiable simulation



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ABSTRACT:

Controlling the evolution of nonequilibrium systems to optimize thermodynamical quantities such as heat, work, and entropy is a key goal for designing nanotechnological devices like artificial molecular machines. Conversely, biological molecular machines have evolved to capitalize on the laws of nonequilibrium physics, in some cases achieving remarkable robustness and efficiency, but precisely *how* this is achieved remains elusive. Classical thermodynamics is ill-equipped to describe the physics of nonequilibrium systems, and new techniques are needed. Here, I introduce one such technique: repurposing the tools used in machine learning optimizations -- in particular, automatic differentiation -- to find optimal control protocols for nonequilibrium systems. In particular, I'll demonstrate the successful use of automatic differentiation to optimize Monte Carlo (MC) and Molecular Dynamics (MD) simulations. To illustrate the former case, I'll present how to minimize the entropy production when flipping a "bit" from 0 to 1 (represented by Ising lattice spins). I'll then show how to leverage differentiable MD simulations to minimize the external energy required to unfold a protein or DNA molecule and thereby improve free energy landscape reconstructions. Employing automatic differentiation on these and other systems requires careful consideration of gradient computation, and I'll share challenges we've encountered as well as strategies we've found successful across a range of systems. I'll conclude with a discussion of implications of these successes on other longstanding nonequilibrium physics questions.

BIO: After earning her BSc and MSc in Physics at the University of Alberta, Megan completed her DPhil in Theoretical Physics at the University of Oxford as a Rhodes Scholar. Her research, pursued in collaboration with DNA nanotechnologists, used molecular simulations to explore the response of DNA nanomachines to forces. As a Schmidt Science Postdoctoral Fellow, Megan worked at Harvard University to apply machine learning techniques to study non-equilibrium biological systems. Now an assistant Professor at the University of Calgary in the Biological Sciences Department, Megan seeks to improve our understanding of how nature has harnessed the laws of physics to drive processes like robust self-assembly and molecular energy transduction, ultimately leading to better rational design of synthetic, self-assembling nanomachines.

TUESDAY, SEPTEMBER 12, 2023
2:30 pm – 3:30 pm
Building 2, Room 449

http:math.mit.edu/seminars/pms

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