Thesis Projects in Generative AI for Molecular Simulations

Molecular simulations are an important tool in biology, chemistry, material science, and physics. It has the potential to give us atom-resolution insights into how properties of matter arise, how drugs bind their target, or how proteins shift into disease inducing states. However, a significant issue with current simulation technologies is that it is extremely computationally expensive to conduct such simulation. In our research group, we are developing generative AI to address this problem, and we recently established a platform called ITO (implicit transfer operator, see figure below), which allows us to speed up simulations by orders of magnitude.

We are looking for driven and ambitious students to join our team to develop this platform into an impactful technology. In this connection we have several projects available including:

1. Extend ITO to generalize across different physical conditions for example, changing temperatures or changing pressure.
2. Extend ITO to account for periodic boundary conditions to allow for simulation of bulk liquids and materials.

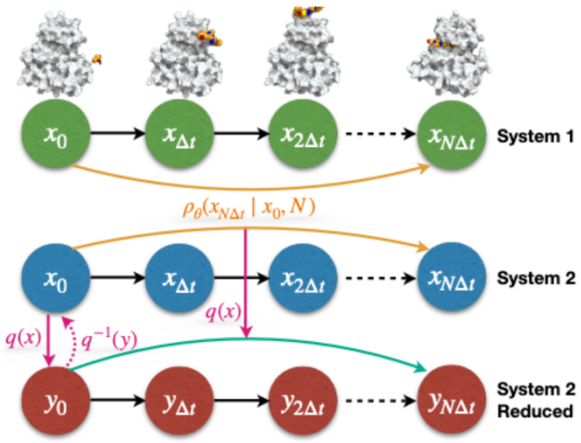

Figure 1: Implicit transfer operator illustration, showing how conventional simulations work (black arrows) and how ITO enable much larger steps (orange and blue lines), thereby speeding up simulations of long timescale events, such as drug binding.

Viable candidates will have working experience with a modern machine learning library (pytorch or jax) and be comfortable at least one of these topics: molecular dynamics simulations, machine learning, statistical mechanics, linear algebra, or (stochastic) dynamical systems (e.g. differential equations).

To apply send a brief motivation, CV (with link to github page if applicable), and a list of transcripts (with grades) to simonols@chalmers.se

More details about our work can be found in some of our recent publications:
https://arxiv.org/abs/2305.18046
https://www.science.org/doi/full/10.1126/science.aaw1147
https://cloud.ml.jku.at/s/sKtfdFpoTp9F7sJ