CSC Seminar

SPEAKER

Simon Olsson

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TITLE

Accelerating Molecular Simulations with Generative Models

ABSTRACT

Generative modeling is a powerful technique to learn probability distributions from data. Many properties and quantities of interest in the sciences are often expressed as expectation values for a certain probability distribution, most prominently in statistical physics. Focusing on molecular sciences, I will in this talk, detail how we are developing Generative AI to improve molecular dynamics simulations. I will focus on our work on Implicit Transfer Operators — a long time-scale Molecular Dynamics surrogate model closing the time-scale gap between numerical simulations and biological processes.

Bio: Simon Olsson is an Associate Professor at Chalmers University of Technology in Gothenburg, Sweden, specializing in machine learning, computational biology, and molecular modeling. His research focuses on developing machine learning approaches to speed up numerical simulations and tackle inverse design problems. Before joining Chalmers he was a postdoctoral researcher at FU Berlin, ETH Zurich and IRB Bellinzona. He has a PhD in bioinformatics from the University of Copenhagen.

Thursday, January 30, 2025 at 2 pm
seminar room Prigogine