School of Data Science
香港城市大學
City University of Hong Kong

SDSC SEMINAR

Machine-learning-based Modeling of Multi-scale Dynamical Processes with Molecular Fidelity

Date: 23 August 2024 (Friday)

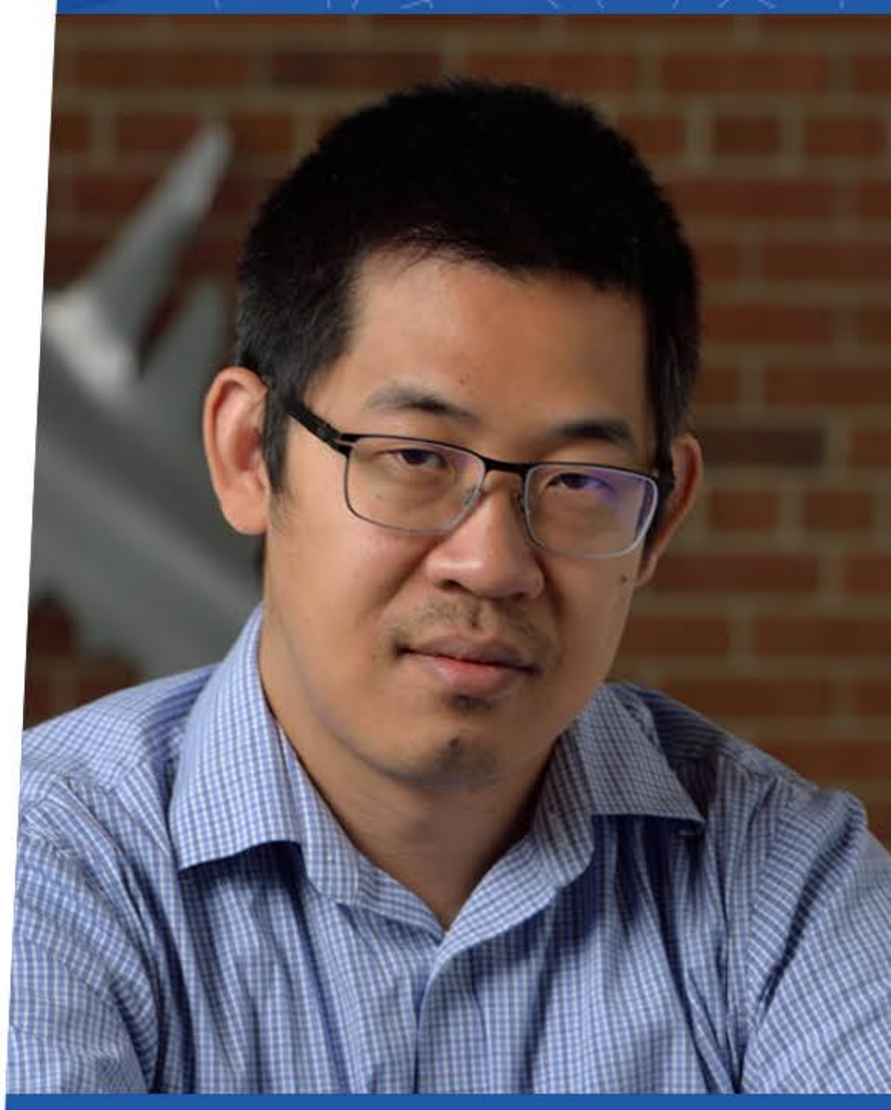
Time: 2:00pm - 3:00pm

Venue: Rm 6-209, Lau Ming Wai Academic Building

Zoom: https://cityu.zoom.us/j/87514446514

ABSTRACT

One essential challenge in the computational modeling of multiscale systems is the availability of reliable and interpretable closures that faithfully encode the micro-dynamics. For systems without clear scale separation, there generally exists no such a simple set of macro-scale field variables onto which we can project and predict the dynamics in a self-determined way. We introduce a machine-learning-based approach that enables us to systematically pass the micro-scale physical laws onto the macro-scale. The non-Newtonian hydrodynamics of polymeric fluids is used as an example to illustrate the essential idea. To faithfully retain molecular fidelity, we establish a micro-macro correspondence via a set of encoders for the micro-scale polymer configurations and their macro-scale counterparts, a set of nonlinear conformation tensors. The dynamics of these conformation tensors, with a new form of the objective tensor derivative, can be derived from the micro-scale model. Unlike our conventional wisdom about ML modeling, the training only uses time-discrete samples. The final model, named the deep non-Newtonian model (DeePN2), retains a multi-scaled nature with clear physical interpretation and strictly preserves the frame-indifference constraints. We show that DeePN2 can faithfully capture the broadly overlooked viscoelastic differences arising from the specific molecular structural mechanics without human intervention.



Professor Huan LEI

GUEST SPEAKER'S PROFILE

Professor Huan LEI got his Ph.D. in applied mathematics at Brown University. Prior to that, he obtained his B.S. from the University of Science and Technology of China. He is currently an assistant professor in the Department of Computational Mathematics, Science and Engineering at Michigan State University. His research mainly focuses on developing physics interpretable and structure-preserving machine-learning methods for computational modeling of multiscale problems. He is the recipient of the National Science Foundation (NSF) CAREER award.

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All are welcome