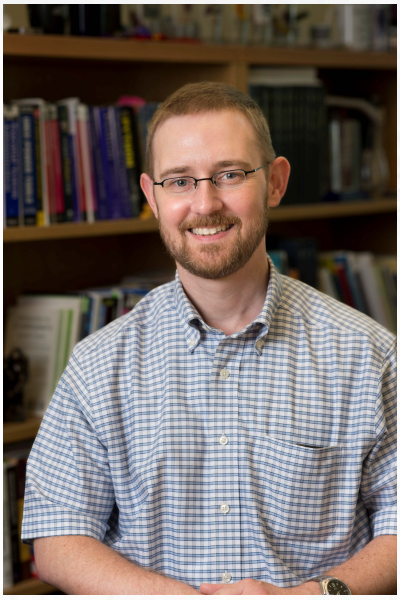
HAJIM SCHOOL OF ENGINEERING AND APPLIED SCIENCES
UNIVERSITY of ROCHESTER



The Department of Chemical Engineering Presents:

JOHN KITCHIN

Professor, Dept. of Chemical Engineering, Carnegie Mellon University

Machine-learning frameworks in molecular simulation and its potential impact on science and engineering

ABSTRACT: We use models in science and engineering extensively. We use them to make predictions about the behavior of systems, to optimize designs, and to understand why systems behave the way they do. Most of our models are built from physical principles, and the parameters in the models are usually determined from measured data. That data is often expensive to gather, but the model is then cheap to evaluate. The accuracy of these models depends both on the depth of understanding we have, and the quality of the data, and when we hit the limit of our understanding it is difficult to make better models. Machine learning offers a path forward to build models that are not necessarily based on physics, but which more accurately predict outputs.

We are interested in building models that allow us to perform molecular simulations that require many (hundreds of thousands) of calculations. These are not practical with quantum chemical calculations, which are too expensive to run at this scale. Existing molecular force fields are efficient enough for this, however, they lack the accuracy required to obtain meaningful results. I will present how we are using machine learning in conjunction with quantum chemical calculations to develop efficient models that can be used to simulate effects such as segregation, diffusion, etc., which can only be probed using simulation methods such as Monte Carlo and molecular dynamics.

Machine learning has more to offer science and engineering than just model development. I will also discuss some aspects of how machine learning works, particularly the role that automatic differentiation has in machine learning. This has implications for many types of scientific programming, and may enable new ways to think about science and engineering problem solving.

BIO: John Kitchin completed his B.S. in Chemistry at North Carolina State University. He completed a M.S. in Materials Science and a PhD in Chemical Engineering at the University of Delaware in 2004 under the advisement of Dr. Jingguang Chen and Dr. Mark Barteau. He received an Alexander von Humboldt postdoctoral fellowship and lived in Berlin, Germany for 1 ½ years studying alloy segregation with Karsten Reuter and Matthias Scheffler in the Theory Department at the Fritz Haber Institut. Professor Kitchin began a tenure-track faculty position in the Chemical Engineering Department at Carnegie Mellon University in January of 2006. He is currently a Full Professor. At CMU, Professor Kitchin works in the areas of alloy catalysis and molecular simulation. He was awarded a DOE Early Career award in 2010 to investigate multifunctional oxide electrocatalysts for the oxygen evolution reaction in water splitting using experimental and computational methods. He received a Presidential Early Career Award for Scientists and Engineers in 2011. He recently completed a sabbatical in the Accelerated Science group at Google learning to apply machine learning to scientific and engineering problems.

Wednesday, September 25 3:25PM

Goergen Hall Room 101 (Sloan Auditorium)