CHEMICAL ENGINEERING

SEMINAR SERIES

JOHN KITCHIN

Monday, April 09, 2018

Professor, Chemical Engineering
Carnegie Mellon University

Machine-learning frameworks in computational catalysis and its potential impact on science and engineering

ABSTRACT: Model building has been a core activity in chemical engineering from the beginning. Historically these models have either been derived from physical insight, or by empirical observation. Continuous advances in computer hardware and software, as well as in experimental instrumentation have led to a significant increase in the use of machine learning as a new approach to model building in scientific research. In this approach, models are built from data using flexible functions, or using algorithms. In this talk, I will use our work in computational catalysis to illustrate how machine learning can be used to augment expensive computations to solve research problems.

In catalysis, we often use density functional theory (DFT), a first-principles physics based simulation, to compute properties of catalyst surfaces and reactions. These computations are too expensive to use directly in other simulations such as molecular dynamics or Monte Carlo simulations, and so a variety of coarse-graining approaches have been developed to build reduced-order models that can be used. For example, in the last decade there has been the development of DFT-trained neural networks to create atomistic models that can be used in molecular dynamics or Monte Carlo simulations. We have used this approach to study coverage dependent oxygen adsorption on Pd(111) surfaces and segregation in AuPd alloy surfaces, which we will discuss in this talk.

The current approaches used in machine learning model building have significant implications for science and engineering, and may lead to new ways to solve problems. For example, nearly all the modern machine learning frameworks use automatic differentiation to enable the model regression. This means that derivatives of the model do not need to be derived by hand, and are available as part of the model. These

derivatives often have physical meaning, e.g. forces or stresses in molecular simulations, or they are related to fluxes, or they are part of constraints, e.g. the Gibbs-Duhem relations in thermodynamics. Thus, it becomes possible in some cases to build some physics into a machine learning model. I will show some examples of how machine learning frameworks can be used to solve some engineering problems that aren,Äôt usually thought of as machine learning problems.

BIOGRAPHY: 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 1½ 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 is currently on sabbatical in the Accelerated Science group at Google learning to apply machine learning to scientific and engineering problems.

RECEPTION 3:30 • LECTURE 4:00 – 5:00
PHYSICS ASTRONOMY BLDG. PAA A 118

CHEMICAL ENGINEERING
UNIVERSITY of WASHINGTON
Knowledge and solutions for a changing world