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Subject: [nist-ai] TODAY - MGI.Seminar Series: The Open Force Field Initiative: Better force fields through open, data-driven science -- Shirts, University of Colorado Boulder [August 19, 2019, 11 AM EDT, G: 101/LCTR A, B: 2-0113 (VTC)]
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MGI.Seminar Series

Monday, August 19, 2019
11:00 AM EST, 101/LCTR A (w/ VTC to Boulder 2-0113)

The Open Force Field Initiative: Better force fields through open, data-driven science

Prof. Michael R. Shirts

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Abstract

Physical modeling of biologically relevant molecular entities is a powerful tool for predicting molecular properties and function, interpreting experiments, and designing new small molecules, biomolecules or polymers with therapeutic utility. While molecular simulation has benefited from recent massive increases in computational power, improvements in molecular mechanics force fields have lagged behind. As a result, the utility of physical modeling is limited by the uncertain accuracy and restricted domain of applicability of current force fields. Despite a revolution in data availability and ubiquity of computing resources, we lack technologies to draw on the wealth of available experimental and quantum chemical data to rapidly and systematically improve force fields.

The Open Force Field Initiative (OpenFF) is a collaboration focused on the development of 1) extensible, open source toolkits for constructing, applying, and evaluating force fields; 2) the curation of public datasets necessary to build high-accuracy biomolecular (and biocompatible) force fields; and 3) the generation of improved molecular force fields for biomolecular and other soft matter applications.

In this talk, I will discuss recent efforts by OpenFF to simplify the existing force field framework, put force field development in an explicitly data-driven, Bayesian context, reduce the cost of exploring properties as a function of parameter space, put and gather the data needed to make this effort possible, as well as the current status of our initial force field parameterization effort.

Bio

Dr. Shirts is an associate professor of Chemical and Biological Engineering at the University of Colorado Boulder. He received his A.B. in chemistry from Harvard and his Ph.D. in Chemistry from Stanford, where he was a Fannie and John Hertz Fellow. At Stanford, he helped found the Folding@Home distributed computing platform, which allows hundreds of thousands of volunteers to contribute their spare CPU cycles to solve biophysical problems, and was afterwards an NIH NRSA Fellow at Columbia University. Dr. Shirts was previously an assistant and then associate professor of chemical engineering at the University of Virginia, where he was awarded an ACS Computers in Chemistry Young Investigator award and an NSF CAREER award. He is a founding and managing editor of the Living Journal of Computational Molecular Science. His current work involves two main focuses. First, developing classical molecular simulation tools for more robust and useful scientific discovery and molecular engineering, and second, understanding in collaboration with experimentalists how small molecular changes create large-scale structure and function changes in biological and soft materials.

Speaker Schedule

If you would like to meet the speaker please contact Fred Phelan (frederick.phelan@nist.gov, x6761) to schedule.

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