Applied Math Seminar scheduled on Friday, October 25, 2019, 11-12pm, LO1328

Speaker: Dr. Matthew Spellings (University of Michigan)

Title: **Scaling Colloidal Self-assembly Simulations using Machine Learning**

Abstract:

Over the last several years, researchers have designed and catalogued a host of methods to synthesize colloidal- and nanoscale particles with a variety of attributes. Internal aspects of building blocks—such as particle shape and surface coating—as well as characteristics of the assembly environment—such as depletant concentration and temperature—all influence which ordered structure (if any) will form *via* self-assembly. Because the three-dimensional configuration of particles plays an enormous role in determining the physical properties of the assembled systems, self-assembly simulations are often used to identify the important conditions required to form a particular structure or predict which structures will assemble; however, robustly and automatically characterizing structures in three dimensions can be challenging. In this talk, I will discuss methods to incorporate machine learning into both the experimental design and simulation analysis components of the self-assembly design loop in order to increase our scientific throughput by orders of magnitude. These methods promise to open up many types of new studies to analysis that were previously intractable due to limitations of computational power or scale.

About the speaker:

After studying chemical engineering at Vanderbilt University, Matthew Spellings went on to receive his Ph.D. from the University of Michigan. Matthew's research interests include colloidal- and nanoscale self-assembly, software design, data visualization, programming languages, heterogeneous computing, and machine learning.