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Hector D. Ceniceros* (ceniceros@ucsb.edu), Department of Mathematics, University of California, Santa Barbara, CA 93106. *Machine Learning from Polymer Self Consistent Field Theoretic Simulations to Accelerate Phase Discovery.*

Self consistent field theory (SCFT) has been a valuable coarse-grained method for the study of many equilibrium polymer solutions. However, SCFT simulations are computationally expensive and the process of exploring the parameter space for new polymer phases is a formidable task. In this talk, we will discuss our first steps to use machine learning tools to accelerate this process. More specifically, our program consists of two problems: (1) the learning of the free energy map as a function of the model parameters and of the polymer segment density and (2) the determination of a polymer segment density that minimizes a fitness function. We will present different approaches for (1), including simple kernel ridge regression and deep learning and discuss, time permitting, local vs global optimization strategies for (2). (Received September 04, 2019)