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Using machine learning to drive computational discovery in self-organizing material systems[1] CAROLYN PHILLIPS, Argonne National Laboratory, GREGORY VOTH, University of Chicago — In a complex self-organizing system, small changes in the interactions between the system's components can result in different emergent macrostructures or macrobehavior. In chemical engineering and material science, such spontaneously self-assembling systems, using polymers, nanoscale or colloidal-scale particles, and DNA are an attractive way to create materials that are precisely engineered. Computer simulations of such systems are a powerful tool for discovery. However, as the rate at which data can be amassed continues to accelerate, the pace of discovery becomes limited not by the rate at which data can be generated, but can be analyzed. We consider this problem from two ends, using a model particle system that self-assembles simple and complex crystals. First, we show how the ordered states can be discovered in a large data set of simulation results by using a hierarchy of pattern analysis techniques including shape matching and machine learning algorithms. Second, we introduce a learning algorithm, inspired by adaptive mesh refinement, that guides the deployment of computational experiments. This algorithm densely searches the space of the degrees of freedom for a self-organizing system, while targeting certain features, thus, gathering more information for less computational effort. New algorithmic techniques, such as these, for managing the growing volume of simulation data catalyze advancing computational power to be a tool for discovery.

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