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MACHINE LEARNING MATERIALS PHYSICS: A CASE STUDY IN PREDICTING PRECIPITATE MORPHOLOGY

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Machine learning has been effective at detecting patterns and predicting the response of systems that behave free of natural laws. Examples include learning crowd dynamics, recommender systems and autonomous mobility. There also have been applications to the search for new materials that bear relations to big data classification problems. However, when it comes to physical systems governed by conservation laws, the role of machine learning has been more limited. Here, we present our recent work in exploring the role of machine learning methods in discovering, or aiding, the search for physics. Specifically, this talk will focus on using machine learning algorithms to represent high-dimensional free energy surfaces with the goal of identifying precipitate morphologies in alloy systems. Traditionally, this problem is approached by combining phase field models, which impose first-order dynamics, with elasticity, to traverse a free energy landscape in search of minima. Equilibrium precipitate morphologies occur at these minima. Here, we exploit the ability of machine learning methods to represent high-dimensional data, combined with surrogate optimization, sensitivity analysis and uncertainty quantification as an alternate approach to finding minimum energy states. This combination of data-driven methods offers an alternative to the imposition of first-order dynamics via phase field methods, and represents one approach to learning materials physics with machine learning.