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Predicting material microstructure evolution via data-driven machine learning

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Predicting microstructure evolution can be a formidable challenge, yet it is essential to building microstructure-processing-property relationships. Yang et al. offer a new solution to traditional partial differential equation-based simulations: a data-driven machine learning approach motivated by the practical needs to accelerate the materials design process and deal with incomplete information in the real world of microstructure simulation.

The recent rapid rise in data-driven practices in the materials science domain has led to the development of efficient, generalizable, and accurate approaches for several applications, including material property prediction,[1] mining (micro)structure-property and (micro)structure-processing relationships,[2–4] and characterization of material microstructures.[5,6] Central to the materials science domain is linking microstructure to properties and performance, and critical to building such linkages is understanding how microstructures evolve as a function of environmental exposure or processing conditions (e.g., time, temperature, applied stress or strain, irradiation).

Improvements in computational capabilities have been enabled by deep neural networks, improved hardware, and openly available software packages. Computational materials science is a broad field with numerous methods that range in length scale from the atomic scale to continuum. Techniques such as phase field modeling are widely used for predicting microstructure evolution in two- and three-dimensional systems.[7] In addition, density functional theory (DFT), a quantum-based method, has been instrumental in discovering new materials, identifying dopants for alloy strengthening, detailing diffusion mechanisms, and more. However, any computational approach is constrained by the length and timescales of simulations, accuracy, and generalizability (or transferability) between different material systems.[8] Progress in materials science will rely heavily on feedback both from these computational models and validation with experiments. Yet, the scaling of such methods to larger datasets, particularly in three dimensions, can be time consuming and computationally expensive. In the May 14, 2021 issue of *Patterns*, Yang et al.[9] offer a new alternative to partial differential equation (PDE)-based simulations using a data-driven approach employing recurrent neural networks (RNN) in their article "self-supervised learning and prediction of microstructure evolution with recurrent neural networks."

Motivated by the practical need to deal with incomplete information in real world applications of microstructure evolution simulations, RNNs were trained to infer parameters from input image sequences to correctly predict microstructure evolution. The authors demonstrate that even with incomplete information of the PDEs and their solutions, the RNN can be trained to accurately emulate system trajectory. Numerical simulations were used to generate image sequences used as training sets for four classic microstructure evolution phenomena with variable complexity: (1) plane wave propagation, (2) grain growth, (3) spinodal decomposition, and (4) dendritic crystal growth. A convolutional RNN was trained to predict spatiotemporal evolution of material microstructure, building upon several prior works that have cited convolutional NNs (CNNs) as excellent models for representing microstructure image data.[3,10]

The novel architecture presented in this work is intentionally trained with only partial information of the PDE solutions. The challenge of training a neural net to predict long-time evolution behavior based only on short-time data that have much faster dynamics is explored in this work. For both grain growth and spinodal decomposition problems, the RNN was trained with early-stage microstructure images only and was able to accurately predict the much slower evolution at 10-fold larger times. This impressive long-term prediction capability is also computationally efficient when compared to PDE-based simulations. The RNN performance is not limited by numerical stability of PDEs and can make reliable predictions at much larger time steps. RNNs are shown to accelerate predictions by 92 times for spinodal decomposition when run on a GPU, and 7.6 times when run on a CPU, for example.

Several key findings from Yang et al.'s[9] work include that the RNN architecture developed can (1) generalize well beyond training datasets over long time periods up to 10 times the training data's time span, (2) be applied to larger images than the training set with comparable accuracy, (3) predict evolution of microstructures with different morphologies than the training dataset, and (4) employ time steps 1–2 orders of magnitude larger than PDE-based simulations.

This study demonstrates that a well-trained RNN can not only serve as a PDE emulator but also infer implicit material properties from spatiotemporal data and provides a representation of the targeted problems that lowers data demand and improves training and prediction efficiency. The architecture and approach detailed in Yang et al.'s[9] study has wide applicability. In particular, this approach may be applied to the analysis

of both two- and three-dimensional microscopy data collected during *in situ* or *in operando* experimentation to further improve our understanding of the spatiotemporal evolution of material microstructures. This work represents a timely, important advancement in the development of reliable computational methodologies using neural networks that can provide advantages over traditional approaches for predictive materials modeling. Hence, Yang et al.'s[9] approach and findings have implications to a wide range of applications in the materials research community.

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