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Data-Driven Modeling of Lithium-ion Batteries

Lithium-ion batteries (LIBs) could be found ubiquitously in cell phones, laptops, more recently in Electric Vehicles and Energy Storage Systems. Thus far, the current State-of-the-Art in modeling efforts utilizes the "Doyle-Fuller-Newman" (DFN) model, which is a system of partial differential equations. These equations could be solved using the Finite Element Method (FEM). Within the DFN framework, the most common approach is to solve it pseudo-2D which treats the electrode kinetics as a homogenous reaction. With recent advances in tomography, researchers have been able to resolve the 3D microstructure of the active material used in LIBs, which allows for design of new electrode architectures from the structure-performance relationship of the microstructures. Though 3D modeling adds a lot of degrees of freedom so there is a need to model the effect of electrode microstructure on battery operation while being relatively quick to solve. Here we propose a data-driven Machine Learning framework using Convolutional Neural Networks to be able to resolve the electrode microstructure and model galvanostatic operation of LIBs; results indicate up to 10x quicker runtimes than the FEM approach.

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