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A Modularized Modelling, Discretization and Model Order Reduction Workflow for the Simulation of Li-ion Batteries

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A major cause for performance degradation and failure of rechargeable Li-ion batteries is the disposition of a metallic Li-phase at the negative electrode of the battery cell (Li-plating). The process leading to the formation of this additional phase, however, is still poorly understood. It is the aim of the MULTIBAT research project to gain a better insight into the causes of Li-plating with the help of mathematical modelling and numerical simulation. However, since Li-plating is initiated on a micrometer scale at the interface between electrode and electrolyte, battery models which resolve the porous electrode geometry [2] are needed to accurately describe this effect. This in turn leads to high-dimensional nonlinear finite volume discretizations [4] which require substantial computational effort for their solution.

In this contribution we present the simulation workflow that has been established by MULTIBAT to tackle this challenging application problem. Model order reduction plays an integral role in this workflow in order to make the microscale modelling approach computationally feasible for parameter studies and responsive simulation tools. Our workflow is designed from ground up to be modular, allowing different groups to contribute their expertise in the different parts of the modelling and simulation pipeline, and allowing easy adaption of the developed algorithms and tools to similar application problems based on transport processes in materials with microscale structure.

For the model order reduction we have implemented reduced basis approximation algorithms in conjunction with empirical operator interpolation [1] for the nonlinear parts in the system's space differential operator as generic algorithms in our freely available model reduction software library `pyMOR` [3]. Due to `pyMOR`'s interface-based approach, these algorithms can be automatically applied to newly developed battery models in the battery simulation software `BEST`. At the same time, improved reduction algorithms can be used without requiring changes in `BEST`. Moreover, `pyMOR`'s algorithms can be easily reused with other PDE solvers to tackle new application problems.

Besides a presentation of the MULTIBAT workflow, we will also cover the battery model and its reduction in more detail and discuss our current results.

References

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