

An hp -Adaptive Finite Element Method for a Chemo-Mechanical Battery Active Particle Model

Fabian Castelli¹ Willy Dörfler²

Lithium-ion batteries are currently the most prominent electrochemical energy storage systems for everyday mobile devices and also large-scale stationary applications. One reason for the decreasing performance of a battery over its lifetime is mechanical stress in the electrode material. An inhomogeneous lithium distribution due to phase separation causes high mechanical stresses, which can induce particle fracture and thus loss of capacity.

We consider our previously developed Cahn–Hilliard-type phase-field model coupling lithium diffusion, large deformations and phase separation based on a thermodynamically consistent transport theory, see [2,3]. Limitations for the numerical investigation are mainly due to the strongly varying spatial and temporal scales of the underlying phase field model, which require a very fine mesh and time resolution, however, solely at specific stages in space and time.

To overcome these numerical difficulties, we present our general-purpose hp -adaptive finite element solution algorithm with variable-step, variable-order time stepping [1].

We show the functionality of the hp -adaptive solution algorithm at the example of the chemo-mechanical particle model and demonstrate the computational savings for an increasing local polynomial degree range. In particular, we compare the developed method to one with fixed spatial degree and observe reduction of the computational cost.

References:

- [1] G.F. Castelli, W. Dörfler: Comparison of a h - and hp -adaptive finite element solver for chemo-mechanically coupled battery electrode particles. Submitted. 2021.
- [2] G.F. Castelli: Numerical Investigation of Cahn–Hilliard-Type Phase-Field Models for Battery Active Particles. Ph.D. thesis, Karlsruhe Institute of Technology (KIT), 2021.
- [3] G.F. Castelli, L. von Kolzenberg, B. Horstmann, A. Latz, W. Dörfler: Efficient Simulation of Chemical-Mechanical Coupling in Battery Active Particles. *Energy Technol.*, 9(6):2000835, 2021.

¹Karlsruhe Institute of Technology (KIT), Institute of Thermal Process Engineering, Kaiserstr. 12, 76131 Karlsruhe, Germany
fabian.castelli@kit.edu

²Karlsruhe Institute of Technology (KIT), Institute of Applied and Numerical Mathematics, Englerstr. 2, 76131 Karlsruhe, Germany
willy.doerfler@kit.edu