

A Parallel Matrix-Free Preconditioner for Cahn–Hilliard-Type Phase Separation in Battery Particles

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We consider a Cahn–Hilliard-type phase-field model for the description of phase separation in electrode particles of lithium-ion batteries. During lithium insertion, a separation into a lithium poor and a lithium rich phase occurs and the phase transition migrates through the electrode particle. Due to the strongly varying spatial and temporal scales as well as the nonlinearities, this problem is computationally expensive to solve.

In order to solve the model in an efficient way, we employ a finite element discretization in space and implement a variable-step, variable-order time stepping algorithm. We use a gradient recovery estimator as local refinement criterion. For the solution of the linear systems, we extended and implemented a block-preconditioner for the Cahn–Hilliard equation. The blocks of the preconditioner are symmetric positive definite and can be inverted by the CG method with multigrid preconditioning. Therefore, this preconditioner is especially suited for the matrix-free implementation. Moreover, the preconditioner respects the nonlinear and possible anisotropic character of the Cahn–Hilliard model equation.

We validated our implemented Cahn–Hilliard solver on some benchmark examples. The matrix-free preconditioner is robust for the classical Cahn–Hilliard equation and also for the battery application problem. In particular, the number of GMRES steps per time step is practically independent of the mesh level, even for locally refined meshes.

References:

- [1] 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.
- [2] G.F. Castelli, W. Dörfler: Comparison of a h - and hp -adaptive finite element solver for chemo-mechanically coupled battery electrode particles. 2021. (submitted)
- [3] G.F. Castelli, W. Dörfler: Study on an Adaptive Finite Element Solver for the Cahn–Hilliard Equation. In: F.J. Vermolen, C. Vuik (eds.): Numerical Mathematics and Advanced Applications ENUMATH 2019, 245–253, 2021.

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