# Efficient Matrix-Free Simulation of a Cahn-Hilliard-Type Phase-Field Model for Battery Electrode Particles

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We focus on the efficient numerical treatment of a Cahn–Hilliard-type phase-field model arising in the description of phase separation in electrode particles of lithium ion batteries. During lithium insertion, a separation of the concentration profile into a lithium poor and a lithium rich phase evolves and the phase transition migrates through the particle domain. Due to the strongly varying spatial and temporal scales as well as the strong anisotropy of certain electrode materials, this application problem is computationally expensive to solve.

In order to simulate the model efficiently we employ a finite element discretization in space and implement an adaptive solution algorithm based on a variable-step, variable-order time integration scheme and a gradient recovery estimator as local refinement criterion. In addition, for the underlying well-known Cahn–Hilliard equation we propose an extended preconditioner, which is particularly suited for matrix-free computations. Moreover, the preconditioner respects the nonlinear and possible anisotropic character of the Cahn–Hilliard model equation.

The implemented Cahn–Hilliard solver is validated at the example of benchmarks and outperforms existing solvers. It turns out that 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. Furthermore, at the example of extended particle models we demonstrate the capabilities and significance of the implemented adaptive solution algorithm.

References:

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