Abstract

Electrochemical processes are essential in the manufacturing of a very broad range of products. The multi-ion transport and reaction model (MITReM) is used to simulate such electrochemical processes. The governing partial differential equations (PDEs) are discretized in space by a combined finite element and residual-distribution scheme. The discrete system is linearized with Newton's method which results in a series of linear systems. The focus of this work is on the development of a stable and efficient point-based algebraic multigrid (PAMG) method for the solution of the linear systems which arise in the MITReM simulation.

The new PAMG approach makes use of physics-aware smoothing and coarse-grid correction techniques. This means that it, explicitly, takes important physical properties of the PDE system into account.

We introduce a reordering framework which makes it possible to use physics-oriented matrix-based measures for strength of connectivity to derive application-specific point orderings for smoothing. The framework's generality not only allows the determination of suited permutations of the variables for the electrochemical simulations considered, but also for other convection- and/or migration-dominated simulation tasks.

We introduce a heuristic Péclet number to locate areas causing numerical difficulties within the hierarchy of the algebraic multigrid (AMG) method for scalar PDEs as well as systems of PDEs. We investigate several coarse-grid correction techniques which take this information into account and show results for the convection-diffusion equation, the migration-diffusion system and the MITReM.

We motivate the use of the physics-aware PAMG components and apply the approach for a range of geometries and chemical setups with scientific and industrial relevance. Our numerical experiments illustrate, in particular, that physical properties of the underlying problem have to explicitly be considered for constructing efficient and robust AMG-based methods.