Adaptive finite element approaches for microscopic and macroscopic simulations of battery electrodes

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Abstract

Diffusion and heterogeneous reaction processes characterize electrochemical systems like fuel cells, oxygen capturing membranes and batteries. When these processes occur in complex microstructures the physical phenomena have a multiscale character. From the practical point of view usually a macroscopic rather than microscopic quantity is of interest, e.g., the flux over a surface, i.e. the current in case of electrochemical systems. The direct computation of this quantity is typically beyond the computational capacities even of large computer systems. Therefore, a reduction of the problem is necessary.

A possible mathematical simplification of the problem is done by using upscaled models for which so called cell problems have to be solved. Since this part of the model captures the microscopic effects, it needs appropriate numerical methods to describe the microscopic porous electrode microstructures. For the computation of effective diffusion coefficients on complex microstructures we show a 3D adaptive cut-cell implementation based on a level set method and a goal oriented error estimator. The mesh is refined only according to a "macroscopic" quantity of interest. In addition, we present an adaptive finite element method for an homogenized Newman-type battery model.

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