Simulating Lithium-Ion Batteries with Finite Elements

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In this talk we present the numerical treatment of a micro-scale model for Lithium-ion batteries.

The battery is partitioned into $\Omega = \Omega_{\mathrm{an}} \cup \Omega_{\mathrm{e}} \cup \Omega_{\mathrm{ca}}$. The subdomains are representing the anode electrode, the electrolyte and the cathode electrode respectively. The conservation equation for Lithium $\partial_t c = -\nabla \cdot \vec{N}$ and the equation for local charge neutrality $0 = \nabla \cdot \vec{j}$ are decoupled in the electrodes but due to the existence of positively charged Ions in the electrolyte those equations are coupled in this region.

The Li-concentration c and the electrical Potential Φ may have jumps over the interfaces separating electrodes from electrolyte but they are coupled via highly nonlinear Neumann conditions. Additionally suitable boundary conditions are imposed in order to model the discharge of the battery at a constant macroscopic current.

A discretization by implicit Euler in time and H^1-conforming finite elements on triangular meshes in space is presented. Especially the treatment of the nonlinear terms is discussed. The performance of the `Matlab` implementation is demonstrated.

Finally we present how we are planning to integrate other physical effects like two-phase particles, intercalation-induced stress and Joule-heating into the numerical simulation.

References:

[1] A. Latz, J. Zausch, and O. Iliev. Modeling of species and charge transport in li-ion batteries based on non-equilibrium thermodynamics. Technical Report 190, Fraunhofer (ITWM), 2010
[2] J. Newman and K. E. Thomas-Alyea. Electrochemical Systems. Wiley, 2004

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