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Reconstruction of State-Dependant Material Properties and Its Application in Electrochemical Systems

Outlining a computational approach to the solution of an inverse modelling problem concerning the material properties of electrolytes used in Lithium-ion batteries is the main theme of this presentation. The dependence of material properties on the concentration of Lithium ions is reconstructed based on the concentration data obtained from an in-situ NMR imaging experiment. This experiment is modelled by a 1D time-dependent PDE describing the evolution of the concentration of Lithium ions with prescribed initial concentration and fluxes at the boundary. The material properties that appear in this model are reconstructed by solving a variational optimization problem in which the least-square error between the experimental and simulated concentration values is minimized. This optimization problem is solved using an innovative gradient-based method in which the gradients are obtained with adjoint analysis. Steps to obtain gradients through adjoint analysis, validational studies on the computational framework for this reconstruction problem and reconstructed material properties of a lab-manufactured and a commercial battery electrolyte are presented with insights which complement available experimental results.