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COMPUTATIONAL HOMOGENIZATION FOR (LI-ION) BATTERY CELLS.

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The electrochemical and mechanical performance of (Li-ion) batteries strongly depends on the interaction between macro and micro-scale phenomena, in particular within the electrodes. Insertion and extraction of Lithium from electrodes in current commercial batteries take place in active particles, whose size is three order of magnitudes smaller than the battery cell scale. However, directly resolving all scales and modeling all particles in the electrodes is not computationally feasible, even for the largest computational facility available nowadays. Instead, the micro-scale effects are incorporated into the macro-scale problem through homogenization approaches and constitutive models that are derived from homogenization methods.

A multi-scale and multi-physics model of the phenomena that presiede the functioning of batteries is the concern of the present talk. Following recent publications [1], the computational homogenization technique is tailored to model the events that coexist during batteries charging and discharging cycles. At the macro-scale, diffusion-advection equations model the coupling between electrochemistry and mechanics in the whole cell. The multi-component porous electrode, migration, diffusion, and intercalation of Lithium in the active particles, the phase-segregation and swelling of the latter are modeled at the micro-scale. A rigorous thermodynamics setting is stated and scale transitions are formulated.

A novel model for lithiation in active particles [2] is coupled to a Maxwell's equations based formulation for the ionic motion in the (liquid) electrolyte. Image-based modeling techniques have been applied in order to reconstruction the porous electrode microstructure. High-performance computing implementations via Abaqus and deal.II have been carried out. Numerical simulations at the micro-scale will show the potential and the capability of the proposed formulation.

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