Simulation of Lithium-Ion Batteries with the Finite Element Method

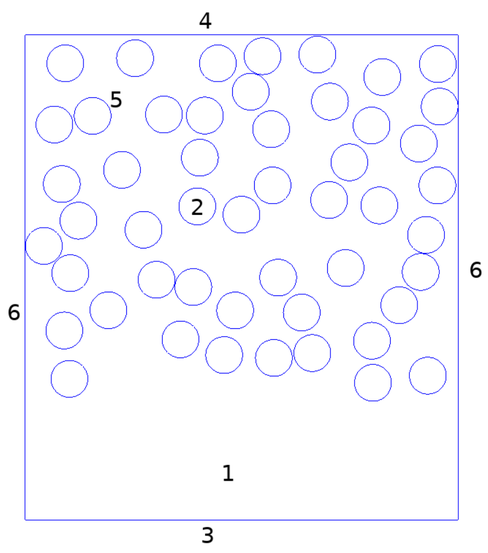
Introduction

- The goal of the project is to simulate the lithium concentration c_{Li} and electrical potential ϕ.
- Cathode particles ($\text{Li}_y\text{Mn}_2\text{O}_4$) submerged into electrolyte polymer matrix
- Solid anode (Li_xC_6) is not included in computational domain, since it is possible to solve for the concentration c_{Li} analytically there.
- Finite Element Method is used to deal with the irregular geometry

References

- C. M. Doyle.
  PhD thesis, University of California at Berkeley, Berkeley, CA, 1995.
- R.E. García, Y.-M. Chiang, W.C. Carter, P. Limthongkul, and C.M. Bishop.
  Microstructural modeling and design of rechargeable lithium-ion batteries.
  Journal of the Electrochemical Society, 152(1):A255–A263, 2005.

Model Domain



Cross section of battery separator and cathode.

1. Electrolyte
2. Electrode particles
3. Electrolyte/Anode interface
4. Positive ohmic contact interface
5. Electrolyte/Particle interface
6. Outer battery wall

Key Parts of Mathematical Model

- Time evolution of lithium concentration c_{Li}:

$$\frac{\partial c_{\text{Li}}}{\partial t} = \underbrace{\nabla \cdot (D_{\text{Li}} \nabla c_{\text{Li}})}_{\text{nonlinear diffusion}} + \underbrace{\nabla \cdot \left(\frac{D_{\text{Li}} z \mathcal{F}}{\mathcal{R} T} c_{\text{Li}} \nabla \phi \right)}_{\text{migration driven by potential gradient}}$$

- Electrical potential ϕ:

$$\underbrace{\frac{\partial \rho}{\partial t} = 0}_{\text{charge conservation}} = \nabla \cdot (\kappa \nabla \phi) + \underbrace{\nabla \cdot \left(\frac{D_{\text{Li}} z \mathcal{F}}{\mathcal{R} T} c_{\text{Li}} \nabla c_{\text{Li}} \right)}_{\text{potential due to Li-ions}}$$

- Partly linearized Butler-Volmer equation (on electrode surfaces):

$$\underbrace{-\kappa \frac{\partial \phi}{\partial \hat{n}}}_{\text{current density}} = \underbrace{i_0(c_{\text{Li}})}_{\text{nonlinear exchange current}} \frac{(\alpha_a + \alpha_c)\mathcal{F}}{\mathcal{R} T} \underbrace{\eta(c_{\text{Li}}, \phi)}_{\text{nonlinear surface overpotential}}$$

Implementation

- Implementation in Netgen/NGSolve `ngsolve.org`
- Description of variational formulation via a Python interface
- Linear Lagrange elements for space discretization
- Crank-Nicholson method for time evolution
- Damped Newton-Raphson method to treat nonlinear relations in each time step
- Separate solving on each domain
- Coupling via interface conditions

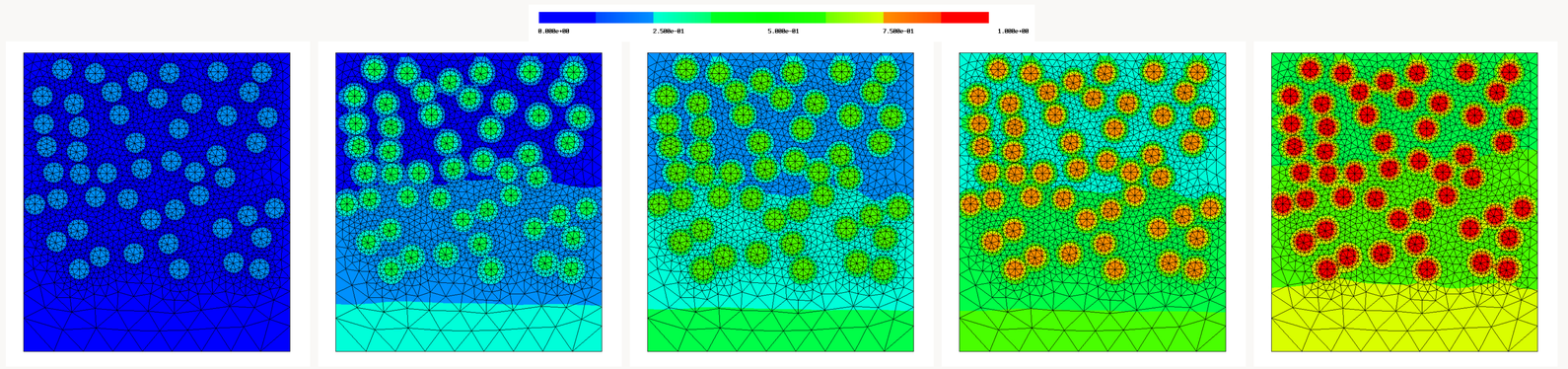
Current Status

- Concentration only
- Partly nonlinear particle/electrolyte interface conditions

Further Work

- Combine potential and concentration model
- Nonlinear diffusivity coefficients
- Nonlinear boundary conditions for anode/electrolyte interface

Results



(a) 0s **(b)** 10s **(c)** 20s **(d)** 30s **(e)** 40s

Figure: Time evolution of lithium concentration c_{Li} (normalized to lithium solubility limit in cathode particles)

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