A fast solver for a Lithium-Ion battery electrode model

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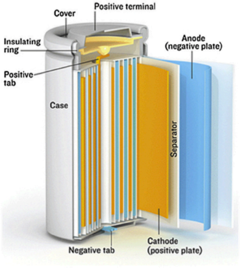
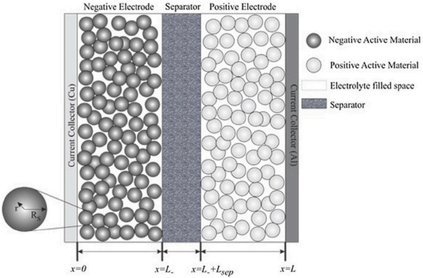
Overview

- Battery Basics
- Pseudo 2D Model
  - Fuller, Doyle, and Newman (1994)
  - Scaled model (with Moyles, Myers, and Hennessey)
- Computational Results
- Fast Solver

Lithium Ion Batteries

Open up the Battery

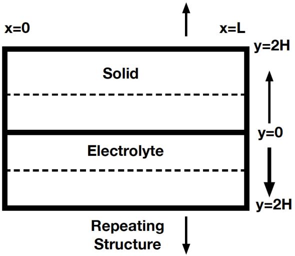




- Negative Electrode: Graphite
- Positive Electrode: Lithium Cobalt Oxide or Lithium Iron Phosphate
- Intercalation: Energetically favourable in the positive electrode
- Electrolyte: Lithium salt in an organic solvent

Pseudo Two Dimensional (P2D) Model

Single Electrode Domain



Solid: intercalated Lithium $c(y, t; x)$ P2D,
potential $\psi(t)$ high solid conductivity
Electrolyte: ionic concentration $u(x, t)$,
potential $\phi(x, t)$
Interface: Flux $j(x, t)$ of Li^+ ions into solid

P2D Model

Ingredients and Scaling

- Intercalated flux $-D_c c_y$.
- Dilute electrolyte flux $-D_u u_x \pm \frac{FD_u}{RT} u\phi_x$.

Scaling:

- Scale x by L, y by H
- Scale ψ and ϕ by RT/F $(RT/F \approx 0.01)$
- Scale c by $c_{\max}$, u by u_{eq}
- Scale t by H^2/D_c, j by $D_c c_{\max}/H$
- $\epsilon = H/L \ll 1$ One ingredient for P2D model structure

P2D Model

Scaling

- Consider current density I for battery operation
- Diffusive flux in the solid $-D_c c_y$ (unscaled) gives a current limit of order

$$I_1 = \frac{FLD_c c_{\max}}{2H^2}$$

- Diffusive flux in the electrolyte gives a current limit of order

$$I_2 = \frac{FD_u u_{eq}}{2L}$$

- Current not limited by surface flux or electrolyte resistance
- P2D scaling: I, I_1 and I_2 have roughly the same magnitude
- Dimensionless parameters:
    - $I/I_1 := \mathcal{I}$
    - $I/I_2 := \mathcal{I}_*$
    - $I_2/I_1 = \mathcal{I}/\mathcal{I}_* = \epsilon^2 \frac{D_u u_{\mathrm{eq}}}{D_c c_{\max}} := \mathcal{D}$

P2D Model

Scaled Asymptotic Equations

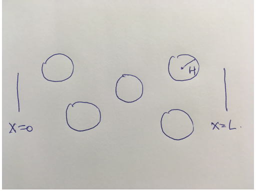
$$I_1 = \frac{FLD_c c_{\max}}{2H^2}, \quad I_2 = \frac{FD_u u_{eq}}{2L}$$
$$I_2/I_1 := \mathcal{D}, \quad I/I_1 := \mathcal{I}$$

$$\begin{aligned}
c_t &= c_{yy} \text{ with } c_y\,|_{y=1} = 0, \quad c_y\,|_{y=0} = j \\
\mathcal{D}u_{xx} &= j/2 \text{ with } \int_0^1 u(x)dx = 1, u_x\,|_{x=0} = 0 \quad ! \\
\mathcal{D}(u\phi_x)_x &= j/2 \text{ with } \phi_x\,|_{x=0} = 0, \quad \phi\,|_{x=1} = 0 \\
j &= R\sqrt{uc(1-c)} \ \exp\{-\psi + \phi\} \text{ with } \int_0^1 j(x)dx = \mathcal{I}
\end{aligned}$$

- If $I \ll \min\{I_1, I_2\}$ then equivalent circuit model Moyles.
- If $\mathcal{D}$ large, then single particle model.
- If $\mathcal{D}$ small, electrolyte only model.
- Otherwise, P2D model is appropriate.

P2D Model

Spherical Particles



Considering spherical particles of radius H with 50% volume fraction, change

$$c_t = c_{yy} \text{ with } c_y\,|_{y=1} = 0, \quad c_y\,|_{y=0} = j$$

to

$$c_t = \frac{1}{r^2}(r^2 c_r)_r \text{ with } c_r\,|_{r=0} = 0, \quad c_r\,|_{r=1} = j/3.$$

D_u should include tortuousity effects.

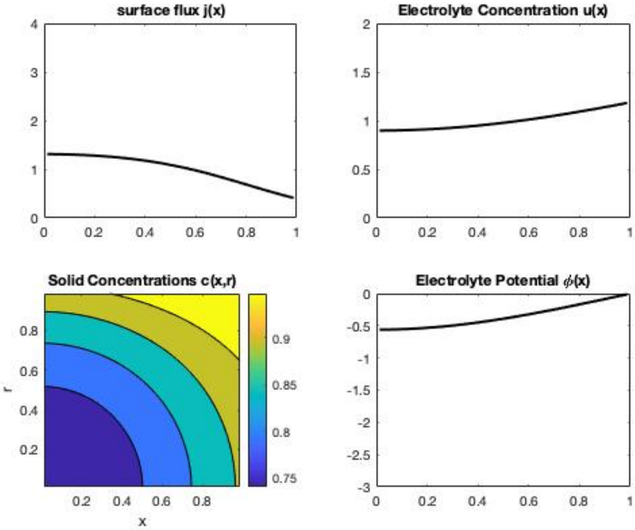
Computations

Implemented the P2D model in MATLAB:

- Cell-centred finite difference method in x and r
- Implicit time stepping (Backward Euler)
- Newton iterations for the resulting nonlinear problems

Computations

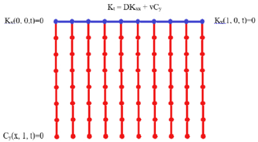
$\mathcal{I} = 1$ and $\mathcal{I}_* = 1$ ($\mathcal{D} = 1$)



Eliminating c from the Jacobian matrix

The Idea

Note coupling only at one end in y (r):



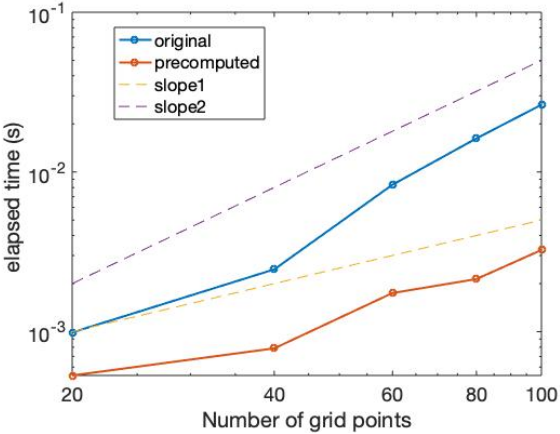
$$
\begin{aligned}
(c - c^n)/k &= c_{yy} \text{ with } c_y\,|_{y=1} = 0, \quad c_y\,|_{y=0} = j \\
j &= R\sqrt{uc(1-c)}\ \exp\{-\psi + \phi\} \text{ with } \int_0^1 j(x)dx = \mathcal{I}
\end{aligned}
$$

$c(0)$ in the expression for j can be found in terms of c^n separately at each x (with a tridiagonal solve in the discrete case).

$O(N)$ unknowns for the channel problem, reduction from $O(N^2)$.

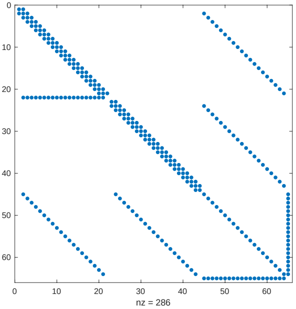
Eliminating c from the Jacobian matrix

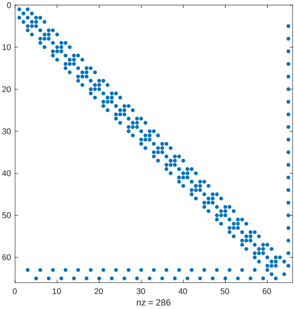
The Speed-Up



Electrolyte Problem Reordering

The Idea

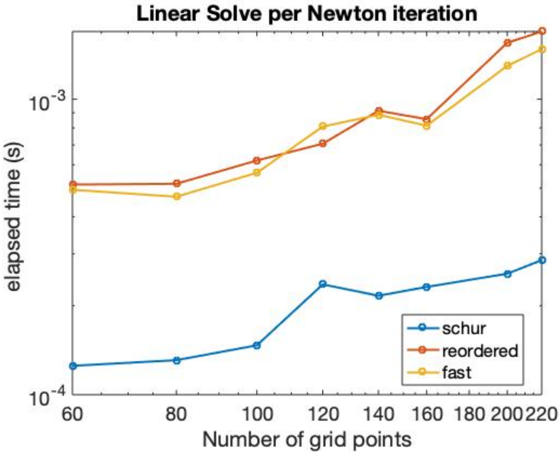




Reorder unknowns, use a Schur complement to reduce the problem to banded solves.

Electrolyte Problem Reordering

The Speed-Up



Summary

- Rechargeable Lithium Ion Battery basics
- Scaled P2D model and Computational results
- Fast solver for P2D model suitable for real time control:
  - Eliminate c variables from the channel problem
  - Reorder the channel variables, Shur complement to banded solves
- Next steps:
  - Adaptive time stepping
  - Implement for “real” model with two electrodes and separator