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MULTIBAT

Reduced Order Modelling of Lithium-Ion Battery Models with Resolved Electrode Geometry

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Gent
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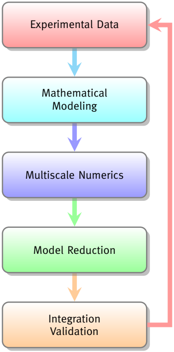
The MULTIBAT Project



- Understand degradation processes in rechargeable Li-Ion Batteries through mathematical modeling and simulation.
- Focus: Li-Plating.

Challenge

Li-plating is initiated at interface between active particles and electrolyte.

$\Rightarrow$ Need pore-scale models which resolve active particle geometry.

$\Rightarrow$ Huge nonlinear discretizations.

- Cannot be solved at cell scale on current hardware.
- **Parameter studies extremely expensive, even on small domains.**

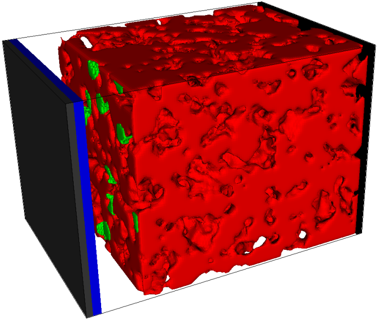
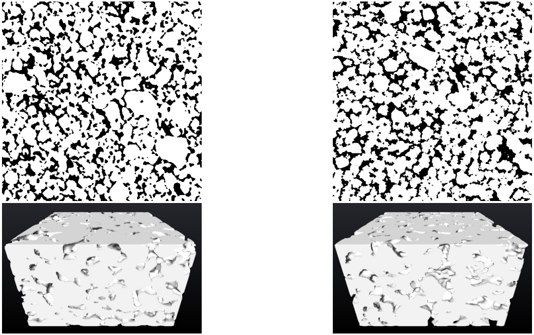


Figure: Simulation of half-cell geometry with plated lithium (green) on $65.6\mu m \times 44\mu m \times 44\mu m$ domain.

Imaging and Stochastic Structure Modeling

Feinauer, Schmidt, Westhoff (Ulm, Accumotive)



- Visual comparison of 2D and 3D cut-outs of experimental data (left) and simulated (right) shows good agreement.

Microscale Modeling

Hein, Latz (DLR at Helmholtz Institute Ulm)

Variables:

c : Li^+ concentration ϕ : electrical potential

Electrolyte:

$$\frac{\partial c}{\partial t} - \nabla \cdot (D_e \nabla c) = 0$$
$$-\nabla \cdot (\kappa \frac{1 - t_+}{F} RT \frac{1}{c} \nabla c - \kappa \nabla \phi) = 0$$

Electrodes:

$$\frac{\partial c}{\partial t} - \nabla \cdot (D_s \nabla c) = 0$$
$$-\nabla \cdot (\sigma \nabla \phi) = 0$$

Coupling: Normal fluxes at interfaces given by Butler-Volmer kinetics

$$j_{inter} = 2k\sqrt{c_e c_s (c_{max} - c_s)} \sinh\left(\frac{\eta}{2RT} \cdot F\right) \qquad \eta = \phi_s - \phi_e - U_0(\frac{c_s}{c_{max}})$$
$$N_{inter} = \frac{1}{F} \cdot j_{inter}$$

Microscale Modeling – Lithium Plating

Hein, Latz (DLR at Helmholtz Institute Ulm)

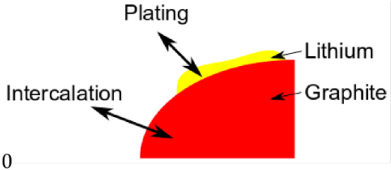
Two possible reaction at negative electrode (Graphite):

- Intercalation $\mathrm{Li}^{+}_{\mathrm{Electrolyte}} + \mathrm{e}^{-}_{\mathrm{Solid}} \rightleftharpoons \mathrm{LiC}_{6,\mathrm{Solid}}$
- Lithium plating $\mathrm{Li}^{+}_{\mathrm{Electrolyte}} + \mathrm{e}^{-}_{\mathrm{Solid}} \rightleftharpoons \mathrm{Li}^{\Theta}_{\mathrm{Solid}}$

Overpotential with lithium reference:

- $\eta_{\mathrm{i}} = \Phi_{\mathrm{Solid}} - \varphi^{\mathrm{Li}^+}_{\mathrm{Electrolyte}} - U_0(c_{\mathrm{Solid}})$
- $\eta_{\mathrm{p}} = \Phi_{\mathrm{Solid}} - \varphi^{\mathrm{Li}^+}_{\mathrm{Electrolyte}}$

Lithium plating if $\eta_{\mathrm{p}} \leq 0$ $\quad \eta_{\mathrm{i}} + U_0(c_{\mathrm{So}}) \leq 0$



Active material and Electrolyte

$$i_{\mathrm{Inter}} = i_{\mathrm{I},0}\left(\exp\left[\frac{F}{2RT}\eta_i\right] - \exp\left[-\frac{F}{2RT}\eta_i\right]\right)$$

$$i_{\mathrm{I},0} = i_{\mathrm{I},00} \cdot \sqrt{c_{\mathrm{E}} \cdot c_{\mathrm{S}} \cdot \left(c_{\mathrm{S}}^{\max} - c_{\mathrm{S}}\right)}$$

Plated Lithium and Electrolyte

$$i_{\mathrm{Li}} = i_{\mathrm{Li},0}\left(\exp\left[\frac{F}{2RT}\eta_{\mathrm{Li}}\right] - \exp\left[-\frac{F}{2RT}\eta_{\mathrm{Li}}\right]\right)$$

$$i_{\mathrm{Li},0} = i_{\mathrm{Li},00} \cdot \sqrt{c_E}$$

Discretization

Iliev, Schmidt, Zausch (Fraunhofer ITWM)

Cell centered **Finite Volume** discretization on voxel grid + **implicit Euler** leads to nonlinear equation systems of the form:

Full Order Model

Find $[c_\mu^{(n)}, \phi_\mu^{(n)}] \in V_h \oplus V_h =: V$ such that

$$\begin{bmatrix} \frac{1}{\Delta t}(c_\mu^{(n+1)} - c_\mu^{(n)}) \\ 0 \end{bmatrix} + A_\mu\left(\begin{bmatrix} c_\mu^{(n+1)} \\ \phi_\mu^{(n+1)} \end{bmatrix}\right) = 0, \qquad c_\mu^{(0)} = c_{\mu,0}.$$

- Numerical fluxes on interfaces = Butler-Volmer fluxes.
- Newton scheme with algebraic multigrid solver.
- Implemented by Fraunhofer ITWM in BEST.
- $\mu \in \mathcal{P}$ indicates dependence on model parameters (e.g. temperature T, charge rate).

Reduced Basis Approximation

Ohlberger, R

Reduced Order Model

Find $[\tilde{c}_\mu^{(n)}, \tilde{\phi}_\mu^{(n)}] \in \tilde{V}_c \oplus \tilde{V}_\phi =: \tilde{V}$ solving projected equation

$$\begin{bmatrix} \frac{1}{\Delta t}(\tilde{c}_\mu^{(n+1)} - \tilde{c}_\mu^{(n)}) \\ 0 \end{bmatrix} + \{P_{\tilde{V}} \circ A_\mu\} \left(\begin{bmatrix} \tilde{c}_\mu^{(n+1)} \\ \tilde{\phi}_\mu^{(n+1)} \end{bmatrix} \right) = 0, \qquad \tilde{c}_\mu^{(0)} = P_{\tilde{V}_c}(c_{\mu,0}).$$

- **Basis generation:** POD of a priori selected solution trajectories, separately for c and ϕ (different scales).
- **POD (=Proper Orthogonal Decomposition):** truncated singular value decomposition of snapshot matrix (a.k.a. principal component analysis)
- **Future:**
  - efficient a posteriori error bound $\longrightarrow$ POD-Greedy
  - localized MOR ($\longrightarrow$ LRBMS, ArbiLoMod)

Empirical Operator Interpolation (a.k.a. DEIM, EIM)

Problem: Still expensive to evaluate

$$P_{\tilde{V}} \circ A_\mu : \tilde{V} \longrightarrow V \longrightarrow \tilde{V}.$$

Solution:

- Use locality of finite volume operators:

  to evaluate M DOFs of $A_\mu([c,\phi])$ wee need $M' \leq C \cdot M$ DOFs of $[c,\phi]$.

- Approximate

$$A_\mu \approx \mathcal{I}_M[A_\mu] := I_M \circ \tilde{A}_{M,\mu} \circ R_{M'},$$

where

$R_{M'}: V \to \mathbb{R}^{M'}$	restriction to M' DOFs needed for evaluation
$\tilde{A}_{M,\mu}: \mathbb{R}^{M'} \to \mathbb{R}^M$	A_μ restricted to M interpolation DOFs
$I_M: \mathbb{R}^M \to V$	linear combination with interpolation basis

Empirical Operator Interpolation (2)

Empirical Operator Interpolation

Given M interpolation DOFs (magic points) and corresponding interpolation basis, approximate:

$$A_\mu \approx \mathcal{I}_M[A_\mu] := I_M \circ \tilde{A}_{M,\mu} \circ R_{M'}.$$

Basis Generation:

- Compute operator evaluations on solution snapshots (including Newton stages).
- Iteratively extend interpolation basis with worst-approximated evaluation. Choose new interpolation DOF where new vector is maximal (**EI-GREEDY**).
- Interpolate Butler-Volmer part of A_μ and $1/c \cdot \nabla c$ separately (ϕ-part of A_μ vanishes for solutions).
- Future: Build RB and interpolation basis simultaneously using error estimator to select snapshots (POD-EI-GREEDY).

Full Reduction

Reduced Order Model with EI

Find $[\tilde{c}_\mu^{(n)}, \tilde{\phi}_\mu^{(n)}] \in \tilde{V}_c \oplus \tilde{V}_\phi = \tilde{V}$ solving projected equation

$$\begin{bmatrix} \frac{1}{\Delta t}(\tilde{c}_\mu^{(n+1)} - \tilde{c}_\mu^{(n)}) \\ 0 \end{bmatrix} + \left\{ (P_{\tilde{V}} \circ I_M) \circ \tilde{A}_{M,\mu} \circ R_{M'} \right\} \left(\begin{bmatrix} \tilde{c}_\mu^{(n+1)} \\ \tilde{\phi}_\mu^{(n+1)} \end{bmatrix} \right) = 0, \quad \tilde{c}_\mu^{(0)} = P_{\tilde{V}_c}(c_{\mu,0}).$$

Offline/Online decomposition

- Precompute the linear operators $P_{\tilde{V}} \circ I_M$ and $R_{M'}$ w.r.t. basis of $\tilde{V}$.
- Effort to evaluate $(P_{\tilde{V}} \circ I_M) \circ \tilde{A}_{M,\mu} \circ R_{M'}$ w.r.t. this basis:

$$\mathcal{O}(NM) + \mathcal{O}(M) + \mathcal{O}(CMN),$$

where $N := \dim \tilde{V}$.

Numerical Results

Model:

- Half-cell with plated Li
- μ = discharge current
- 2.920.000 DOFs

Reduction:

- Snapshots: 3
- $N = 98 + 47$
- $M = 710 + 774$
- Rel. err.: $< 1.5 \cdot 10^{-3}$

Timings:

- Full model: $\approx$ 13h
- Projection: $\approx$ 9h
- Red. model: $\approx$ 5m
- Speedup: **154**

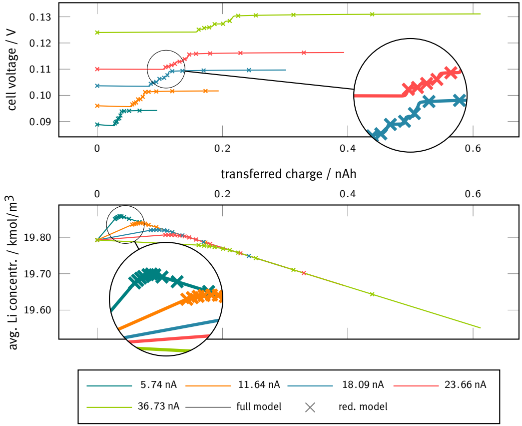


Figure: Validation of reduced order model output for random discharge currents; solid lines: full order model, markers: reduced order model.

Outlook: Localized RB Approximation

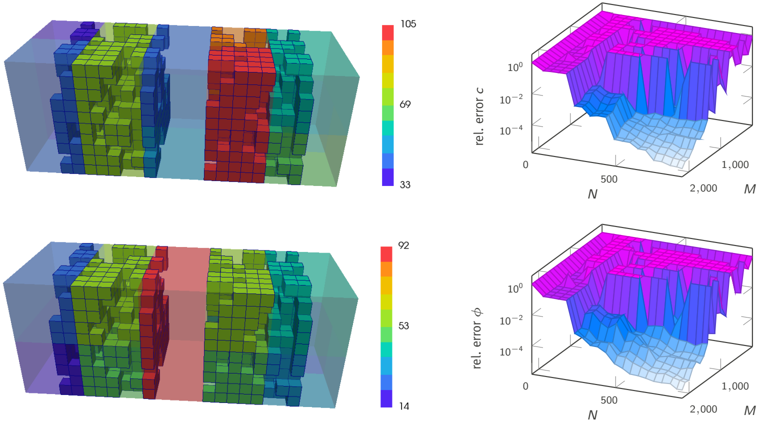
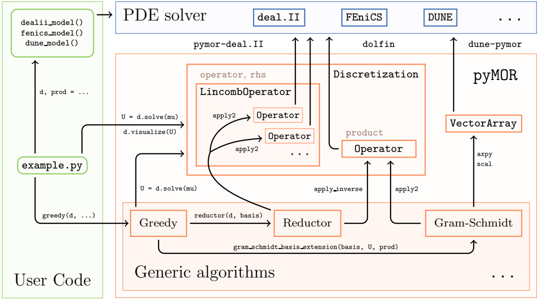


Figure: First experiments on small battery geometry; left: local RB dimensions, right: error for varying N, M; top: Li-concentration c, bottom: electrical potential ϕ.

pyMOR – Model Order Reduction with Python



- Quick prototyping with Python.
- Seamless integration with high-performance PDE solvers including FEniCS, deal.II, NGSolve, DUNE.
- Out of box MPI support for reduction algs. and PDE solvers.
- BSD-licensed, fork us on Github!

Thank you for your attention!

MULTIBAT: Unified Workflow for fast electrochemical 3D simulations of lithium-ion cells combining virtual stochastic microstructures, electrochemical degradation models and model order reduction
arXiv:1704.04139, 2017.

Localized Reduced Basis Approximation of a Nonlinear Finite Volume Battery Model with Resolved Electrode Geometry.
In: Model Reduction of Parametrized Systems, Springer, 2017.

pyMOR – Generic Algorithms and Interfaces for Model Order Reduction
SIAM J. Sci. Comput., 38(5), 2016.
`http://www.pymor.org/`

My homepage
`http://stephanrave.de/`