Efficient Reduced Order Simulation of Pore-Scale Lithium-Ion Battery Models

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The MULTIBAT Project

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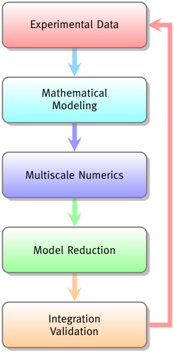


- Understand degradation processes in rechargeable Li-Ion Batteries through mathematical modeling and simulation.
- Focus: Li-Plating.

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.**

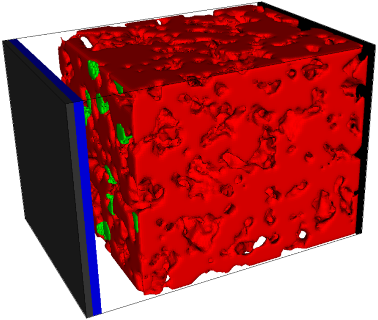
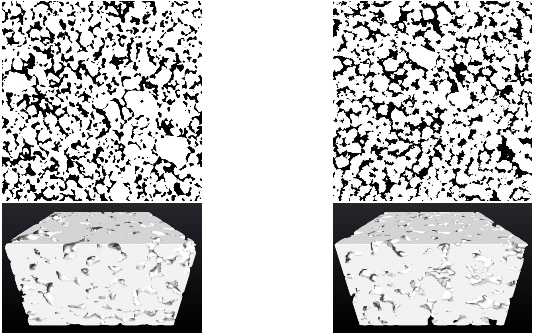


Figure: Simulation of half-cell geometry with plated lithium (green) on $65.6\mu m \times 44\mu m \times 44\mu m$ domain.

Stochastic Structure Modeling [Feinauer, Schmidt, Westhoff (Ulm)]



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

Microscale Modeling [Hein, Latz (HIU)]

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

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

Microscale Modeling – Lithium Plating

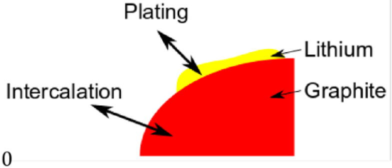
Two possible reaction at negative electrode (Graphite):

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

Overpotential with lithium reference:

- $\eta_i = \Phi_{Solid} - \varphi^{Li^+}_{Electrolyte} - U_0(c_{Solid})$
- $\eta_p = \Phi_{Solid} - \varphi^{Li^+}_{Electrolyte}$

Lithium plating if $\eta_p \leq 0$ $\quad \eta_i + U_0(c_{So}) \leq 0$



Active material and Electrolyte

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

$$i_{I,0} = i_{I,00} \cdot \sqrt{c_E \cdot c_S \cdot (c_S^{max} - c_S)}$$

Plated Lithium and Electrolyte

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

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

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

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

- 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 (Münster)]

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

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

- **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)
- **More advanced:** Use greedy search to select snapshot parameters.

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).
- More advanced: 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
- $\mu =$ discharge current
- 2.920.000 DOFs

Reduction:

- Snapshots: 3
- $N = 178 + 67$
- $M = 924 + 997$
- Rel. err.: $< 4.5 \cdot 10^{-3}$

Timings:

- Full model: $\approx$ 15.5h
- Projection: $\approx$ 14h
- Red. model: $\approx$ 8m
- Speedup: **120**

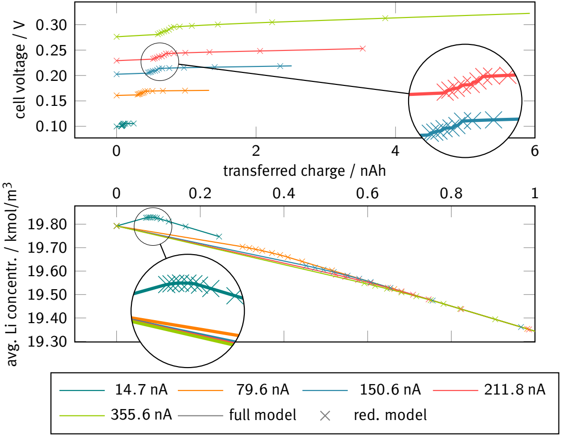


Figure: Validation of reduced order model output for random discharge currents; solid lines: full order model, markers: reduced order model.

Semi-Heuristic Error Estimate [Hain, Ohlberger, Radic, Urban, 2018]

Idea: Use extended ROM as surrogate for FOM solution:

$$[\hat{c}_\mu^n, \hat{\varphi}_\mu^{(n)}] \in \hat{V}_c \oplus \hat{V}_\varphi \supset \tilde{V}_c \oplus \tilde{V}_\varphi$$

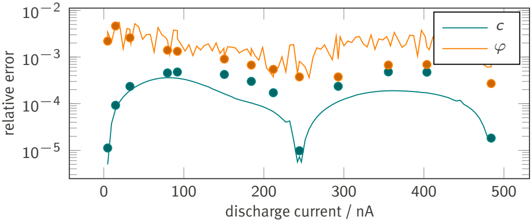
Saturation Assumtion:

$$\|\hat{c}_\mu^{(n)} - c_\mu^{(n)}\| \leq \Theta \cdot \|\tilde{c}_\mu^{(n)} - c_\mu^{(n)}\|, \qquad \|\hat{\varphi}_\mu^{(n)} - \varphi_\mu^{(n)}\| \leq \Theta \cdot \|\tilde{\varphi}_\mu^{(n)} - \varphi_\mu^{(n)}\|$$

Error Estimate:

$$\|\tilde{c}_\mu^{(n)} - c_\mu^{(n)}\| \leq \frac{1}{1-\Theta} \cdot \|\tilde{c}_\mu^{(n)} - \hat{c}_\mu^{(n)}\|, \quad \|\tilde{\varphi}_\mu^{(n)} - \varphi_\mu^{(n)}\| \leq \frac{1}{1-\Theta} \cdot \|\tilde{\varphi}_\mu^{(n)} - \hat{\varphi}_\mu^{(n)}\|$$

- $\hat{N} - N = 28 + 30$
- $\Theta := 0$
- max rel overest:
  1.08 / 3.46
- min rel underest:
  2.89 / 1.45



Outlook: Localized RB Approximation

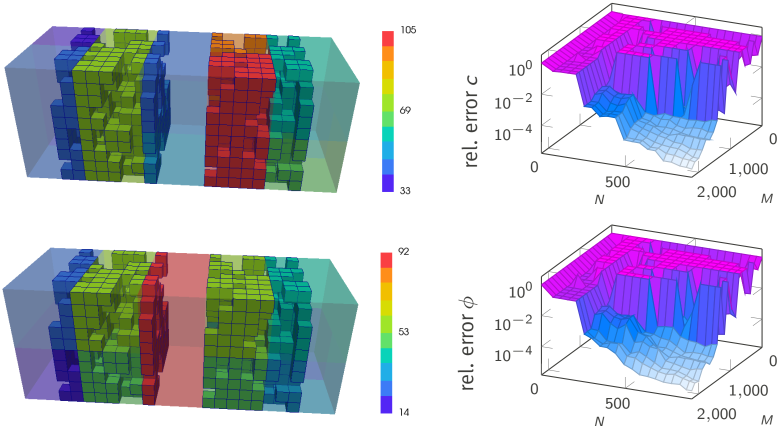
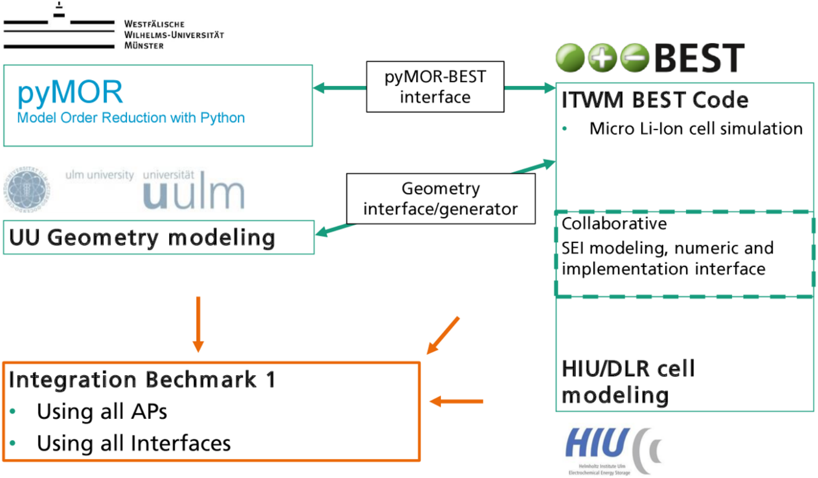


Figure: First experiments on small battery geometry; left: local RB dimensions, right: error for varying N, M; top: Li-concentration c, bottom: electrical potential ϕ.

Software Interfaces in MULTIBAT



Software Interfaces in MULTIBAT

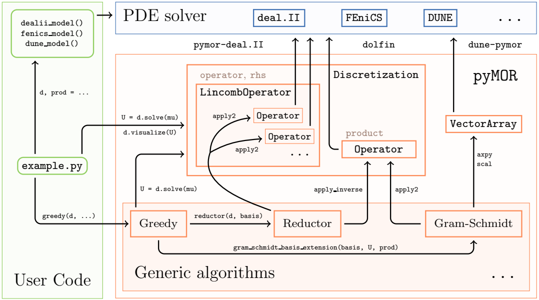
Interfaces allow us to:

- easily exchange Dune solver with BEST.
- independently develop MOR algorithms.
- easily apply MOR algorithms to updated models in BEST.
- reuse MOR algorithms for other problems.

Integration Bechmark 1
- Using all APs
- Using all Interfaces

modeling

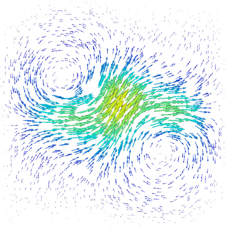
pyMOR – Model Order Reduction with Python



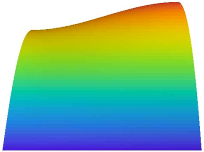
- Quick prototyping with Python.
- Seamless integration with high-performance PDE solvers.
- Out of box MPI support for reduction algs. and PDE solvers.
- BSD-licensed, fork us on Github!

pyMOR – Some More Applications

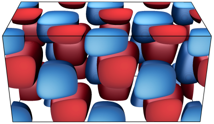
Linear elasticity
(deal.II)



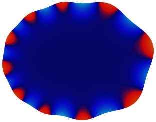
Nonlinear diffusion
(FEniCS)



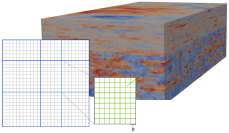
MPI distributed transport
problem (DUNE)



Free boundary problem
(NGSolve)



Localized RB Multiscale
Method (DUNE)



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
J. Comp. Sci., 2018.

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/`

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