A Model Reduction Framework for Efficient Simulation of Li-Ion Batteries

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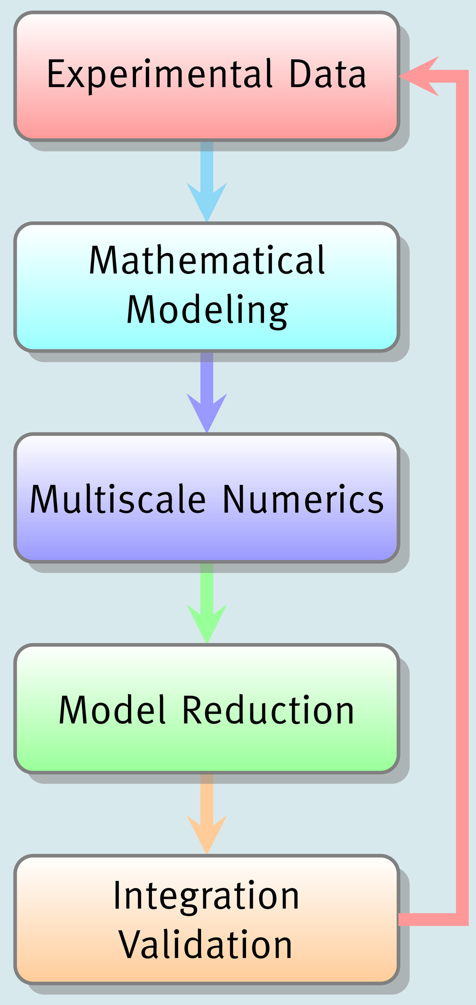
The MULTIBAT Project

A major cause for the failure of rechargeable lithium-ion batteries is the deposition of metallic lithium at the negative battery electrode (**Li-plating**). Once established, this metallic phase can grow in the form of dendrites to the positive electrode, ultimately short-circuiting the cell. As Li-plating is initiated at the interface between active electrode particles and the electrolyte, understanding of this phenomenon is only gained through physical models accounting for effects on the **micrometer-scale**.

Microscale models, however, require highly resolved meshes in the model discretization, leading to computationally expensive **high-dimensional**, **non-linear** discrete problems. Thus, it is desirable to combine microscale modeling with **model order reduction** strategies which are able to reduce the computation time while at the same time keeping the microscopic features of the model.



The goal of the **MULTIBAT** project is to develop

- stochastic electrode geometries based on tomography data (provided by industry partner Deutsche ACCUmotive).
- microscale models of cell dynamics including Li-plating.
- multiscale schemes for numerical simulation.
- **model order reduction methods for resulting discrete problems.**
- **simulation software integrating developed models and algorithms.**

Project Partners

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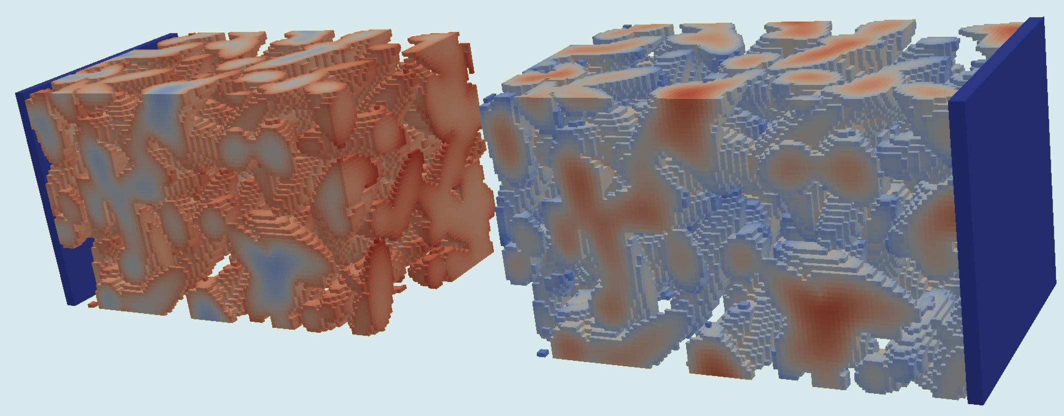
Microscale Battery Model [1]



Simulation of microscale model with DUNE-MULTIBAT. Coloring indicates Li^+ concentration

Governing Equations

On each subdomain (anode, cathode, electrolyte):

$$\frac{\partial c}{\partial t} - \nabla \cdot (\alpha(c,\phi)\nabla c + \beta(c,\phi)\nabla\phi) = 0$$

$$-\nabla \cdot (\gamma(c,\phi)\nabla c + \delta(c,\phi)\nabla\phi) = 0$$

(c: Li^+ concentration, ϕ: electric potential)

Butler-Volmer kinetics at electrode/electrolyte interface

Electric current density j at interface:

$$2k\sqrt{c_e c_s (c_{max} - c_s)} \sinh\left(\frac{\phi_s - \phi_e - U_0(\frac{c_s}{c_{max}})}{2RT} \cdot F\right)$$

Li^+ flux at interface: $\frac{1}{F} \cdot j$

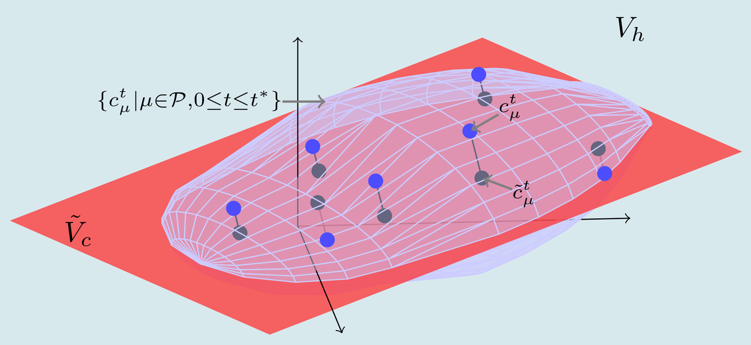
Discretization

The microscale model is discretized by a cell-centered finite volume scheme, incorporating interface conditions into the numerical flux [2]. Implicit Euler time-stepping leads to

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

with $c_\mu^{(t)}, \phi_\mu^{(t)} \in V_h$. μ indicates parameter dependence (e.g. temperature, charge rate).

Reduced Basis Projection



In a preparatory **Offline-Phase**, reduced spaces $\tilde{V}_c, \tilde{V}_\phi \subseteq V_h$ are computed from solutions of $(*)$ for selected parameters $\mu \in \mathcal{P}$. In the **Online-Phase**, reduced solutions can then be computed quickly for arbitrary new parameters via Galerkin projection onto $\tilde{V}_c, \tilde{V}_\phi$.

Online-Phase

Compute reduced solution by solving projected equations

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

for $\tilde{c}_\mu^{(t)} \in \tilde{V}_c, \tilde{\phi}_\mu^{(t)} \in \tilde{V}_\phi, \tilde{V} = \tilde{V}_c \oplus \tilde{V}_\phi$

(Use empirical interpolation [3] to quickly evaluate $P_{\tilde{V}} \circ A_\mu$.)

Offline-Phase

Build $\tilde{V}_c, \tilde{V}_\phi$ using iterative greedy algorithm:

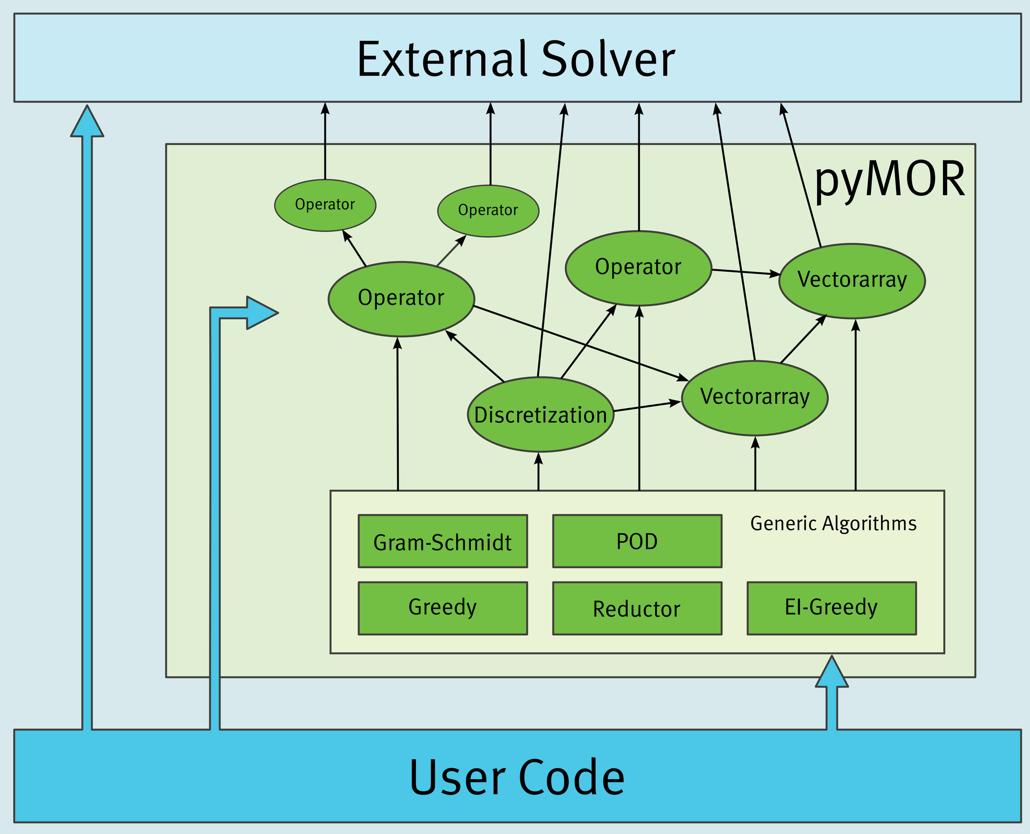
function GREEDY($\mathcal{S}_{train} \subset \mathcal{P}$, ε, $\tilde{V}_c^0$, $\tilde{V}_\phi^0$)
  $\tilde{V}_c, \tilde{V}_\phi \leftarrow \tilde{V}_c^0, \tilde{V}_\phi^0$
  while $\max_{\mu \in \mathcal{S}_{train}}$ ERR-EST(RB-SOLVE(μ), μ) $> \varepsilon$ **do**
    $\mu^* \leftarrow \arg\max_{\mu \in \mathcal{S}_{train}}$ ERR-EST(RB-SOLVE(μ), μ)
    $\tilde{V}_c, \tilde{V}_\phi \leftarrow$ BASIS-EXT($\tilde{V}_c, \tilde{V}_\phi$, SOLVE($\mu^*$))
  return $\tilde{V}_c, \tilde{V}_\phi$

pyMOR – Model Order Reduction with Python

pyMOR is a software library developed at the University of Münster for building model order reduction applications with the Python programming language.

Features

- Modern, object oriented design.
- Completely open source (BSD-licensed).
- Simple abstract interfaces for easy integration with external PDE solvers.
- All algorithms generic in terms of these interfaces:
  - RB-projection of arbitrary operators supporting nested affine decompositions
  - empirical interpolation of arbitrary operators
  - basis generation
  - orthonormalization algorithms, time-stepping, ...
- NumPy/SciPy-based discretizations for getting started easily.
- Adds interactive Python shell to your solver.



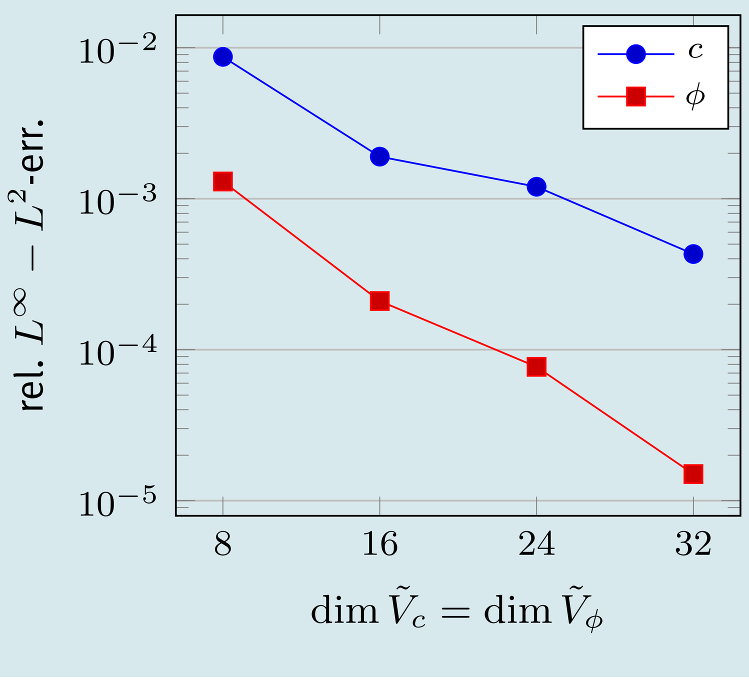
External Solvers

BEST	Battery simulation software developed at Fraunhofer ITWM (pyMOR bindings currently under development).
Dune–MULTIBAT	Prototype implementation of battery model based on the DUNE [4] numerics environment (pyMOR bindings fully functional).
Dune–pyMOR	Generic interface classes for DUNE-based solvers.

Add your solver!

http://www.pymor.org

Numerical Results



To explore the potential of the Reduced Basis Method for microscale battery simulations, the quality of the RB-projection was evaluated with pyMOR and DUNE-MULTIBAT for a small 3D test problem with porous electrode geometry. We observed rapid error decay w.r.t. the dimensions of the reduced spaces $\tilde{V}_c, \tilde{V}_\phi$ (see figure).

- Domain: $48\mu m \times 24\mu m \times 24\mu m$
- Grid: $40 \times 20 \times 20$
- Time-stepping: 20 steps of $30s$
- Charge rate: $[10^{-4}, 10^{-3}]A/cm^2$
- Temperature: $[250, 350]K$

- $\mathcal{S}_{train}$: 3×3 equidistant params
- Errors estimation: 20 random params
- ERR-EST: True error
- BASIS-EXT: POD of projection error trajectories [3]

References

[1] Latz, A., Zausch, J.: Thermodynamic consistent transport theory of li-ion batteries. Journal of Power Sources **196**(6), 3296 – 3302 (2011)

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[3] Drohmann, M., Haasdonk, B., Ohlberger, M.: Reduced basis approximation for nonlinear parametrized evolution equations based on empirical operator interpolation. SIAM J. Sci. Comput. **34**(2), A937–A969 (2012)

[4] Bastian, P., Blatt, M., Dedner, A., Engwer, C., Klöfkorn, R., Ohlberger, M., Sander, O.: A Generic Grid Interface for Parallel and Adaptive Scientific Computing. Part I: Abstract Framework. Computing **82**(2–3), 103–119 (2008)

http://www.uni-muenster.de/math/num/ag_ohlberger

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