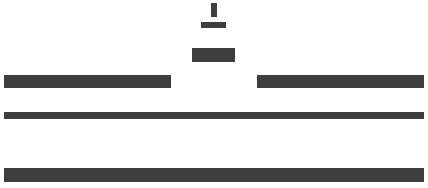

Westfälische
Wilhelms-Universität
Münster

A Modularized Modeling, Discretization and Model Order Reduction Workflow

for the Simulation of Li-ion Batteries

living.knowledge
WWU Münster

M. Ohlberger,
S. Rave, S. Schmidt

MoRePaS III
Trieste
October 15, 2015

Outline

- The MULTIBAT Project
- Reduction of Microscale Battery Models
- Software Implementation

The MULTIBAT Project

ulm university universität ulm

DLR Institute of Technical Thermodynamics

MULTIBAT

SPONSORED BY THE
Federal Ministry of Education and Research

Fraunhofer ITWM

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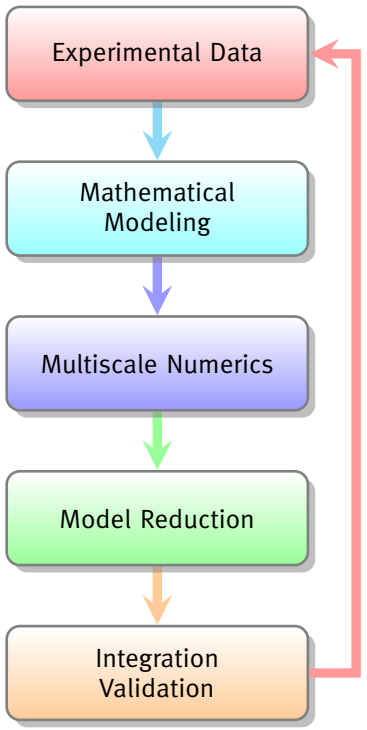


- Understand degradation processes in rechargeable Li-Ion Batteries through mathematical modeling and simulation.
- Focus: Li-Plating.

Problem Setting

- Li-plating initiated at interface between active particles and electrolyte.
- Need microscale models which resolve active particle geometry.
- Huge nonlinear discrete models.
  - Cannot be solved at cell scale on current hardware.
  - **Parameter studies extremely expensive, even on small domains.**

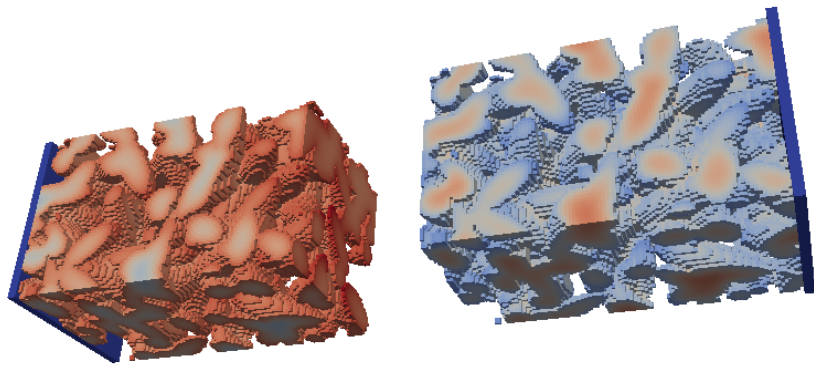
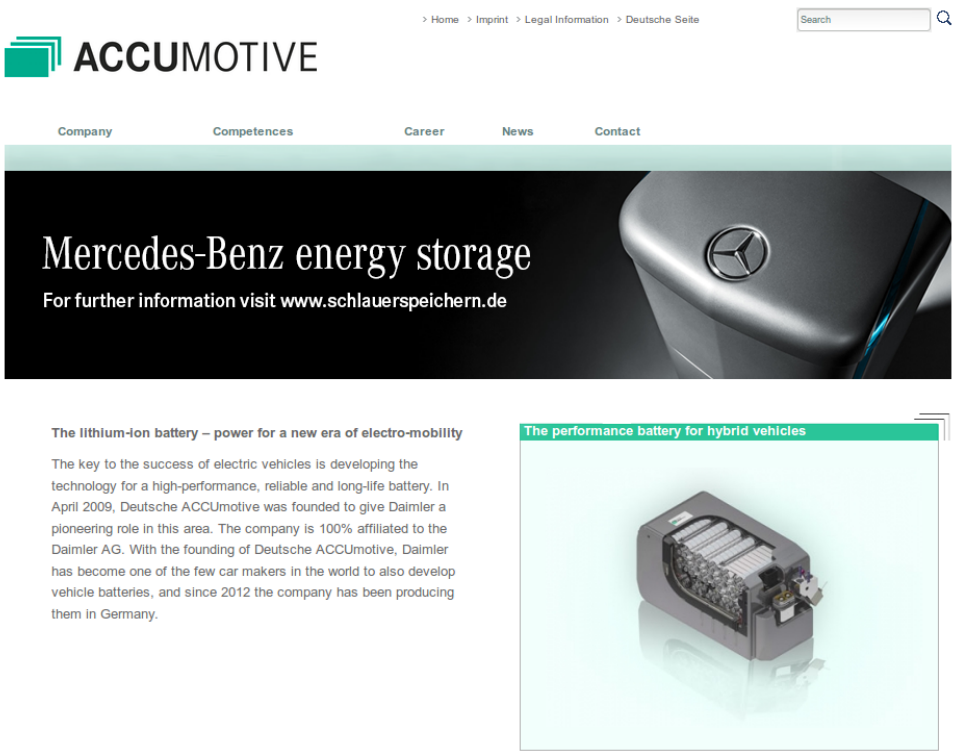


Figure : Simulation of microscale battery model on $246\mu m \times 60\mu m \times 60\mu m$ domain with random electrode geometry.

Our Industry Partner

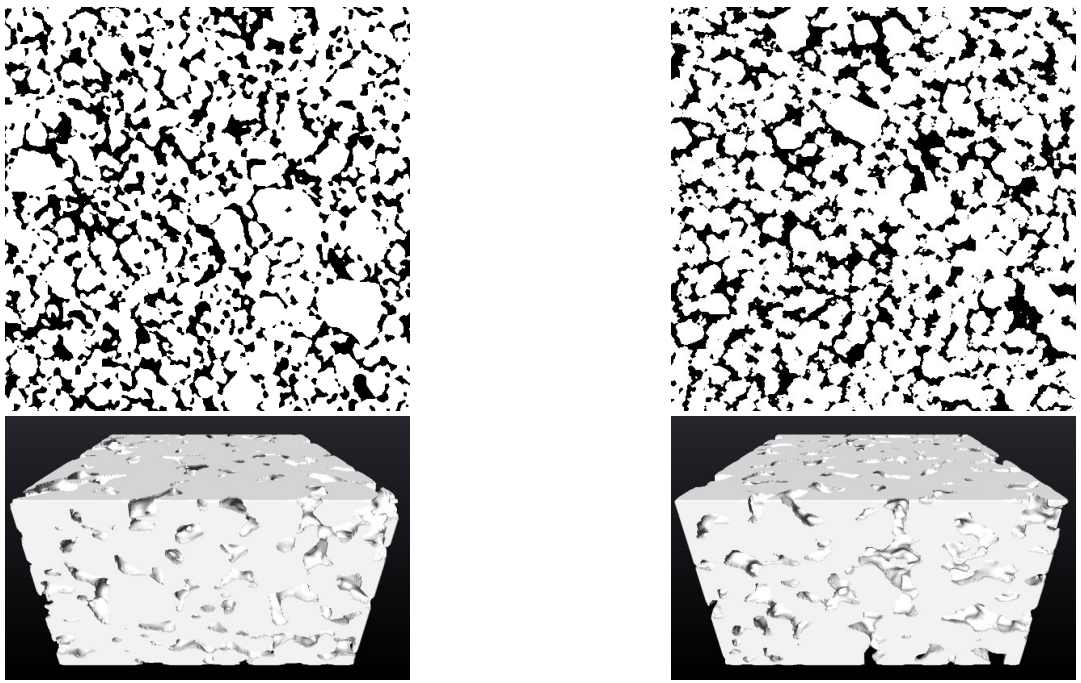


Provides:

- synchrotron imaging data of battery electrodes
- industrial know-how

Imaging and Stochastic Structure Modeling

Voker Schmidt, Julian Feinauer (Ulm, Accumotive)

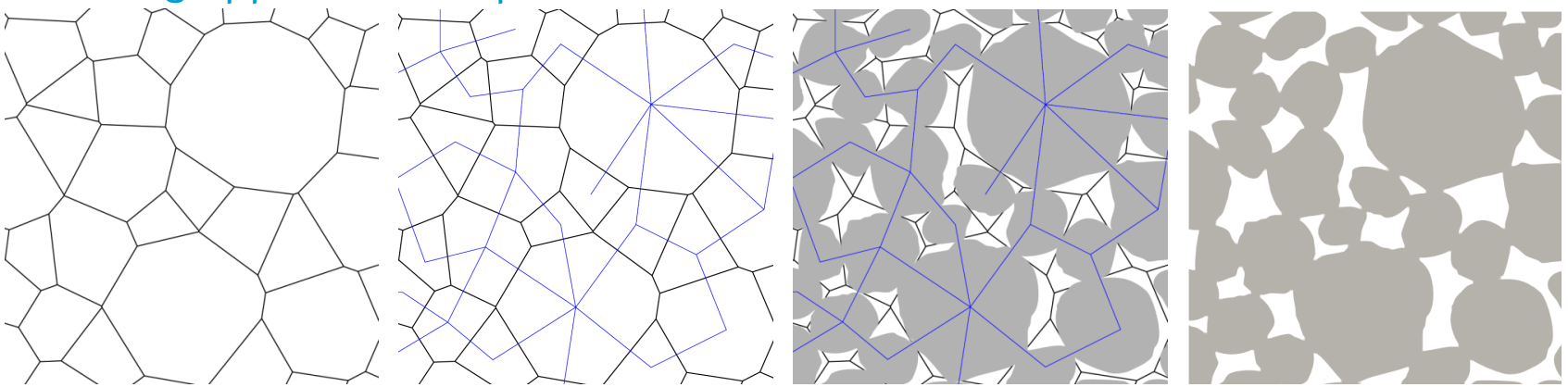


- Visual comparison of 2D and 3D cut-outs of experimental data (left) and simulated (right) shows good agreement.

Imaging and Stochastic Structure Modeling

Voker Schmidt, Julian Feinauer (Ulm, Accumotive)

Modeling Approach: Complete Simulation Model



- Create realization φ of the random Laguerre tesselation.
- Construct the connectivity graph.
- For each Laguerre cell $C \in \varphi$:
  - Define constraints $A \cdot c = b$ for particle placed in centroid x of C.
  - Sample coefficients c that fulfill $A \cdot c = b$ form $\mathcal{N}(\mu, \Sigma)$.
  - Reconstruct particle from coefficients c.
- Smooth structure with morphological closing.

Basic Microscale Model

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

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

$$N_{se} = \frac{1}{F} \cdot j_{se}$$

Modeling of Lithium Plating

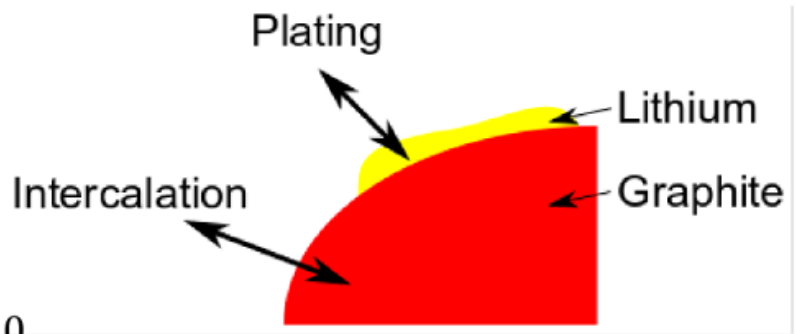
Arnulf Latz, Simon Hein (DLR at Helmholtz Institute Ulm)

Two possible reaction at negative electrode (Graphite):

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

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

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

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

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

Oleg Iliev, Sebastian Schmidt, Jochen Zausch (Fraunhofer ITWM)

- Cell centered finite volume on voxel grid + implicit Euler:

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

- 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).

Reduction of Microscale Battery Models

Model Reduction

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

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

- **Basis generation:** POD of a priori selected solution trajectories, separately for c and ϕ (different scales).

- **Next steps:**
  - better a priori choices for snapshot set (instead of equidistant μ)
  - efficient a posteriori error bound $\rightarrow$ POD-Greedy
  - localized MOR ($\rightarrow$ LRBMS)

Empirical Operator Interpolation

Problem: Still expensive to evaluate

$$P_{\tilde{V}} \circ A_\mu : \tilde{V}_c \oplus \tilde{V}_\phi \longrightarrow V_h \oplus V_h \longrightarrow \tilde{V}_c \oplus \tilde{V}_\phi.$$

Solution:

- Use locality of finite volume operators:
  to evaluate M DOFs of $A_\mu(c, \phi)$ need only $M' \leq C \cdot M$ DOFs of (c, ϕ).
- Approximate

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

where

$R_{M'}$:	Restriction to M' DOFs needed for evaluation
$\tilde{A}_{M,\mu}$:	A_μ restricted to M interpolation DOFs
I_M:	Interpolation operator

Empirical Operator Interpolation (2)

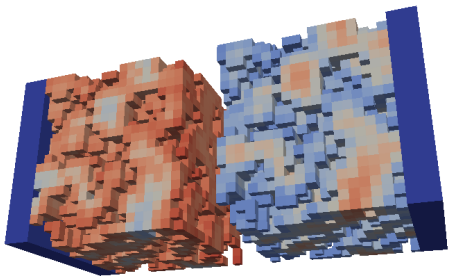
$$P_{\tilde{V}} \circ A_\mu \approx P_{\tilde{V}} \circ (I_M \circ \tilde{A}_{M,\mu} \circ R_{M'}) =: P_{\tilde{V}} \circ \mathcal{I}_M[A_\mu]$$

Basis Generation:

- Compute operator evaluations on solution snapshots (including Newton stages).
- Iteratively extend interpolation basis with worst-approximated evaluation. Choose new interplation 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 interplation basis simultaneously using error estimator to select snapshots (POD-EI-GREEDY).

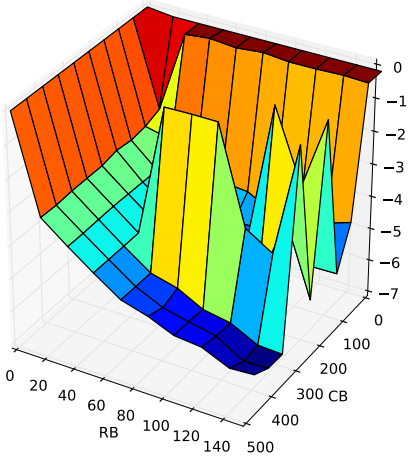
First Results

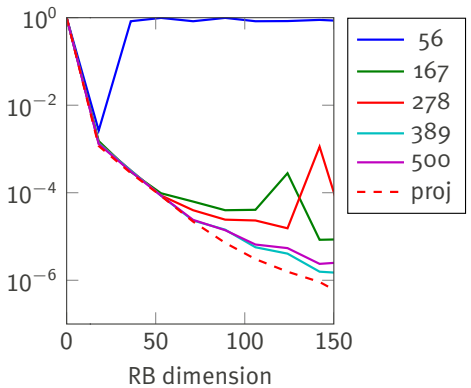
- Geometry (36,800 DOFs):



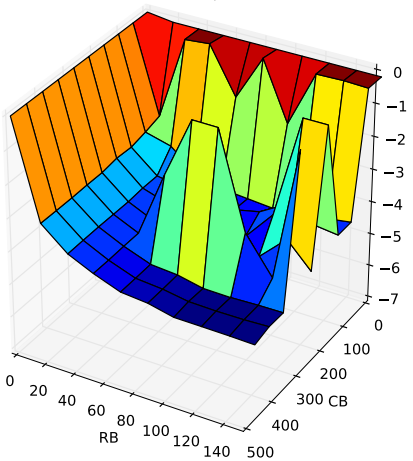
- Dune –based solver.
- Charge rate $\in [0.1C, 1C]$, constant temperature.
- 10 snapshots for training.
- Time for solution $\approx$ 1000s.
- Time for red. solution $\approx$ 40s. (dim $RB = 50$, dim $CB = 278$)
- Speedup: $\times$25

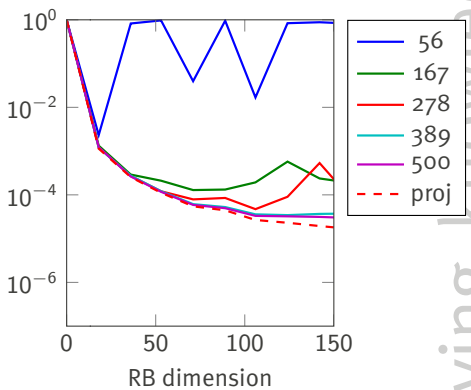
$L^\infty - L^2$ err., concentration, training set





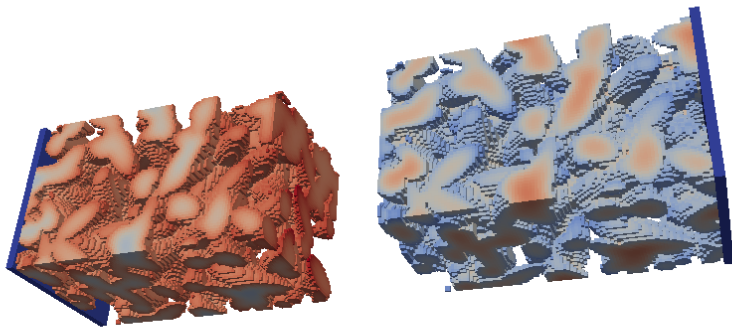
$L^\infty - L^2$ err., concentration, random params.





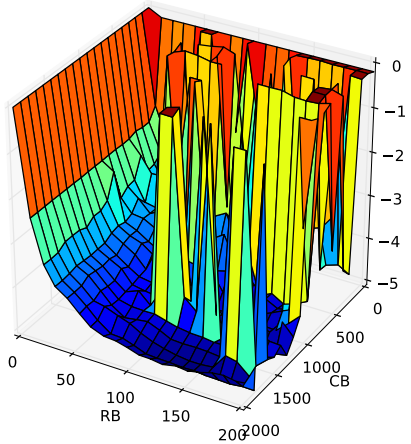
More Results

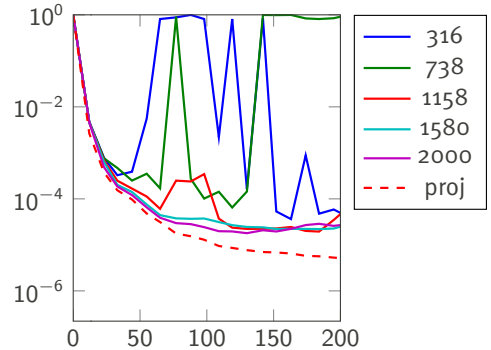
- Geometry (1,771,200 DOFs):



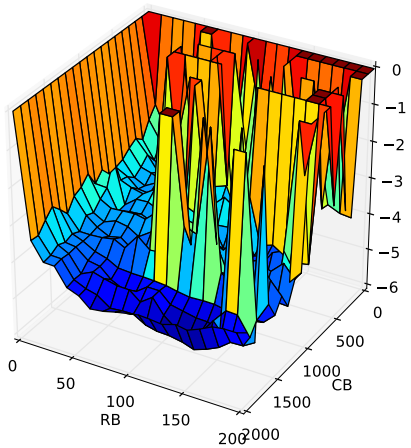
- Dune –based solver.
- Charge rate $\in [0.1C, 1C]$, constant temperature.
- 17 snapshots for training.
- Time for solution $\approx$ 15h.
- Time for red. solution $\approx$ 156s (dim $RB = 55$, dim $CB = 1580$).
- Speedup: $\times$340

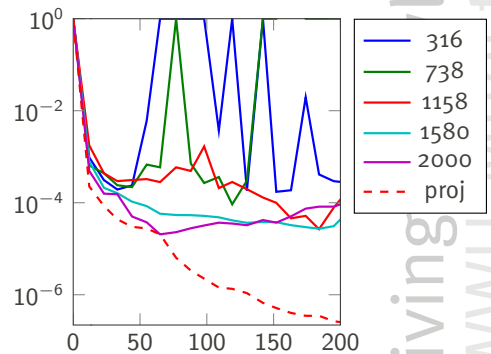
$L^\infty - L^2$ err., concentration, random params.





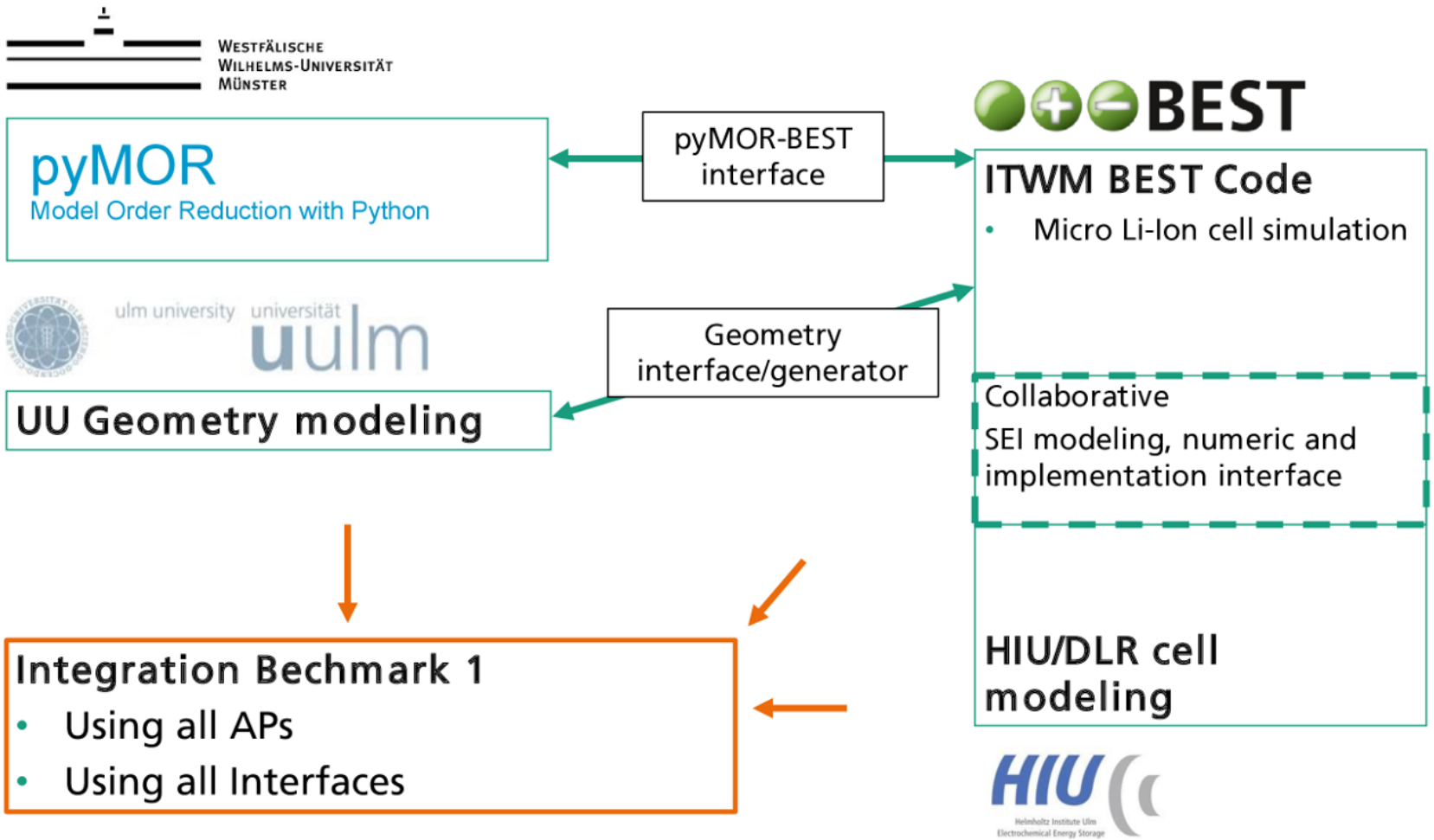
$L^\infty - L^2$ err., potential, random params.





Software Implementation

Software Interfaces in MULTIBAT



Software Interfaces in MULTIBAT

Interfaces allow us to:

- easily exchange 

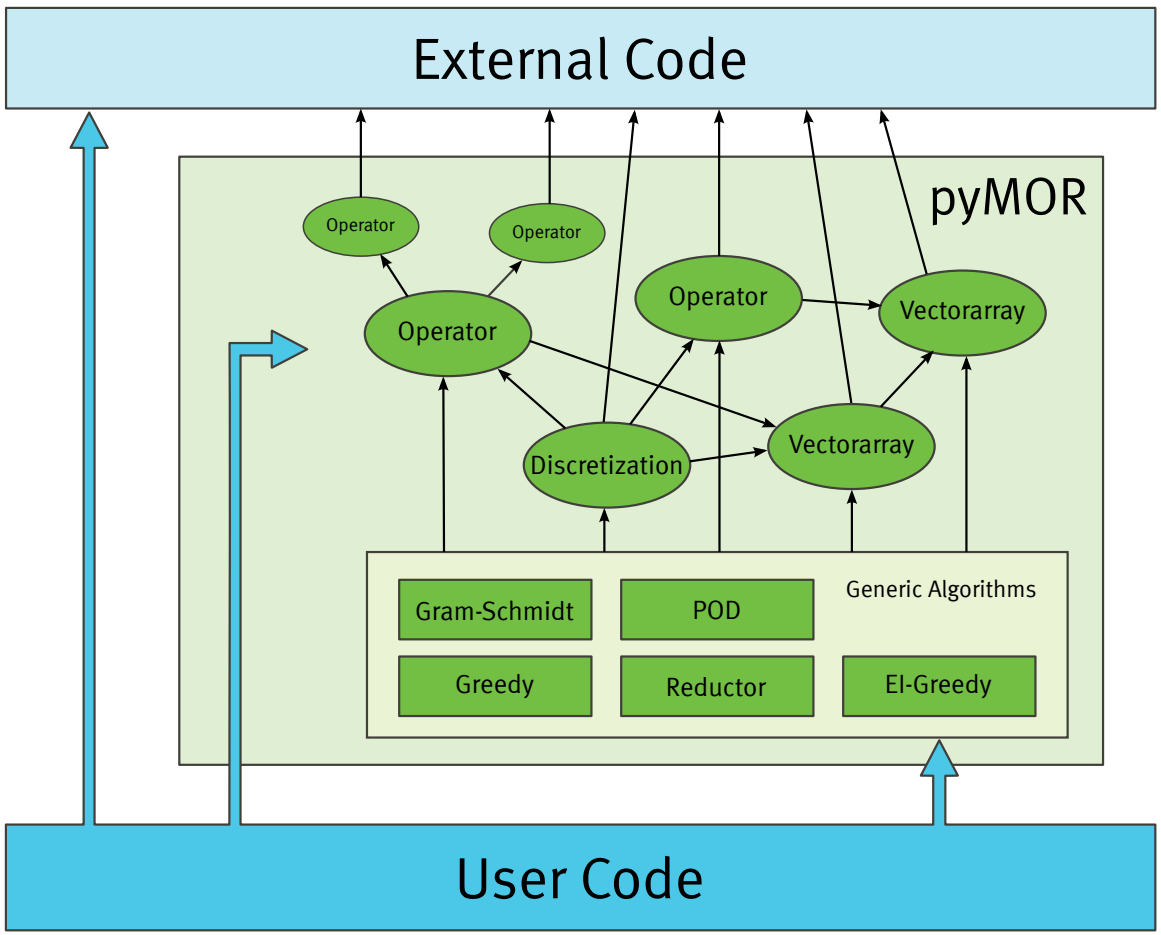
solver with BEST.
- independently develop MOR algorithms.
- easily apply MOR algorithms to updated models in BEST.
- reuse MOR algorithms for other problems.

- Using all APs
- Using all Interfaces

pyMOR

- Python-based MOR library (in particular reduced basis method).
- BSD license, `http://www.pymor.org/`.
- `VectorArray`, `Operator`, `Discretization` interfaces for tight integration of external solvers.
- Generic algorithms based on these interfaces:
  - RB-Projection, EI, error estimation
  - Greedy, EI-Greedy, POD, Gram-Schmidt
  - Timestepping, (iterative linear solvers)
- Small `NumPy`/`SciPy`-based discretization toolkit for easy prototyping.

Interfacing external PDE-solvers



New: Now with FEniCS Support

- Directly interfaces FEniCS LA backend, no copies needed.
- Use same MOR code with both backends!
- Only 150 SLOC for bindings.
- Thermal block demo:
  30 SLOC FEniCS +
  15 SLOC wrapping for pyMOR.
- Easily increase FEM order, etc.

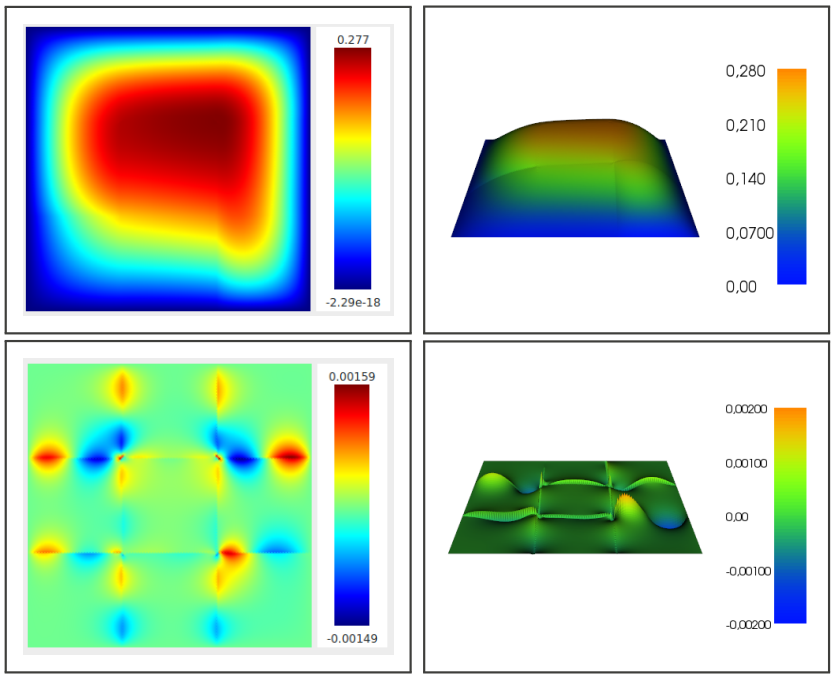


Figure : 3x3 thermal block problem
top: red. solution, bottom: red. error
left: pyMOR solver, right: FEniCS solver

New: Tools for interfacing MPI parallel solvers

- Automatically make sequential bindings MPI aware.
- Reduce HPC-Cluster models without thinking about MPI at all.
- Interactively debug MPI parallel solvers.

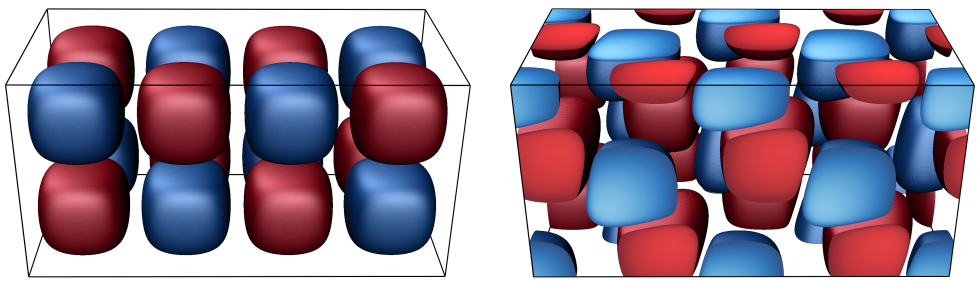


Figure : FV solution of 3D Burgers-type equation ($27.6 \cdot 10^6$ DOFs, 600 timesteps) using Dune.

Table : Time (s) needed for solution using `DUNE` / `DUNE` with `pyMOR` timestepping.

`MPI` ranks	1	2	3	6	12	24	48	96	192
`DUNE`	17076	8519	5727	2969	1525	775	395	202	107
`pyMOR`	17742	8904	6014	3139	1606	816	418	213	120
overhead	3.9%	4.5%	5.0%	5.7%	5.3%	5.3%	6.0%	5.4%	11.8%

People Involved

with pyMOR

Mario Ohlberger

Rene Milk

Stephan Rave

Felix Schindler

Andreas Buhr

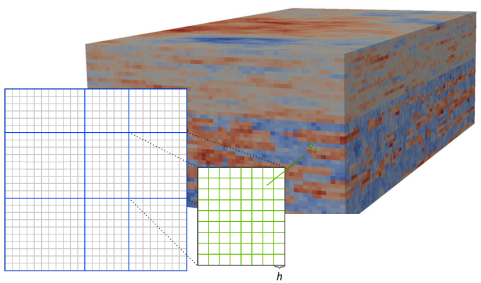
Michael Laier

Falk Meyer

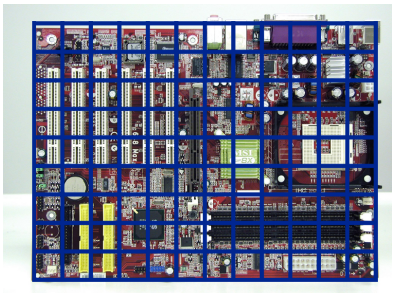
Michael Schaefer

Main Projects

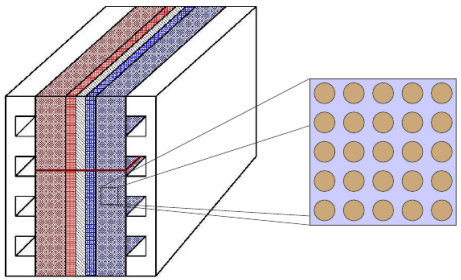
using pyMOR



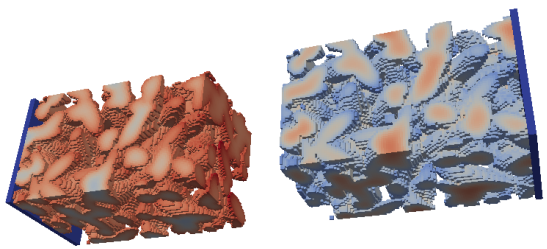
Localized Reduced Basis MultiScale method



Reduction of Maxwell's equations allowing
Arbitrary Local Modifications



Reduced basis approximation for multiscale
optimization problems



Reduction of microscale Li-ion battery models

Thank you for your attention!

AG Ohlberger
`http://wwwmath.uni-muenster.de/num/ohlberger/`

pyMOR – Model Order Reduction with Python
`http://www.pymor.org/`
arXiv:1506.07094

MULTIBAT
`http://j.mp/multibat`