Westfälische
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Reduced Basis Approximation of Microscale Lithium-Ion Battery Models

from Theory to Implementation

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SimTech MOR-Seminar
Stuttgart
December 2, 2015

Outline

1. Theory of reduced basis methods
   - Abstract problem formulation
   - Reduced basis approximation for coercive, affinely decomposed problems
   - Proof of (sub-)exponential convergence
2. Reduced basis approximation of microscale Li-ion battery models
   - The MULTIBAT project
   - Current results
   - Software implementation

Theory of Reduced Basis Methods

Abstract Problem Formulation

Consider parametric problems

$$\Phi : \mathcal{P} \to V, \qquad s : V \to \mathbb{R}^S$$

where

- $\mathcal{P} \subset \mathbb{R}^P$ *compact* set (parameter domain)
- V Hilbert space (solution state space, $\dim V \gg 0$, possibly $\dim V = \infty$)
- Φ maps parameters to solutions
- s maps state vectors to quantities of interest

Objective

Compute

$$s \circ \Phi : \mathbb{R}^P \to V \to \mathbb{R}^S$$

for many $\mu \in \mathcal{P}$ or quickly for unknown single $\mu \in \mathcal{P}$.

Abstract Problem Formulation

Objective

Compute

$$s \circ \Phi : \mathbb{R}^P \to V \to \mathbb{R}^S.$$

- When Φ, s sufficiently smooth, quickly computable low-dimensional approximation of $s \circ \Phi$ should exist.
- Could use interpolation scheme. However:
  - How to choose interpolation points?
  - Error control?!
- State space approximation:
  - Find $\Phi_N : \mathcal{P} \to V_N$ s.t. $\Phi \approx \Phi_N$ and $\dim V_N =: N \ll \dim V$.
  - Can assume $V_N \subset V$ (orthogonal projection)
  - Approximate $s \circ \Phi \approx s \circ \Phi_N$.

State Space Approximation

Main questions

1. Do good approximation spaces V_N exist?
2. How to find a good approximation space V_N?
3. How to construct a quickly-evaluable $\Phi_N : \mathcal{P} \to V_N$?
4. How to control the approximation errors $\Phi(\mu) - \Phi_N(\mu)$, $s(\Phi(\mu)) - s(\Phi_N(\mu))$?

- We answer these questions for the archetypical class of

  linear, coercive, affinely decomposed problems.

Linear, coercive, affinely decomposed problem.

Linear, coercive problem

$\Phi(\mu) = u_\mu \in V$ is the solution of variational problem

$$a_\mu(u_\mu, v) = f(v) \qquad \forall v \in V,$$

where $a_\mu : V \times V \to \mathbb{R}$ is continuous, coercive bilinear form, $f \in V'$.
Moreover, $s : V \to \mathbb{R}^S$ is linear and continuous.

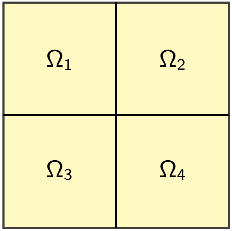
Linear, coercive, affinely decomposed problem

Additionally:

$$a_\mu = \sum_{q=1}^{Q} \theta_q(\mu) a_q \qquad \forall \mu \in \mathcal{P},$$

where $\theta_q : \mathcal{P} \to \mathbb{R}$ continuous, $a_q : V \times V \to \mathbb{R}$ continuous bilinear form, $(1 \leq q \leq Q)$.

Model Problem



$$\Omega = \bigcup_{i=1}^{4} \Omega_i, \quad \mathcal{P} = [\alpha, 1]^4, \ \alpha > 0$$

$$a_\mu(x) = \sum_{i=1}^{4} \mu_i \cdot \chi_{\Omega_i}(x), \qquad x \in \Omega, \mu \in \mathcal{P}$$

$$f \in L^2(\Omega)$$

Thermal block problem

For $\mu \in \mathcal{P}$, find $u_\mu \in H_0^1(\Omega)$ s.t.

$$-\nabla \cdot (a_\mu \nabla u_\mu) = f$$

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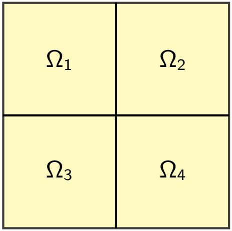

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For $\mu \in \mathcal{P}$, find $u_\mu \in H_0^1(\Omega)$ s.t.

$$\sum_{k=1}^{4} \mu_k \int_{\Omega_k} \nabla u_\mu \cdot \nabla v = \int_\Omega f \cdot v \qquad \forall v \in H_0^1(\Omega)$$

3. Definition of Φ_N

Full order problem

$\Phi(\mu) = u_\mu \in V$ is the solution of variational problem

$$a_\mu(u_\mu, v) = f(v) \qquad \forall v \in V,$$

where $a_\mu : V \times V \to \mathbb{R}$ is continuous, coercive bilinear form, $f \in V'$.

Reduced order problem

For given $V_N \subset V$, let $\Phi_N(\mu) := u_{\mu,N} \in V_N$ be the Galerkin projection of u_μ onto V_N, i.e.

$$a_\mu(u_{\mu,N}, v) = f(v) \qquad \forall v \in V_N.$$

- Since a_μ is coercive, $u_{\mu,N}$ is well-defined.

3. Definition of Φ_N

Theorem (Céa)

Let c_μ denote the coercivity constant of a_μ. Then

$$\|u_\mu - u_{\mu,N}\| \leq \frac{\|a_\mu\|}{c_\mu} \inf_{v \in V_N} \|u_\mu - v\|.$$

- $u_{\mu,N}$ is quasi-optimal approximation of u_μ in V_N.
- For badly conditioned ($\|a_\mu\|/c_\mu \gg 0$) or non-coercive a_μ use Petrov-Galerkin projection!

3. Definition of Φ_N

Let $\varphi_1, \cdots, \varphi_N$ be a basis of V_N. Then $u_{\mu,N} = \sum_{l=1}^{N} \varphi_l \cdot \underline{u}_{\mu,N,l}$, where

$$\sum_{q=1}^{Q} \mu_q \cdot \left[a_q(\varphi_l, \varphi_k)\right]_{k,l} \cdot \underline{u}_{\mu,N,l} = \left[f(\varphi_k)\right]_k \tag{1}$$

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Proposition

If $\left[a_q(\varphi_l, \varphi_k)\right]_{k,l}$ are pre-computed, (1) can be solved with effort $\mathcal{O}(QN^2 + N^3)$.

Warning

Using solution snapshots $u_{\mu_1}, \ldots, u_{\mu_N}$ as basis for V_N leads to (really!) badly conditioned reduced system matrices! Orthonormalize!

4. Error control

Define residual $\mathcal{R}_\mu(u) \in V'$ as

$$\mathcal{R}_\mu(u)[v] := f(v) - a_\mu(u, v).$$

Then

$$\begin{aligned} \|u_\mu - u_{\mu,N}\|^2 &\leq c_\mu^{-1} a_\mu(u_\mu - u_{\mu,N},\ u_\mu - u_{\mu,N}) \\ &= c_\mu^{-1} \mathcal{R}_\mu(u_{\mu,N})[u_\mu - u_{\mu,N}] \leq c_\mu^{-1} \|\mathcal{R}_\mu(u_{\mu,N})\| \, \|u_\mu - u_{\mu,N}\|. \end{aligned}$$

Proposition

The quantity $\Delta_\mu(u_{\mu,N}) := c_\mu^{-1} \cdot \|\mathcal{R}(u_{\mu,N})\|$ is a reliable and effective a posteriori estimate for the model reduction error:

$$\|u_\mu - u_{\mu,N}\| \leq \Delta_\mu(u_{\mu,N}) \leq \|a_\mu\| \cdot c_\mu^{-1} \cdot \|u_\mu - u_{\mu,N}\|.$$

4. Error control

We have

$$\|\mathcal{R}_\mu(u_{\mu,N})\|^2 = \left\| f + \sum_{q=1}^{Q} \sum_{n=1}^{N} \underline{u}_{\mu,N,n} a_q(\varphi_n, \cdot) \right\|^2.$$

Note that V' is a Hilbert space via the Riesz isomorphism.

Thus, we can pre-compute all $(1 + QN)^2$ cross-terms in the scalar-product evaluation. Online effort: $\mathcal{O}((1 + QN)^2) = \mathcal{O}(Q^2 N^2)$.

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However, bad numerical stability (half machine precision). Better approach:

Stable estimator decomposition (Buhr, R, 2014)

Project $\mathcal{R}_\mu$ onto V_N and $\mathrm{span}\{f, a_q(\varphi_n, \cdot)\}$ w.r.t. orthonormal bases.

4. Error control

Simple output error bound

We have

$$|s \circ \Phi(\mu) - s \circ \Phi_N(\mu)| \leq \|s\| \cdot \Delta_\mu(u_{\mu,N}).$$

- Not very effective: Typically, error decays at faster rate than $\Delta_\mu(u_{\mu,N})$.
- When a_μ symmetric and $s = f$ ('compliant' case):

$$0 \leq s \circ \Phi(\mu) - s \circ \Phi_N(\mu) \leq c_\mu \cdot \Delta_\mu(u_{\mu,N})^2.$$

- For general a_μ, s: Improved estimates via dual weighted residual approach.
- If unknown, c_μ can be replaced by arbitrary lower bound $0 < \alpha_\mu \leq c_\mu$ ($\rightarrow$ sucessive constraint method).

1. Existence of good V_N

Definition

The *Kolmogorov N-width* $d_N(\Phi(\mathcal{P}))$ of $\Phi(\mathcal{P})$ is given as

$$d_N(\Phi(\mathcal{P})) = \inf_{\substack{V_N \subseteq V \\ \text{lin subsp.} \\ \dim V_N \leq N}} \sup_{u \in \Phi(\mathcal{P})} \inf_{v \in V_N} \|u - v\|.$$

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- Cannot beat N-width with any V_N.
- For elliptic problems with fixed operator and arbitrary RHS in some unit ball: Polynomial decay of d_N.
- Hope for exponential decay of $d_N(\Phi(\mathcal{P}))$.

1. Existence of good V_N

Proposition (Cohen, DeVore, 2014)

Let $F : V \times X \longrightarrow W$ holomorphic map between Banach spaces and $\mathcal{P} \subseteq X$.
If for all $\mu \in \mathcal{P}$

- $\Phi(\mu) := u_\mu$ is the unique solution of $F(u_\mu, \mu) = 0$
- $\partial_u F(u_\mu, \mu) : V \longrightarrow W$ is invertible,

then there is holomorphic extension $\Phi : \mathcal{O} \longrightarrow V$ with $\mathcal{P} \subseteq \mathcal{O}$ open.

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Implicit function theorem (for complex Banach spaces).

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Implicit function theorem (for complex Banach spaces).

- For affinely decomposed, linear coercive problems:

$$F : V \times \mathbb{C}^Q \to V', \quad F(u, \underline{z})[v] := \sum_{q=1}^{Q} z_q \cdot a_q(u, v) - f$$

1. Existence of good V_N

Corollary

There are $C, c > 0$ s.t.

$$d_N(\Phi(\mathcal{P})) \leq Ce^{-cN^{1/Q}}$$

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Proof

- $\hat{\mathcal{P}} := \{(\theta_1(\mu), \ldots, \theta_Q(\mu) \mid \mu \in \mathcal{P}\} \subset \mathbb{C}^Q$ is compact ($\mathcal{P}$ cpct., θ_q cont.)
- $\hat{\Phi} : \hat{\mathcal{P}} \to V$, $\hat{\Phi}[\theta_1(\mu), \ldots, \theta_Q(\mu)] := \Phi(\mu)$ has holom. ext. to $\hat{\mathcal{P}} \subset \mathcal{O}$.

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- Thus, $\hat{\Phi}$ can be extended as multivariate power series for any $z \in \hat{\mathcal{P}}$.
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- By compactness of $\hat{\mathcal{P}}$, finitely many power series expansions suffice to represent any $\hat{\mathcal{P}}(z)$, $z \in \hat{\mathcal{P}}$.
- $V_N :=$ span{first $k(N)$ coeffs. in expansions}.

2. Construction of V_N

Definition (weak greedy sequence)

Let $0 < \gamma \leq 1$ and $s_1, s_2, \ldots \in \Phi(\mathcal{P})$ be such that

$$\inf_{v \in V_{N-1}} \|s_N - v\| \geq \gamma \cdot \sup_{u \in \Phi(\mathcal{P})} \inf_{v \in V_{N-1}} \|u - v\| \qquad V_N := \operatorname{span}\{s_1, \ldots s_N\}$$

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Theorem (DeVore, Petrova, Wojtaszczyk, 2013)

Let (s_n) be a weak greedy series for $\Phi(\mathcal{P})$ with param. γ. Assume there are $C, c, \alpha > 0$ such that

$$d_N(\Phi(\mathcal{P})) \leq Ce^{-cN^\alpha}.$$

Then with $V_N := \operatorname{span}\{s_1, \ldots s_N\}$ we have

$$\sup_{u \in \Phi(\mathcal{P})} \inf_{v \in V_N} \|u - v\| \leq \sqrt{2C}\gamma^{-1} e^{-c' N^\alpha}, \qquad c' = 2^{-1-2\alpha} c.$$

2. Construction of V_N

Greedy algorithm with error estimator

Choose snapshots $s_N := u_{\mu_N}$ where μ_N is such that

$$\mu_N = \operatorname*{arg\,max}_{\mu \in \mathcal{P}} \Delta_\mu(u_{\mu,N-1})$$

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Then

$$\begin{aligned}\inf_{v \in V_{N-1}} \|s_N - v\| &\geq \|a_\mu\|^{-1} \cdot c_\mu \cdot \|u_{\mu_N} - u_{\mu_N,N-1}\| \\ &\geq \|a_\mu\|^{-2} \cdot c_\mu^2 \cdot \Delta_\mu(u_{\mu_N,N-1}) \\ &\geq \|a_\mu\|^{-2} \cdot c_\mu^2 \cdot \Delta_\mu(u_{\mu,N-1}) \geq \|a_\mu\|^{-2} \cdot c_\mu^2 \inf_{v \in V_{N-1}} \|u_\mu - v\|\end{aligned}$$

Proposition

The greedy algorithm with error estimator generates a weak greedy sequence with parameter $\inf_{\mu \in \mathcal{P}} \|a_\mu\|^{-2} \cdot c_\mu^2$.

Summary

- Using the greedy algorithm with error estimator we obtain spaces V_N such that

$$\sup_{\mu\in\mathcal{P}} \inf_{v\in V_N} \|u_\mu - v\| \leq \sqrt{2C} \cdot \max_{\mu\in\mathcal{P}}(\|a_\mu\|^2 \cdot c_\mu^{-2}) \cdot e^{-c' N^{1/Q}} \tag{2}$$

- For these spaces, the following a priori bound holds:

$$\sup_{\mu\in\mathcal{P}} \|u_\mu - u_{\mu,N}\| \leq \sqrt{2C} \cdot \max_{\mu\in\mathcal{P}}(\|a_\mu\|^3 \cdot c_\mu^{-3}) \cdot e^{-c' N^{1/Q}} \tag{3}$$

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- Replace $\mathcal{P}$ by sufficiently dense but finite training set $\mathcal{S} \subset \mathcal{P}$.
  Note that (2), (3) are then only guaranteed to hold for $\mu \in \mathcal{S}$.

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- Replace $\mathcal{P}$ by sufficiently dense but finite training set $\mathcal{S} \subset \mathcal{P}$.
Note that (2), (3) are then only guaranteed to hold for $\mu \in \mathcal{S}$.
- There should be a computationally feasible basis generation algorithm for which (2), (3) are maintained on all of $\mathcal{P}$ ...

Reduced Basis Approximation of Microscale Li-Ion Battery Models

The MULTIBAT Project

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DLR Institute of Technical Thermodynamics

MULTIBAT

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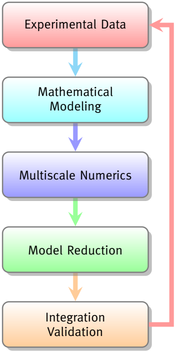


- Understand degradation processes in rechargeable Li-Ion Batteries through mathematical modeling and simulation.
- Focus: Li-Plating.

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.**

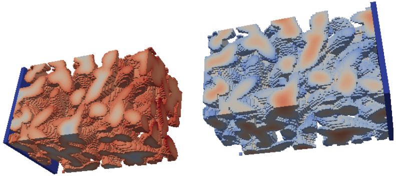
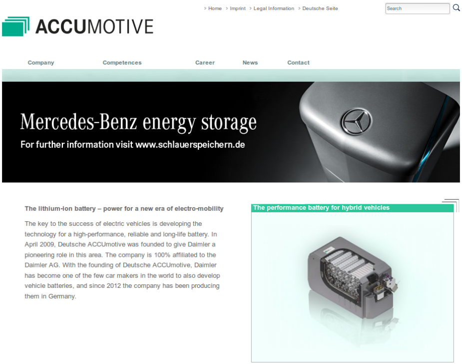


Figure : Simulation of microscale battery model on $246\mu m \times 60\mu m \times 60\mu m$ domain with random electrode geometry.

Our Industry Partner

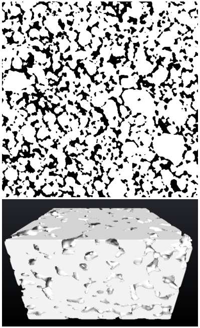


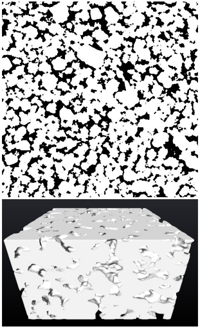
Provides:

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

Imaging and Stochastic Structure Modeling

Voker Schmidt, Julian Feinauer (Ulm, Accumotive)



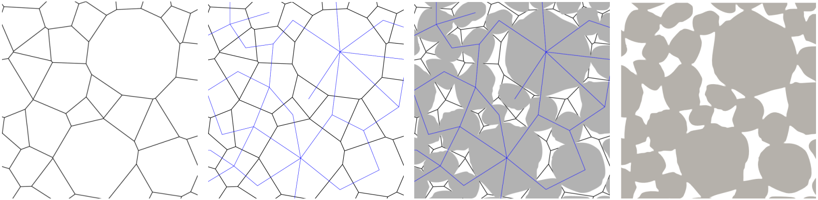


- Visual comparison of 2D and 3D cut-outs of experimental data (left) and simulated (right) shows good agreement.

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)

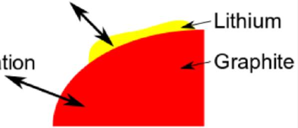
Two possible reaction at negative electrode (Graphite):

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

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

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

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:

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

- 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

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

- **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)
  - effective a posteriori error bound $\to$ POD-Greedy
  - localized MOR ($\to$ 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)

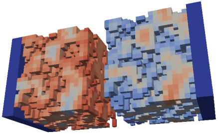
$$P_{\tilde{V}} \circ A_\mu \approx P_{\tilde{V}} \circ (I_M \circ \tilde{A}_{M,\mu} \circ R_{M'}) =: P_{\tilde{V}} \circ \mathcal{I}_M[A_\mu]$$

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).

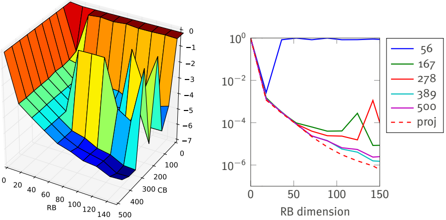
First Results

- Geometry (36,800 DOFs):

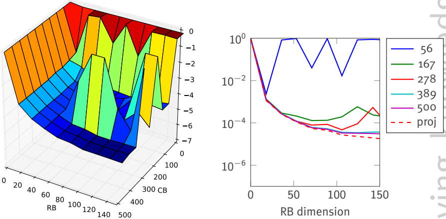


- Dune –based solver.
- Charge rate $\in [0.1C, 1C]$, constant temperature.
- 10 snapshots for training.
- Time for solution $\approx 1000s$.
- Time for red. solution $\approx 40s$. (dim $RB = 50$, dim $CB = 278$)
- Speedup: $\times 25$

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

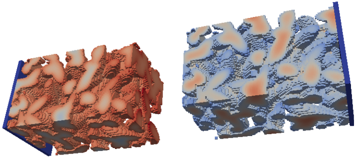


$L^\infty - L^2$ err., concentration, random params.



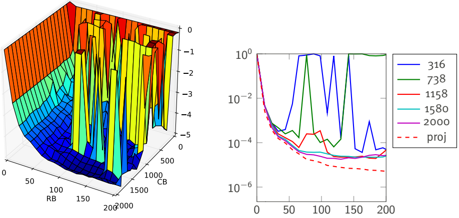
More Results

- Geometry (1,771,200 DOFs):

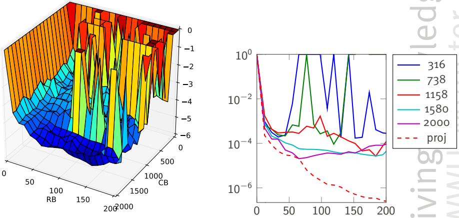


- Dune –based solver.
- Charge rate $\in [0.1C, 1C]$, constant temperature.
- 17 snapshots for training.
- Time for solution $\approx$ 15h.
- Time for red. solution $\approx$ 156s (dim $RB = 55$, dim $CB = 1580$).
- Speedup: $\times 340$

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

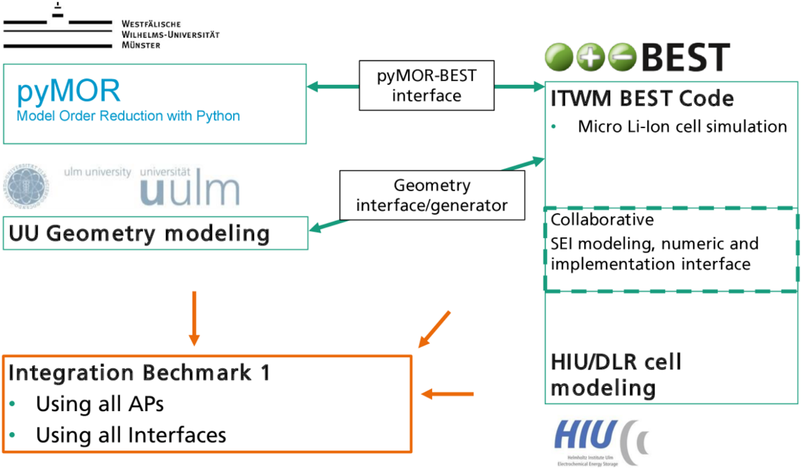


$L^\infty - L^2$ err., potential, random params.



Software Implementation

Software Interfaces in MULTIBAT



Software Interfaces in MULTIBAT

Interfaces allow us to:

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

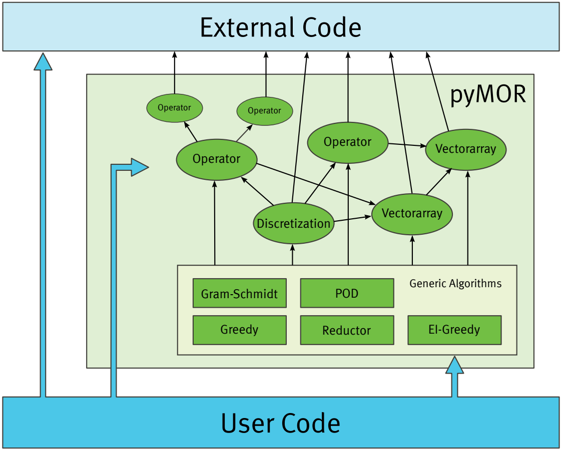
- Using all APs
- Using all Interfaces

HIU
Helmholtz Institute Ulm
Electrochemical Energy Storage

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 (now with `gmsh` support) 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.

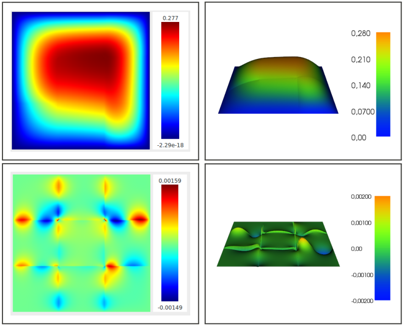


Figure : 3x3 thermal block problem
top: red. solution, bottom: red. error
left: pyMOR solver, right: FEniCS solver

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.

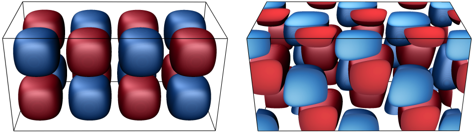


Figure : FV solution of 3D Burgers-type equation ($27.6 \cdot 10^6$ DOFs, 600 timesteps) using 

.

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

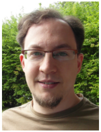
Stephan Rave

Felix Schindler

Andreas Buhr

Michael Laier

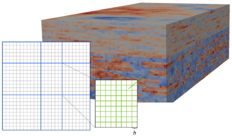
Falk Meyer



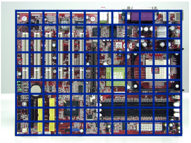
Michael Schaefer

Main Projects

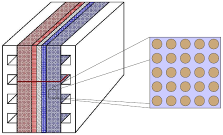
using pyMOR



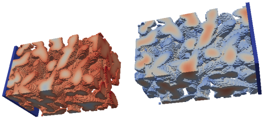
Localized Reduced Basis MultiScale method



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!

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

Reduced Basis Methods: Success, Limitations and Future Challenges
arXiv:1511.02021

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

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

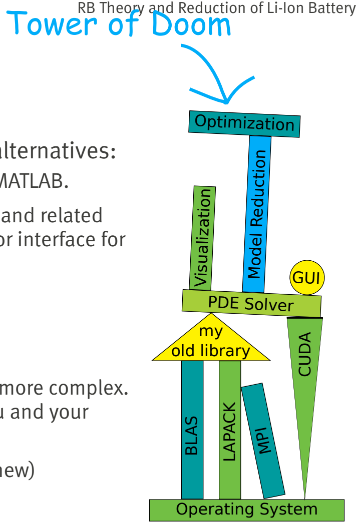
What if you don't like pyMOR?

I don’t like pyMOR because . . .

- I prefer MATLAB.
- I prefer procedual-style programming.
- it’s too complicated.
- does not implement anything I need.
- it’s not written by myself.

Suggestions

- Try not to reinvent the wheel. Look for alternatives:
  - RBMatlab: Reduced Basis toolbox for MATLAB.
  - modred: Python-based library for POD and related methods, parallel algorithms and vector interface for handling large datasets.
  - `http://modelreduction.org/`
- When writing your own code:
  - Scientific software is getting more and more complex. Defining proper interfaces will help you and your co-workers.
  - Consider implementing (or defining a new) OpenInterfaces standard!



OpenInterfaces

- Common interfaces for scientific computing, e.g.:
  - problem description interface for ODEs / PDEs and control problems
  - high-level ODE / PDE solver interface
  - solver solution interface
  - internal solver algorithm and data structure interface
- Tools for bridging the language barrier. Easy interoperability between

  C++, Python, Matlab, Julia, Fortran, R
- Specification freely available and published under open licenses.
- Community driven development process.

Join us! — http://www.openinterfaces.org/

" {Christian Himpe, R}