



Westfälische
Wilhelms-Universität
Münster

Model Order Reduction for Electrochemistry Simulations



Outline

- ▶ The reduced basis method in a nutshell.
- ▶ Reduced basis approximation of microscale Li-ion battery models.
- ▶ Software design.
- ▶ Distributed hierarchical POD computation.



The Reduced Basis Method in a Nutshell

Abstract Problem Formulation

Consider parametric problems

$$\Phi : \mathcal{P} \rightarrow V, \quad s : V \rightarrow \mathbb{R}^S$$

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 (*hard* to compute).
- ▶ s maps state vectors to quantities of interest.

Objective

Compute

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

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

Abstract Problem Formulation

Objective

Compute

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

- ▶ 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 $\Phi_N : \mathcal{P} \rightarrow V_N$ s.t. $\Phi \approx \Phi_N$ and $\dim V_N =: N \ll \dim V$.
 - ▶ W.l.g. 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 $\Phi_N : \mathcal{P} \rightarrow V_N$?
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 basic class of

linear, coercive, affinely decomposed problems.

Problem Class

Linear, coercive problem

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

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

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

Linear, coercive, affinely decomposed problem

Additionally:

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

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

3. Definition of Φ_N

Full order problem

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

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

where $a_\mu : V \times V \rightarrow \mathbb{R}$ 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.

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

- ▶ 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

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

Proposition

Let $\varphi_1, \dots, \varphi_N$ be a basis of V_N . If $[a_q(\varphi_l, \varphi_k)]_{k,l}$ are precomputed, reduced problem can be solved with effort $\mathcal{O}(QN^2 + N^3)$.

4. Error Control

Proposition

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

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

Have $\|\mathcal{R}_\mu(u_{\mu,N})\|^2 = \left\| f + \sum_{q=1}^Q \sum_{n=1}^N \underline{u}_{\mu,N,n} a_q(\varphi_n, \cdot) \right\|^2$. Thus, can precompute all cross-terms in inner product evaluation with effort $\mathcal{O}((1 + QN)^2) = \mathcal{O}(Q^2 N^2)$.

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

Stable estimator decomposition (Buhr, R, 2014)

Project \mathcal{R}_μ onto V_N and $\text{span}\{f, a_q(\varphi_n, \cdot)\}$ 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 $0 < \alpha_\mu \leq c_\mu$ (→ successive 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

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

Theorem

For linear, coercive, affinely decomposed probelems there are $C, c > 0$ s.t.

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

Proof

- ▶ Φ is holomorphic due to implicit function theorem.
- ▶ Use coefficients of truncated power series expansions as basis.

2. Construction of V_N

Definition (weak greedy sequence)

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

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

Then (s_n) is called weak greedy sequence for $\Phi(\mathcal{P})$ with parameter γ .

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

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

Then with $V_N := \text{span}\{s_1, \dots, s_N\}$ we have

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

2. Construction of V_N

Greedy algorithm with error estimator

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

$$\mu_N = \arg \max_{\mu \in \mathcal{P}} \Delta_{\mu}(u_{\mu, N-1})$$

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

1. Do good approximation spaces V_N exist?

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

2. How to find a good approximation space V_N ?

Greedy algorithm with error estimator

3. How to construct a quickly-evaluable $\Phi_N : \mathcal{P} \rightarrow V_N$?

Galerkin projection

4. How to control the approximation errors $\Phi(\mu) - \Phi_N(\mu)$,
 $s(\Phi(\mu)) - s(\Phi_N(\mu))$?

Residual-based error estimator



Reduced Basis Approximation of Microscale Li-Ion Battery Models

The MULTIBAT Project



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MULTIBAT



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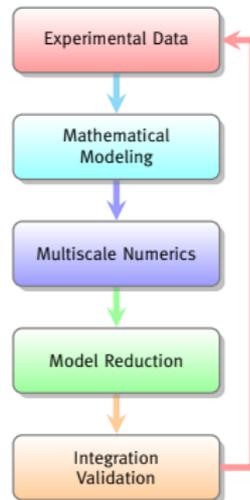
Federal Ministry
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Fraunhofer
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- ▶ Understand degradation processes in rechargeable Li-Ion Batteries through mathematical modeling and simulation.
- ▶ Focus: Li-Plating.

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.**

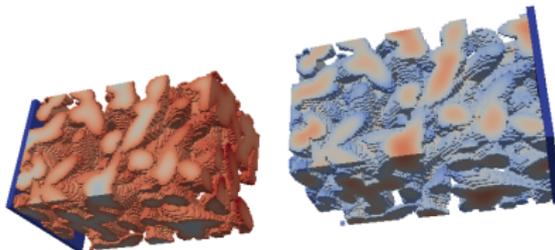


Figure: Simulation of microscale battery model on $246\mu\text{m} \times 60\mu\text{m} \times 60\mu\text{m}$ domain with random electrode geometry.

Our Industry Partner



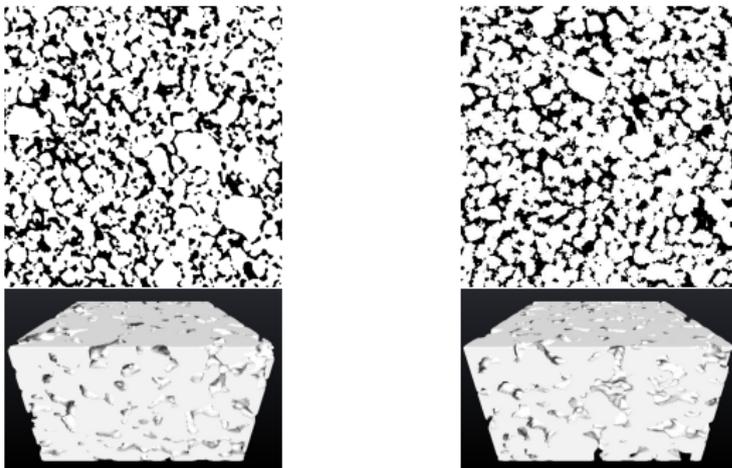
The screenshot shows the ACCUMOTIVE website. At the top, there is a navigation bar with links for Home, Imprint, Legal Information, and Deutsche Seite, along with a search bar. Below the navigation bar, there is a main banner for Mercedes-Benz energy storage with the text "Mercedes-Benz energy storage" and "For further information visit www.schlauerspeichern.de". To the right of the text is an image of a Mercedes-Benz car battery. Below the banner, there are two columns of text. The left column is titled "The lithium-ion battery – power for a new era of electro-mobility" and discusses the company's role in developing high-performance, reliable, and long-life batteries. The right column is titled "The performance battery for hybrid vehicles" and features an image of a battery pack.

Provides:

- ▶ synchrotron imaging data of battery electrodes
- ▶ industrial insights

Imaging and Stochastic Structure Modeling

Voker Schmidt, Julian Feinauer (Ulm, Accumotive)

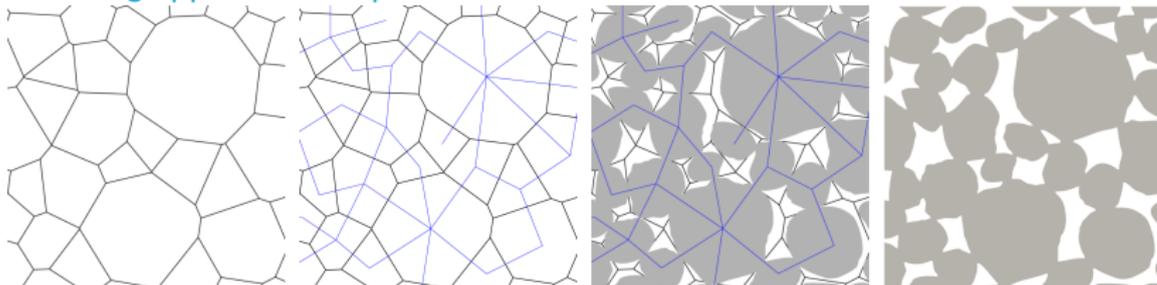


- ▶ Visual comparison of 2D and 3D cut-outs of experimental data (left) and simulated (right) shows good agreement.

Imaging and Stochastic Structure Modeling

Voker Schmidt, Julian Feinauer (Ulm, Accumotive)

Modeling Approach: Complete Simulation Model



- ▶ Create realization φ of the random Laguerre tessellation.
- ▶ 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 $A \cdot c = b$ from $\mathcal{N}(\mu, \Sigma)$.
 - ▶ Reconstruct particle from coefficients c .
- ▶ Smooth structure with morphological closing.

Basic Microscale Model

Variables:

c : Li^+ concentration

ϕ : electrical potential

Electrolyte:

$$\begin{aligned} \frac{\partial c}{\partial t} - \nabla \cdot (D_e \nabla c) &= 0 \\ -\nabla \cdot \left(\kappa \frac{1-t_+}{F} RT \frac{1}{c} \nabla c - \kappa \nabla \phi \right) &= 0 \end{aligned}$$

Electrodes:

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

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

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

Modeling of Lithium Plating

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

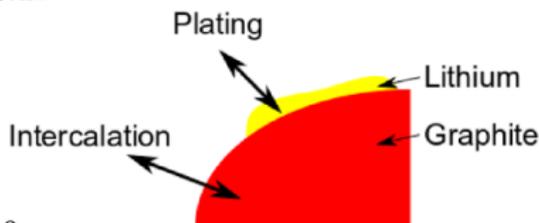
Two possible reaction at negative electrode (Graphite):

- Intercalation $\text{Li}_{\text{Electrolyte}}^+ + e_{\text{Solid}}^- \rightleftharpoons \text{LiC}_{6,\text{Solid}}$
- Lithium plating $\text{Li}_{\text{Electrolyte}}^+ + e_{\text{Solid}}^- \rightleftharpoons \text{Li}_{\text{Solid}}^{\ominus}$

Overpotential with lithium reference:

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

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



Active material and Electrolyte

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

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

Plated Lithium and Electrolyte

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

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

Discretization

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

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

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

- ▶ 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).

Model Order 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 \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

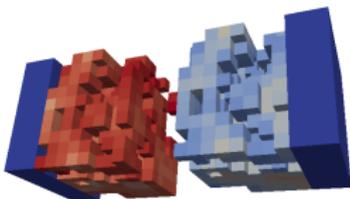
Empirical Operator Interpolation (2)

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

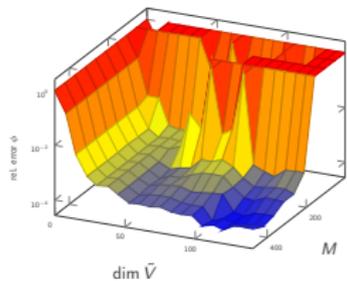
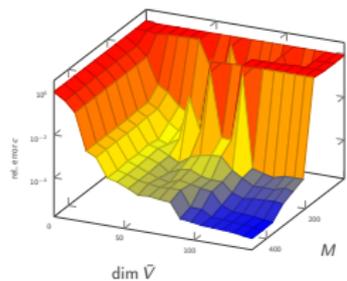
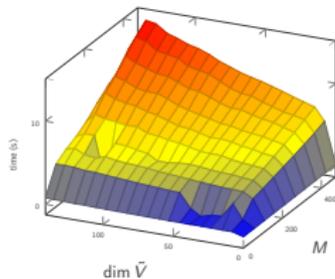
Basis Generation:

- ▶ Compute operator evaluations on solution snapshots (including Newton stages).
- ▶ Iteratively extend interpolation basis with worst-approximated evaluation. Choose new 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).

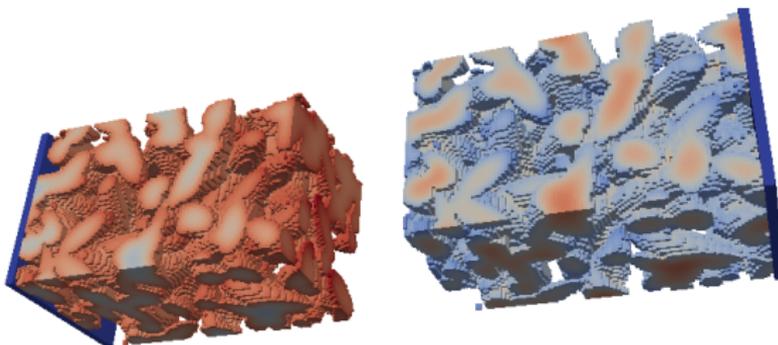
Experiments



- ▶ 4.600 DOFs, 20 snapshots
- ▶ $T = 298K, I \in [0.1C, 1C]$



Experiments

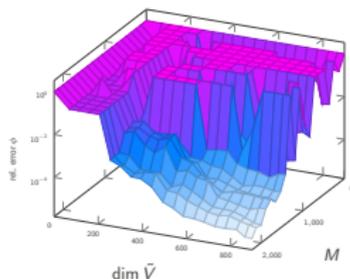
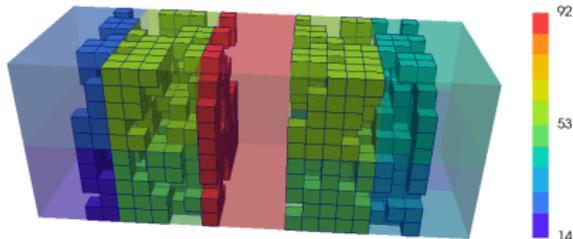
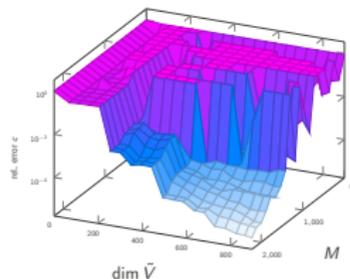
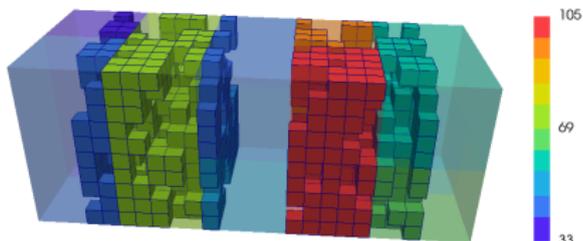


- ▶ 1.749.600 DOFs, solution time: 6.5h.
- ▶ Only 2 solution snapshots.

dim \tilde{V}	11	21	30	40
rel. error c	$9.26 \cdot 10^{-3}$	$3.96 \cdot 10^{-3}$	$3.05 \cdot 10^{-3}$	$2.93 \cdot 10^{-3}$
rel. error ϕ	$2.07 \cdot 10^{-3}$	$1.50 \cdot 10^{-3}$	$1.46 \cdot 10^{-3}$	$1.26 \cdot 10^{-3}$
time (s)	82	81	79	81
speedup	279	285	290	283

Localized Reduced Basis Approximation

- First experiments on small geometry (no enrichment, no parallelization).





Software Design

Software Interfaces in MULTIBAT



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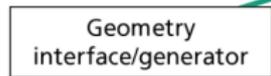
ITWM BEST Code

- Micro Li-Ion cell simulation



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UU Geometry modeling



Collaborative
SEI modeling, numeric and
implementation interface

HIU/DLR cell
modeling

Integration Benchmark 1

- Using all APs
- Using all Interfaces



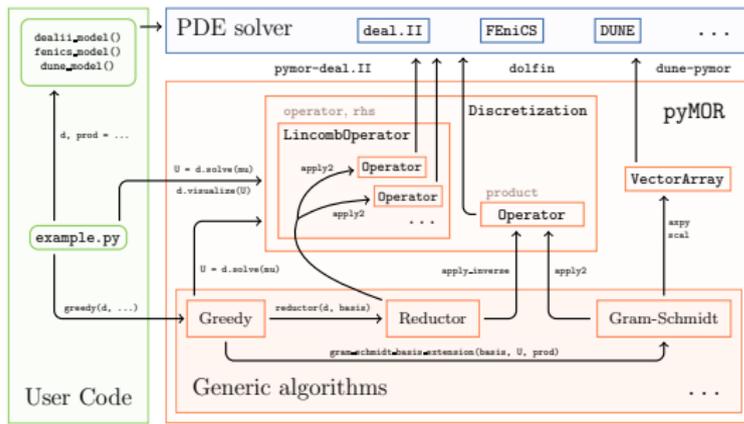
Software Interfaces in MULTIBAT

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 – Model Reduction with Python



- ▶ Quick prototyping with Python.
- ▶ Seamless integration with high-performance PDE solvers.
- ▶ Comes with small NumPy/SciPy-based discretization toolkit for getting started quickly.
- ▶ BSD-licensed, fork us on Github!

FEniCS Support included

- ▶ 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.

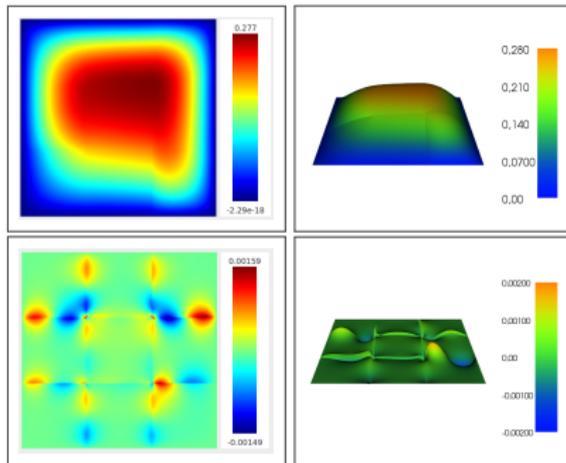


Figure: 3x3 thermal block problem
top: red. solution, bottom: red. error
left: pyMOR solver, right: FEniCS solver

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.

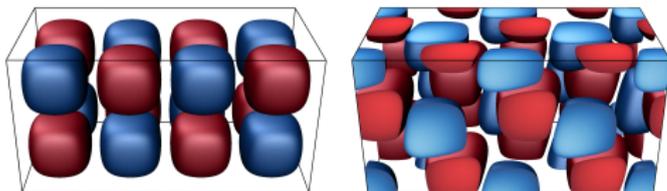


Figure: FV solution of 3D Burgers-type equation
($27.6 \cdot 10^6$ DOFs, 600 timesteps) using 

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



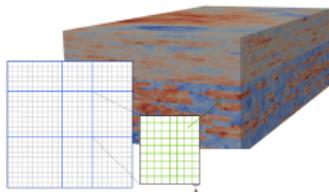
Falk Meyer



Michael Schaefer

Main Projects

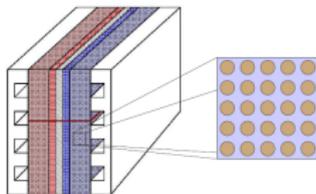
using pyMOR



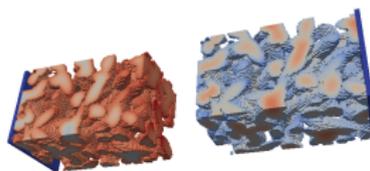
Localized Reduced Basis MultiScale method



Reduction of Maxwell's equations allowing
Arbitrary Local Modifications



Reduced basis approximation for multiscale
optimization problems

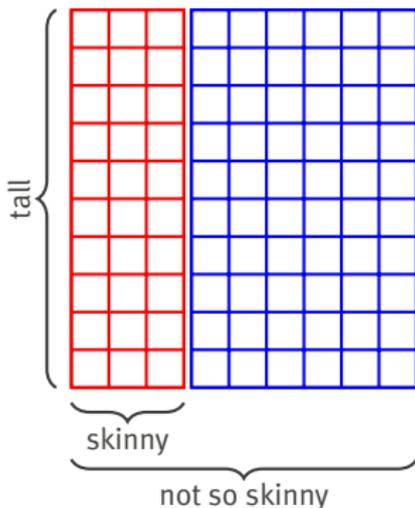


Reduction of microscale Li-ion battery models



Distributed hierarchical POD computation

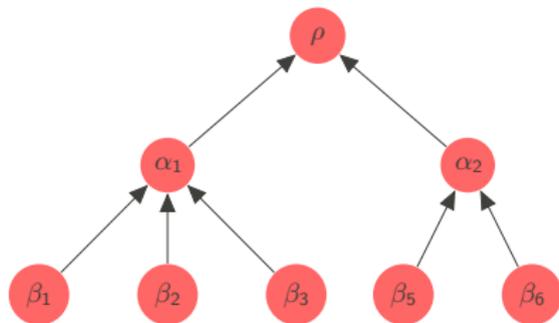
Are your tall and skinny matrices not so skinny anymore?



- ▶ Computational effort for POD scales (at least) quadratically with number of snapshots.
- ▶ Hard to parallelize.
- ▶ Really slow if data does not fit into RAM.
- ▶ **Idea:** PODs of PODs!

HAPOD – Hierarchical Approximate POD

Himpe, Leibner, R



- ▶ Input: Assign snapshot vectors to leaf nodes β_i as input.
- ▶ At each node:
 1. Perform POD of input vectors with given local error tolerance.
 2. Scale POD modes by singular values.
 3. Send scaled modes to parent node as input.
- ▶ Output: POD modes at root node ρ .

HAPOD – Hierarchical Approximate POD

Himpe, Leibner, R

Theorem (Error and mode bounds)

Choose local POD error tolerances $\varepsilon_{\mathcal{T}}$ for l^2 -mean approximation error as:

$$\varepsilon_{\mathcal{T}}(\rho) := \frac{\sqrt{|\mathcal{S}|}}{\sqrt{M_{\rho}}} \cdot (1 - \omega) \cdot \varepsilon^*, \quad \varepsilon_{\mathcal{T}}(\alpha) := \frac{\sqrt{|\mathcal{S}_{\alpha}|}}{\sqrt{M_{\alpha} \cdot (L - 1)}} \cdot \omega \cdot \varepsilon^*.$$

Then:

$$\frac{1}{|\mathcal{S}|} \sum_{s \in \mathcal{S}} \|s - P(s)\|^2 \leq (\varepsilon^*)^2 \quad \text{and} \quad |\text{HAPOD}[\mathcal{S}, \varepsilon_{\mathcal{T}}]| \leq |\text{POD}(\mathcal{S}, (1 - \omega) \cdot \varepsilon^*)|.$$

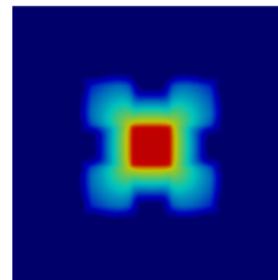
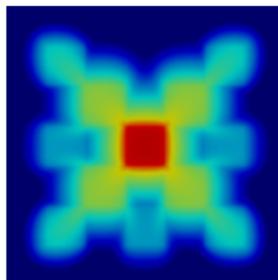
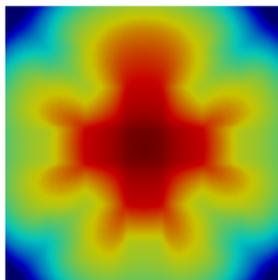
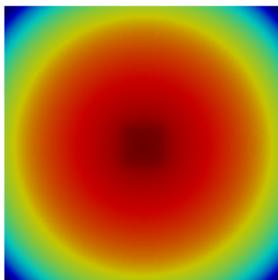
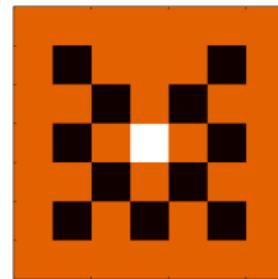
Moreover:

$$\begin{aligned} |\text{HAPOD}[\mathcal{S}, \varepsilon_{\mathcal{T}}](\alpha)| &\leq |\text{POD}(\mathcal{S}_{\alpha}, (L - 1)^{-1/2} \cdot \omega \cdot \varepsilon^*)| \\ &\leq \min_{N \in \mathbb{N}} (d_N(\mathcal{S}) \leq (L - 1)^{-1/2} \cdot \omega \cdot \varepsilon^*), \end{aligned}$$

HAPOD – Example

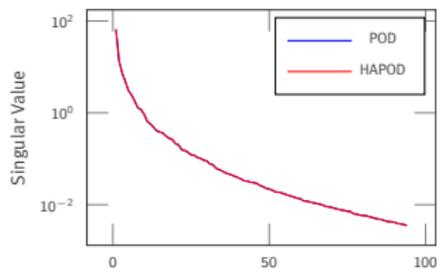
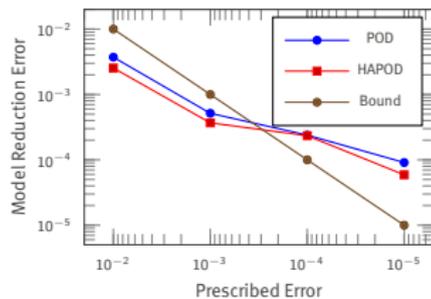
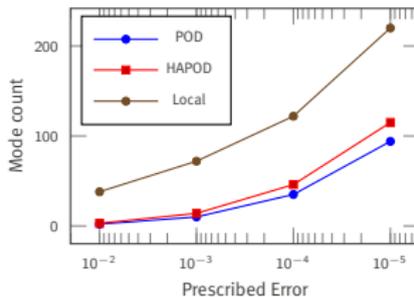
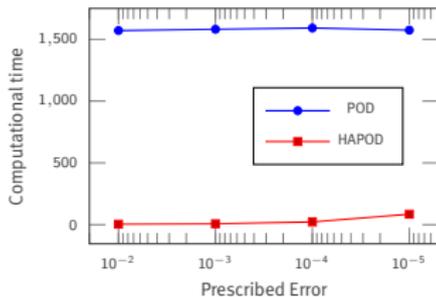
Himpe, Leibner, R

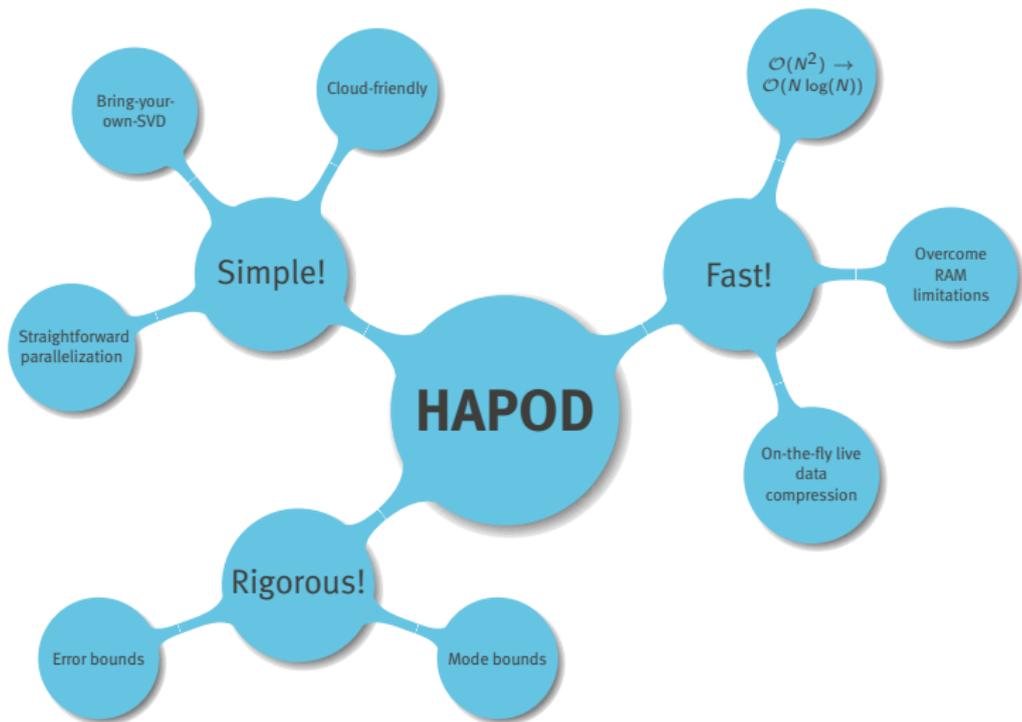
- ▶ 2D neutron transport equation.
- ▶ Moment closure/FV approximation.
- ▶ Varying absorption and scattering coefficients.
- ▶ Distributed snapshot and HAPOD computation on PALMA cluster (125 cores).



HAPOD – Example

Himpe, Leibner, R







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