WWU MÜNSTER

Model Order Reduction of Large-Scale Systems

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MM Mathematics Münster Cluster of Excellence

Outline

1. Introduction to Reduced Basis Methods
2. HAPOD – Hierarchical Approximate POD
3. Localized Reduced Basis Additive Schwarz Methods
4. Two-Scale Reduced Basis Localized Orthogonal Decomposition
5. Model Order Reduction with pyMOR

Not featured:

- Model order reduction of problems with moving shocks/boundaries via nonlinear approximation.

Introduction to Reduced Basis Methods

Reduced Basis Methods for Elliptic Problems

Parametric linear elliptic problem (full order model)

For given parameter $\mu \in \mathcal{P}$, find $u_h(\mu) \in V_h$ s.t.

$$
\begin{aligned}
a(u_h(\mu), v_h; \mu) &= f(v_h) \qquad\qquad \forall v_h \in V_h \\
y_h(\mu) &= g(u_h(\mu))
\end{aligned}
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Parametric linear elliptic problem (reduced order model)

For given $V_N \subset V_h$, let $u_N(\mu) \in V_N$ be given by Galerkin proj. onto V_N, i.e.

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RB Methods – Computing V_N

Weak greedy basis generation

function $\textsc{Weak-Greedy}(\mathcal{S}_{train} \subset \mathcal{P}, \varepsilon)$
    $V_N \leftarrow \{0\}$
    while $\max_{\mu\in\mathcal{S}_{train}} \textsc{Err-Est}(\textsc{ROM-Solve}(\mu), \mu) > \varepsilon$ **do**
        $\mu^* \leftarrow \text{arg-max}_{\mu\in\mathcal{S}_{train}} \textsc{Err-Est}(\textsc{ROM-Solve}(\mu), \mu)$
        $V_N \leftarrow \text{span}(V_N \cup \{\textsc{FOM-Solve}(\mu^*)\})$
    end while
    return V_N
end function

Err-Est

Use residual-based error estimate w.r.t. FOM (finite dimensional $\rightsquigarrow$ can compute dual norms).

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- Use dual weighted residual approach for improved convergence w.r.t to output $y_N(\mu)$.

RB Methods – Online Efficiency

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Affine decomposition

Assume that a_μ can be written as

$$a(u, v; \mu) = \sum_{q=1}^{Q} \theta_q(\mu) a_q(u, v).$$

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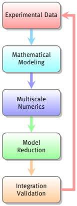
Offline/Online splitting

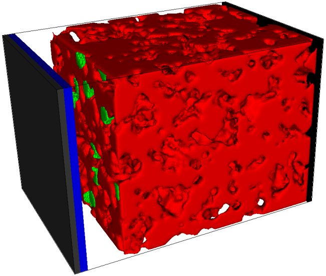
By pre-computing

$$a_q(\varphi_i, \varphi_j),\ f(\varphi_i),\ g(\varphi_i)$$

for a reduced basis $\varphi_1, \dots, \varphi_N$ of V_N, solving ROM becomes independent of dim V_h.

Example: RB Approximation of Li-Ion Battery Models





MULTIBAT: Gain understanding of degradation processes in rechargeable Li-Ion Batteries through mathematical modeling and simulation at the pore scale.

FOM:

- 2.920.000 DOFs
- Simulation time: ≈ 15.5h

ROM:

- Snapshots: 3
- dim $V_N = 245$
- Rel. err.: $< 4.5 \cdot 10^{-3}$
- Reduction time: ≈ 14h
- Simulation time: ≈ 8m
- Speedup: 120

HAPOD – Hierarchical Approximate POD

Computing V_N with POD

Offline phase

Basis for V_N is computed from **solution snapshots** $u_{\mu_s}(t)$ of full order problem via:

- Proper Orthogonal Decomposition (POD)
- POD-Greedy (= greedy search in μ + POD in t)

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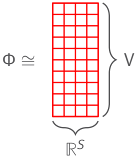
POD (a.k.a. PCA, Karhunen–Loève decomposition)

Given Hilbert space V, $\mathcal{S} := \{v_1, \dots, v_S\} \subset V$, the k-th POD mode of $\mathcal{S}$ is the k-th left-singular vector of the mapping

$$\Phi\colon \mathbb{R}^S \to V, \qquad e_s \to \Phi(e_s) := v_s$$

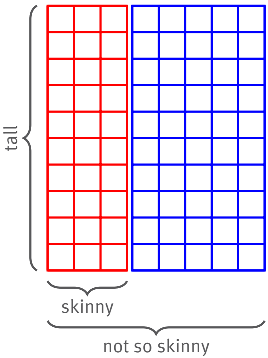


Optimality of POD

Let V_N be the linear span of first N POD modes, then:

$$\sum_{s\in\mathcal{S}} \|s - P_{V_N}(s)\|^2 = \sum_{m=N+1}^{|\mathcal{S}|} \sigma_m^2 = \min_{\substack{X\subset V\\ \dim X\leq N}} \sum_{s\in\mathcal{S}} \|s - P_X(s)\|^2$$

Are your tall and skinny matrices not so skinny anymore?



POD of large snapshot sets:

- large computational effort
- parallelization?
- data > RAM $\Longrightarrow$ disaster

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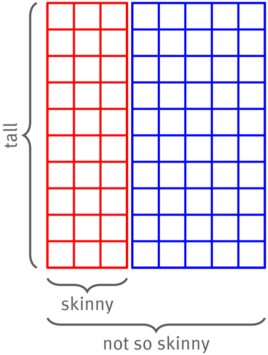

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Solution: PODs of PODs!

Disclaimer

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  We are aware of:
  [Qu, Ostrouchov, Samatova, Geist, 2002], [Paul-Dubois-Taine, Amsallem, 2015], [Brands, Mergheim, Steinmann, 2016], [Iwen, Ong, 2017].

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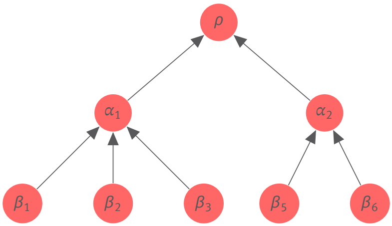
  [Qu, Ostrouchov, Samatova, Geist, 2002], [Paul-Dubois-Taine, Amsallem, 2015], [Brands, Mergheim, Steinmann, 2016], [Iwen, Ong, 2017].
- Our contributions:
  1. Formalization for arbitrary trees of worker nodes.
  2. Extensive theoretical error and performance analysis.
  3. A recipe for selecting local truncation thresholds.
  4. Extensive numerical experiments for different application scenarios.
- Can be trivially extended to low-rank approximation of snapshot matrix by keeping track of right-singular vectors.

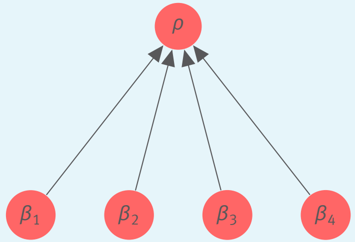
HAPOD – Hierarchical Approximate POD



- Input: Assign snapshot vectors to leaf nodes β_i as input.
- At each node α:
  1. Perform POD of input vectors with given local ℓ^2-error tolerance $\varepsilon(\alpha)$.
  2. Scale POD modes by singular values.
  3. Send scaled modes to parent node as input.
- Output: POD modes at root node ρ.

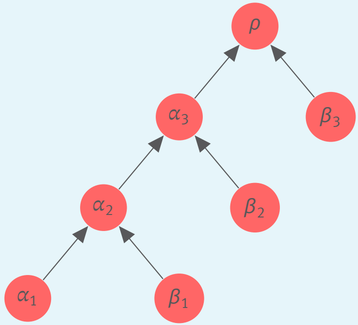
HAPOD – Special Cases

Distributed HAPOD



- Distributed, communication avoiding POD computation.

Incremental HAPOD



- On-the-fly compression of large trajectories.

HAPOD – Some Notation

Trees

$\mathcal{T}$	the tree
$\rho_{\mathcal{T}}$	root node
$\mathcal{N}_{\mathcal{T}}(\alpha)$	nodes of $\mathcal{T}$ below or equal node α
$\mathcal{L}_{\mathcal{T}}$	leafs of $\mathcal{T}$
$L_{\mathcal{T}}$	depth of $\mathcal{T}$

HAPOD

$\mathcal{S}$	snapshot set
$D\colon \mathcal{S} \to \mathcal{L}_{\mathcal{T}}$	snapshot to leaf assignment
$\varepsilon(\alpha)$	error tolerance at α
$\lvert \mathrm{HAPOD}[\mathcal{S}, \mathcal{T}, D, \varepsilon](\alpha) \rvert$	number of HAPOD modes at α
$\lvert \mathrm{POD}(\mathcal{S}, \varepsilon) \rvert$	number of POD modes for error tolerance ε
P_α	orth. proj. onto HAPOD modes at α
$\tilde{\mathcal{S}}_\alpha$	snapshots at leafs below α

HAPOD – Theoretical Analysis

Theorem (Error bound[1])

$$\sum_{s\in\widetilde{\mathcal{S}}_\alpha} \|s - P_\alpha(s)\|^2 \leq \sum_{\gamma\in\mathcal{N}_{\mathcal{T}}(\alpha)} \varepsilon(\gamma)^2.$$

[1] For special cases in appendix of [Paul-Dubois-Taine, Amsallem, 2015].

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Theorem (Mode bound)

$$\Big|\mathrm{HAPOD}[\mathcal{S}, \mathcal{T}, D, \varepsilon](\alpha)\Big| \leq \Big|\mathrm{POD}\Big(\widetilde{\mathcal{S}}_\alpha, \varepsilon(\alpha)\Big)\Big|.$$

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Theorem (Mode bound)

$$\left|\mathrm{HAPOD}[\mathcal{S},\mathcal{T},D,\varepsilon](\alpha)\right| \leq \left|\mathrm{POD}\left(\widetilde{\mathcal{S}}_\alpha, \varepsilon(\alpha)\right)\right|.$$

But how to choose ε in practice?

- Prescribe error tolerance ε^* for final HAPOD modes.
- Balance quality of HAPOD space (number of additional modes) and computational efficiency ($\omega \in [0,1]$).
- Number of input snapshots should be irrelevant for error measure (might be even unknown a priori). Hence, control ℓ^2-*mean* error $\frac{1}{|\mathcal{S}|}\sum_{s\in\mathcal{S}}\|s - P_{\rho_\mathcal{T}}(s)\|^2$.

[1] For special cases in appendix of [Paul-Dubois-Taine, Amsallem, 2015].

HAPOD – Theoretical Analysis

Theorem (ℓ^2-mean error and mode bounds)

Choose local POD error tolerances $\varepsilon(\alpha)$ *for* ℓ^2*-approximation error as:*

$$\varepsilon(\rho_{\mathcal{T}}) := \sqrt{|S|} \cdot \omega \cdot \varepsilon^*, \qquad \varepsilon(\alpha) := \sqrt{\tilde{\mathcal{S}}_\alpha} \cdot (L_{\mathcal{T}} - 1)^{-1/2} \cdot \sqrt{1 - \omega^2} \cdot \varepsilon^*.$$

Then:

$$\frac{1}{|\mathcal{S}|} \sum_{s \in \mathcal{S}} \|s - P_{\rho_{\mathcal{T}}}(s)\|^2 \leq \varepsilon^{*2} \quad \textit{and} \quad |\operatorname{HAPOD}[\mathcal{S}, \mathcal{T}, D, \varepsilon]| \leq |\overline{\operatorname{POD}}(\mathcal{S}, \omega \cdot \varepsilon^*)|,$$

where $\overline{\operatorname{POD}}(\mathcal{S}, \varepsilon) := \operatorname{POD}(\mathcal{S}, |\mathcal{S}| \cdot \varepsilon)$.

Moreover:

$$|\operatorname{HAPOD}[\mathcal{S}, \mathcal{T}, D, \varepsilon](\alpha)| \leq |\overline{\operatorname{POD}}(\tilde{\mathcal{S}}_\alpha, (L_{\mathcal{T}} - 1)^{-1/2} \cdot \sqrt{1 - \omega^2} \cdot \varepsilon^*)|$$

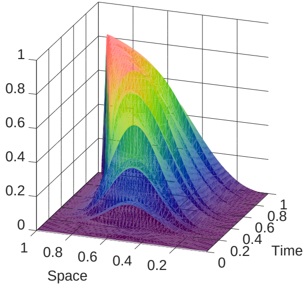
Incremental HAPOD Example

Compress state trajectory of forced inviscid Burgers equation:

$$\begin{aligned} \partial_t z(x,t) + z(x,t)\cdot\partial_x z(x,t) &= u(t)\exp(-\frac{1}{20}(x-\frac{1}{2})^2), & (x,t) &\in (0,1)\times(0,1),\\ z(x,0) &= 0, & x &\in [0,1],\\ z(0,t) &= 0, & t &\in [0,1], \end{aligned}$$

where $u(t) \in [0, 1/5]$ iid. for 0.1% random timesteps, otherwise 0.

- Upwind finite difference scheme on uniform mesh with $N = 500$ nodes.
- 10^4 explicit Euler steps.
- 100 sub-PODs, $\omega = 0.75$.
- All computations on Raspberry Pi 1B single board computer (512MB RAM).



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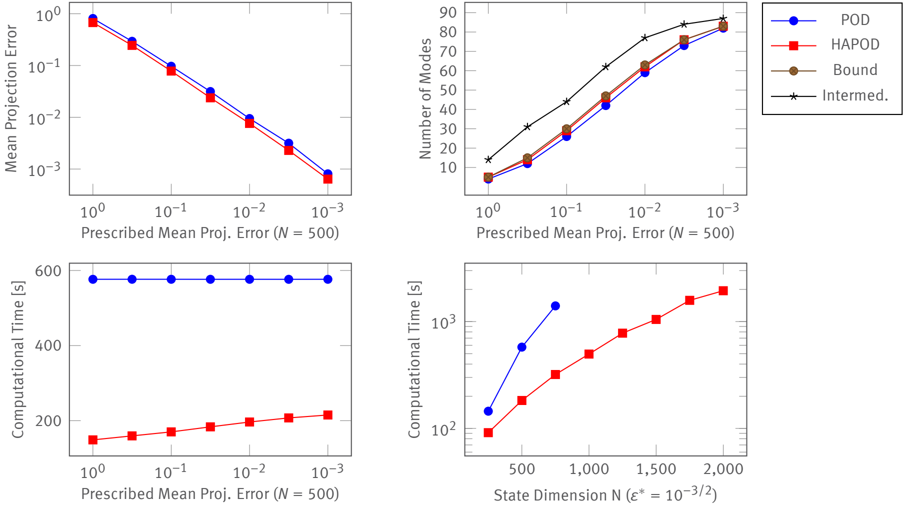
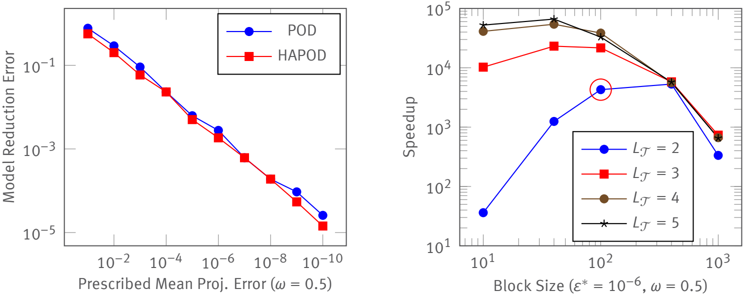


Distributed HAPOD Example

Distributed computation and POD of empirical cross Gramian:

$$\widehat{W}_{X,ij} := \sum_{m=1}^{M} \int_0^\infty \langle x_i^m(t), y_m^j(t) \rangle \, dt \in \mathbb{R}^{N \times N}$$

- 'Synthetic' benchmark model[2] from MORWiki with parameter $\theta = \frac{1}{10}$.
- Partition $\widehat{W}_X$ into 100 slices of size 10.000 × 100.



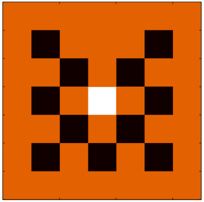
[2] See: http://modelreduction.org/index.php/Synthetic_parametric_model

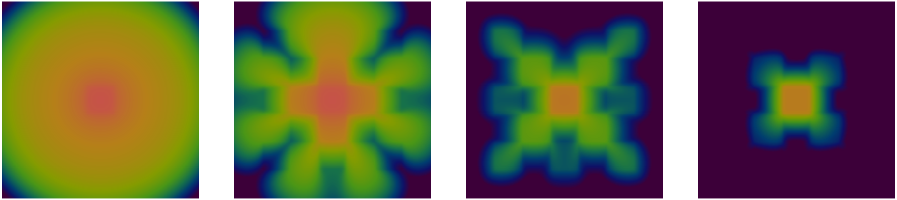
HAPOD – HPC Example

Neutron transport equation

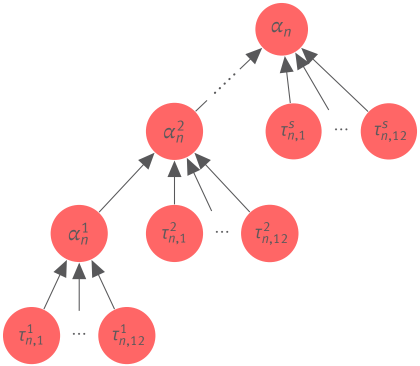
$$\partial_t \psi(t,\mathbf{x},\mathbf{v}) + \mathbf{v}\cdot\nabla_{\mathbf{x}}\psi(t,\mathbf{x},\mathbf{v}) + \sigma_t(\mathbf{x})\psi(t,\mathbf{x},\mathbf{v}) = \frac{1}{|V|}\sigma_s(\mathbf{x})\int_V \psi(t,\mathbf{x},\mathbf{w})\,\mathrm{d}\mathbf{w} + Q(\mathbf{x})$$

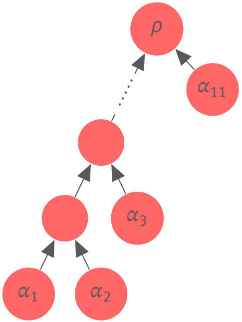
- Moment closure/FV approximation.
- Varying absorbtion and scattering coefficients.
- Distributed snapshot and HAPOD computation on PALMA cluster (125 cores).





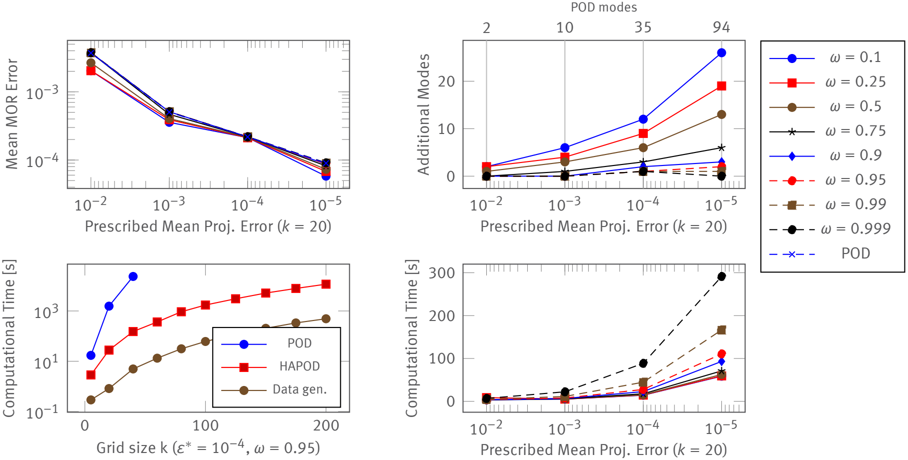
HAPOD – HPC Example





- HAPOD on compute node n. Time steps are split into s slices. Each processor core computes one slice at a time, performs POD and sends resulting modes to main MPI rank on the node.
- Incremental HAPOD is performed on MPI rank 0 with modes collected on each node.

HAPOD – HPC Example

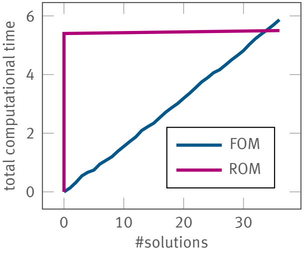


- $\approx 39.000 \cdot k^3$ doubles of snapshot data (≈ 2.5 terabyte for $k = 200$).

Localized Reduced Basis Additive Schwarz Methods

RB Method – Caveats

- Offline time too large in not-so-many-query scenarios?
- $\mathcal{P}$ too large?



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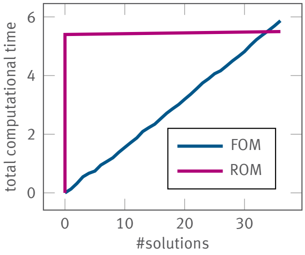

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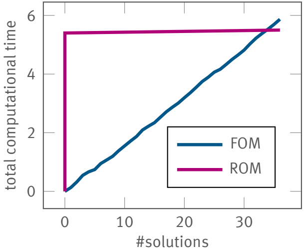

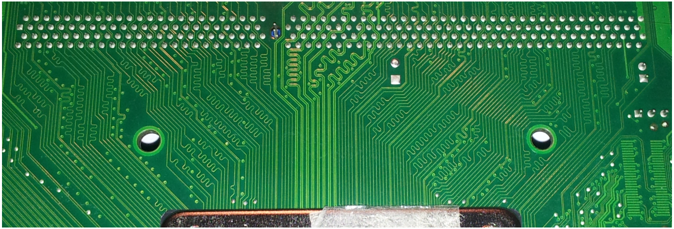

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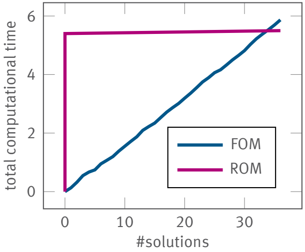

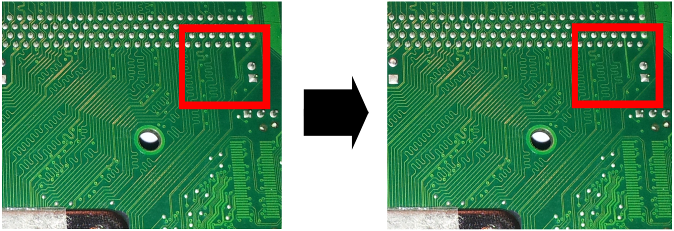

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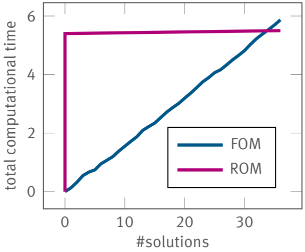
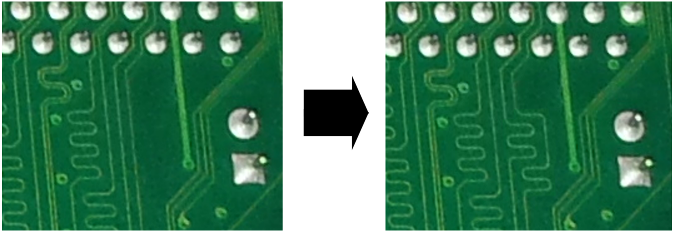




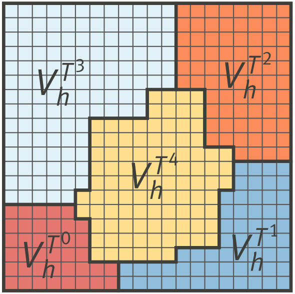
Localized RB Methods for Elliptic Problems

Idea of the **LRBMS**: given a finely-resolved grid τ_h [ALBRECHT ET AL., 2012]

- decompose approximation space into *local* spaces $V_h = \bigoplus_{T \in \mathcal{T}_H} V_h^T$
- associated with subdomains $T \in \mathcal{T}_H$

  independent local discretizations and approximation spaces (CG or DG)

  and global SWIPDG coupling [ERN, STEPHANSEN, ZUNINO, 2009]



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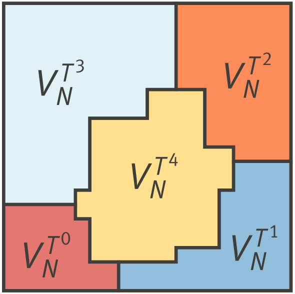
- reduced *broken* space $V_N = \bigoplus_{T \in \mathcal{T}_H} V_N^T$



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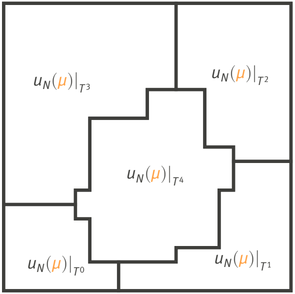
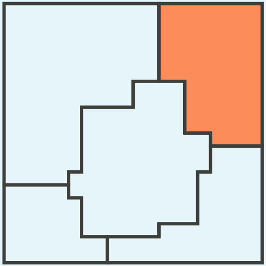
- larger V_N, but sparse ROM system matrices
- initialization of V_N^T:
  - empty
  - global solution snapshots
  - **local training**



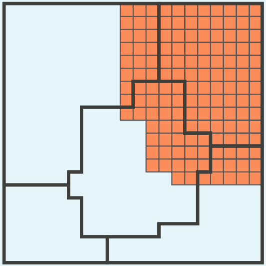
Offline Initialization of V_N

Training algorithm (adapted from [Buhr, Engwer, Ohlberger, R, 2017]) for all $T \in \mathcal{T}_H$



Offline Initialization of V_N

Training algorithm (adapted from [Buhr, Engwer, Ohlberger, R, 2017]) for all $T \in \mathcal{T}_H$



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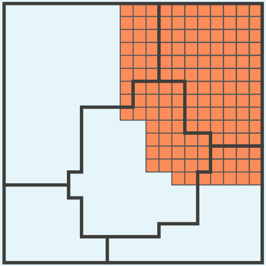

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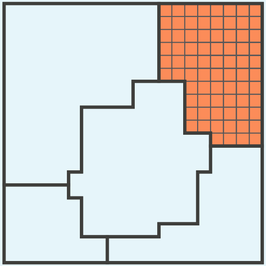

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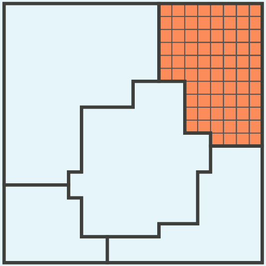

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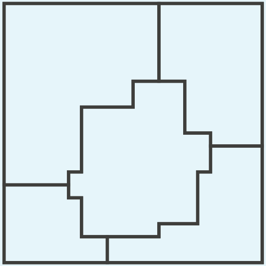
Enrichment algorithm for some $\mu \in \mathcal{P}$



- compute reduced solution $u_N(\mu)$
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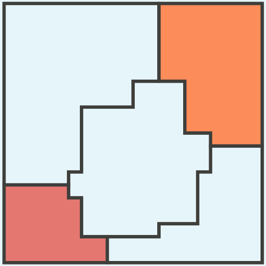

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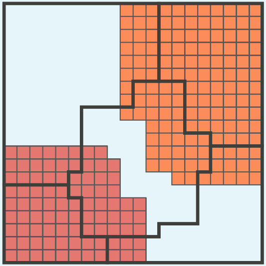

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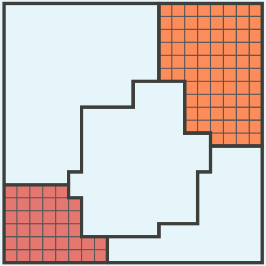

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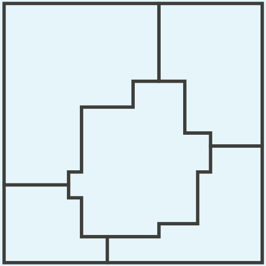

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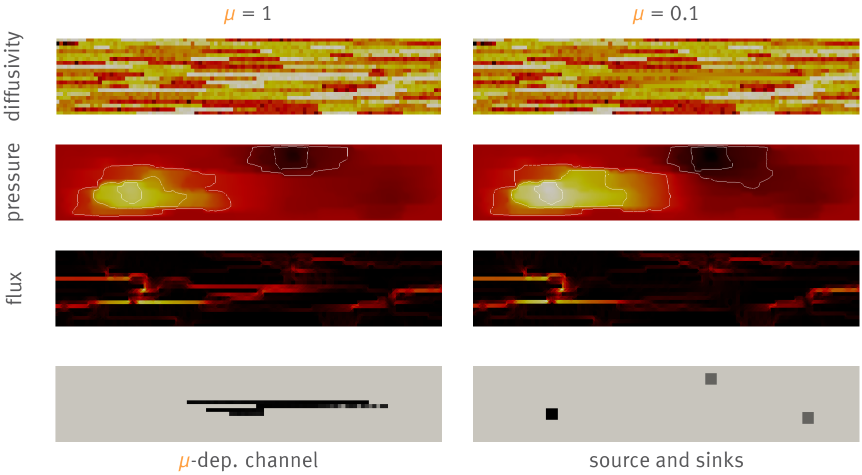
- iterate until $\eta_{h,N}(u_{\mu,N}) \leq \Delta$, return $u_N(\mu)$

$\dim V_h(T^\delta)$ |

LRBMS with online enrichment: Example SPE10



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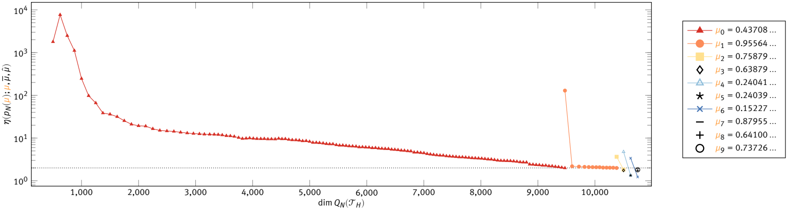
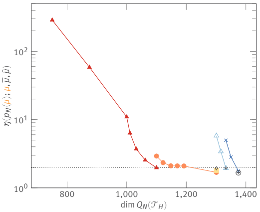
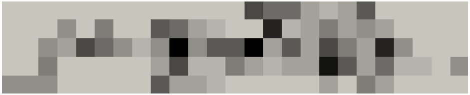


Convergence history of LRBMS with initially empty V_N



LRBMS initialized with 2 solution snapshots



Distribution of local basis size after online enrichment.

Related Approaches (incomplete)

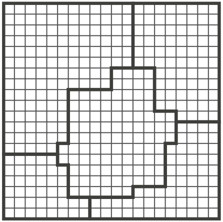
- Reduced Basis Element Method
  [Maday, Ronquist, 2002]

- Port-Reduced Static Condensation Reduced Basis Element Method
  [Eftang, Patera, 2013]

- Generalized Multiscale Finite Element Methods
  [Efendiev, Galvis, Hou 2013]

- Reduced Basis Hybrid Method
  [Iapichino, Quarteroni, Rozza, Volkwein, 2014]

- ArbiLoMod, a Simulation Technique Designed for Arbitrary Local Modifications
  [Buhr, Engwer, Ohlberger, R, 2017]



Questions

- Where should be enriched?
- How fast will enrichment converge?
- Which training method to combine with enrichment?
- How to balance training and enrichment?

Goal: Minimize total number of local V_h-dependent computations/communication events.

Connections with Domain Decomposition Methods

- Local enrichment function $\varphi_h(\mu)|_T$

$$
\begin{aligned}
a(\varphi_h(\mu), v_h; \mu) &= f(v_h) && \text{in } T^\delta \\
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corresponds to subdomain solution in Restricted Additive Schwarz (RAS) method.

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  locally(!) adaptive [Spillane, 2016] RAS multi-preconditioned CG [Bridson, Greif, 2006]

- Moreover:

  offline training of V_N

  $\cong$

  construction of coarse space

  e.g. DtN [Nataf et al., 2011], GenEO [Spillane et al., 2014], SHEM [Gander, Loneland, Rahman, 2015]

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3. In each iteration compute solution $u_N(\mu)$ via Galerkin projection onto $V_N^0 \oplus V_N^T$.
4. Use RB estimator $\eta_{h,N}(u_N(\mu);\mu)$ to locally enrich V_N^T whith AS corrections where needed:

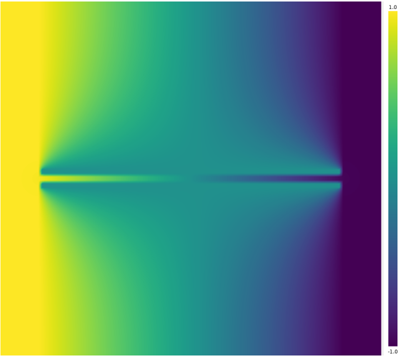
$$\eta_{h,N}(u_N(\mu);\mu)^2 := C(\mu)^2 \sum_{T \in \mathcal{T}_H} \left(\sup_{v_h \in V_h^T} \frac{f(v_h) - a(u_N(\mu), v_h; \mu)}{\|v_h\|} \right)^2$$

where, with C_{stab} the stability constant of decomposition $V_h = V_N^0 + \sum_{T \in \mathcal{T}_H} V_h^T$:

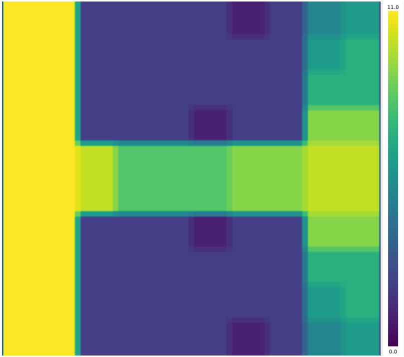
$$C(\mu) \leq C_{inf\text{-}sup}(\mu) \cdot C_{stab}$$

Simple Experiment (without μ, local non-parametric changes)

Solution (contrast: 10^5)



Number of local solutions (max=11)



- 10 × 10 subdomains
- 4 elements overlap
- 6 GenEO basis functions per domain

- enrich where $\|\mathcal{R}|_T\| \geq 0.5/|\mathcal{T}_H| \cdot \|\mathcal{R}\|$
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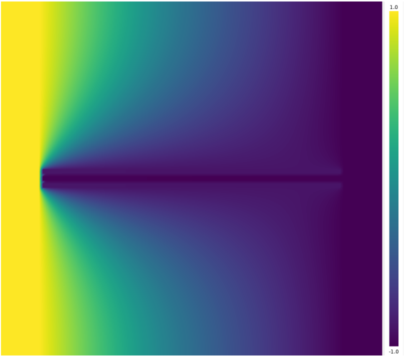

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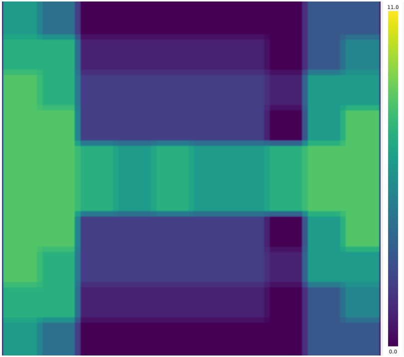

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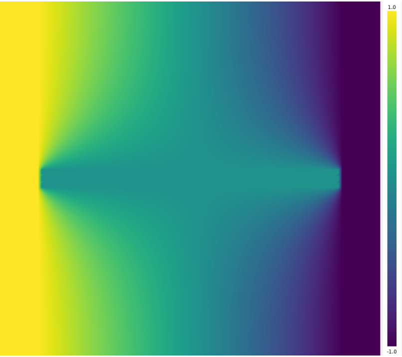

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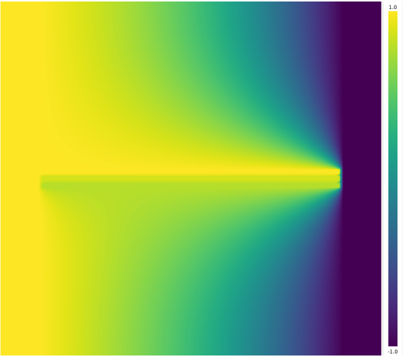

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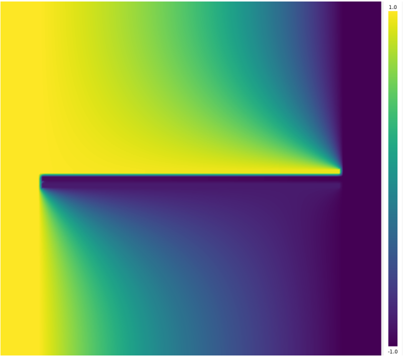

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Some Remarks

- Communication of V_h-dependet data only with neighbors of enriched subdomains.
- localized enrichment $\cong$ flexible multi-preconditioned projected CG with full orthogonalization.
- More iterations but less work.

	iterations	local solutions
PCG	118	11800
PCG + RB solution as initial value	84	8400
enrich localized (keep solutions in V_N^T)	**38**	**1803**
enrich everywhere (keep solutions in V_N^T)	36	3600
enrich localized (keep updates in V_N^T)	33	1718
enrich everywhere (keep updates in V_N^T)	29	2900

Two-Scale Reduced Basis Localized Orthogonal Decomposition

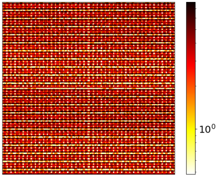
Multiscale Model Problem

Parameterized diffusion equation

For a fixed parameter $\mu \in \mathcal{P}$ find u_μ s.t.

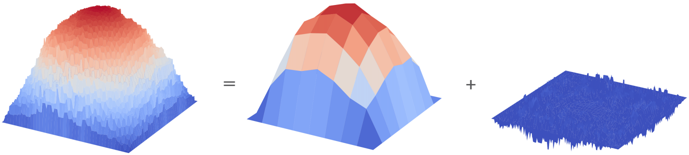
$$\begin{aligned} -\nabla \cdot A_\mu \nabla u_\mu &= f, && \text{in } \Omega, \\ u_\mu &= 0, && \text{on } \partial\Omega, \end{aligned} \qquad \text{or in weak form} \qquad a_\mu(u_\mu, v) = F(v), \quad \forall v \in V$$

- Parameter space $\mathcal{P} \subset \mathbb{R}^m$, $m \in \mathbb{N}$
- Bounded Lipschitz domain $\Omega \subset \mathbb{R}^d$, Hilbert space V.
- $f \in L^2(\Omega)$, bilinear form a_μ and functional $F \in V'$.
- Homogeneous Dirichlet boundary conditions.
- $A_\mu \in L^\infty(\Omega, \mathbb{R}^{d \times d})$ symmetric and uniformly elliptic: $0 < \alpha \leq A_\mu \leq \beta < \infty$.
- Possibly high variations in A_μ (e.g. due to soil composition).



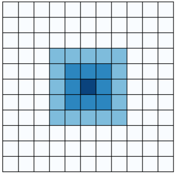
Multiscale Orthogonal Decomposition

- Fine mesh $\mathcal{T}_h$ and coarse mesh $\mathcal{T}_H$ with maximal element diameter $H \gg h$, FE spaces V_h and $V_H := V_h \cap \mathcal{P}_1(\mathcal{T}_H)$.
- Interpolation operator $\mathcal{I}_H: V_h \to V_H$ (e.g. L^2-projection).
- Finescale space $V^\mathrm{f} := \ker(\mathcal{I}_H) = \{v \in V_h \,|\, \mathcal{I}_H(v) = 0\}$, decomposition $V = V_H + V^\mathrm{f}$.



- Finescale correction $\mathcal{Q}_\mu: V_H \to V^\mathrm{f}$ defined by $$a_\mu(\mathcal{Q}_\mu v_H, v^\mathrm{f}) = a_\mu(v_H, v^\mathrm{f}), \qquad \forall\, v^\mathrm{f} \in V^\mathrm{f}.$$
- Multiscale space $V_\mu^\mathrm{ms} := (I - \mathcal{Q}_\mu)V_H$.
- a-orthogonal decomposition $V_h = V_\mu^\mathrm{ms} \oplus_a V^\mathrm{f}$.

Localization



- Truncated finescale space $V^{\mathrm{f}}(U_k(T)) := \left\{ v \in V^{\mathrm{f}} \,\middle|\, v|_{\Omega \setminus U_k(T)} = 0 \right\}$.
- For each $T \in \mathcal{T}_H$, define localized correctors $\mathcal{Q}_k^T v_H \in V^{\mathrm{f}}(U_k(T))$

$$a_{U_k(T)}(\mathcal{Q}_k^T v_H, v^{\mathrm{f}}) = a_T(v, v^{\mathrm{f}}), \qquad \forall\, v^{\mathrm{f}} \in V^{\mathrm{f}}(U_k(T)),$$

- Localized corrector operator $\mathcal{Q}_k = \sum_{T \in \mathcal{T}_H} \mathcal{Q}_k^T$.
- LOD space $V_k^{\mathrm{ms}} := \{\lambda_x - \mathcal{Q}_k \lambda_x \,|\, x \in \mathcal{N}_H\}$

Lemma [Målqvist/Peterseim ’14]

The correctors $\mathcal{Q}$ decay exponentially, e.g.

$$\|\mathcal{Q} - \mathcal{Q}_k\| \leq C_{\mathcal{Q}} k^{d/2} \theta^k \|\mathcal{Q}\|,$$

where $0 < \theta < 1$ and $C_{\mathcal{Q}}$ depends on α/β but not on the variations of A_μ.

Petrov Galerkin Formulation [Elfverson/Ginting/Henning '15]

Petrov–Galerkin LOD method

Find $u_H^{\text{ms}} \in V_k^{\text{ms}}$ such that

$$a(u_k^{\text{ms}}, v) = F(v), \qquad \forall\, v \in V_H.$$

- No interaction between correctors required.
- Reduced memory consumption.
- Still similar convergence results.

Convergence theorem

$$\left\|u_{h,\mu} - u_{H,k,\mu}\right\|_{L^2} + \left\|u_{h,\mu} - u_{H,k,\mu}^{\text{ms}}\right\|_1 \lesssim (H + \theta^k k^{d/2})\|f\|_{L^2(\Omega)}$$

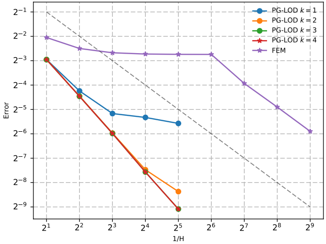


Figure: Energy error $|||u_\varepsilon - u_{H,k}^{\text{ms}}|||$ for the PG–LOD and $|||u_\varepsilon - u_h|||$ for the FEM for 1d model problem from **[Peterseim'16]**.

Two-Scale Formulation of the LOD

Two-Scale space

$$\mathfrak{V} := V_H \oplus V^{\mathrm{f}}_{h,k,T_1} \oplus \cdots \oplus V^{\mathrm{f}}_{h,k,T_{|\mathcal{T}_H|}}$$

$$|||\mathfrak{u}|||_1^2 := \|u_H\|_1^2 + \sum_{T \in \mathcal{T}_H} \left\|u^{\mathrm{f}}_T\right\|_1^2$$

Two-Scale Formulation of the LOD

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Two-scale bilinear form

$$\mathfrak{B}_\mu(\mathfrak{u}, \mathfrak{v}) := a_\mu(u_H - \sum_{T\in\mathcal{T}_H} u^{\mathrm{f}}_T, v_H) + \rho^{1/2} \sum_{T\in\mathcal{T}_H} a_\mu(u^{\mathrm{f}}_T, v^{\mathrm{f}}_T) - a^T_\mu(u_H, v^{\mathrm{f}}_T),$$

Two-Scale Formulation of the LOD

Two-Scale space

$$\mathfrak{V} := V_H \oplus V^{\mathrm{f}}_{h,k,T_1} \oplus \cdots \oplus V^{\mathrm{f}}_{h,k,T_{|\mathcal{T}_H|}}$$

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Proposition

The two-scale solution $\mathfrak{u}_\mu \in \mathfrak{V}$ of

$$\mathfrak{B}_\mu(\mathfrak{u}_\mu, \mathfrak{v}) = F(v_H) \qquad \forall \mathfrak{v} \in \mathcal{V}.$$

is uniquely determined and given by $\mathfrak{u}_\mu = \left[u_{H,k,\mu},\ \mathcal{Q}^{T_1}_{k,\mu}(u_{H,k,\mu}),\ \ldots,\ \mathcal{Q}^{T_{|\mathcal{T}_H|}}_{k,\mu}(u_{H,k,\mu})\right]$.

Two-scale Stability Estimate

Proposition

Let $\rho := C_{\text{ovl}} \cdot \kappa$, then $\mathfrak{B}_\mu$ is $|||\cdot|||_{a,\mu}$-$|||\cdot|||_1$-continuous and inf-sup stable with the following bounds on the respective constants:

$$\sup_{0\neq\mathfrak{u}\in\mathfrak{V}} \sup_{0\neq\mathfrak{v}\in\mathfrak{V}} \frac{\mathfrak{B}_\mu(\mathfrak{u},\mathfrak{v})}{|||\mathfrak{u}|||_{a,\mu}\cdot|||\mathfrak{v}|||_1} \leq \beta^{1/2} \quad \text{and} \quad \inf_{0\neq\mathfrak{u}\in\mathfrak{V}} \sup_{0\neq\mathfrak{v}\in\mathfrak{V}} \frac{\mathfrak{B}_\mu(\mathfrak{u},\mathfrak{v})}{|||\mathfrak{u}|||_{a,\mu}\cdot|||\mathfrak{v}|||_1} \geq \gamma_k/\sqrt{5}.$$

where

$$|||\mathfrak{u}|||^2_{a,\mu} := \|u_H - \sum_{T\in\mathcal{T}_H} u_T^{\mathrm{f}}\|^2_{a,\mu} + \rho \sum_{T\in\mathcal{T}_H} \|\mathcal{Q}^T_{k,\mu}(u_H) - u_T^{\mathrm{f}}\|^2_{a,\mu}$$

Error Bound

$$\left\{\|u_{H,k,\mu} - u_H\|_1^2 + \rho \sum_{T\in\mathcal{T}_H} \|\mathcal{Q}^T_{k,\mu}(u_H) - u_T^{\mathrm{f}}\|_1^2\right\}^{1/2} \leq \sqrt{5} C_{\mathcal{I}_H} \alpha^{-1/2} \gamma_k^{-1} \sup_{\mathfrak{v}\in\mathfrak{V}} \frac{\mathfrak{F}(\mathfrak{v}) - \mathfrak{B}_\mu(\mathfrak{u},\mathfrak{v})}{|||\mathfrak{v}|||_1}$$

$$\leq \sqrt{15} C_{\mathcal{I}_H} (C_{\text{ovl}} + 1)^{1/2} \kappa^{1/2} \gamma_k^{-1} \beta^{1/2} \left\{\|u_{H,k,\mu} - u_H\|_1^2 + \rho \sum_{T\in\mathcal{T}_H} \|\mathcal{Q}^T_{k,\mu}(u_H) - u_T^{\mathrm{f}}\|_1^2\right\}^{1/2}.$$

Two-Scale Reduced Basis Approach

Stage 1 (for each $T \in \mathcal{T}_H$)

ROM:

$$a_\mu(\mathcal{Q}^{T,rb}_{k,\mu}(v_H), v^{\mathrm{f}}_T) = a^T_\mu(v_H, v^{\mathrm{f}}_T), \qquad \forall v^{\mathrm{f}}_T \in V^{\mathrm{f},rb}_{k,T}.$$

Output:

$$\mathbb{K}^{rb}_\mu := \sum_{T \in \mathcal{T}_H} \mathbb{K}^{rb}_{T,\mu}, \qquad \left(\mathbb{K}^{rb}_{T,\mu}\right)_{ji} := \left(A_\mu(x_T\nabla - \nabla \mathcal{Q}^{T,rb}_{k,\mu})\phi_i\,,\, \nabla\phi_j\right)_{U_k(T)}$$

Error bound:

$$\|\mathcal{Q}^T_{k,\mu}(v_H) - \mathcal{Q}^{T,rb}_{k,\mu}(v_H)\|_{a,\mu} \leq \alpha^{-1/2} \sup_{v^{\mathrm{f}}_T \in V^{\mathrm{f}}_{h,k,T}} \frac{a^T_\mu(v_H, v^{\mathrm{f}}_T) - a_\mu(\mathcal{Q}^{T,rb}_{k,\mu}(v_H), v^{\mathrm{f}}_T)}{\|v^{\mathrm{f}}_T\|_1}.$$

Basis generation: weak greedy algorithm

Two-Scale Reduced Basis Approach

Stage 2

ROM:

$$\mathfrak{u}_\mu^{rb} := \operatorname*{arg\,min}_{\mathfrak{u}\in\mathfrak{V}^{rb}} \sup_{\mathfrak{v}\in\mathfrak{V}} \frac{\mathfrak{F}(\mathfrak{v}) - \mathfrak{B}_\mu(\mathfrak{u},\mathfrak{v})}{|||\mathfrak{v}|||_1}.$$

Error bound:

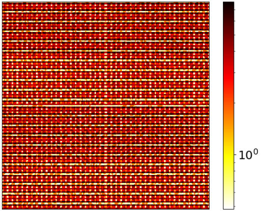
$$\left\{\|u_{H,k,\mu} - u_H\|_1^2 + \rho \sum_{T\in\mathcal{T}_H} \|\mathcal{Q}_{k,\mu}^T(u_H) - u_T^{\mathrm{f}}\|_1^2\right\}^{1/2} \leq \sqrt{5}C_{\mathcal{I}_H}\alpha^{-1/2}\gamma_k^{-1} \sup_{\mathfrak{v}\in\mathfrak{V}} \frac{\mathfrak{F}(\mathfrak{v}) - \mathfrak{B}_\mu(\mathfrak{u},\mathfrak{v})}{|||\mathfrak{v}|||_1}$$

Basis generation: weak greedy algorithm; snapshots computed with:

$$\mathbb{K}_\mu^{rb} \cdot \underline{u}_{H,k,\mu} = \mathbb{F}$$

$$\mathfrak{u}_\mu := \left[u_{H,k,\mu}, \mathcal{Q}_{k,\mu^*}^{T_1,rb}(u_{H,k,\mu}), \dots, \mathcal{Q}_{k,\mu^*}^{T,rb}(u_{H,k,\mu})\right]$$

Numerical Experiment



- $\mathcal{P} := [1, 5]^3$
- $|\mathcal{T}_h| = 67,108,864$
- $|\mathcal{T}_H| = 4,096$
- $1,024$ processes
- $\kappa \approx 16$
- Stage 2 greedy until Stage 1 error dominates.

tolerance ε_1	10^{-1}		10^{-2}	
method	RBLOD	TSRBLOD	RBLOD	TSRBLOD
$t_1^{\text{offline}}(T)$	4994	4052	10393	11241
t_1^{offline}	26008	20382	48379	53279
t_2^{offline}	-	5754	-	10385
t^{offline}	26008	26136	83403	63665
cum. size St.1	147473	94417	278528	193289
av. size St.1	9.00	23.05	17.00	47.19
size St.2	-	10	-	18
t^{LOD}	484.58		493.06	
t^{online}	3.93	0.0006	4.62	0.001
speed-up w.r.t LOD	123.15	8.32e5	106.79	4.93e5
$e_{\text{LOD}}^{H^1,\text{rel}}$	6.40e-4	1.99e-3	2.56e-5	2.04e-5
$e_{\text{LOD}}^{L^2,\text{rel}}$	1.74e-4	1.95e-3	1.86e-6	8.86e-6

Model Order Reduction with pyMOR

pyMOR main developers

Linus Balicki

René Fritze

Petar Mlinarić

Stephan Rave

Felix Schindler

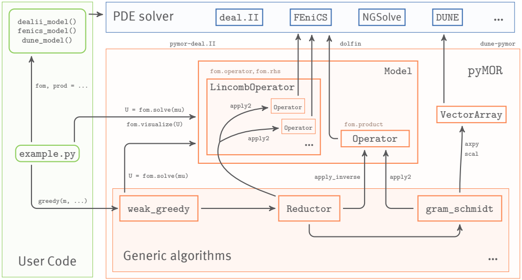
pyMOR – Model Order Reduction with Python

Goal

One library for algorithm development *and* large-scale applications.

- Started late 2012, 20k lines of Python code, 6k single commits.
- BSD-licensed, fork us on GitHub!
- Quick prototyping with Python 3.
- Comes with small `NumPy`/`SciPy`-based discretization toolkit for getting started quickly.
- Seamless integration with high-performance PDE solvers.

Generic Algorithms and Interfaces for MOR



- VectorArray, Operator, Model classes represent objects in solver's memory.
- No communication of high-dimensional data.
- Tight, low-level integration with external solver.
- No MOR-specific code in solver.

Implemented Algorithms

- Gram-Schmidt, POD, HAPOD.
- Greedy basis generation with different extension algorithms.
- Automatic (Petrov-)Galerkin projection of arbitrarily nested affine combinations of operators.
- Interpolation of arbitrary (nonlinear) operators, EI-Greedy, DEIM.
- A posteriori error estimation.
- System theory methods: balanced truncation, IRKA, ...
- Iterative linear solvers, eigenvalue computation, Newton algorithm, time-stepping algorithms.
- New! Non-intrusive MOR using artificial neural networks.

Feature Tour: FEniCS Support

- Directly interfaces FEniCS LA backend, no copies needed.
- Use same MOR code as with builtin discretization toolkit!
- Builtin support for empirical interpolation.
- Thermal block demo:
  30 SLOC FEniCS +
  15 SLOC wrapping for pyMOR.
- Easily increase FEM order, etc.

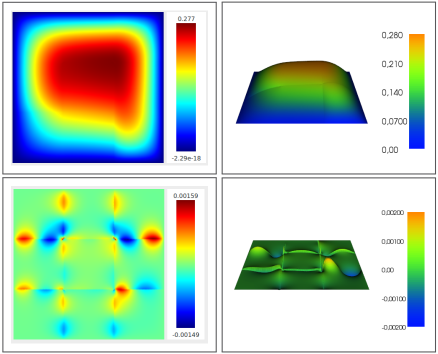


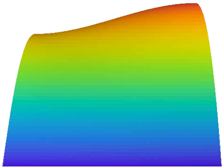
Figure: 3x3 thermal block problem
top: red. solution, bottom: red. error
left: pyMOR solver, right: FEniCS solver

Feature Tour: Empirical Interpolation with FEniCS

Nonlinear Poisson problem from FEniCS docs (for $\mu = 1$)

$$
\begin{aligned}
-\nabla \cdot \{(1 + \mu u^2(x, y)) \cdot \nabla u(x, y)\} &= x \cdot \sin(y) && \text{for } x, y \in (0, 1) \\
u(x, y) &= 1 && \text{for } x = 1 \\
\nabla u(x, y) \cdot n &= 0 && \text{otherwise}
\end{aligned}
$$

- `mesh = UnitSquareMesh(100, 100); V = FunctionSpace(mesh, "CG", 2)`.
- Time for solution: ≈ 3.4 s.
- $\mu \in [1, 1000]$, RB size: 2, EI DOFs: 5, rel. error $\approx 10^{-6}$.



- Local operator evaluation implemented using `dolfin.SubMesh`.
- Speedup: 80.
- See `fenics_nonlinear` demo.

Feature Tour: deal.II Support

- `pymor-deall.II` support module
  `https://github.com/pymor/pymor-deal.II`
- Python bindings for
  - `dealii::Vector`,
  - `dealii::SparseMatrix`.
- pyMOR wrapper classes.
- MOR demo for linear elasticity example from tutorial.

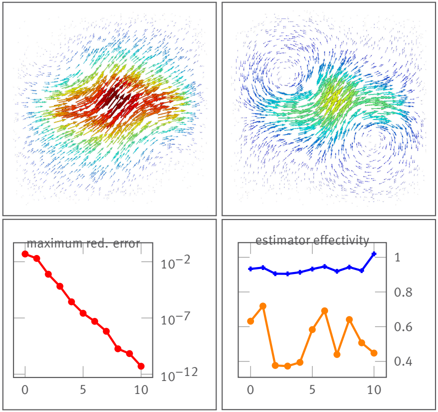


Figure: top: Solutions for $(\mu, \lambda) = (1, 1)$ and $(\mu, \lambda) = (1, 10)$, bottom: red. errs. and max./min. estimator effectivities vs. dim V_N.

Feature Tour: NGSolve Support

- Based on NGS-Py Python bindings for NGSolve.
- pyMOR wrappers for vector and matrix classes.
- 3d thermal block demo included.
- Joint work with Christoph Lehrenfeld.

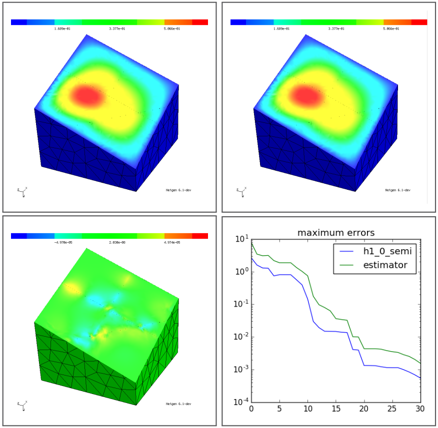


Figure: 3d thermal block problem
top: full/red. sol., bottom: err. for worst approx. μ and max. red. error vs. dim V_N.

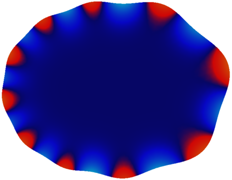
Feature Tour: MOR for an NGSolve Free Boundary Problem

[Lehrenfeld, R, 19]

Osmotic cell swelling model [Lippoth, Prokert, 2012]

Given $\Omega(0) \subset \mathbb{R}^d$, $u(0) \in H^1(\Omega(0))$ and coefficients $u_{\text{ext}}, \alpha, \beta, \gamma \in \mathbb{R}$, the **concentration** $u(t)$ and **normal velocity** w_Γ of $\Gamma(t)$ is given by:

$$
\begin{aligned}
\partial_t u - \alpha \Delta u &= 0 && \text{in } \Omega(t), \\
w_\Gamma u + \alpha \partial_{\mathbf{n}} u &= 0 && \text{on } \Gamma(t), \\
-\beta\kappa + \gamma(u - u_{\text{ext}}) &= w_\Gamma && \text{on } \Gamma(t).
\end{aligned}
$$



- ALE formulation $\rightarrow$ diffusion coeffs nonlinear in deformation field Ψ
- Empirical interpolation w.r.t. Ψ.

Feature Tour: 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.

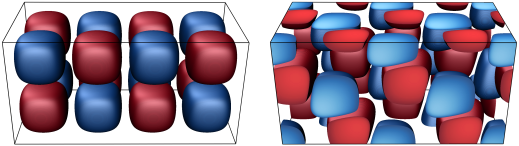


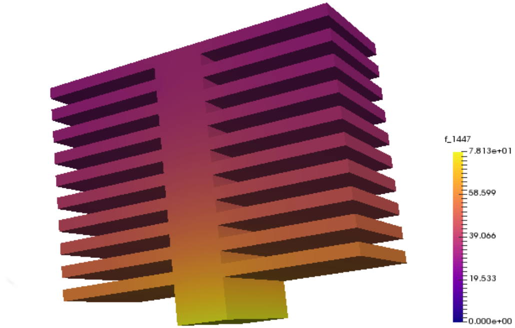
Figure: FV solution of 3D Burgers-type equation ($27.6 \cdot 10^6$ DOFs, 600 time steps) using Dune.

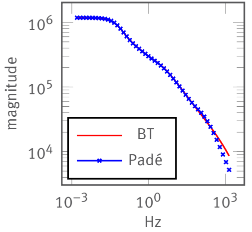
Table: Time (s) needed for solution using DUNE / DUNE with pyMOR timestepping.

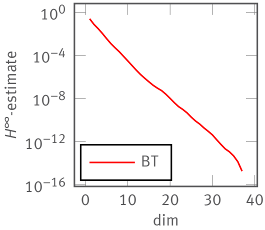
MPI ranks	1	2	3	6	12	24	48	96	192
DUNE	17076	8519	5727	2969	1525	775	395	202	107
pyMOR	17742	8904	6014	3139	1606	816	418	213	120
overhead	3.9%	4.5%	5.0%	5.7%	5.3%	5.3%	6.0%	5.4%	11.8%

Feature Tour: System-Theoretic MOR with FEniCS

- MPI distributed heatsink model with FEniCS
- Heat conduction with Robin boundary
- Input: heat flow at base
- Output: temperature at base
- MOR: Balanced truncation and Padé approximation







System-Theoretic MOR with FEniCS – Implementation

Model assembly with FEniCS

```
def discretize():
    domain = ...
    mesh = ms.generate_mesh(domain, RESOLUTION)
    subdomain_data = ...

    V = df.FunctionSpace(mesh, 'P', 1)
    u = df.TrialFunction(V)
    v = df.TestFunction(V)
    ds = df.Measure('ds', domain=mesh, subdomain_data=boundary_markers)

    A = df.assemble(- df.Constant(100.) * df.inner(df.grad(u), df.grad(v)) * df.dx
    - df.Constant(0.1) * u * v * ds(1))
    B = df.assemble(df.Constant(1000.) * v * ds(2))
    E = df.assemble(u * v * df.dx)
```

System-Theoretic MOR with FEniCS – Implementation

pyMOR wrapping

```
# def discretize (cont.)
    # monkey patch apply_inverse_adjoint, assuming symmetriy
    FenicsMatrixOperator.apply_inverse_adjoint = FenicsMatrixOperator.apply_inverse

    space = FenicsVectorSpace(V)
    A = FenicsMatrixOperator(A, V, V)
    B = VectorOperator(space.make_array([B]))
    C = B.H
    E = FenicsMatrixOperator(E, V, V)
    fom = LTIModel(A, B, C, None, E)
    return fom
```

System-Theoretic MOR with FEniCS – Implementation

pyMOR wrapping

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    # monkey patch apply_inverse_adjoint, assuming symmetriy
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    C = B.H
    E = FenicsMatrixOperator(E, V, V)
    fom = LTIModel(A, B, C, None, E)
    return fom
```

MPI wrapping

```
from pymor.tools import mpi
if mpi.parallel:
    from pymor.models.mpi import mpi_wrap_model
    fom = mpi_wrap_model(discretize, use_with=True)
else:
    fom = discretize()
```

System-Theoretic MOR with FEniCS – Implementation

Balanced Truncation

```
reductor = BTReductor(fom)
bt_rom = reductor.reduce(10)

bt_rom.mag_plot(np.logspace(-2, 4, 100), Hz=True)
```

Padé approximation

```
k = 10
V = arnoldi(fom.A, fom.E, fom.B, [0] * r)
W = arnoldi(fom.A, fom.E, fom.C, [0] * r, trans=True)
pade_rom = LTIPGReductor(fom, W, V, False).reduce()

pade_rom.mag_plot(np.logspace(-2, 4, 100), Hz=True)
```

Thank you for your attention!

Feinauer, Hein, R, Schmidt, Westhoff, et al., *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. 31, 2019.

Himpe, Leibner, R, *Hierarchical Approximate Proper Orthogonal Decomposition*, SISC 40(5), 2018.

Buhr, Engwer, Ohlberger, R, *ArbiLoMod, a Simulation Technique Designed for Arbitrary Local Modifications*, SISC, 39(4), 2017.

Gander, R, *Localized Reduced Basis Additive Schwarz Methods*, arXiv 2103.10884, 2021.

Milk, R, Schindler, *pyMOR – Generic Algorithms and Interfaces for Model Order Reduction*, SISC 38(5), 2016.

```
pip3 install pymor
```