Two-Scale Reduction of LOD Multiscale Models

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Model Reduction and Surrogate Modeling (MORE)

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Mathematics Münster
Cluster of Excellence

Outline

1. **LOD**
2. **RBLOD**
3. **TS LOD**
4. **TSRBLOD**

where

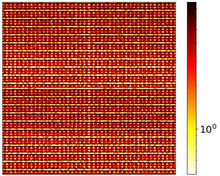
- LOD = Localized Orthogonal Decomposition
- RB = Reduced Basis
- TS = Two-Scale

Multiscale Model Problem

Parameterized diffusion equation

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

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

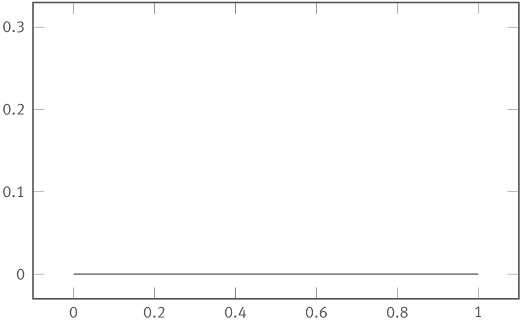


- Parameter space $\mathcal{P} \subset \mathbb{R}^p, p \in \mathbb{N}$.
- Bounded Lipschitz domain $\Omega \subset \mathbb{R}^d$.
- Homogeneous Dirichlet boundary conditions, $V := H^1_0(\Omega)$.
- $A_\mu \in L^\infty(\Omega, \mathbb{R}^{d\times d})$ symmetric and uniformly elliptic:

$$0 < \alpha \leq A_\mu \leq \beta < \infty.$$

- $f \in L^2(\Omega)$.
- Rapid change of $A_\mu(x)$, but not too high contrast $\kappa := \beta/\alpha$.

Need for Numerical Multiscale Methods



Toy example: For $\varepsilon \ll 1$, find $u_\varepsilon \in H^1_0((0,1))$ s.t.

$$-\left(A\left(\frac{x}{\varepsilon}\right)u_\varepsilon'(x)\right)' = 1$$
$$A(y) = 1 + 0.9\sin(2\pi y).$$

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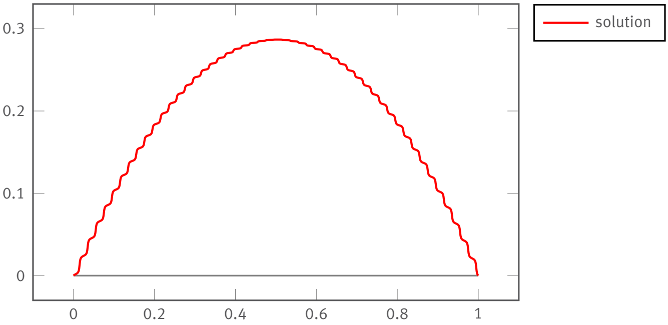

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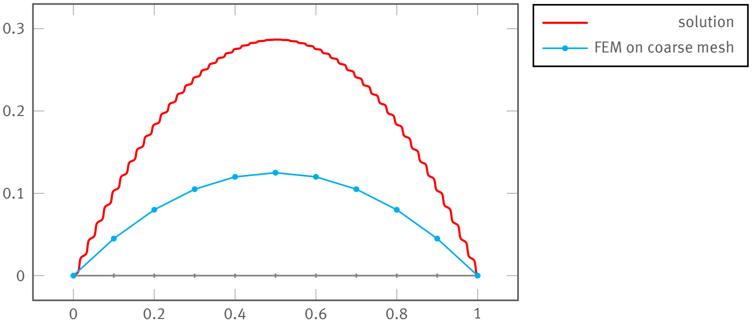

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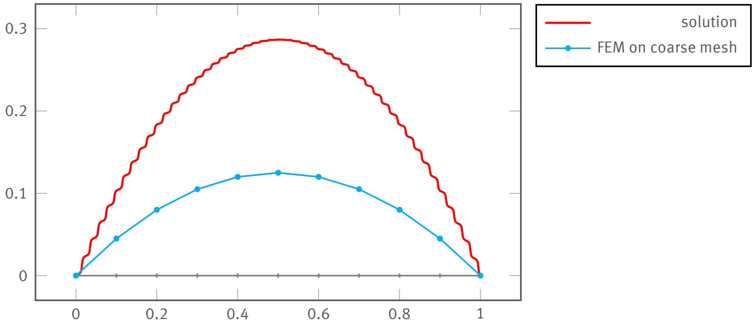

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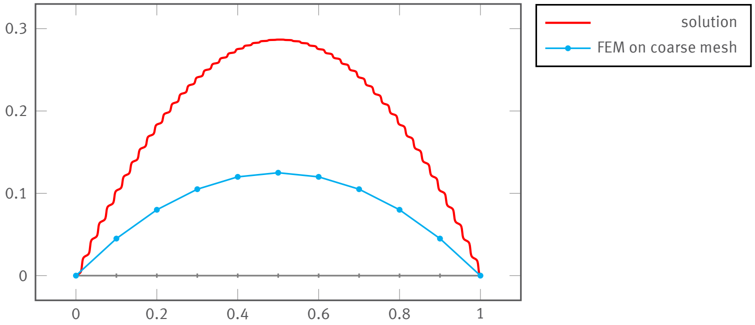

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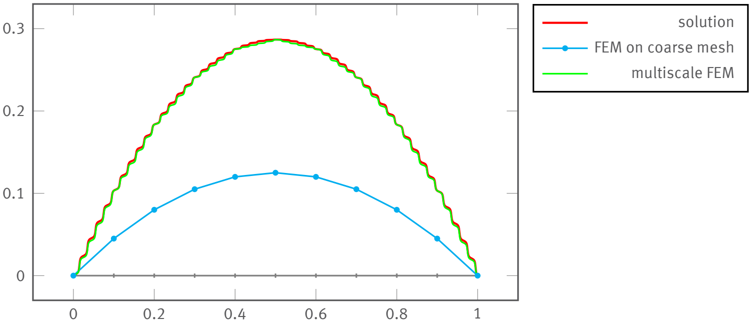

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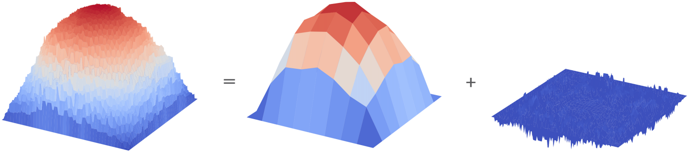
Multiscale Orthogonal Decomposition

- Fine mesh $\mathcal{T}_h$ and coarse mesh $\mathcal{T}_H$ with maximal element diameter $H \gg h$, FE spaces V_h and $V_H := V_h \cap \mathcal{P}_1(\mathcal{T}_H)$.
- Quasi-interpolation operator $\mathcal{I}_H : V_h \to V_H$ (e.g. based on local L^2-projections).
- Fine-scale space $V^{\mathrm{f}} := \ker(\mathcal{I}_H) \rightsquigarrow$ decomposition $V_h = V_H + V^{\mathrm{f}}$.



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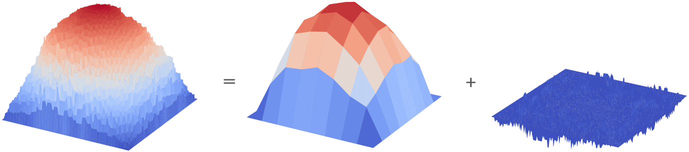

- Fine-scale correction $\mathcal{Q}_\mu : V_H \to V^{\mathrm{f}}$ defined by

$$a_\mu(\mathcal{Q}_\mu(v_H), v^{\mathrm{f}}) = a_\mu(v_H, v^{\mathrm{f}}), \qquad \forall\, v^{\mathrm{f}} \in V^{\mathrm{f}}.$$

- Multiscale space $V^{\mathrm{ms}}_{H,\mu} := (I - \mathcal{Q}_\mu)V_H \rightsquigarrow a_\mu$-orthogonal decomposition $V_h = V^{\mathrm{ms}}_\mu \oplus_{a_\mu} V^{\mathrm{f}}$.

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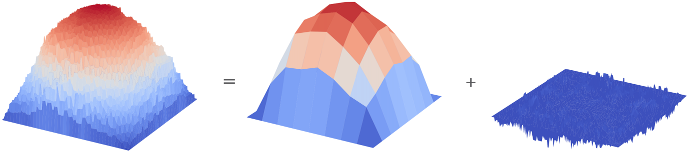

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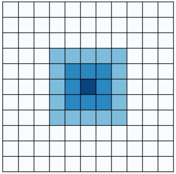
Problem: Computing $\mathcal{Q}_\mu$ as hard as finding $u_{h,\mu}$!

Localization



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

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

- Localized corrector operator $\mathcal{Q}_{k,\mu} = \sum_{T \in \mathcal{T}_H} \mathcal{Q}^T_{k,\mu}$.
- LOD space $V^{\mathrm{ms}}_{H,k,\mu} := (I - \mathcal{Q}_{k,\mu}) V_H = \left\{ \phi_x - \mathcal{Q}_{k,\mu}(\phi_x) \,\middle|\, x \in \mathcal{N}_H \right\}$

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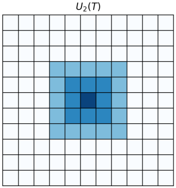

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Lemma [Målqvist/Peterseim '14]

The correctors $\mathcal{Q}_\mu(\phi_x)$ decay exponentially, hence,

$$\|\!|\mathcal{Q}_\mu(\phi_x) - \mathcal{Q}_{k,\mu}(\phi_x)\|\!| \le C_{\mathcal{Q}} k^{d/2}\, \theta^k \|\!|\mathcal{Q}_\mu(\phi_x)\|\!|,$$

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

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

Petrov–Galerkin LOD method

Find $u^{\mathrm{ms}}_{H,k,\mu} \in V^{\mathrm{ms}}_{H,k,\mu}$ such that

$$a_\mu(u^{\mathrm{ms}}_{H,k,\mu}, v) = F(v), \qquad \forall\, v \in V_H.$$

Advantages of PG over Galerkin:

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

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Convergence theorem

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

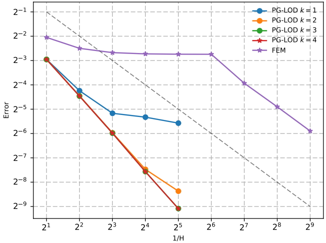

Figure: Energy error $|\!|\!| u - u^{ms}_{H,k,\mu} |\!|\!|$ for the PG–LOD and $|\!|\!| u - u_H |\!|\!|$ for 1d model problem from **[Peterseim'16]**.

RBLOD[1] [Abdulle, Henning, 15]

Idea: Accelerate LOD by applying RB methodology to corrector problems

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

[1] We present here a slight variation of the original work.

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The approximate LOD coarse-scale system matrix $\mathbb{K}^{rb}_\mu$ can then be pre-assembled as

$$\left(\mathbb{K}^{rb}_\mu\right)_{ji} = a_\mu(\varphi_i - \mathcal{Q}^{T,rb}_{k,\mu}(\varphi_i), \varphi_j) = a_\mu(\varphi_i, \varphi_j) - \sum_T \underbrace{a_\mu}_{\sum_{q=1}^Q \theta_q(\mu) a^q} \Big(\underbrace{\mathcal{Q}^{T,rb}_{k,\mu}(\varphi_i)}_{\sum_{n=1}^{N_T} c_n \psi^T_n \in V^{\mathrm{f},rb}_{k,T}}, \varphi_j\Big) \qquad (\star)$$

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Benefit: $\mathbb{K}^{rb}_\mu$ can be assembled independently of $\dim V_h$!

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Shortcomings:

- Size of $\mathbb{K}^{rb}_\mu$ still depends on dim V_H, which might be large.
- Rigorous a posteriori error control for RBLOD solution?
- Apply RB to coarse-scale problem? $(\star)$ leads to large dim V_H-dependent affine decomposition!

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Two-Scale Formulation of the LOD in homogenization: [Allaire, 92], for HMM: [Ohlberger, 05]

Two-scale space

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

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

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Two-scale bilinear form

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

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Proposition

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

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

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 $\rho := C_{\mathrm{ovl}} \cdot \kappa$, 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 γ_k is the PG–LOD inf-sup constant and

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

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Error Bound

$$|||\mathfrak{u}_\mu - \mathfrak{u}|||_{a,\mu} \leq \sqrt{5}\gamma_k^{-1} \sup_{\mathfrak{v}\in\mathfrak{V}} \frac{\mathfrak{F}(\mathfrak{v}) - \mathfrak{B}_\mu(\mathfrak{u},\mathfrak{v})}{|||\mathfrak{v}|||_1} \leq \sqrt{5}\,\underbrace{\gamma_k^{-1}\beta^{1/2}}_{\sim\kappa^{1/2}}|||\mathfrak{u}_\mu - \mathfrak{u}|||_{a,\mu}.$$

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Error Bound

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

Two-Scale Reduced Basis Approach

Idea: Accelerate LOD by applying RB methodology to two-scale problem

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

Since we only have inf-sup stability of $\mathfrak{B}_\mu$, use as ROM:

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

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Benefits:

- ROM independent from dim V_h and dim V_H.
- $\mathfrak{B}_\mu$ has same affine decomposition as a_μ.
- Rigorous a posteriori error bounds.

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

Since we only have inf-sup stability of $\mathfrak{B}_\mu$, use as ROM:

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

Benefits:

- ROM independent from dim V_h and dim V_H.
- $\mathfrak{B}_\mu$ has same affine decomposition as a_μ.
- Rigorous a posteriori error bounds.

Snapshots: LOD solutions with correctors.

Caveat: Need to solve fine-scale corrector problems in each greedy iteration.

Two-Stage Two-Scale Reduced Basis Approach

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

FOM:

$$a_\mu(\mathcal{Q}^T_{k,\mu}(v_H), v^f_T) = a^T_\mu(v_H, v^f_T), \qquad \forall v^f_T \in V^f_{h,k,T}.$$

ROM:

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

Outputs:

$$a_\mu(\mathcal{Q}^{T,rb}_{k,\mu}(v_H), \phi_j), \qquad a^T_\mu(\phi_i, \mathcal{Q}^{T,rb}_{k,\mu}(v_H))$$

Error bound:

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

Basis generation: weak greedy algorithm w. error tolerance ε_1

Two-Stage Two-Scale Reduced Basis Approach

Stage 2

FOM:

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

ROM:

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

Error bound:

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

Basis generation: 'weak' greedy algorithm w. error tolerance ε_2

Snapshots:

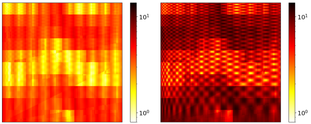
$$\mathbb{K}_\mu^{rb} \cdot \underline{u}_{H,k,\mu^*} = \mathbb{F}$$

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

Numerical Experiment 1

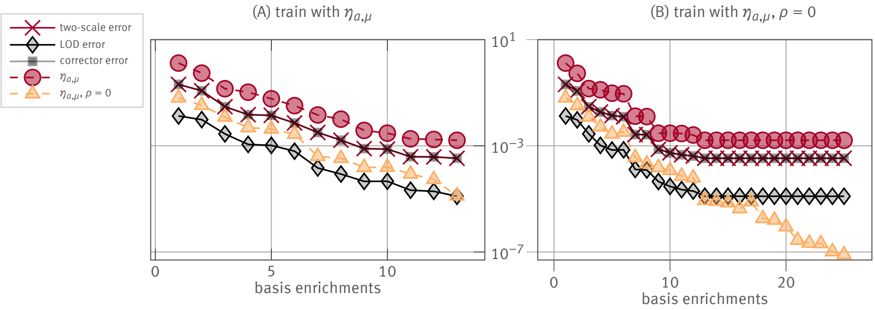
[Abdulle/Henning'15]

- $\mathcal{P} := [0, 5]$
- $A_\mu = \sum_{q=1}^{Q} \theta_q(\mu) A_q$ with $Q = 4$
- $|\mathcal{T}_h| = 65,536$
- $\varepsilon_1 = \varepsilon_2 = 0.001$
- two samples of A_μ:



$\|\mathcal{T}_H\|$	$2^3 \times 2^3$		$2^4 \times 2^4$		$2^5 \times 2^5$	
method	RBLOD	TSRBLOD	RBLOD	TSRBLOD	RBLOD	TSRBLOD
$t_{1,\mathrm{av}}^{\mathrm{offline}}(T)$	41	61	39	61	33	55
t_1^{offline}	71	106	67	102	63	98
t_2^{offline}	-	8	-	56	-	472
t^{offline}	71	114	67	158	63	570
cum. size St.1	2346	1670	8718	6134	31810	22189
av. size St.1	9.16	26.09	8.51	23.96	7.77	21.67
size St.2	-	8	-	9		9
t^{LOD}	0.69		0.49		0.90	
t^{online}	0.0610	0.0003	0.2272	0.0003	1.0462	0.0003
speed-up LOD	11	2506	2	1536	1	2714
$e_{\mathrm{LOD}}^{H^1,\mathrm{rel}}$	1.97e-5	7.30e-4	5.08e-5	2.94e-4	1.11e-4	4.21e-4
$e_{\mathrm{LOD}}^{L^2,\mathrm{rel}}$	4.89e-6	2.71e-4	6.77e-6	1.03e-4	7.70e-6	1.32e-4
$e_{\mathrm{FEM}}^{L^2,\mathrm{rel}}$	2.46e-2	2.46e-2	9.05e-3	9.05e-3	3.98e-3	3.98e-3
$e_{\text{LOD-FEM}}^{L^2,\mathrm{rel}}$	2.46e-2		9.05e-3		3.98e-3	

Numerical Experiment 1: Stage 1 error in Stage 2 training



- **left plot:** $\eta_{a,\mu}$ detects dominant Stage 1 error and aborts enrichment.
- **right plot:** Ignoring Stage 1 error contributions leads to overfitted ROMs without further error decay.

Numerical Experiment 2

- $A_\mu = \sum_{q=1}^{3} \mu_q A_q$
- $\mathcal{P} := [1, 5]^3$
- $|\mathcal{T}_h| = 67,108,864$
- $|\mathcal{T}_H| = 4,096$
- $\kappa \approx 16$
- 1,024 processes
- $\varepsilon_1 = 0.01$ and $\varepsilon_2 = 0.02$.

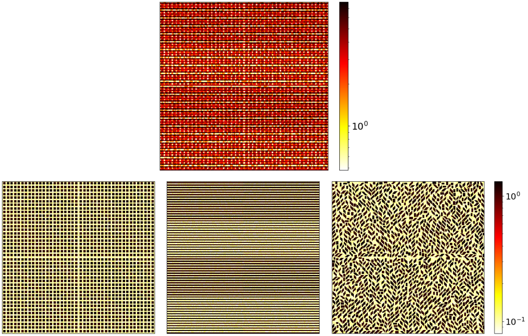


Figure: Coefficient A_μ on **4 coarse elements** for $\mu = (1, 2, 3)^T$ (top center) and A_q for all $q = 1, \dots, 3$ (bottom).

Numerical Experiment 2

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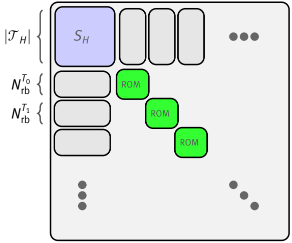
method	RBLOD	TSRBLOD
$t_1^{\text{offline}}(T)$	10278	11289
t_1^{offline}	49436	54837
t_2^{offline}	-	9206
t^{offline}	49436	64043
cum. size St.1	278528	193289
av. size St.1	17.00	47.19
size St.2	-	16
storage	409MB	28KB
t^{LOD} (parallel)	515	
t^{online} (sequential)	4.39	0.0005
speed-up w.r.t LOD	117	9.57e5
$e_{\text{LOD}}^{H^1,\text{rel}}$	1.95e-5	4.43e-4
$e_{\text{LOD}}^{L^2,\text{rel}}$	2.36e-5	4.49e-4

Some Remarks

- $\mathfrak{B}_\mu$ has a sparse block structure and never needs to be assembled.
- Stage 1 can be performed in parallel without communication.
- Stage 2 completely dim V_h independent.



Block structure of $\mathfrak{B}_\mu$ w.r.t. Stage 2 full-order space.

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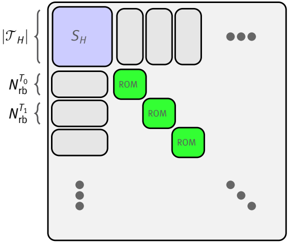
- ε_1 can be chosen small to ensure stage 2 greedy succeeds (only offline time affected).
- Adaptive strategies for locally decreasing ε_1 easily possible.



Block structure of $\mathfrak{B}_\mu$ w.r.t. Stage 2 full-order space.

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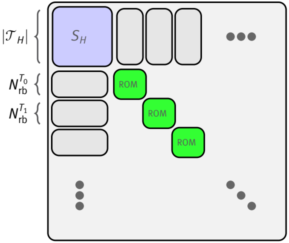
- Stage 1 can be performed in parallel without communication.
- Stage 2 completely dim V_h independent.
- ε_1 can be chosen small to ensure stage 2 greedy succeeds (only offline time affected).
- Adaptive strategies for locally decreasing ε_1 easily possible.
- Error analysis also applies in the RBLOD case.
- Can be extended to other problem classes.



Block structure of $\mathfrak{B}_\mu$ w.r.t. Stage 2 full-order space.

Thank you for your attention!

Keil, Rave, *An Online Efficient Two-Scale Reduced Basis Approach for the Localized Orthogonal Decomposition*, arXiv:2111.08643, 2021.