# Online-Adaptive Localized Reduced Basis Approximation of Parameterized Parabolic Problems

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# Outline

1. A Localized Reduced Basis Method for Elliptic Problems.
2. A General Parabolic A Posteriori Error Estimate.
3. A Localized Reduced Basis Method for Parabolic Problems.

# A Localized Reduced Basis Method for Elliptic Problems

# Parametric Model Order Reduction

Consider time-dependent parametric problems

$$\Phi_h : \mathcal{P} \to L^2([0,T]; V_h), \qquad s : L^2([0,T]; V_h) \to \mathbb{R}^S$$

where

- $\mathcal{P} \subset \mathbb{R}^P$ parameter domain.
- $V_h$ "truth" solution state space, $\dim V_h \gg 0$.
- $\Phi_h$ maps parameters to solutions (*hard* to compute).
- $s$ maps state vectors to quantities of interest.

## Objective

Compute

$$s \circ \Phi_h : \mathbb{R}^P \to L^2([0,T]; V_h) \to \mathbb{R}^S$$

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

# Reduced Basis Methods: Three Basic Ideas

## Objective

Compute
$$s \circ \Phi_h : \mathbb{R}^P \to L^2([0, T]; V_h) \to \mathbb{R}^S$$

**When $\Phi_h$, $s$ sufficiently smooth,** quickly computable low-dimensional approximation of $s \circ \Phi_h$ should exist.

- **Idea 1:** State space projection:
  - Define approximation $\Phi_N : \mathcal{P} \to L^2([0, T]; V_N)$, $N := \dim V_N \ll \dim V_h$, via (Petrov-)Galerkin projection.
  - Approximate $s \circ \Phi_h \approx s \circ \Phi_N$.
- **Idea 2:** Construct $V_N$ from PODs of solution snapshots $\Phi_h(\mu_1), \ldots, \Phi_h(\mu_k)$.
- **Idea 3:** Select $\mu_1, \ldots, \mu_k$ iteratively via offline greedy search over $\mathcal{P}$ using quickly computable surrogate $\eta(\Phi_N(\mu), \mu) \geq \|\Phi_h(\mu) - \Phi_N(\mu)\|$ (POD-Greedy).

**+ affine decomposition / hyper-reduction (EIM, DEIM, GEIM, Gappy POD, ...)**

# Example: RB Approximation of Li-Ion Battery Models

ulm university universität uulm

Institute of Technical Thermodynamics

MULTIBAT

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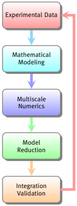
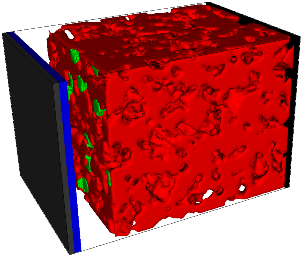


**MULTIBAT:** Gain understanding of degradation processes in rechargeable Li-Ion Batteries through mathematical modeling and simulation at the pore scale.

Full order model:

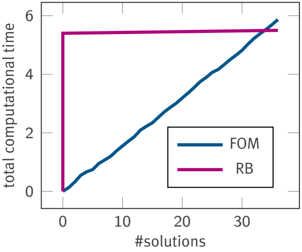
- 2.920.000 DOFs
- Simulation time: $\approx$ 13h

Reduced order model:

- Snapshots: 3
- $\dim V_N = 145$
- Rel. err.: $< 1.5 \cdot 10^{-3}$
- Reduction time: $\approx$ 9h
- Simulation time: $\approx$ 5m
- Speedup: **154**

# Caveats

- Offline time too large in not-so-many-query scenarios?
- $\mathcal{P}$ too large?
- $\Phi_h$ accurate for all $\mu \in \mathcal{P}$?
- $\Phi_h$ actually computable?




Some solutions:

- online-adaptivity of $V_N$
- $\mathcal{P}$-localization of $V_N$
- $\mathcal{P}$-adaptivity of $V_h$
- $\Omega$-localization of $V_N$

**Wanted**

Efficient a posteriori error indicators:

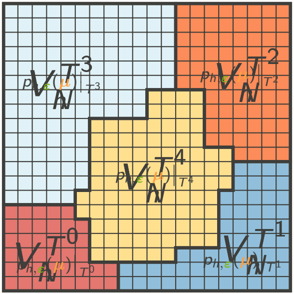
- ROM to FOM/true error
- localized in $\mathcal{P}$ / $\Omega$

# Localized RB Methods for Elliptic Problems

Idea of the **LRBMS:** given a *multi-purpose highly-resolved* grid $\tau_h$

- decompose approximation space into *local* spaces $V_h = \bigoplus_{T \in \mathcal{T}_H} V_h^T$
- associated with *arbitrary* (connected) subdomains $T \in \mathcal{T}_H$
  independent local discretizations and approximation spaces (CG or DG)
  and global SWIPDG coupling [Ern, Stephansen, Zunino, 2009]
- build local reduced spaces $V_N^T \subset V_h^T$
- reduced *broken* space $V_N = \bigoplus_{T \in \mathcal{T}_H} V_N^T$

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



# Localized A Posteriori Error Estimate

## Error Estimate

[Ohlberger, Schindler, 2014],[Ern, Stephansen, Vohralík, 2010]

$$|\!|\!| p(\mu) - \tilde{p}(\mu) |\!|\!|_{\mu}^2 \leq \eta(\tilde{p}(\mu);\mu)^2 := \sum_{T\in\mathcal{T}_H} \eta_{nc}^T(\tilde{p}(\mu))^2 + \eta_r^T(\tilde{p}(\mu))^2 + \eta_{df}^T(\tilde{p}(\mu);\mu)^2$$

where

- nonconformity estimator: $I_{OS}[\cdot] \in H_0^1(\Omega)$
  $\eta_{nc}^T(\tilde{p}(\mu);\mu) := |\!|\!| \tilde{p}(\mu) - I_{OS}[\tilde{p}(\mu)] |\!|\!|_{\mu,T}$
- residual estimator: $-\sigma(\mu)\nabla_h\cdot \approx R_h[\cdot] \in H_{\mathrm{div}}(\Omega)$
  $\eta_r^T(\tilde{p}(\mu)) := (C_P^T/c_\sigma^T)^{1/2} h_T \|f - \nabla\cdot R_h[\tilde{p}(\mu);\mu]\|_{L^2,T}$
- diffusive flux estimator:
  $\eta_{df}^T(\tilde{p}(\mu);\mu) := \left\|(\sigma(\mu))^{-1/2}(\sigma(\mu)\nabla_h\tilde{p}(\mu) + R_h[\tilde{p}(\mu);\mu])\right\|_{L^2,T}$

- provides an estimate on
  - discretization error: $\tilde{p}(\mu) = p_h(\mu)$
  - full error: $\tilde{p}(\mu) = p_N(\mu)$
- include $1 \in \tilde{V}_N^T$ for each $T \in \mathcal{T}_H$.

# Localized A Posteriori Error Estimate – Remarks

## Estimate on ROM-/FOM-approximation vs. analytical solution

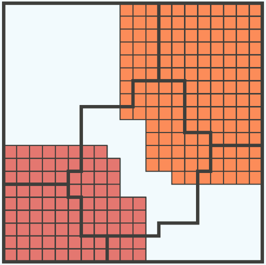
- key ingredient: diffusive flux reconstruction $R_h$, locally conservative w.r.t. $\mathcal{T}_H$
- fully computable upper bound
- offline/online decomposable (under some assumptions on $\sigma(\mu)$)
- localized w.r.t. subdomains $T \in \mathcal{T}_H$
- locally efficient (with a factor of $H/h$)

$\Rightarrow$ local mesh refinement ([Ali, Steih, Urban, 2016], [Yano, 2015], [Yano, 2016]), if discretization insufficient

$\Rightarrow$ local basis enrichment, if reduced space insufficient

# Online-Adaptive Enrichment of $V_N$

## LRBMS: online — for some $\mu \in \mathcal{P}$



- compute reduced solution $p_N(\mu)$
- estimate error $\eta_{h,N}(\mu)$
- if $\eta_{h,N}(\mu) > \Delta$, start intermediate local enrichment phase:
  - compute local error indicators
  - mark subdomains for enrichment: $\mathcal{X} = \mathtt{mark}(\mathcal{T}_H)$
  - solve corrector problem on overlapping subdomain $T^\delta \supset T$ for all $T \in \mathcal{X}$:

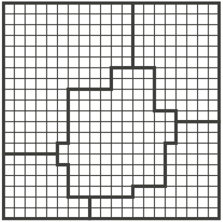
$$b(\varphi_h(\mu), q_h; \mu) = (f, q_h) \qquad \text{in } T^\delta$$
$$\varphi_h(\mu) = p_N(\mu) \qquad \text{on } \partial T^\delta$$

  - extend local reduced basis for all $T \in \mathcal{X}$:

$$V_N^T := \mathtt{gram\_schmidt}(\{V_N^T \cup \varphi_h(\mu)|_T\})$$

  - update reduced quantities
  - compute updated reduced solution $p_N(\mu)$ and $\eta_{h,N}(\mu)$
- iterate until $\eta_{h,N}(p_N(\mu)) \leq \Delta$, return $p_N(\mu)$

# Related Approaches



- Reduced basis element Method
  [Maday, Ronquist, 2002]
- Reduced basis hybrid Method
  [Iapichino, Quarteroni, Rozza, Volkwein, 2014]
- Port-reduced static condensation Reduced basis element Method
  [Eftang, Patera, 2013]
- ArbiLoMod, a Simulation Technique Designed for Arbitrary Local Modifications
  [Buhr, Engwer, Ohlberger, R, 2017]

# A General Parabolic A Posteriori Error Estimate

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# Parabolic Parametric Problems

## Model

For a Gelfand triple $V \subset H \subset V'$, an end time $T > 0$ and $\mu \in \mathcal{P}$,
find $p(\mu, \cdot) \in L^2(0, T; V)$ with $\partial_t p(\mu, \cdot) \in L^2(0, T; V')$, $p(\mu, 0) = p_0(\mu) \in V$, s.t.

$$< \partial_t p(\mu, t), q > \; + b(p(\mu, t), q; \mu) = (f, q)_H \qquad \forall q \in V, t \in [0, T].$$

## Approximation

Consider $\tilde{V} \subset H$, find an approximation $\tilde{p}(\mu, \cdot) \in L^2(0, T; \tilde{V})$, $\partial_t \tilde{p}(\mu, \cdot) \in L^2(0, T; \tilde{V})$, s.t.

$$\big(\partial_t \tilde{p}(\mu, t), \tilde{q}\big)_H + b(\tilde{p}(\mu, t), \tilde{q}; \mu) = (f, \tilde{q})_H \qquad \forall \tilde{q} \in \tilde{V}, t \in [0, T].$$

## FEM/DG

$$V = H_0^1(\Omega) \subset L^2(\Omega) = H$$
$$\tilde{V} = V_h(\tau_h) \subset L^2(\Omega)$$

## RB

$$V = H = V_h(\tau_h)$$
$$\tilde{V} = V_N \subset V_h(\tau_h)$$

## LRBMS

$$V = H_0^1(\Omega) \subset L^2(\Omega) = H$$
$$\tilde{V} = V_N \subset V_h(\tau_h)$$

# Elliptic Reconstruction

[Makridakis, Nochetto, 2003]

## Definition

Given $\tilde{p} \in \tilde{V}$, define the *elliptic reconstruction* $\mathcal{E}(\tilde{p}; \mu) \in V$, as the solution of

$$b(\mathcal{E}(\tilde{p}; \mu), q; \mu) = \big(\tilde{B}(\tilde{p}; \mu) + f - \tilde{\Pi}(f), q\big)_H \qquad \text{for all } q \in V. \qquad \text{(ELL)}$$

where

| | | | |
|---|---|---|---|
| $\tilde{B}(\tilde{p}; \mu) \in \tilde{V}$ | $H$-Riesz representative of $b(\tilde{p}, \cdot; \mu)$: | $(\tilde{B}(\tilde{p}; \mu), \tilde{q})_H = b(\tilde{p}, \tilde{q}; \mu)$ | $\forall \tilde{q} \in \tilde{V}$ |
| $\tilde{\Pi}(f) \in \tilde{V}$ | $H$-orthogonal projection of $f$: | $(\tilde{\Pi}(\tilde{p}), \tilde{q})_H = (\tilde{p}, \tilde{q})_H$ | $\forall \tilde{q} \in \tilde{V}$ |

## Proposition

$\tilde{p} \in \tilde{V}$ is the $\tilde{V}$-Galerkin approximation of the solution $\mathcal{E}(\tilde{p}; \mu) \in V$ of (ELL).

## Proof

$$\begin{aligned}\big(\tilde{B}(\tilde{p}; \mu) + f - \tilde{\Pi}(f), \tilde{q}\big)_H &= \big(\tilde{B}(\tilde{p}; \mu), \tilde{q}\big)_H + \big(f, \tilde{q}\big)_H - \big(\tilde{\Pi}(f), \tilde{q}\big)_H \\ &= b(\tilde{p}, \tilde{q}; \mu) \qquad \forall \tilde{q} \in \tilde{V}\end{aligned}$$

# Elliptic Reconstruction

[Makridakis, Nochetto, 2003]

## Definition

Given $\tilde{p} \in \tilde{V}$, define the *elliptic reconstruction* $\mathcal{E}(\tilde{p};\mu) \in V$, as the solution of

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where

$\tilde{B}(\tilde{p};\mu) \in \tilde{V}$ $H$-Riesz representative of $b(\tilde{p}, \cdot;\mu)$: $(\tilde{B}(\tilde{p};\mu), \tilde{q})_H = b(\tilde{p}, \tilde{q};\mu) \quad \forall \tilde{q} \in \tilde{V}$

$\tilde{\Pi}(f) \in \tilde{V}$ $H$-orthogonal projection of $f$: $(\tilde{\Pi}(\tilde{p}), \tilde{q})_H = (\tilde{p}, \tilde{q})_H \quad \forall \tilde{q} \in \tilde{V}$

## Proposition

$\tilde{p} \in \tilde{V}$ is the $\tilde{V}$-Galerkin approximation of the solution $\mathcal{E}(\tilde{p};\mu) \in V$ of (ELL).

$\Rightarrow$ We can estimate $\|\mathcal{E}(\tilde{p}) - \tilde{p}\|$ by *any* a posteriori estimate on the elliptic problem (ELL)!

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# Parabolic Estimate

## Error identity

For arbitrary $\tilde{p}(t) \in \tilde{V}$ and $\mathcal{R}_T(\tilde{p};\mu)(t) \in \tilde{V}$ the $H$-Riesz representative of the time-stepping:

$$< \partial_t(p(\mu,t) - \tilde{p}(\mu,t)), q > + b(p(\mu,t) - \mathcal{E}(\tilde{p}(\mu,t), q;\mu) = (-\mathcal{R}_T[\tilde{p};\mu](t), q) \quad \forall q \in V$$

## Abstract estimate

[Georgoulis, Lakkis, Virtanen, 2011][Ohlberger, R, Schindler, 2017]

Let $C := (3|||b|||_\mu + 2)^{1/2}$ and $C^b_{H,V,\mu}$, s.t. $\|q\|_H \leq C^b_{H,V,\mu} |||q|||_\mu \quad \forall q \in V$. Then

$$\begin{aligned}
\|p(\mu) - \tilde{p}\|_{L^2(0,T,|||\cdot|||_\mu)} \leq\ & \left\|p(\mu,0) - \tilde{p}^c(0)\right\|_H \\
+\ & C\left\|\tilde{p}^d\right\|_{L^2(0,T;|||\cdot|||_\mu)} + 2\left\|\partial_t\tilde{p}^d\right\|_{L^2(0,T;|||\cdot|||_{\mu,-1})} \\
+\ & (C+1)\left\|\mathcal{E}(\tilde{p};\mu) - \tilde{p}\right\|_{L^2(0,T;|||\cdot|||_\mu)} \\
+\ & 2C^b_{H,V,\mu}\left\|\mathcal{R}_T[\tilde{p}]\right\|_{L^2(0,T;H)}
\end{aligned}$$

$$\begin{matrix} \tilde{p} = & \tilde{p}^c & + & \tilde{p}^d \\ \Cap & \Cap & & \Cap \\ \tilde{V} & V & & \tilde{V} \end{matrix}$$

$\Rightarrow$ bound $|||\mathcal{E}(\tilde{p}(t);\mu) - \tilde{p}(t)||| \leq \eta_{\text{ell}}(\tilde{p})$ by an elliptic estimate on (ELL)

# Parabolic Estimate

## Abstract estimate

[Georgoulis, Lakkis, Virtanen, 2011][Ohlberger, R, Schindler, 2017]

$$\|p(\mu) - \tilde{p}\|_{L^2(0,T,|||\cdot|||_\mu)} \leq \left\|p(\mu,0) - \tilde{p}^c(0)\right\|_H + C\left\|\tilde{p}^d\right\|_{L^2(0,T;|||\cdot|||_\mu)} + 2\left\|\partial_t\tilde{p}^d\right\|_{L^2(0,T;|||\cdot|||_{\mu,-1})} + (C+1)\left\|\mathcal{E}(\tilde{p};\mu) - \tilde{p}\right\|_{L^2(0,T;|||\cdot|||_\mu)} + 2C^b_{H,V,\mu}\left\|\mathcal{R}_T[\tilde{p}]\right\|_{L^2(0,T;H)}$$

$$\tilde{p} = \tilde{p}^c + \tilde{p}^d, \quad \tilde{p} \in \tilde{V}, \quad \tilde{p}^c \in V, \quad \tilde{p}^d \in \tilde{V}$$

## FEM/DG

$$V = H^1_0(\Omega) \subset L^2(\Omega) = H$$
$$\tilde{V} = V_h(\tau_h) \subset L^2(\Omega)$$

$\Rightarrow$ discretization error

## RB

$$V = H = V_h(\tau_h)$$
$$\tilde{V} = V_N \subset V_h(\tau_h)$$

$\Rightarrow$ ROM error

## LRBMS

$$V = H^1_0(\Omega) \subset L^2(\Omega) = H$$
$$\tilde{V} = V_N \subset V_h(\tau_h)$$

$\Rightarrow$ ROM + discretization error

# Parabolic Estimate - Time Discrete Version

## Corollary

Let $\tilde{V} \subseteq V$, $p_0(\mu) \in \tilde{V}$ and

$$\left(\frac{1}{\Delta t}(p^{n+1}(\mu) - p^{n+1}(\mu)), q\right)_H + b(p^{n+1}(\mu), q; \mu) = (f, q)_H \qquad \forall q \in V,$$

$$\left(\frac{1}{\Delta t}(\tilde{p}^{n+1}(\mu) - \tilde{p}^{n+1}(\mu)), \tilde{q}\right)_H + b(\tilde{p}^{n+1}(\mu), \tilde{q}; \mu) = (f, \tilde{q})_H \qquad \forall \tilde{q} \in \tilde{V}.$$

Then:

$$\sum_{n=1}^{N} \|p^n(\mu) - \tilde{p}^n(\mu)\|_\mu \leq \sum_{n=1}^{N} \|\mathcal{E}(\tilde{p}^n(\mu); \mu) - \tilde{p}^n(\mu)\|_\mu$$

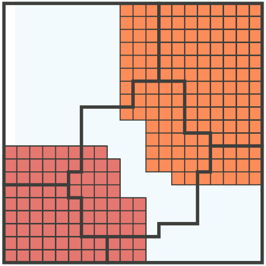
# A Localized Reduced Basis Method for Parabolic Problems

# Parabolic LRBMS

- Use same space decomposition $V_h = \bigoplus_{T \in \mathcal{T}_H} V_h^T$ as in elliptic case.
- Same SWIPDG coupling as in elliptic case.
- Block diagonal mass matrix.
- Use parabolic estimate with localized elliptic estimator.

# Online-Adaptive Enrichment of $V_N$

## Parabolic LRBMS: online — for some $\mu \in \mathcal{P}$



- compute reduced solution $p_N(\mu, t)$
- estimate error $\eta_{h,N}(\mu)$
- if $\eta_{h,N}(\mu) > \Delta$, start intermediate local enrichment phase:
  - compute local error indicators
  - mark subdomains for enrichment: $\mathcal{X} = \mathtt{mark}(\mathcal{T}_H)$
  - solve corrector problem on overlapping subdomain $T^\delta \supset T$ for all $T \in \mathcal{X}$:

$$(\partial_t \varphi_h(\mu, t), q_h)_H + b(\varphi_h(\mu, t), q_h; \mu) = (f, q_h) \qquad \text{in } T^\delta$$
$$\varphi_h(\mu, t) = p_N(\mu, t) \qquad \text{on } \partial T^\delta$$
$$\varphi_h(\mu, 0) = p_h(\mu, 0)$$

  - extend local reduced basis for all $T \in \mathcal{X}$:

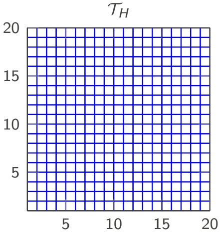
$$V_N^T := V_N^T \oplus \mathtt{pod}(\{\varphi_h(\mu, t)|_T - \Pi_{V_N^T} \varphi_h(\mu, t)|_T \mid t \in [0, T]\})$$

  - update reduced quantities
  - compute updated reduced solution $p_N(\mu)$ and $\eta_{h,N}(\mu)$
- iterate until $\eta_{h,N}(p_N(\mu)) \leq \Delta$, return $p_N(\mu)$

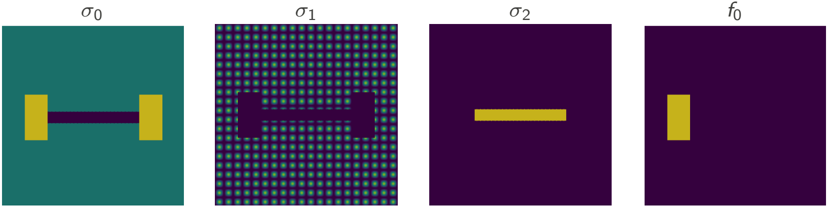
# A First Experiment

Solve for $t \in [0,1]$, $\Omega := [0,1]^2$, $\mu \in \mathcal{P} := [0,1] \times [0.1, 100]$:

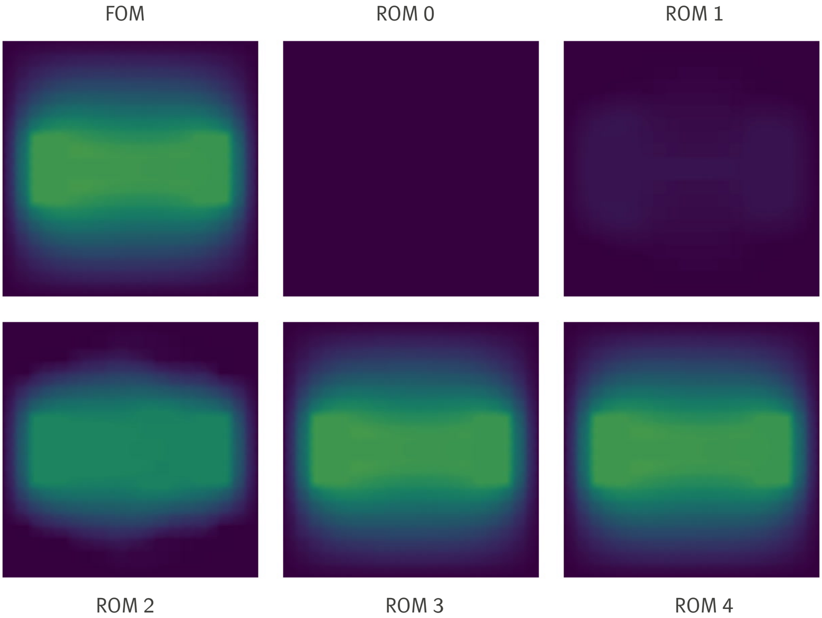
$$\partial_t p(\mu, t) - \nabla \cdot [(\sigma_0 + \mu_1\sigma_1 + \mu_2\sigma_2)\nabla p(\mu, t)] = \sin(4\pi t)^2 f_0$$
$$p(\mu, t)|_{\partial\Omega} = 0$$
$$p(\mu, 0) = 0$$




- dim $V_h = 960000$, $\Delta t = 0.01$, 1 layer oversampling

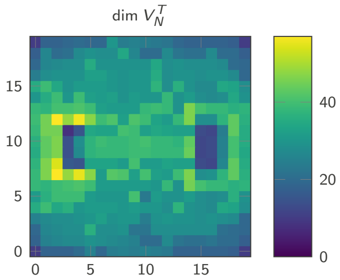


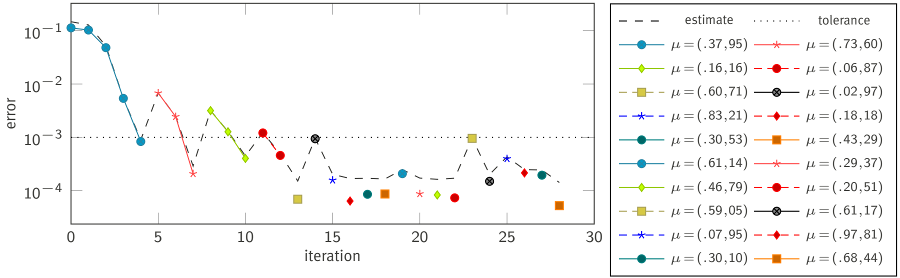
# Experiment: First Online Enrichment ($\mu = [0.37, 95]$)



# Experiment: Convergence

- Solve for 20 random $\mu \in \mathcal{P}$.
- Enrich until $\eta_{h,N}(\mu) < \Delta := 0.001$.
- $\eta_{ell,h,N} := \|\mathcal{E}(p_N(\mu)) - p_N(\mu)\|_{L^2([0,T];|||\cdot|||_\mu)}$



# Outlook

- Use online-efficient estimator for $\eta_{ell,h,N}$.
- Remove obsolete subspaces of $V_N^T$.
- Time localization of enrichment problems.
- Scale to $> 10^8$ DOFs.

# Thank you for your attention!

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