Reduced basis methods for the resolution of parameter-dependent PDEs
MS13

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1 Reminders

- Reduced Basis Methods
- POD-Galerkin
- POD + TP VF

2 aposteriori errors

Reduced Basis Methods (RBM)

$PDE : \boldsymbol{\mu} \to u(\boldsymbol{\mu})$

$\boldsymbol{\mu} \in \mathcal{G}$: Parameter

$u(\boldsymbol{\mu})$: Solution $u_h(\boldsymbol{\mu};\ \mathbf{x}) = \sum_{i=1}^{\mathcal{N}} u_i(\boldsymbol{\mu}) w_i(\mathbf{x})$,

$$\begin{cases} -\nabla \cdot \big(a(\boldsymbol{\mu})\nabla u\big) = f(\boldsymbol{\mu}) & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega. \end{cases}$$

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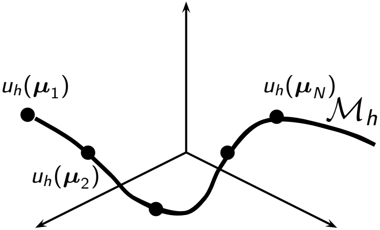
Solution manifold

Solution manifold: $\mathcal{M} = \{u(\boldsymbol{\mu}) |\ \boldsymbol{\mu} \in \mathcal{G}\}$
HF solution manifold: $\mathcal{M}_h = \{u_h(\boldsymbol{\mu}) |\ \boldsymbol{\mu} \in \ \mathcal{G}\}$

How can we reduce the manifold complexity?

Reduced space

V^N Reduced space



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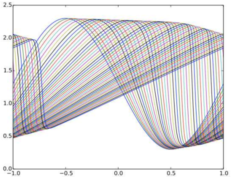

Fig. 1: Snapshots of the solution to the unsteady viscous Burger equation with $u_0 = \lambda$
$\lambda = 1.3$, $\nu = 4$, $\varepsilon = 0.04$

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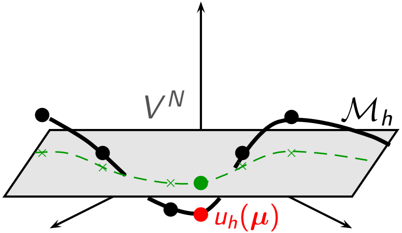

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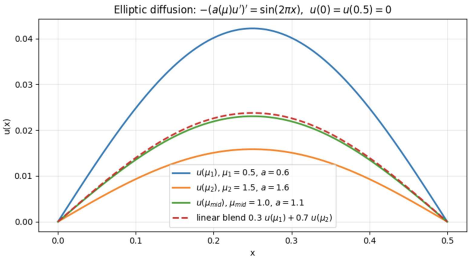

$$V_N = \mathrm{Span}\{u_1, u_2, \ldots u_N\}$$

where $u_1, \ldots, u_N$ = snapshots

Reduced Basis Methods (RBM)

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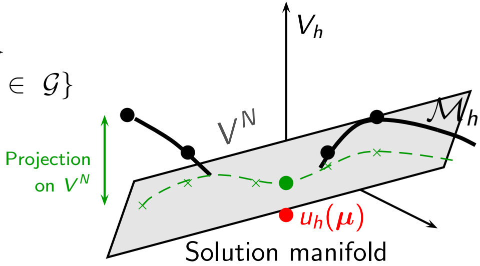

Reduced space

V^N Reduced space

Projection on V^N:

$$\boxed{\inf_{v_N \in V^N} \|u_h - v_N\|_{V_h}.}$$

Exponential decay

$$\boxed{\forall N > 1, \quad d_N(\mathcal{M}, V) \leq Ce^{-\tau N}.}$$

Kolmogorov N-width $=$ error from the **linear** space that best fit the solution manifold:

$$\boxed{?}$$

Reduced Basis Methods

- **Offline** Construction of a reduced space V_N spanned by a reduced basis $\rightarrow$???
- **Online** Computation of the reduced coefficients α $\rightarrow$???

Reduced Basis Methods

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Reduced basis Galerkin approximation

Assume the weak formulation of the HF problem yields the discretized system

$$\mathbf{A}(\boldsymbol{\mu})\mathbf{u}(\boldsymbol{\mu}) = \mathbf{l}(\boldsymbol{\mu})$$

then

$$a\left(u_N(\boldsymbol{\mu}), v_N; \boldsymbol{\mu}\right) = \ell\left(v_N; \boldsymbol{\mu}\right)$$

gives a new system to solved:

$$\boxed{\mathbf{P}^T\mathbf{A}(\boldsymbol{\mu})\mathbf{P}\ \alpha(\boldsymbol{\mu}) = \mathbf{P}^T\mathbf{l}(\boldsymbol{\mu}),} \tag{G-RB}$$

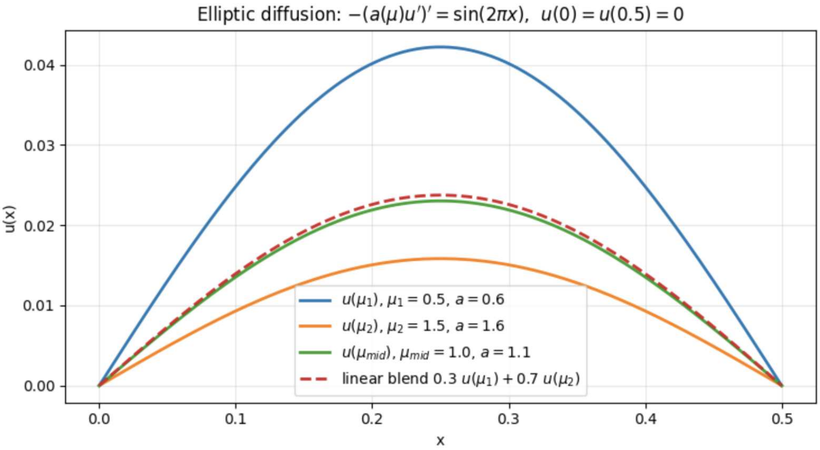
where $\mathbf{P} \in \mathbb{R}^{\mathcal{N}\times N}$. Now, we get a system where the inversion cost is in $\mathcal{O}(N^3)$ since dimensions : $\mathbf{P}^T\mathbf{A}(\boldsymbol{\mu})\mathbf{P} \in \mathbb{R}^{N\times N}$ and $\mathbf{P}^T b \in \mathbb{R}^N$!

Reduced basis Galerkin approximation

Assembling cost with the affine operators:
$\mathcal{O}(N^2 Q^a + N Q^l)$ with

$$\mathbf{P}^T \mathbf{A}(\boldsymbol{\mu}) \mathbf{P} = \sum_{q=1}^{Q^a} \theta_q^a(\boldsymbol{\mu}) \underbrace{\mathbf{P}^T \mathbf{A}_q \mathbf{P}}_{\text{precomputed offline}} , \quad \mathbf{P}^T \mathbf{l}(\boldsymbol{\mu}) = \sum_{q=1}^{Q^l} \theta_q^l(\boldsymbol{\mu}) \underbrace{\mathbf{P}^T \mathbf{l}_q}_{\text{precomputed offline}} .$$

POD: Continuous version



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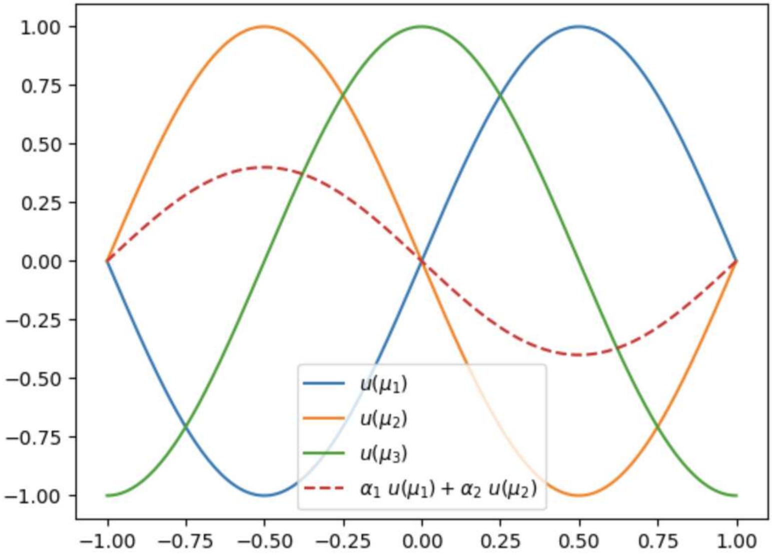


POD: Continuous version

How many snapshots do we need to represent our data?

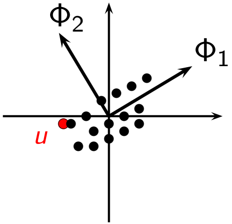
POD: Continuous version

Suppose we need M snapshots, the POD compresses our data by using $N \leq M$ basis functions!

POD: Continuous version

We want to approximate $u(\mathbf{x}, \boldsymbol{\mu})$ by $\sum_{k=1}^{N} a_k(\boldsymbol{\mu})\Phi_k(\mathbf{x})$.

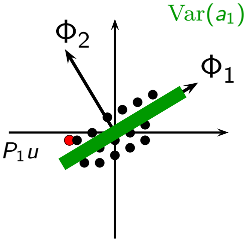
Let us consider $\boldsymbol{\mu}$ a random variable and u centered ($\mathbb{E}_{\boldsymbol{\mu}}[u] = 0$).
POD = PCA: We want to find the axes that best represent the data!



$$\boxed{\min_{\|\Phi_i\|=1} \mathbb{E}[\| u - \sum_{k=1}^{N} a_k(\boldsymbol{\mu})\ \Phi_k \|^2].}$$

POD: Continuous version

How do we find the reduced basis?



$$Var(a_1) = \mathbb{E}[a_1^2] - (\mathbb{E}[a_1])^2 = \mathbb{E}[a_1^2]$$

$$a_1 = (u, \Phi_1), \ \ \|\Phi_1\| = 1.$$

$$\boxed{\min_{\|\Phi_1\|=1} \mathbb{E}[\|u - (u,\Phi_1)\Phi_1\|^2] \text{ or } \max_{\|\Phi_1\|=1} \mathbb{E}[|(u,\Phi_1)|^2] \text{ or } C\Phi_1 = \lambda_1 \Phi_1}$$

Link between regularity and eigenvalues

One can show that the more regularizing the operator C is, the faster its eigenvalues decay!

Exercise: Transport equation

Let $T_h : L^2(0,1) \to L^2(0,1)$ be the transport operator defined by $(T_h x)(t) = x(t-h)$, with periodic boundary conditions on $(0,1)$ and a fixed shift $h \in (0,1)$.

1. Show that T_h is a bounded linear operator on $L^2(0,1)$ and that $\|T_h x\|_{L^2} = \|x\|_{L^2}$.
2. Compute the adjoint T_h and show that $T_h^* = T_{-h}$.
3. Show that $T_h^* T_h = I$, where I is the identity operator.
4. Deduce that the singular values of T_h satisfy $\sigma_n = 1 \quad$ for all n.
5. Conclude that T_h is not compact and does not regularize.

Link between regularity and eigenvalues

Solution

1. Linearity is immediate. Moreover, $\| T_h x\|^2_{L^2(0,1)} = \int_0^1 |x(t-h)|^2\, dt = \int_0^1 |x(t)|^2 dt$, due to periodicity. Hence $\| T_h x\|_2 = \|x\|_2$ for all x, so T_h is bounded and $\| T_h\| = 1$.

2. Adjoint. For $x, y \in L^2(0,1)$, $(T_h x, y) = \int_0^1 x(t-h)\,\overline{y(t)}\, dt$.
Let $u = t - h$. Using periodicity, $\int_0^1 x(t-h)\,\overline{y(t)}\, dt = \int_0^1 x(u)\,\overline{y(u+h)}\, du = (x,\ T_{-h} y)$, since $(T_{-h} y)(u) = y(u+h)$. Therefore $T_h^* = T_{-h}$.

3. Using $T_h^* = T_{-h}$, for any x,
$(T_h^* T_h x)(t) = (T_{-h} T_h x)(t) = (T_h x)(t+h) = x((t+h)-h) = x(t)$. Hence $T_h^* T_h = I$.

4. Singular values. By definition, the singular values are the square roots of the eigenvalues of $T_h^* T_h$ (counted with multiplicity). Since $T_h^* T_h = I$, all eigenvalues equal 1, with infinite multiplicity. Thus $\sigma_n(T_h) = 1, \qquad \forall n \in \mathbb{N}$.

Link between regularity and eigenvalues

Solution

5.

- Let $e_k(t) = e^{2\pi ikt}$. Then $\{e_k\}$ orthonormal family
- $T_h\ e_k(t) = e_k(t-h) = e^{-2\pi ikh}\ e_k(t)$. So, $\{T_h e_k\}$ is also orthonormal: no converging subsequence.
- Moreover, T_h is an isometry (unitary), so it does not attenuate high frequencies and therefore does not regularize.

Snapshot POD

$$\boxed{\mathbb{E}[(u,\Phi)u] = \lambda\Phi, \text{ i. e. } C\Phi = \lambda\Phi}.$$

$$\Leftrightarrow \frac{1}{N_{train}} \sum_{k=1}^{N_{train}} u(\mathbf{x},\boldsymbol{\mu}_k) \sum_{j=1}^{N_{train}} \alpha_j \mathbf{C}_{k,j} = \lambda \sum_{k=1}^{N_train} \alpha_k u(\mathbf{x},\boldsymbol{\mu}_k)$$

gives for one $k = i$

$$\boxed{\frac{1}{N_{train}} \sum_{j=1}^{N_{train}} \mathbf{C}_{i,j}\alpha_j = \lambda\alpha_i.}$$

Discretization: Snapshot POD algorithm

1: Collect snapshots $u(\cdot, \mu_i)$, $i = 1, \ldots, N_{train}$
2: Assemble snapshot matrix S
3: Compute correlation matrix $C = S^T S$ or $C = S^T M S$ (M= mass matrix)
4: Solve $C\alpha_i = \lambda_i \alpha_i$, $i = 1, \ldots, N_{train}$
5: Sort the eigenvalues
6: Retrieve first N eigenvalues/eigenvectors
7: Build POD modes $\Phi_i = \frac{1}{\sqrt{\lambda_i}} S\alpha_i$, $i = 1, \ldots, N$

How do we choose N? $\lambda_1 >= \lambda_2 >= \ldots >= 0$

$$\boxed{\mathbb{E}[\|u - P_N u\|^2] = \sum_{k>N} \mathbb{E}[a_k^2] = \sum_{k>N} \lambda_k}$$

Relativ Information Content (RIC) must be close to 0:

$1 - \sum_{k=1}^{N} \lambda_k / \sum_{k=1}^{N_{train}} \lambda_k$

Finite Volume schemes

- Hyperbolics problems: `Finite Volume Methods for Hyperbolic Problems, Randall J. LeVeque`
- `Finite volume methods, R Eymard, T Gallouët, R Herbin`

TP VF5-TPFA

Notations

Mesh ($\mathcal{T}$) size: h

Sets of edges: $\mathcal{F}, \mathcal{F}_{ext}, \mathcal{F}_{int}, \mathcal{F}_K$

Normals: $\mathbf{n}_K, \mathbf{n}_{K\sigma}, \mathbf{n}_{KL}$

Volumes / Measures/Distances: $|K|, |\sigma|, d_{K\sigma}, d_{L\sigma}, d_{KL}$

Finite Volume Methods

Based on the conservation form of the PDE

Integrate the balance equation on each cell κ and apply Stokes' formula:

$$\sum_{\text{edges of } \kappa} \text{outward flux} = \int_{\kappa} \text{source.}$$

Approximate each flux and write the discrete balance equation obtained.

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Based on the conservation form of the PDE $\rightarrow$ Flux: total outward flux $=$ the total internal source

Integrate the equation on each cell κ and apply Stokes' formula:

$$\int_K f(\mathbf{x})\ d(\mathbf{x}) = -\int_K \nabla \cdot (a(\boldsymbol{\mu})\nabla u) = \sum_{\sigma \in \mathcal{F}_K} \underbrace{-\int_\sigma a(\boldsymbol{\mu})\nabla u(\mathbf{x}) \cdot \mathbf{n}_{K,\sigma}\ d_\gamma(\mathbf{x})}_{\overline{F}_{K,\sigma}}$$

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Flux balance:

$$\sum_{\sigma \in \mathcal{F}_K} \overline{F}_{K,\sigma} = \int_K f(\mathbf{x})\ d(\mathbf{x}).$$

Flux conservativity:

$$\overline{F}_{K,\sigma} + \overline{F}_{L,\sigma} = 0 \text{ if } \sigma = K|L.$$

We want to find $u_h = (u_K)_{K \in \mathcal{T}} \in \mathbb{R}^{\mathcal{T}}$
Define $u_h \to F_{K,\sigma}(u_h)$ that approximates the flux and find $u_h \in \mathbb{R}^{\mathcal{T}}$ such that
$|K| f_K = \sum_{\sigma \in \mathcal{F}_K} F_{K,\sigma} \forall K \in \mathcal{T}.$

TP VF5-TPFA

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Case of an interior edge $\sigma \in \mathcal{E}_{int},\ \sigma = K|L$

$$x_L - x_K = d_{KL}\,\mathbf{n}_{KL}.$$

If $x \in \sigma$,

$$(\nabla u(x)) \cdot \mathbf{n}_{KL} = \frac{u(x_L) - u(x_K)}{d_{KL}} + \mathcal{O}(h).$$

$$\Longrightarrow \overline{F}_{K,\sigma} = \underbrace{-\overline{A(\boldsymbol{\mu})}|\sigma|\frac{u(x_L) - u(x_K)}{d_{KL}}}_{F_{K,\sigma}(u_h)} + \mathcal{O}(h^2)$$

where $\overline{A}$ is the harmonic average: $\overline{A} = \frac{A(x_L)A(x_K)d_{KL}}{A(x_L)d_{K,\sigma} + A(x_K)d_{L,\sigma}}$

TP VF5-TPFA

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.

Case of a boundary edge $\sigma \in \mathcal{E}_{ext}$

$$x_\sigma - x_K = d_{K\sigma}\, \mathbf{n}_{K\sigma}.$$

$$(\nabla u(x))\cdot \mathbf{n}_{K\sigma} \approx \frac{u(x_\sigma) - u(x_K)}{d_{K\sigma}} = \frac{0 - u(x_K)}{d_{K\sigma}} \qquad \text{(boundary condition)}$$

$$\Longrightarrow \overline{F}_{K,\sigma} = \underbrace{-|\sigma| A_K \frac{-u(x_K)}{d_{K\sigma}}}_{F_{K,\sigma}(u_h)} + \mathcal{O}(h^2)$$

TP VF5-TPFA

Find $u_h = (u_K)_{K \in \mathcal{T}_h}$ such that for all K in $\mathcal{T}_h$:

$$\sum_{\sigma \in F_K \cap F_{int}} \tau_\sigma (u_K - u_L) + \sum_{\sigma \in F_K \cap F_{ext}} \tau_\sigma u_K = \int_K f(x)dx$$

with Dirichlet boundary $u = 0$ on $\partial\Omega$, where $\tau_\sigma = |\sigma| \frac{A_K \ A_L}{A_L \ d_{K,\sigma} + A_K \ d_{L,\sigma}}$ on F_{int} and $\tau_\sigma = |\sigma| \frac{A_K}{d_{K,\sigma}}$ on F_{ext}

We take here $\Omega = [0,1] \times [0,1]$ with a cartesian mesh.
$A(x,y;\mu) = 2\mu_1 + \mu_2 \ sin(x+y) \ cos(xy)$
$f(x,y;\mu) = \mu_3(1-y) + \mu_4 x \ (1-x)$

POD-based Reduced Order Model with TPFA

- Complete the function `assemble_tpfa`. The TPFA solver must return the cell centers, the matrix M, and the vector b such that $Mu = b$.
- Generate a training dataset:

  Use $N_{train} = 10$ snapshots and sample random parameters $\boldsymbol{\mu}$ with components in $[0, 1]$.
  Solve the full-order TPFA system for each sampled parameter.
  Store the resulting solutions as a snapshots list.
- Using the discrete L^2 inner product $(u, v)_{L^2} = \sum_K |K| \, u_K v_K$,

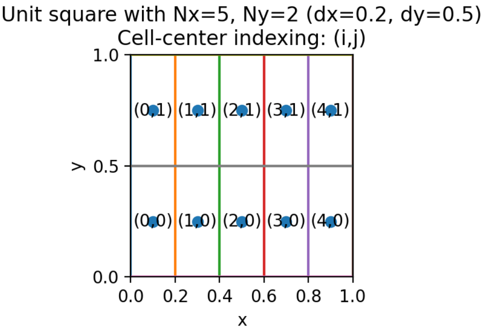
  Assemble the snapshot correlation matrix.
  Compute the reduced basis with a Proper Orthogonal Decomposition (POD).
  Verify that the reduced basis is orthonormal with respect to $(\cdot, \cdot)_{L^2}$.
- Determine how many modes N are sufficient using the Relative Information Content.
- Write a function that computes the ROM projection coefficients of a given full-order solution u.
- Consider a new parameter $\boldsymbol{\mu}$. Write a function that computes the reduced-order approximation of the solution without computing the HF solution.
- Show that the obtained reduced system has the form $\widetilde{M}a = \widetilde{b}$, where $\widetilde{M}$ is of size $N \times N$ and $\widetilde{b}$ is of size N.

TP VF5-TPFA

POD-based Reduced Order Model with TPFA

- Test the reduced model for $\boldsymbol{\mu} = (0.6, 0.5, 0.2, 0.8)$.
- Compare the errors $\|u_{\mathrm{ref}} - u\|_{L^2}$ and $\|u_{\mathrm{ref}} - u_N\|_{L^2}$, where u_{ref} is a refined solution.

TP



Unit square with Nx=5, Ny=2 (dx=0.2, dy=0.5)
Cell-center indexing: (i,j)
(0,1)
(1,1)
(2,1)
(3,1)
(4,1)
(0,0)
(1,0)
(2,0)
(3,0)
(4,0)
y
x
0.0
0.5
1.0
0.0
0.2
0.4
0.6
0.8
1.0

TP Kolmogorov

TP2:

with Kolmogorov n width not small: $u(x, \mu) = tanh(\frac{x-\mu}{\delta})$.

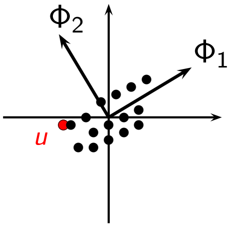
Reduced Basis Methods

- ◇ **Offline** Construction of a reduced space V_N spanned by a reduced basis.
- ◇ **Online** Computation of the reduced coefficients $\boldsymbol{\alpha}$.

The optimal reduced space V^N may not be found
Two main algorithms to find approximated reduced spaces: **the Proper Orthogonal Decomposition (POD)** or **greedy algorithms**.

1. Reminders
   - Reduced Basis Methods
   - POD-Galerkin
   - POD + TP VF
2. aposteriori errors

Computable error bound



$$\boxed{d_N(\mathcal{M}_h, V_h) = \inf_{\substack{V^N \subset V_h \\ \dim(V^N)=N}} \sup_{u_h \in \mathcal{M}_h} \inf_{v_N \in V^N} \|u_h - v_N\|_{V_h} = \varepsilon.}$$

POD reminder: $V_N = \mathrm{Span}\{\Phi_1, \ldots, \Phi_N\}$, where

$$V_N = \inf_{\substack{V^N \subset V^M \\ \dim(V^N)=N}} \mathbb{E}[\|u - P_N u\|_V^2]$$

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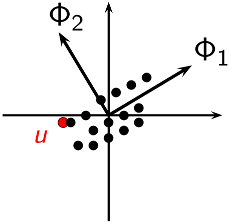

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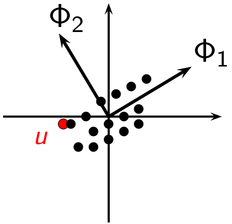
$$\frac{1}{M}\sum_{i=1}^{M} \|u_h(\mu_i) - P_N(u_h(\mu_i))\|_V^2 = \sum_{k=N+1}^{M} \lambda_k$$

Computable error bound



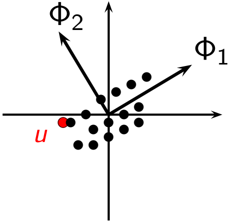
$$\boxed{d_N(\mathcal{M}_h, V_h) = \inf_{\substack{V^N \subset V_h \\ \dim(V^N)=N}} \sup_{u_h \in \mathcal{M}_h} \inf_{v_N \in V^N} \|u_h - v_N\|_{V_h} = \varepsilon.}$$

$$\frac{1}{M}\sum_{i=1}^{M} \|u_h(\mu_i) - P_N(u_h(\mu_i))\|_V^2 = \sum_{k=N+1}^{M} \lambda_k$$

$$\|u_h(\mu_m) - P_N(u_h(\mu_m))\|_V^2 \leq \sum_{i=1}^{M} \|u_h(\mu_i) - P_N(u_h(\mu_i))\|_V^2 = M \sum_{k=N+1}^{M} \lambda_k$$

Thus, at the points $\{\mu_m\}_{1\leq m\leq M}$, we know that the error is bounded by $\delta > 0$

Computable error bound



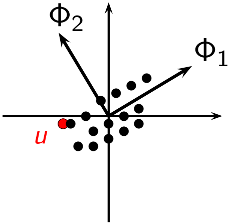
$$\boxed{d_N(\mathcal{M}_h, V_h) = \inf_{\substack{V^N \subset V_h \\ \dim(V^N)=N}} \sup_{u_h \in \mathcal{M}_h} \inf_{v_N \in V^N} \|u_h - v_N\|_{V_h} = \varepsilon.}$$

What about $\|u_h(\mu) - P_N(u_h(\mu))\|_V$ for $\mu \notin \{\mu_m\}_{1 \leq m \leq M}$????

or

$\|u_h(\mu) - u_N(\mu)\|_V$ for any μ, including $\mu \in \{\mu_m\}_{1 \leq m \leq M}$, since in practice the RB approximation is not optimal, i.e., $u_N(\mu) \neq P_N(u_h(\mu))$????

Computable error bound



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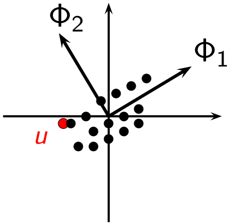
Like FEM Cea's lemma, under some assumptions (a coercive ...)

$$\|u_h - u_N\|_V \leq \frac{\gamma(\mu)}{\alpha(\mu)} \inf_{v_N \in V_N} \|u_h - v_N\|_V$$

but in practice $\inf_{v_N \in V_N} \|u_h - v_N\|_V$ is not computable!

Computable error bound



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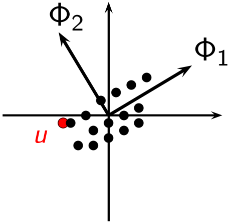
We want a bound that depends only on the RB approximation u_N :

Computable error bound



$$\boxed{d_N(\mathcal{M}_h, V_h) = \inf_{\substack{V^N \subset V_h \\ \dim(V^N)=N}} \ \sup_{u_h \in \mathcal{M}_h} \ \inf_{v_N \in V^N} \|u_h - v_N\|_{V_h} = \varepsilon.}$$

We want a bound that depends only on the RB approximation u_N :

aposteriori bound !!!

Aposteriori

The aposteriori error bound measures the RB method fiability:

$$\|u(\boldsymbol{\mu}) - u_N(\boldsymbol{\mu})\|_V \leq \underbrace{\|u(\boldsymbol{\mu}) - u_h(\boldsymbol{\mu})\|_V}_{=\mathcal{O}(h^s)} + \underbrace{\|u_h(\boldsymbol{\mu}) - u_N(\boldsymbol{\mu})\|_V}_{\leq \Delta_N(\boldsymbol{\mu})}$$

There are many different types of a posteriori error estimation:

- residual-based estimates
- averaging-based estimates
- equilibrated fluxes estimates
- equilibrated residual estimates
- hierarchical estimates
- heuristic estimates

Computable error bound

Theorem: Banach-Necas-Babuska

Let $a : V \times W$ continuous bilinear form and $f : W \to \mathbb{R}$ continuous linear form
The problem

$$\text{find } u \in V,\ a(u,w) = f(w),\ \forall w \in W$$

is well-posed iff

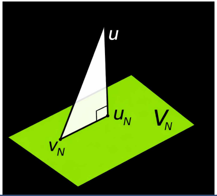
$$\exists \alpha_{sta} > 0, \forall v \in V, \sup_{w \in W \setminus \{0\}} \frac{a(v,w)}{\|w\|_W} \geq \alpha_{sta} \|v\|_V.$$

The following estimate holds true:

$$\boxed{\|u\|_V \leq \frac{1}{\alpha_{sta}} \|f\|_{W'}}$$

The dual space of V is $V' := \mathcal{L}(V, \mathbb{R})$ the space of continuous linear forms.
Norm: $\|g\|_{V'} = \sup_{v \in V, v \neq 0} \frac{|g(v)|}{\|v\|_V}$

Computable error bound



Reminder: Galerkin condition

The error e_N is orthogonal to the test space V_N in the energy inner product induced by $a(\cdot, \cdot)$:

$$\boxed{a(e_N, v_N) = a(u - u_N, v_N) = 0, \ \forall v_N \in V_N.}$$

Consider the weak residual $r(v) = \ell(v) - a(u_N, v)$. Then

$$r(v_N) = a(u, v_N) - a(u_N, v_N) = a(e_N, v_N) = 0, \ \forall v_N \in V_N.$$

In other words, the residual vanishes on the test space.

Computable error bound

The following estimate holds true:

$$\boxed{\|u\|_V \leq \frac{1}{\alpha_{sta}} \|f\|_{W'}}$$

And thus:
the following estimate holds true:

$$\|u - u_N\| = \|e\|_V \leq \frac{1}{\alpha_{sta}} \|r\|_{W'}$$

Computable error bound

Theorem: Banach-Necas-Babuska

Let $a : V_h \times W_h$ continuous bilinear form and $f_h : W_h \to \mathbb{R}$ continuous linear form
The H-F problem

$$\text{find } u_h \in V_h,\ a(u_h, w_h) = f(w_h),\ \forall w_h \in W_h$$

is well-posed iff

$$\exists \alpha_{sta} > 0, \forall v_h \in V_h, \sup_{w_h \in W_h \setminus \{0\}} \frac{a(v_h, w_h)}{\|w_h\|_W} \geq \alpha_{sta} \|v_h\|_V.$$

The following estimate holds true:

$$\boxed{\|u_h\|_V \leq \frac{1}{\alpha_{sta}} \|f_h\|_{W'}}$$

Computable error bound

$\alpha_{sta} = \inf_{v_h \in V_h} \sup_{w_h \in V_h} \frac{a(v_h, w_h)}{\|v_h\|_V \|w_h\|_V} > 0$ is the "inf-sup stability constant"

$$\mathbf{A} : V \to V'$$

With HF basis $\{w_i\}_{i=1}^{\mathcal{N}}$, we know that:
$a(u, v) = \mathbf{v}^T \mathbf{A} \mathbf{u}$, with $\mathbf{A}_{ij} = a(w_j, w_i)$, and $(u, v) = \mathbf{v}^T \mathbf{M} \mathbf{u}$ with $\mathbf{M}_{ij} = (w_j, w_i)$.

$\alpha_{sta} = \inf_{v_h \in V_h} \sup_{w_h \in V_h} \frac{\mathbf{w_h}^T \mathbf{A} \ \mathbf{v_h}}{\|\mathbf{v_h}\|_V \|\mathbf{w_h}\|_V} = \inf_{v_h \in V_h} \frac{\|\mathbf{A} \mathbf{v_h}\|_{V'}}{\|\mathbf{v_h}\|_V} > 0$ is the "inf-sup stability constant"

$$\forall u_h \in V_h, \ \|\mathbf{A} \mathbf{u_h}\|_{V'} \geq \alpha_{sta} \|\mathbf{u_h}\|_V$$

Computable error bound

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$$\forall u_h \in V_h, \ \|\mathbf{A} \mathbf{u_h}\|_{V'} \geq \alpha_{sta} \|\mathbf{u_h}\|_V$$

Computable error bound

$$\forall u_h \in V_h, \ \|\mathbf{Au_h}\|_{V'} \geq \alpha_{sta}\|\mathbf{u_h}\|_V$$

Coercivity?

- a can be asymetric
- $a(u,u)$ can be 0

Stokes:

$$(u \ \ p)\begin{pmatrix} A & B^T \\ B & 0 \end{pmatrix}\begin{pmatrix} u \\ p \end{pmatrix} = u^T A u + \underbrace{2p^T B u}_{\text{can be negative!}}$$

Coercivity $\Leftrightarrow u = \underset{v \in V}{min} J(v) = \frac{1}{2}a(v,v) - l(v)$ (Convexity, unique minimum: Lax-Milgram)

Computable error bound

$$\forall u_h \in V_h, \ \|\mathbf{Au_h}\|_{V'} \geq \alpha_{sta}\|\mathbf{u_h}\|_V$$

Going back to $V_N \subset V_h$:

consider the weak residual $r(v) = \ell(v) - a(u_N, v)$. Then

$$\begin{aligned} V_N' \ni \mathbf{r_N} &= \mathbf{l} - \mathbf{Au_N} \\ &= \mathbf{Au_h} - \mathbf{Au_N} = \mathbf{Ae_N} \end{aligned}$$

- ◇ From continuity, $\|\mathbf{Aw}\|_{V'} \leq \gamma\|\mathbf{w}\|_V$
- ◇ From inf-sup condition, $\|\mathbf{Aw}\|_{V'} \geq \alpha_{sta}\|\mathbf{w}\|_V$

Thus, with $\mathbf{w} = \mathbf{e_N}$,

$$\boxed{\frac{1}{\gamma}\|\mathbf{r_N}\|_{W'} \leq \|\mathbf{e_N}\|_V \leq \frac{1}{\alpha_{sta}}\|\mathbf{r_N}\|_{V'}}$$

Computable error bound

$$\forall u_h \in V_h,\ \|\mathbf{Au_h}\|_{V'} \geq \alpha_{sta}\|\mathbf{u_h}\|_V$$

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Aposteriori

We are going to use $\|u_h(\boldsymbol{\mu}) - u_N(\boldsymbol{\mu})\|_V \leq \frac{1}{\alpha_{sta}(\boldsymbol{\mu})} \|r_N(\boldsymbol{\mu})\|_{V'}$

> "A posteriori numerical analysis based on the method of equilibrated fluxes", M. Vohralik

`https://who.rocq.inria.fr/Martin.Vohralik/Enseig/APost/a`$_p$*osteriori.pdf*

Aposteriori

An *a posteriori error estimator* is a function $\Delta_N : \mathcal{G} \to \mathbb{R}^+$ satisfying the following properties:

Robustness:

$$\forall \boldsymbol{\mu} \in \mathcal{G}, \qquad \|u_h(\boldsymbol{\mu}) - u_N(\boldsymbol{\mu})\|_V \leq \Delta_N(\boldsymbol{\mu}).$$

Efficiency (and local efficiency):

$$\forall \boldsymbol{\mu} \in \mathcal{G}, \quad \exists K(\boldsymbol{\mu}) > 0 \quad \text{such that} \quad \Delta_N(\boldsymbol{\mu}) \leq K(\boldsymbol{\mu})\|u_h(\boldsymbol{\mu}) - u_N(\boldsymbol{\mu})\|_V$$

Asymptotic exactness: the effectivity index $I_{eff} = \frac{\Delta_N(\boldsymbol{\mu})}{\|u_h - u_N\|} \underset{N\to\infty}{\rightarrow} 1$

Guaranteed upper bound: The function Δ_N can be evaluated for all $\boldsymbol{\mu} \in \mathcal{G}$ without evaluating $u_h(\boldsymbol{\mu})$ (fully computable from $u_N(\boldsymbol{\mu})$).

Small evaluation cost: Can be evaluated locally (only performing calculations in the element K or in its neighborhood $\mathcal{I}_K$)

Error components identification: Distinguish and estimate separately the different error components

Aposteriori

We are going to use

$$\boxed{\Delta_N(\boldsymbol{\mu}) = \frac{1}{\alpha_{sta}(\boldsymbol{\mu})}\|r_N(\boldsymbol{\mu})\|_{V'} = \frac{1}{\alpha_{sta}(\boldsymbol{\mu})}\|\mathbf{l} - \mathbf{Au_N}\|_{V'}}$$

An *a posteriori error estimator* is a function $\Delta_N : \mathcal{G} \to \mathbb{R}^+$ satisfying the following properties:

- **Robustness:** ☒ $\forall \boldsymbol{\mu} \in \mathcal{G}, \qquad \|e_N(\boldsymbol{\mu})\|_V \leq \Delta_N(\boldsymbol{\mu})$.
- **Efficiency (and local efficiency):** ☒ Since $\alpha\Delta \leq e_N\gamma$, we take $K = \frac{\gamma}{\alpha}$
- **Asymptotic exactness:** ☒ the effectivity index $I_{eff} = \frac{\Delta_N(\boldsymbol{\mu})}{\|u_h - u_N\|} \underset{N\to\infty}{\to} 1$
- **Guaranteed upper bound:** ☒ Without evaluating $u_h(\boldsymbol{\mu})$
- **Small evaluation cost:** local residual (useful for raffinement / mesh adaptation)
- **Error components identification:** Distinguish and estimate separately the different error components (e.g. algebraic error, linked to solver imprecision)

Aposteriori

We are going to use

$$\boxed{\Delta_N(\boldsymbol{\mu}) = \frac{1}{\alpha_{sta}(\boldsymbol{\mu})}\|r(u_N(\boldsymbol{\mu}))\|_{V'} = \frac{1}{\alpha_{sta}(\boldsymbol{\mu})}\|\mathbf{l} - \mathbf{A}\mathbf{u}_\mathbf{N}\|_{V'}}$$

The aposteriori error bound measures the RB method fiability:

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There are many different types of a posteriori error estimation:

- residual-based estimates
- averaging-based estimates
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Aposteriori

Two key ingredients:

- ⋄ Dual norm of the residual: Offline-online computation strategy
- ⋄ Inf-sup $\alpha_{sta}(\boldsymbol{\mu})$ not efficiently computable but one can compute $\alpha_{LB}(\boldsymbol{\mu})$ such that

$$\forall \boldsymbol{\mu} \in \mathcal{G}, \alpha_{sta}(\boldsymbol{\mu}) \geq \alpha_{LB}(\boldsymbol{\mu})$$

Case of coercivity: $\alpha^* = \underset{v \neq 0}{inf} \frac{a(v,v)}{\|v\|_V^2}$

Remark: When $\alpha_{sta}(\boldsymbol{\mu})$ becomes small, $K(\boldsymbol{\mu}) = \frac{\gamma}{\alpha}$ becomes too big! Overestimate RB approximation.

Dual norm of the residual

Let's get back to our sheep

linear second-order parameter dependent problem

$$\begin{cases} -\nabla \cdot \big(a(\boldsymbol{\mu})\nabla u\big) = f(\boldsymbol{\mu}) & \text{dans } \Omega, \\ u = 0 & \text{sur } \partial\Omega. \end{cases}$$

$\alpha_{LB} = \alpha_{min}$

Dual norm of the residual

Reminder: Riesz representation Theorem

$$\forall r \in V', \quad \exists! z \in V \text{ such that } r(v) = (z, v)_V \quad \forall v \in V,$$

and we define the norm on V' :

$$\|r\|_{V'}^2 = r(z) = (z, z)_V.$$

Thus, since in our setting $V = H_0^1(\Omega)$, thus $(z, z)_V = z^T \mathbf{K} z = r^T \mathbf{K}^{-1} r$, where $\mathbf{K}$ is the stiffness matrix.

Dual norm of the residual

$$\mathbf{A}(\boldsymbol{\mu}) = \sum_q \theta_q^a(\boldsymbol{\mu})\mathbf{A}_q \quad \text{and} \quad \mathbf{l}(\boldsymbol{\mu}) = \sum_q \theta_q^l(\boldsymbol{\mu})\mathbf{l}_q$$

Reduced basis Galerkin approximation

Assume the weak formulation of the HF problem yields the discretized system

$$\mathbf{A}(\boldsymbol{\mu})\mathbf{u}(\boldsymbol{\mu}) = \mathbf{l}(\boldsymbol{\mu})$$

then

$$a\left(u_N(\boldsymbol{\mu}), v_N; \boldsymbol{\mu}\right) = \ell\left(v_N; \boldsymbol{\mu}\right)$$

gives a new system to solved:

$$\boxed{\mathbf{P}^T\mathbf{A}(\boldsymbol{\mu})\mathbf{P}\,\alpha(\boldsymbol{\mu}) = \mathbf{P}^T\mathbf{l}(\boldsymbol{\mu}),} \tag{G-RB}$$

where $\mathbf{P} \in \mathbb{R}^{\mathcal{N}\times N}$. Now, we get a system where the inversion cost is in $\mathcal{O}(N^3)$ since dimensions : $\mathbf{P}^T\mathbf{A}(\boldsymbol{\mu})\mathbf{P} \in \mathbb{R}^{N\times N}$ and $\mathbf{P}^T b \in \mathbb{R}^N$!

Reduced basis Galerkin approximation

Assembling cost with the affine operators:
$\mathcal{O}(N^2 Q^a + N Q^l)$ with

$$\mathbf{P}^T \mathbf{A}(\boldsymbol{\mu}) \mathbf{P} = \sum_{q=1}^{Q^a} \theta_q^a(\boldsymbol{\mu}) \underbrace{\mathbf{P}^T \mathbf{A}_q \mathbf{P}}_{\text{precomputed offline}} \quad , \quad \mathbf{P}^T \mathbf{l}(\boldsymbol{\mu}) = \sum_{q=1}^{Q^l} \theta_q^l(\boldsymbol{\mu}) \underbrace{\mathbf{P}^T \mathbf{l}_q}_{\text{precomputed offline}} \quad .$$

Dual norm of the residual

$$\mathbf{A}(\boldsymbol{\mu}) = \sum_q \theta_q^a(\boldsymbol{\mu})\mathbf{A}_q \quad \text{and} \quad \mathbf{l}(\boldsymbol{\mu}) = \sum_q \theta_q^l(\boldsymbol{\mu})\mathbf{l}_q$$

$$\begin{aligned}
\|\mathbf{A}(\boldsymbol{\mu})\mathbf{u_N}(\boldsymbol{\mu}) - \mathbf{l}(\boldsymbol{\mu})\|_{V'}^2 = &\sum_{q=1}^{Q^\ell}\sum_{k=1}^{Q^\ell} \theta_q^\ell(\boldsymbol{\mu})\theta_k^\ell(\boldsymbol{\mu}) \boxed{\mathbf{l_k}^T\mathbf{K}^{-1}\mathbf{l_q}} \\
&+ \sum_{q=1}^{Q^a}\sum_{k=1}^{Q^a} \theta_q^a(\boldsymbol{\mu})\theta_k^a(\boldsymbol{\mu})\, \boldsymbol{\alpha}(\boldsymbol{\mu})^T \boxed{\mathbf{P}^T\mathbf{A}_k^T\mathbf{K}^{-1}\mathbf{A}_q\mathbf{P}}\, \boldsymbol{\alpha}(\boldsymbol{\mu}) \\
&- 2\sum_{q=1}^{Q^\ell}\sum_{k=1}^{Q^a} \theta_q^\ell(\boldsymbol{\mu})\theta_k^a(\boldsymbol{\mu})\, \boldsymbol{\alpha}(\boldsymbol{\mu})^T \boxed{\mathbf{P}^T\mathbf{A}_k^T\mathbf{K}^{-1}\mathbf{l}_q}.
\end{aligned}$$

Online complexity: since the boxed quantities are precomputed offline and $\alpha(\boldsymbol{\mu}) \in \mathbb{R}^N$ is known, the computational cost is

$$\mathcal{O}\left((Q^\ell)^2 + (Q^a)^2N^2 + Q^\ell Q^a N\right).$$

We solve systems like $\mathbf{K}w = \mathbf{l_q}$ and $\mathbf{K}w = \mathbf{A_q P}$

Aposteriori

We are going to use

$$\boxed{\Delta_N(\boldsymbol{\mu}) = \frac{1}{\alpha_{sta}(\boldsymbol{\mu})}\|r_N(\boldsymbol{\mu})\|_{V'} = \frac{1}{\alpha_{sta}(\boldsymbol{\mu})}\|\mathbf{l} - \mathbf{A}\mathbf{u}_\mathbf{N}\|_{V'}}$$

An *a posteriori error estimator* is a function $\Delta_N : \mathcal{G} \to \mathbb{R}^+$ satisfying the following properties:

Robustness: ☒ $\forall \boldsymbol{\mu} \in \mathcal{G}, \qquad \|e_N(\boldsymbol{\mu})\|_V \leq \Delta_N(\boldsymbol{\mu})$.

Efficiency (and local efficiency): ☒ Since $\alpha\Delta \leq e_N\gamma$, we take $K = \frac{\gamma}{\alpha}$

Asymptotic exactness: ☒ the effectivity index $I_{eff} = \frac{\Delta_N(\boldsymbol{\mu})}{\|u_h - u_N\|} \underset{N\to\infty}{\longrightarrow} 1$

Guaranteed upper bound: ☒ Without evaluating $u_h(\boldsymbol{\mu})$

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Aposteriori

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$$\begin{cases} -\nabla \cdot \big(a(\boldsymbol{\mu})\nabla u\big) = f(\boldsymbol{\mu}) & \text{dans } \Omega, \\ u = 0 & \text{sur } \partial\Omega. \end{cases}$$

$\alpha_{LB} = \alpha_{min}$

$$\Delta_N = \frac{1}{\alpha}\sum_K \eta_K$$

where

$$\eta_K^2 = \left(h_K^2\|f + \Delta u_N\|_{L^2(K)}^2 + \sum_{e\subset\partial K} h_e\|[[\nabla u_N \cdot \mathbf{n}]]\|_{L^2(e)}^2\right)$$

Aposteriori

$$\Delta_N = \frac{1}{\alpha}\sum_K \eta_K \text{ where } \eta_K^2 = \left(h_K^2\|f+\Delta u_N\|^2_{L^2(K)} + \sum_e h_e\|[[\nabla u_N\cdot \mathbf{n}]]\|^2_{L^2(e)}\right)$$

Proof:

$r(v) = \ell(v) - a(u_N, v)$. Then with $\Omega = \cup_K K$,

$$\begin{aligned} r(v) &= \sum_K \Big(\int_K fv - \int_K (\nabla u_N, \nabla v)\Big) \\ &= \sum_K \Big(\int_K fv + \int_K \Delta u_N \cdot v - \int_{\partial K} (\nabla u_N \cdot n) v\Big) \\ &= \sum_K \underbrace{\int_K (f+\Delta u_N) v}_{\text{element residual}} - \sum_K \underbrace{\int_{\partial K} (\nabla u_N \cdot n) v}_{\text{flux continuity default}} \end{aligned}$$

Aposteriori

By C-S and Poincare:
$|\int_K (f+\Delta u_N)v| \leq \|f+\Delta u_N\|_{L^2(K)}\|v\|_{L^2(K)} \leq Ch_K\|f+\Delta u_N\|_{L^2(K)}\|\nabla v\|_{L^2(K)}$
and by trace inequality,
$|\int_e (\nabla u_N \cdot n)v| \leq \|\nabla u_N \cdot \mathbf{n}\|_{L^2(e)}\|v\|_{L^2(e)} \leq Ch_e^{1/2}\|\nabla u_N \cdot \mathbf{n}\|_{L^2(e)}\|\nabla v\|_{L^2(K)}$

$$|r(v)| \leq \Big(\sum_K Ch_K\|f+\Delta u_N\|_{L^2(K)} + Ch_e^{1/2}\|\nabla u_N \cdot \mathbf{n}\|_{L^2(e)}\Big)\|\nabla v\|_{L^2(K)}$$

Thus $(A+B \leq \sqrt{2}(A^2+B^2)^{1/2} \Leftrightarrow)$,
$|r(v)| \leq \big(\sum Ch_K^2\|f+\Delta u_N\|_{L^2(K)}^2 + Ch_e\|\nabla u_N \cdot \mathbf{n}\|_{L^2(e)}^2\big)^{1/2}\|\nabla v\|_{L^2(K)}$

$$\|r\|_{V'} = \sup_{v\neq 0}\frac{|r(v)|}{\|v\|_V}$$

thus

$$\Delta_N = \frac{1}{\alpha}\sum_K \eta_K \ \text{ where } \ \eta_K^2 = \Big(h_K^2\|f+\Delta u_N\|_{L^2(K)}^2 + \sum_e h_e\|[[\nabla u_N \cdot \mathbf{n}]]\|_{L^2(e)}^2\Big)$$

Aposteriori

The error in K depends not only on the residual inside K but also on nearby elements: so the estimator uses a patch residual.

$$\Delta_N = \frac{1}{\alpha_{sta}}(\eta_1 + \eta_2)$$

where

$$\eta_1^2 = \sum_{K' \in I_K} h_K'^2 \|f + \Delta u_N\|^2_{L^2(K')} \quad \text{and} \quad \eta_2 = \sum_{e \in \mathcal{F}_K} h_e \|(\nabla u_N) \cdot n_e\|_{L^2(e)^2}$$

Aposteriori

Two key ingredients:

- Dual norm of the residual: Offline-online computation strategy ☒
- Inf-sup $\alpha_{sta}(\boldsymbol{\mu})$ not efficiently computable but one can compute $\alpha_{LB}(\boldsymbol{\mu})$ such that

$$\forall \boldsymbol{\mu} \in \mathcal{G}, \alpha_{sta}(\boldsymbol{\mu}) \geq \alpha_{LB}(\boldsymbol{\mu})$$

$\alpha_{LB}(\boldsymbol{\mu})$

$$\alpha_{sta}(\boldsymbol{\mu}) = \inf_{v_h \in V_h, v_h \neq 0} \frac{\|\mathbf{A}(\boldsymbol{\mu})\mathbf{v_h}\|_{V'}}{\|\mathbf{v_h}\|_V}.$$

Thus $\forall v_h \in V_h$,

$$\alpha_{sta}(\boldsymbol{\mu})^2 \|\mathbf{v_h}\|_V^2 := \alpha_{sta}(\boldsymbol{\mu})^2 \mathbf{v_h}^T \mathbf{M_V} \mathbf{v_h} \leq \|\mathbf{A}(\boldsymbol{\mu})\mathbf{v_h}\|_{V'}^2 := (\mathbf{A}(\boldsymbol{\mu})\mathbf{v_h})^T \mathbf{M_V}^{-1} (\mathbf{A}(\boldsymbol{\mu})\mathbf{v_h})$$

$$\alpha_{sta}^2 = \inf_{v_h \in V_h, v_h \neq 0} \frac{\mathbf{v_h}^T \mathbf{A}(\boldsymbol{\mu})^T \mathbf{M}_V^{-1} \mathbf{A}(\boldsymbol{\mu})\mathbf{v_h}}{\mathbf{v_h}^T \mathbf{M_V} \mathbf{v_h}}$$

$\alpha_{sta}(\boldsymbol{\mu})$ is the square root of the smallest eigenvalue of the problem

$$\mathbf{A}^T \mathbf{M_V}^{-1} \mathbf{A}(\boldsymbol{\mu})\mathbf{v_h} = \lambda \mathbf{M_V}\ \mathbf{v_h}$$

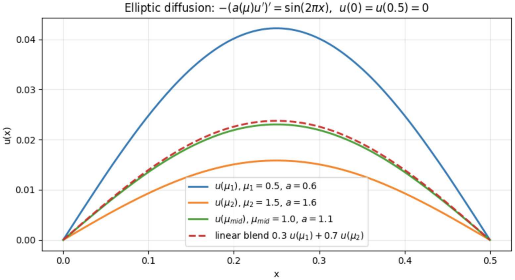
Aposteriori

$$\mathbf{A}^T \mathbf{M_V}^{-1} \mathbf{A} \mathbf{v_h} = \lambda \mathbf{M_V}\ \mathbf{v_h}$$

eigenvalue of size $\mathcal{N}$ but one can find a minorant of α_{sta} efficiently computable.

TP Aposteriori

TP3: Kolmogorov very small



TP4: same PDE with a posteriori

TP Kolmogorov

FEM with Kolmogorov n width not small: Burgers equation:
Viscous Burgers (1D) with periodic BC using scikit-fem

$$u_t + \nu u u_x - \varepsilon u_x x = 0 \; in \; (0, T] \times [-1, 1]$$
$$u(0, x) = u_0(x) = \lambda + sin(x)$$
$$u \; periodic \; at \; x = -1 \; and \; x = 1$$

Time stepping: IMEX (explicit convection, implicit diffusion)
$(M + dt\varepsilon \; K)u^{n+1} = Mu^n - dtF(u^n)$ where $F_i(u^n) = \int \nu v_i(u^n)(u^n)_x dx$