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

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Introduction

- ◇ Understand the purpose of reduced basis methods and how they work
- ◇ Get a non-exhaustive overview of existing methods
- ◇ Implement different methods to gain better insight
- ◇ Understand the limitations and in some cases, how to overcome them

Introduction

Course objectives: Become familiar with reduced basis methods and implement it (during TP sessions).

6 lectures/TP sessions on Tuesday afternoons

February 17: introduction + reduced basis approximation,
February 24: approximation space using POD, TP (start),
March 10: error estimation, TP (continuation),
March 17: approximation space using the Greedy algorithm, TP (continuation),
Deadline for TP 1 report (50% of the grade): Monday, March 24, 11:59 PM,
March 24: RB method for nonlinear PDEs, TP (start),
March 31: extensions / open topics, TP (continuation),
April 7: Oral presentations (50% of the grade).

TP sessions in Python, individually or in pairs, on

linear PDEs (TP),
non-linear PDEs (TP).

Introduction

linear second-order parameter dependent problem

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

$u(\mathbf{x};\mu) \in V$: Unknowns,

$\mu \in \mathcal{G}$: Variable parameter,

$f \in L^2(\Omega)$,

$a : \mathcal{G} \times \Omega \to \mathcal{M}_d(\mathbb{R})$ is measurable, bounded, uniformly elliptic.

Introduction

◇ **Main goal**

The objective of RBM is to find **very quickly accurate approximations** of parameter-dependent functions of the generic form

$$u : \Omega \times \mathcal{G} \to \mathbb{R},$$

– $\Omega \in \mathbb{R}^d$: the spatial domain,

– $\mathcal{G} \subset \mathbb{R}^{N_p}$: the parameter domain, with N_p the number of parameters.
$\mu = (\mu_1, \ldots, \mu_{N_p}) \in \mathcal{G}$: the varying parameter.

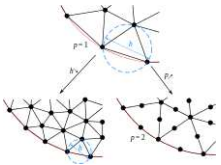
$$\mathcal{L}(\mu)(u(\mu)) = F(\mu), \text{ in } \Omega,$$
$$+ \text{ boundary conditions on } \partial\Omega.$$

Introduction

Usually, classical methods such as

- ◇ Finite Difference Method (FDM)
- ◇ Finite Volume schemes (FV)
- ◇ Finite Element Method (FEM)

are used to provide an accurate approximation.
This consists in solving the problem in a subspace $V_h \subset V$, where h is the mesh size.
Discrete approximations: $u_h \in V_h$.



Introduction

Finite Difference Methods

Mostly based on Taylor expansions of (smooth) solutions.

Cartesian geometry only (at least without any additional tools).

"Replace" derivatives by differential quotients:

$$\frac{\partial u}{\partial x} \rightsquigarrow \frac{u_{i+1} - u_i}{\Delta x}, \qquad \frac{\partial^2 u}{\partial x^2} \rightsquigarrow \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2}.$$

Finite Volume Methods

Based on the conservation form of the PDE

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

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

Approximate each flux and write the discrete balance equation obtained.

Finite Element Methods

Based on a variational formulation of the PDE.

Solve the formulation on a suitable finite-dimensional subspace of the energy space.

Piecewise polynomials: Finite Elements / Fourier-like basis: Spectral Methods

Introduction

Let's get back to our sheep

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Introduction

We know how to solve this PDE with arbitrary accuracy, for instance using **Galerkin finite elements**.

Let $\{w_i\}_{1 \leq i \leq \mathcal{N}}$ be a finite element approximation basis (Lagrange P^1 hat functions). Then

$$u_h = \sum_{i=1}^{\mathcal{N}} u_i w_i$$

(where the u_i are $\mathcal{N}$ real coefficients) defines a finite element approximation.

Finite element linear system (Galerkin approximation)

The vector

$$\mathbf{u} = (u_1, \ldots, u_{\mathcal{N}})^T \in \mathbb{R}^{\mathcal{N}}$$

is the solution of a linear system

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

where $\mathbf{A}(\boldsymbol{\mu}) \in \mathbb{R}^{\mathcal{N} \times \mathcal{N}}$ and $\mathbf{f}(\boldsymbol{\mu}) \in \mathbb{R}^{\mathcal{N}}$.

Introduction

In practice: the finite element approximation basis $\{w_i\}_{1 \leq i \leq \mathcal{N}}$ relies on

- ◇ a mesh (partition of Ω into tetrahedra),
- ◇ for Lagrange P^1 finite elements, the number of degrees of freedom $\mathcal{N}$ equals the number of vertices.

Convergence of the finite element method

Provided that *"sufficiently uniform"* meshes are used,

$$\|u_h - u\|_{H^1} = \mathcal{O}(h^s),$$

where h denotes the mesh size and s the order of convergence.

Arbitrary accuracy can be achieved. We speak of **High Fidelity (HF)** when the prescribed accuracy is considered satisfactory. In general, $\mathcal{N}$ is large.

Reduced basis methods

Specific contexts: requiring the evaluation of the PDE solution for a *very large number of parameter values*

- parametric studies,
- sensitivity analysis,
- uncertainty quantification,
- real-time simulations,
- etc.

Despite the use of HPC, associated computational costs might be prohibitive, especially for large-scale problems.

Reduced basis methods

How to reduce the computational costs of parameter-dependent problems?

Reduced Basis Methods (RBM)

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

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

$u(\boldsymbol{\mu})$: Solution

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

Reduced Basis Methods (RBM)

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

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

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

$$\begin{cases} \text{where } \mathbf{u}(\boldsymbol{\mu}) = (u_1(\boldsymbol{\mu}), \ldots, u_{\mathcal{N}}(\boldsymbol{\mu}))^T \in \mathbb{R}^{\mathcal{N}} \\ \text{ is the solution of a linear system} \\ \mathbf{A}(\boldsymbol{\mu})\mathbf{u}(\boldsymbol{\mu}) = \mathbf{f}(\boldsymbol{\mu}). \end{cases}$$

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Aim of the reduced basis methods (RBM)

Solve the PDE as quickly as possible when it has to be evaluated for many parameter values

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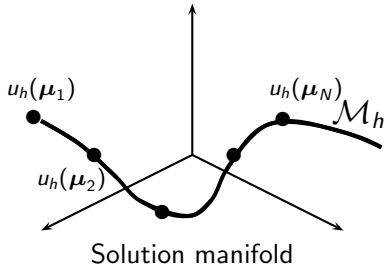

Solution manifold

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

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

Does the manifold have a favorable mathematical property that we could exploit?

Reduced space

V^N Reduced space

Reduced Basis Methods (RBM)

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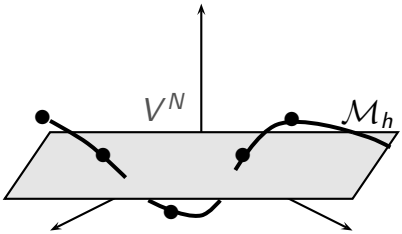

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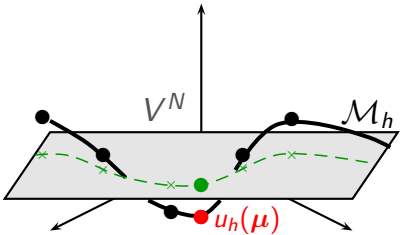

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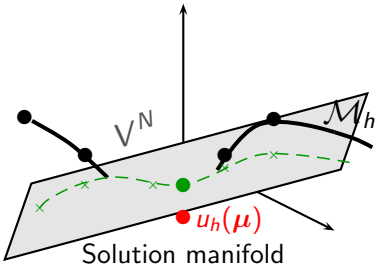

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Reduced space

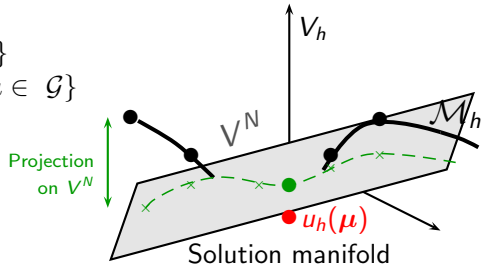
V^N Reduced space

Projection on V^N:

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

We look for the reduced **linear** space that best fit the solution manifold:

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



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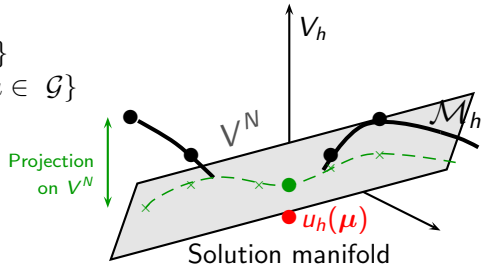

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Reduced Basis Methods (RBM)

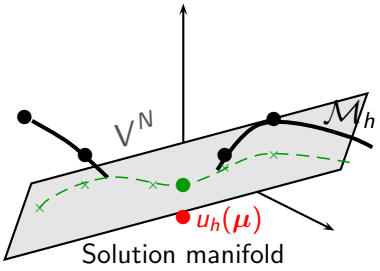
Kolmogorov N-width:

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

Favorable case:
The Kolmogorov N-width is "sufficiently small", for some N "not too large". Typically, exponential decay

$$\exists, \tau, C > 0, \ \forall N > 1, \quad d_N(\mathcal{M}, V) \leq Ce^{-\tau N}.$$

Few a priori results (first result due to Maday, Patera, and Turinici (2002))
Large number of a posteriori results, covering a wide range of applications (elliptic, parabolic, and some—but not all—hyperbolic equations).



Reduced Basis Methods

If we have N small enough, such that $d_N(\mathcal{M}_h, V_h) = \varepsilon$, and if we find the minimizing space V_N, then
$\forall \boldsymbol{\mu} \in \mathcal{G},\ \exists \boldsymbol{\alpha}(\boldsymbol{\mu}) = (\alpha_1(\boldsymbol{\mu}), \ldots, \alpha_N(\boldsymbol{\mu})) \in \mathbb{R}^N$ such that

$$\|u_h(\boldsymbol{\mu}) - \sum_{n=1}^{N} \alpha_n(\boldsymbol{\mu}) \Phi_n\|_V \leq \varepsilon,$$

with $\{\Phi_n\}_{1 \leq n \leq N}$ a basis of V^N, called **the reduced basis**.

Reduced Basis Methods

A reduced basis method is:

- ◇ **A reduced space spanned by a reduced basis:** how to build the infimum space V^N (or to approach it)?
- ◇ **An approximation (in the reduced space):** how to find the N coefficients $(\alpha_1(\boldsymbol{\mu}), \ldots, \alpha_N(\boldsymbol{\mu})) \in \mathbb{R}^N$ such that

$$u_N(\boldsymbol{\mu}) = \sum_{n=1}^{N} \alpha_n(\boldsymbol{\mu}) \Phi_n$$

be the best approximation of $u(\boldsymbol{\mu})$ on V^N?

$u_N(\boldsymbol{\mu}) \in V^N$ is called **the reduced basis approximation.**

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Remarks: The best coefficients are the projection coefficients of $u_h(\boldsymbol{\mu})$:

$$\alpha_n(\boldsymbol{\mu}) = (u_h(\boldsymbol{\mu}), \Phi_n).$$

But of course, we don't want to compute $u_h(\boldsymbol{\mu})$ ...

Reduced basis methods

- Galerkin-POD[a]
- Petrov-Galerkin RBM[b]
- EIM[c]
- POD-DL-ROM[d]
- 2-grid method[e]
- POD-I[f] (Reg, NN)
- PBDW[g]
- PGD[h]
- Surrogate problems[i]
- Operator inference[j]

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[a] J.L. Lumley. *The structure of inhomogeneous turbulent flows.* 1967

[b] K. Carlberg, M. Barone, H. Antil. *Galerkin v. least-squares Petrov-Galerkin projection in nonlinear model reduction.* 2017

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Reduced basis methods: https://reducedbasis.github.io

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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**.

In general, greedy algorithms are more efficient if they are combined with **aposteriori errors**.

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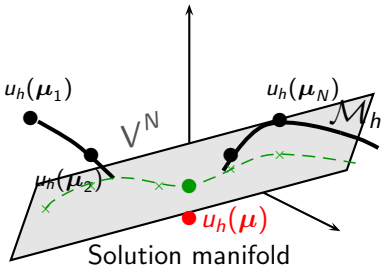
Reduced Basis Methods

In both cases, the set of basis functions is derived from HF solutions for several well chosen parameter values, $\{u_h(\boldsymbol{\mu}_1), \ldots, u_h(\boldsymbol{\mu}_N)\}$, called **the snapshots**.



Sum up

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- Resolution by a classical discretization method (FEM/FV ...)
  A system of size dependent of the number of degrees of freedom $\mathcal{N}$ needs to be solved!
  How to decrease the High-Fidelity (HF) code execution runtimes when we need to solve the problem for **many different parameter values**?

  ROM: Reduce the dimension of the algebraic system arizing from the discretization of a PDE.

- RBM: The solution is obtained with a projection of the HF problem onto a reduced subspace.
- How to obtain the reduced basis?
  POD (TP1) /Greedy algorithms (TP2)
- How to project the HF problem onto the reduced space?

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POD-Galerkin

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Exercise

1. Write the weak formulation of the problem.
2. Prove that the problem is well-posed under some conditions.

POD-Galerkin

Context: $V_N \subset V$ is a subspace of dimension N.

Definition
The Galerkin reduced-basis approximation is the function $u_N(\boldsymbol{\mu}) \in V_N$ satisfying the weak form

$$\forall v_N \in V_N, \qquad a\left(u_N(\boldsymbol{\mu}), v_N; \boldsymbol{\mu}\right) = \ell\left(v_N; \boldsymbol{\mu}\right).$$

Exercise

Show that if $a(\cdot, \cdot; \boldsymbol{\mu}) : V \times V \to \mathbb{R}$ is coercive, then the Galerkin reduced-basis approximation exists and is unique.

POD-Galerkin

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

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

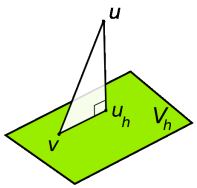
then

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

gives a new system to solved:

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

where $\mathbf{P} \in \mathbb{R}^{\mathcal{N}\times N}$.



G-RB proof

FEM recall: Standard FEM Galerkin condition

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

$$\boxed{a(e_h, v_h) = a(u - u_h, v_h) = 0, \ \forall v_h \in V_h.}$$

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

$$r(v_h) = a(u, v_h) - a(u_h, v_h) = a(e_h, v_h) = 0, \ \forall v_h \in V_h.$$

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

POD-Galerkin

Let $\mathbf{P} = [\Phi_1, \ldots, \Phi_N] \in \mathbb{R}^{N \times \mathcal{N}}$, i.e. $\Phi_j = \sum_{i=1}^{\mathcal{N}} P_{ij} w_i$ and $P = (P_{ij}) \in \mathbb{R}^{N \times \mathcal{N}}$.
$u_N(\boldsymbol{\mu}) = \sum_{n=1}^{N} \alpha_n(\boldsymbol{\mu}) \Phi_n = \mathbf{P}\boldsymbol{\alpha}(\boldsymbol{\mu}),\ \boldsymbol{\alpha} = \boldsymbol{\alpha}(\boldsymbol{\mu}) \in \mathbb{R}^N,\ \mathbf{r}(\boldsymbol{\alpha}) = \mathbf{l}(\boldsymbol{\mu}) - \mathbf{A}(\boldsymbol{\mu})(\mathbf{P}\boldsymbol{\alpha})$.

RB Galerkin condition

1. The residual is orthogonal to the test space V_N : , $\forall v_N \in V_N$.
2. With HF basis $\{w_i\}_{i=1}^{\mathcal{N}}$, we know that:

$$\ell(v_N) = \mathbf{v_N}^T \mathbf{l}, \quad a(u_N, v_N) = \mathbf{v_N}^T \mathbf{A} \mathbf{u_N},\ \forall v_N \in V_N \subset V_h,$$

with $\mathbf{A}_{ij} = a(w_j, w_i)$, $\mathbf{l}_i = \ell(w_i)$
So $r(v_N) = \mathbf{v_N}^T \mathbf{r}$. Thus, $\forall v_N \in V_N$, $\mathbf{v_N}^T \mathbf{r}(\alpha) = 0$.

3. But $v_N \in V_N$, so $v_N = \mathbf{P}\beta$ with $\beta \in \mathbb{R}^N$, and $(\mathbf{P}\beta)^T(\mathbf{l}(\mu) - \mathbf{A}(\mu)(\mathbf{P}\alpha(\mu))) = 0$.
True for all $\beta \in \mathbb{R}^N$: $\mathbf{P}^T(\mathbf{l}(\mu) - \mathbf{A}(\mu)\mathbf{P}\alpha(\mu)) = 0$. Thus,

$$\mathbf{P}^T \mathbf{A}(\mu)\mathbf{P}\ \alpha(\mu) = \mathbf{P}^T \mathbf{l}(\mu).$$

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POD-Galerkin

Interpretation: With the standard RB Galerkin projection, we look for $\boldsymbol{\alpha}$ that minimizes the error in the energy norm.

$$u_N = \arg \min_{v_N \in V_N} \|u - v_N\|_a$$

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 $\mathbf{P}^T b \in \mathbb{R}^N$!

Remarks

- ◇ Other projections can be considered (e.g. Petrov-Galerkin projection $\mathbf{W}^T\mathbf{A}\mathbf{P}\boldsymbol{\alpha} = \mathbf{W}^T\mathbf{I}$ with a test basis $\mathbf{W} \neq \mathbf{P}$).
- ◇ In (G-RB), we first need to assemble $\mathbf{A}(\boldsymbol{\mu}) \in \mathbb{R}^{\mathcal{N}\times\mathcal{N}}$.

Exercise

Consider the PDE model and derive an offline/online strategy to overcome the complexity of the assembly process.

Affine operator
definition

the bilinear for $a(\cdot,\cdot;\ \boldsymbol{\mu}) : V \times V \to \mathbb{R}$ is affine if there exist

- Q^a functions $\theta_q^a : \mathcal{G} \to \mathbb{R},\ 1 \leq q \leq Q^a$ bounded (i.e. $\theta_q^a(\mathcal{G})$),
- Q^a functions $a_q : V \times V \to \mathbb{R},\ 1 \leq q \leq Q^a$

such that

$$\forall \boldsymbol{\mu} \in \mathcal{G},\ \forall (u,v) \in V \times V, a(u,v;\ \boldsymbol{\mu}) = \sum_{q=1}^{Q^a} \theta_q^a(\boldsymbol{\mu}) a_q(u,v).$$

$\mathbf{A}(\boldsymbol{\mu}) = \sum_{q=1}^{Q^a} \theta_q^a(\boldsymbol{\mu}) \mathbf{A}_q.$

And surprisingly for l ...
definition
the linear for $l(\cdot;\ \boldsymbol{\mu}) : V'$ is affine if there exist

- $\diamond$ Q^l functions $\theta_l^a : \mathcal{G} \to \mathbb{R},\ 1 \leq q \leq Q^l$ bounded (i.e. $\theta_q^l(\mathcal{G})$),
- $\diamond$ Q^l functions $l_q : V',\ 1 \leq q \leq Q^l$

such that

$$\forall \boldsymbol{\mu} \in \mathcal{G},\ \forall v \in V, a(v;\ \boldsymbol{\mu}) = \sum_{q=1}^{Q^l} \theta_q^l(\boldsymbol{\mu}) l_q(v).$$

$\mathbf{l}(\boldsymbol{\mu}) = \sum_{q=1}^{Q^l} \theta_q^l(\boldsymbol{\mu}) \mathbf{l}_q.$

POD-Galerkin

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-Galerkin

Visit `https://reducedbasis.github.io/docs/pod/` for the reduced basis Galerkin approximation of the Navier-Stokes problem.

Sum up

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- Resolution by a classical discretization method (FEM/FV ...)
  A system of size dependent of the number of degrees of freedom $\mathcal{N}$ needs to be solved!
  How to decrease the High-Fidelity (HF) code execution runtimes when we need to solve the problem for **many different parameter values**?

ROM: Reduce the dimension of the algebraic system arizing from the discretization of a PDE.

- RBM: The solution is obtained with a projection of the HF problem onto a reduced subspace.
- How to obtain the reduced basis?
  POD (TP1) /Greedy algorithms (TP2)
- How to project the HF problem onto the reduced space?
  Galerkin projections

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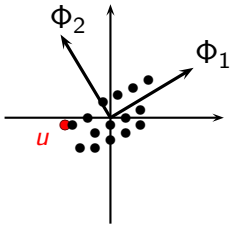
POD

Chapter 2
POD + TP FV

POD: Continuous version

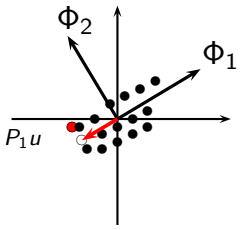
We want to approximate $u(\mathbf{x}, \boldsymbol{\mu})$ by $\sum_{k=1}^{N} a_k(\boldsymbol{\mu})\Phi_k(\mathbf{x})$.

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!



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

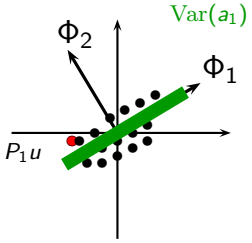
POD: Continuous version



Snapshot projection over Φ_1: $(u, \Phi_1)\Phi_1$

POD: Continuous version

How do we find the reduced basis?



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

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

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

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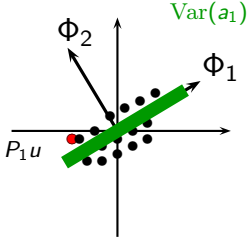

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POD: Continuous version

We want to approximate $u(\mathbf{x}, \boldsymbol{\mu})$ by $\sum_{k=1}^{N} a_k(\boldsymbol{\mu})\Phi_k(\mathbf{x})$,
with $\Phi_k \in L^2(\Omega)$ + orthonormality $\int_\Omega \Phi_i(\mathbf{x})\Phi_j(\mathbf{x})\, d\mathbf{x} = \delta_{ij}$.

We look for $\Phi_i,\ i = 1, \ldots, N$ that maximize the average projection:

$$\max_{\|\Phi_i\|=1} \mathbb{E}[|(u, \Phi_i)|^2].$$

With $\Phi_1 \in V$ where V is a real Hilbert space, one can show that this maximization problem is equivalent to a spectral problem

$$\boxed{C\Phi_1 = \lambda_1 \Phi_1}$$

(assuming that the dominated convergence theorem can be applied).

POD: Continuous version

Proof

Lagrangian: $J[\Phi_1] = \mathbb{E}[|(u, \Phi_1)|^2] - \lambda(\|\Phi_1\|^2 - 1)$.

Directional derivative (with a small variation Ψ):

$J[\Phi + \delta\Psi] = \mathbb{E}[|(u, \Phi + \delta\Psi)|^2] - \lambda(\|\Phi + \delta\Psi\|^2 - 1)$.

$\frac{d}{d\delta} J[\Phi + \delta\Psi]_{|\delta=0} = 0$.

- $(u, \Phi + \delta\Psi) = (u, \Phi) + \delta(u, \Psi)$,
  so $(u, \Phi + \delta\Psi)^2 = (u, \Phi)^2 + 2\delta(u, \Phi)(u, \Psi) + O(\delta^2)$
  and with average:
  $\mathbb{E}[(u, \Phi + \delta\Psi)^2] = \mathbb{E}[(u, \Phi)^2] + 2\delta\mathbb{E}[(u, \Phi)(u, \Psi)] + O(\delta^2)$
  So $\frac{d}{d\delta}\mathbb{E}[(u, \Phi + \delta\Psi)^2]_{|\delta=0} = 2\mathbb{E}[(u, \Phi)(u, \Psi)]$
- $(\Phi + \delta\Psi, \Phi + \delta\Psi) = (\Phi, \Phi) + 2\delta(\Phi, \Psi) + O(\delta^2)$, so
  $\frac{d}{d\delta}(\Phi + \delta\Psi, \Phi + \delta\Psi)_{|\delta=0} = 2(\Phi, \Psi)$.

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POD: Continuous version

Proof

Altogether, we obtain:

$$\boxed{\mathbb{E}[(u,\Phi)(u,\Psi)] - \lambda(\Phi,\Psi) = 0}$$

Let C be such that $(C\Phi,\Psi) = \mathbb{E}[(u,\Phi)(u,\Psi)]$. Then

$$(C\Phi,\Psi) = \lambda(\Phi,\Psi), \forall \Psi.$$

Since true for all Ψ, we obtain:

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

We can prove that C is a positive linear compact self-adjoint operator: the problem is well-posed.

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Spectral theorem (Compact Self-Adjoint Operator)
Let V be a separable Hilbert space and let $C : V \to V$ be a compact, positive, self-adjoint operator. Then there exists an orthonormal basis $\{\Phi_n\}_{n\in\mathbb{N}}$ of V and a sequence of real numbers $(\lambda_n)_{n\in\mathbb{N}} \geq 0$ such that, for all $n \in \mathbb{N}$,

$$C\Phi_n = \lambda_n \Phi_n.$$

Moreover, $\lim_{n\to\infty} \lambda_n = 0$.

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- Assume that there exists λ_n such that $\lim_{n\to\infty} \lambda_n \neq 0$.
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  C compact $\Rightarrow (C\Phi_{n_k})$ admit a convergent subsequence
- (Φ_n) orthonormal $\Rightarrow \|\Phi_n - \Phi_m\| = \sqrt{2} \quad$ for $n \neq m$.
  For the subsequence: $\|C\Phi_{n_{k'_k}} - C\Phi_{m_{k'_k}}\| = \|\lambda_{n_{k'_k}}\Phi_{n_{k'_k}} - \lambda_{m_{k'_k}}\Phi_{m_{k'_k}}\| \nrightarrow 0 \quad$ if $|\lambda_{n_k}| \geq \varepsilon$.

This contradicts the compactness of C.

Snapshot POD

Spectral theorem (Compact Self-Adjoint Operator)
Let V be a separable Hilbert space and let $C : V \to V$ be a compact, positive, self-adjoint operator. Then there exists an orthonormal basis $\{\Phi_n\}_{n\in\mathbb{N}}$ of V and a sequence of real positive numbers $(\lambda_n)_{n\in\mathbb{N}}$ such that, for all $n \in \mathbb{N}$,

$$C\Phi_n = \lambda_n \Phi_n.$$

Moreover, $\lim_{n\to\infty} \lambda_n = 0$.

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

One can prove that C is a positive linear compact self-adjoint operator: one unique solution equal to the largest eigenvalue of the problem!
$(C\Phi, \Phi) = \mathbb{E}[|(u, \Phi)|^2] = \lambda$
$\max_{\|\Phi_1\|=1} \mathbb{E}[|(u, \Phi_1)|^2] = \lambda_1$

POD energy error

$\lambda_1 >= \lambda_2 >= ... >= 0$

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

Proof:
Since $\{\Phi_k\}$ is an orthonormal basis of V, $u(\boldsymbol{\mu}) = \sum_{k=1}^{\infty} a_k(\boldsymbol{\mu})\Phi_k$.

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

In fact, one can show that the more regularizing the operator C is, the faster its eigenvalues decay!

Link between regularity and eigenvalues

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

Exercise

Let $A : L^2(0,1) \to L^2(0,1)$ be defined by $(Ax)(t) = \int_0^t x(s)\, ds$.

1. Determine the adjoint operator A^*.

2. Define $C = A^*A$. Show that C is a compact, positive, and self-adjoint operator on $L^2(0,1)$.

3. Let σ denote a singular value of A, and let $x \neq 0$ satisfy $Cx = A^*Ax = \sigma^2 x$.

(a) Show that A^*Ax is twice differentiable and compute $(A^*Ax)''(t)$.

(b) Deduce that x satisfies the differential equation $x(t) + \sigma^2 x''(t) = 0$.

4. Using the appropriate boundary conditions, determine the general form of the eigenfunctions $x(t)$.

5. Deduce the explicit expression of the singular values σ_n of A and determine their asymptotic behaviour as $n \to \infty$.

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

Thus $\sigma = 1$ No decrease! **No efficient basis functions for transport and advection-dominated regime**

- No regularity gain
- No compacity
- No decrease in POD eigenvalues
- No efficient basis functions

What can we do in that case?

- shifted POD
- transport maps
- nonlinear reduced bases
- POD + autoencoders

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- No efficient basis functions

What can we do in that case?

Transport:

$$\begin{cases} \text{shifted POD: } u(x,t) = \sum_k \sum_n a_{k,n}(t)\Phi_{k,n}(\mathbf{x} - \mathbf{s}_k(t)) \\ \text{transport maps: } u(x,t) = \sum_n a_n(t)\Phi_n(T_t(\mathbf{x})) \end{cases}$$

Nonlinear dynamics:

$$\begin{cases} \text{nonlinear reduced bases: } = \mathrm{F(u)} \leftrightarrow \dot{a} = Aa + H(a \otimes a) \\ \text{POD+autoencoders } [1](\mathrm{t},\mu) \rightarrow NN \rightarrow a(t,\mu) \rightarrow u \simeq Va \end{cases}$$

[1] POD_DL_ROM: https://reducedbasis.github.io/docs/poddlrom/

Sheep model

Let's get back to our sheep

linear second-order parameter dependent problem

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

$u(\mathbf{x}; \boldsymbol{\mu}) \in V$: Unknowns,

$\boldsymbol{\mu} \in \mathcal{G}$: Variable parameter,

How do we construct the reduced basis with the POD in practice?

Snapshot POD

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

$\Leftrightarrow \int_\Omega R(\mathbf{x}, \mathbf{x}')\ \Phi(\mathbf{x}')d\mathbf{x}' = \lambda\Phi(\mathbf{x})$, with $R(\mathbf{x}, \mathbf{x}') = \mathbb{E}[u(\mathbf{x})u(\mathbf{x}')]$, which is the spatial continuous covariance operator.

Snapshot POD

The space of the modes is contained into the snapshots' span.

$$R(\mathbf{x},\mathbf{x}') = \mathbb{E}[u(\mathbf{x})u(\mathbf{x}')] \simeq \frac{1}{N_{train}} \sum_{k=1}^{N_t rain} u(\mathbf{x},\boldsymbol{\mu}_k)u(\mathbf{x}',\boldsymbol{\mu}_k).$$

$$\text{so} \int_\Omega R(\mathbf{x},\mathbf{x}')\ \Phi(\mathbf{x}')d\mathbf{x}' \simeq \frac{1}{N_{train}} \sum_{k=1}^{N_{train}} u(\mathbf{x},\boldsymbol{\mu}_k) \underbrace{\int_\Omega u(\mathbf{x}',\boldsymbol{\mu}_k)\Phi(\mathbf{x}')d\mathbf{x}'}_{a_k=(u(\boldsymbol{\mu}_k),\Phi)} = \lambda\Phi(\mathbf{x}), \qquad (\mathrm{R})$$

$$\boxed{\text{Therefore } \Phi(\mathbf{x}) = \sum_{k=1}^{N_{train}} \alpha_k u(\mathbf{x},\boldsymbol{\mu}_k).}$$

$$a_k = (u(\boldsymbol{\mu}_k),\Phi) = (u(\boldsymbol{\mu}_k), \textstyle\sum_{j=1}^{N_{train}} \alpha_j u(\boldsymbol{\mu}_j)) = \sum_{j=1}^{N_{train}} \alpha_j \underbrace{(u(\boldsymbol{\mu}_k), u(\boldsymbol{\mu}_j))}_{\mathbf{C}_{k,j}}$$

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

Snapshot POD

The space of the modes is contained into the snapshots' span.

$$R(\mathbf{x},\mathbf{x}') = \mathbb{E}[u(\mathbf{x})u(\mathbf{x}')] \simeq \frac{1}{N_{train}} \sum_{k=1}^{N_t rain} u(\mathbf{x},\boldsymbol{\mu}_k)u(\mathbf{x}',\boldsymbol{\mu}_k).$$

$$\text{so} \int_\Omega R(\mathbf{x},\mathbf{x}')\ \Phi(\mathbf{x}')d\mathbf{x}' \simeq \frac{1}{N_{train}} \sum_{k=1}^{N_{train}} u(\mathbf{x},\boldsymbol{\mu}_k) \underbrace{\int_\Omega u(\mathbf{x}',\boldsymbol{\mu}_k)\Phi(\mathbf{x}')d\mathbf{x}'}_{a_k=(u(\boldsymbol{\mu}_k),\Phi)} = \lambda\Phi(\mathbf{x}), \qquad (\mathsf{R})$$

$$\boxed{\text{Therefore } \Phi(\mathbf{x}) = \sum_{k=1}^{N_{train}} \alpha_k u(\mathbf{x},\boldsymbol{\mu}_k).}$$

$$a_k = (u(\boldsymbol{\mu}_k),\Phi) = (u(\boldsymbol{\mu}_k), \textstyle\sum_{j=1}^{N_{train}} \alpha_j u(\boldsymbol{\mu}_j)) = \sum_{j=1}^{N_{train}} \alpha_j \underbrace{(u(\boldsymbol{\mu}_k), u(\boldsymbol{\mu}_j))}_{\mathbf{C}_{k,j}}$$

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Snaphot POD

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

gives for one $k = i$

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

Thus, $\mathbf{C}\alpha = N_{train}\lambda\alpha = \lambda'\alpha$: the eigenvalues of the spatial covariance operator or the snapshot correlation matrix are the same (up to a factor N_{train})!

Discretization

$$\mathbf{C}\alpha = \lambda'\alpha \tag{C}$$

We impose (α_n) orthonormal.
Let $S = [u_1, \ldots, u_{N_{train}}] \in \mathbb{R}^{\mathcal{N} \times N_{train}}$. Then $\Phi = S\alpha$, and
$\|\Phi\|^2 = (S\alpha, S\alpha) = \alpha^T S^T S\alpha$
But (C) implies that $\|\Phi\|^2 = \lambda'\alpha^T\alpha = \lambda'$

$$\text{Hence } \tilde{\Phi}(\mathbf{x}) = \frac{1}{\sqrt{\lambda'}} \sum_{k=1}^{N_{train}} \alpha_k u(\mathbf{x}, \boldsymbol{\mu}_k) \text{ (after normalization)}$$

Let us denote in the following slides $\Phi = \tilde{\Phi}$ and $\lambda = \lambda'$.

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 $\Phi_i = \frac{1}{\sqrt{\lambda_i}} S\alpha_i,\ i = 1, \ldots, N$

The space of the modes is contained into the snapshots' span: $N \leq N_{train}$
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:
$1 - \sum_{k=1}^{N} \lambda_k / \sum_{k=1}^{N_{train}} \lambda_k$

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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Finite Volume Methods

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

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

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Finite Volume Methods

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:

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

Approximate each flux and write the discrete balance equation obtained.

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: $|K|, |\sigma|, d_{K\sigma}, d_{L\sigma}, d_{KL}$

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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Define $u_h \to F_{K,\sigma}(u_h)$ that approximates the flux and find $u \in \mathbb{R}^{\mathcal{T}}$ such that

$$|K| f_K = \sum_{\sigma \in \mathcal{F}_K} F_{K,\sigma}, \ \forall K \in \mathcal{T}$$

.

TP: VF5-TPFA

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 $u \in \mathbb{R}^{\mathcal{T}}$ such that

$$|K| f_K = \sum_{\sigma\in\mathcal{F}_K} F_{K,\sigma},\ \forall K \in \mathcal{T}$$

.

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

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 $u \in \mathbb{R}^{\mathcal{T}}$ such that

$$|K| f_K = \sum_{\sigma\in\mathcal{F}_K} F_{K,\sigma},\ \forall K \in \mathcal{T}$$

.

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: TPFA (Two-Point Flux Approximation)

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.
$A(x, y; \mu) = 2\mu_1 + \mu_2 \ sin(x + y) \ cos(xy)$
$f(x, y; \mu) = \mu_3(1 - y) + \mu_4 x \ (1 - x)$

TP: VF5-TPFA

POD-based Reduced Order Model with TPFA

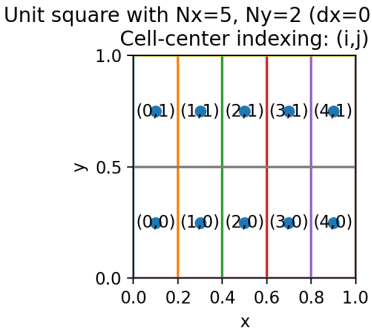
- ◇ Complete the function `assemble_tpfa`. The TPFA solver must return the cell centers, the matrix M, and the vector b such that $Mu = b$.
- ◇ Generate a training dataset:
  - Use $N_{train} = 10$ snapshots and sample random parameters $\boldsymbol{\mu}$ with components in $[0, 1]$.
  - Solve the full-order 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 $\|u_{\text{ref}} - u\|_{L^2}$ and $\|u_{\text{ref}} - u_N\|_{L^2}$, 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)
1.0
0.5
0.0
y
0.0
0.2
0.4
0.6
0.8
1.0
x