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Internship report

Study and implementation of an "a posteriori estimator" for Finite Volume Methods in CFD

Internship report of
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I am highly grateful to **Giovani STABILE** for accepting me as the first (temporary) member of his AI and Reduced Order Methods (ROM) lab and giving me so much of his time. This research project takes part in the DANTE ERC StG project which aims to extend the ROM coupled with AI to Computational Fluids Dynamic and apply it to high-scale simulations.

My focus was on a "a posteriori" error estimator that is presented p.12 which is used in ROM and is based on the Finite Elements Method (FEM) framework. Namely, I tried to formulate the Finite Volumes Methods (FVM) in the FEM framework to make use of this estimator.

This report is divided as follow:
Part 1 is a quick introduction of the FEM.
Part 2 introduces the Certified Reduced Basis Method that is already established for FEM.
Part 3 presents the cell-centered FVM and some error estimators that are used in CFD.
Part 4 presents our work: the merging of a Weak FVM formulation with the RBM.
An **Appendix** and a **Bibliography** are given for standards results and references.

The main result of this report is the connection between a FVM formulation that blends in the FEM framework and the ROM framework p.18.
For further research, the extension of the result may lies in the *Mathematical aspects of discontinuous Galerkin method* [PE12] or the *The Gradient Discretisation Method* [Dro+18], whose links with the problem will not be explicitly addressed in the report.

A longer version of this report with detailed proofs, ideas with Discontinuous Galerkin, Gradient Discretisation, Box Methods and additional material is available here [Lec24b].

For any questions or if you find a mistyping, please contact me or Giovanni:

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Part 1
Finite Element Method

The goal is to approximate the solution of a PDE that lives in an infinite dimensional vector space by the solution of the same PDE restricted to a finite dimensional vector space.
See more in the following book: *The Mathematical Theory of Finite Element Methods*, [BS08].

I - Weak formulation

1) Parametrized Partial Differential Equation

Take any regular set open $\Omega \subset \mathbb{R}^d, d \in \{1,2,3\}$. Define $\partial\Omega := \overline{\Omega} \backslash \Omega$.
We consider field variables $\omega : \Omega \longrightarrow \mathbb{R}^{d_v}$.
Set $(\Gamma_i^D)_{1 \leq i \leq d_v}$ such that $\Gamma^D := \bigcup \Gamma_i^D \subset \partial\Omega$ (not necessary equal).
Define $\mathbb{V}_i := \left\{ v \in \mathbf{H}^1(\Omega, \mathbb{R}) \ / \ v|_{\Gamma_i^D} = 0 \right\}$ $(v : \Omega \to \mathbb{R})$.

$$\mathbb{V} := \prod_{i=1}^{d_v} \mathbb{V}_i \text{ of infinite dimension.}$$

Remark :

$\mathbb{V}_i$ is the space of the $i-th$ coordinate in $\mathbb{R}^{d_v}$ of a solution.

$$v \in \mathbb{V} \Rightarrow v \cong \sum_{i=1}^{d_v} v_i \underbrace{\varphi_i}_{\in \mathbb{V}_i} \Rightarrow \mathbb{V} \cong \left\{ v \in \mathbf{H}^1(\Omega) \ / \ v : \Omega \to \mathbb{R}^{d_v}, v|_{\Gamma^D} = 0 \right\}$$

Note that $\mathbb{V} \subset \mathbf{H}^1$, s.t. if $\langle \cdot | \cdot \rangle_{\mathbb{V}}$ induces $\|\cdot\|_{\mathbb{V}} \sim \|\cdot\|_{\mathbf{H}^1}$, then $(\mathbb{V}, \langle \cdot | \cdot \rangle_{\mathbb{V}})$ is an Hilbert.
We focus on $\mathbb{P} \subset \mathbb{R}^P$ closed set of parameters.

Definition 1.1: Parametrized PDE

Let $f : \mathbb{V} \times \mathbb{P} \to \mathbb{R}$ continuous linear with respect to $\mathbb{V}$.
$\ell : \mathbb{V} \times \mathbb{P} \to \mathbb{R}$ linear with respect to $\mathbb{V}$.
$a : \mathbb{V} \times \mathbb{V} \times \mathbb{P} \to \mathbb{R}$ bilinear coercive continuous symmetric with respect to $\mathbb{V} \times \mathbb{V}$.
We consider

$$\begin{cases} \text{Solve for } u \in \mathbb{V} & a(u, v \ ; \mu) = f(v \ ; \mu) \quad \forall v \in \mathbb{V} \\ \text{Evaluate for } \mu \in \mathbb{P} & s(\mu) := \ell(u \ ; \mu) \end{cases}$$

Let $\alpha(\mu)$ be the coercive constant, $\gamma(\mu)$ the continuous one.
The symmetry and continuity ensure well-posedness of the PDE through Lax-Milgram.

Let $\mu \in \mathbb{P}$, $\mu = (\mu_{[1]}, \ \ldots \ , \mu_{[P]})$, then we define the solution of the PPDE $u(\mu) = (u_1, \ \ldots \ , u_{d_v})$.

Remark :

ℓ is any linear function to define depending on which output correlation we're looking for.

2) Dicretization

Take $\mu \in \mathbb{P}$.
Suppose there exists $\mathbb{V}_\delta \subset \mathbb{V}$ finite dimensional vector space that approximates well $\mathbb{V}$, we search $u_\delta(\mu) \in \mathbb{V}_\delta$ solution of the PPDE on $\mathbb{V}_\delta$.
Let $N_\delta = \dim\left(\mathbb{V}_\delta\right)$ such that $\mathbb{V}_\delta = Vect\left(\{\varphi_i\}_{i=1}^{N_\delta}\right)$.

Definition 1.2: Discretized PDE

Find $u_\delta(\mu)$ such that

$$\begin{cases} a(u_\delta(\mu), v_\delta; \mu) = f(v_\delta; \mu) \quad \forall\ v_\delta \in \mathbb{V}_\delta \\ s_\delta(\mu) = \ell(u_\delta(\mu); \mu) \end{cases}$$

Since $a(u_\delta(\mu), v_\delta; \mu) = f(v_\delta; \mu) = a(u(\mu), v_\delta; \mu)$ there holds

Proposition 1.3: Galerkin's orthogonality

For all v_δ in $\mathbb{V}_\delta$ the following orthogonality holds:

$$a(u_\delta(\mu) - u(\mu), v_\delta; \mu) = 0$$

One important lemma is the following one, which states that the error induced by the solution of the equation is proportional to the best estimation of u we could hope in the discrete space.

Lemma 1.4: Céa's lemma

For all $v_\delta \in \mathbb{V}_\delta$:

$$\|u(\mu) - u_\delta(\mu)\|_{\mathbb{V}} \leq \left(1 + \frac{\gamma(\mu)}{\alpha(\mu)}\right) \inf_{v_\delta \in \mathbb{V}_\delta} \|u(\mu) - v_\delta\|_{\mathbb{V}}$$

$\mathcal{D}$

First note

$$\begin{aligned} \alpha \|u(\mu) - u_\delta(\mu)\|_{\mathbb{V}}^2 \leq a(u(\mu) - u_\delta(\mu), u(\mu) - u_\delta(\mu)) &= a(u(\mu) - u_\delta(\mu), u(\mu)) \\ &= a(u(\mu) - u_\delta(\mu), u(\mu)) - v_\delta) \\ &\leq \gamma \|u(\mu) - u_\delta(\mu)\|_{\mathbb{V}} \|u(\mu) - v_\delta\|_{\mathbb{V}} \end{aligned}$$

Then

$$\begin{aligned} \|u(\mu) - u_\delta(\mu)\|_{\mathbb{V}} &\leq \|u(\mu) - v_\delta\|_{\mathbb{V}} + \|v_\delta - u_\delta(\mu)\|_{\mathbb{V}} \\ &\leq \|u(\mu) - v_\delta\|_{\mathbb{V}} + \frac{\gamma}{\alpha} \|u(\mu) - v_\delta\|_{\mathbb{V}} \\ &= (1 + \frac{\gamma}{\alpha}) \|u(\mu) - v_\delta\|_{\mathbb{V}} \end{aligned}$$

□

The solution of the discrete equation is easy to write and we define the *Truth Solver* or *Full order equation* as follows:

Definition 1.5: Truth Solver

We call the truth solver, the solution of the linear system $A_\delta^\mu u_\delta(\mu) = f_\delta^\mu$ where

$$\begin{cases} (M_\delta)_{i,j} & = & \langle \varphi_i | \varphi_j \rangle_{\mathbb{V}} \\ (A_\delta^\mu)_{i,j} & = & a(\varphi_i, \varphi_j\ ; \mu) \\ (f_\delta^\mu)_i & = & f(\varphi_i\ ; \mu) \\ (\ell_\delta^\mu)_i & = & \ell(\varphi_i\ ; \mu) \end{cases}$$

Remark :

M_δ is the mass matrix that can have a role for defining the property of the space or of the functions. It will not have a role in our report.

II - Solution approximation

1) Finite Elements

We cut Ω in N_e disjoints subspaces $\Omega^{(e)}$ and we set N_i nodes that constitutes the nodal basis, we note $(x_i)_{i \le N_i}$ their coordinates.
A subspace $\Omega^{(e)}$ is called a Finite Element, the set of all the Finite Elements is called the mesh. To have a well defined method, we need to do some assumptions on the geometry of a finite element:
- Each element is a star shapped open set
- Each element is polygonal

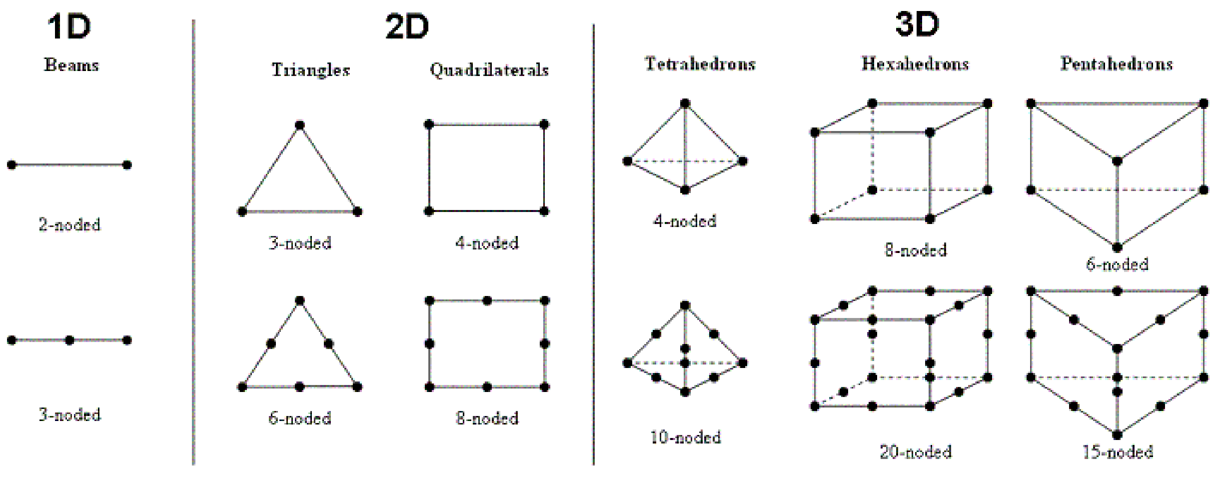

Figure 1: Polygonal elements in 1D, 2D, 3D

Most importantly, the diameter of an element controls the polynomial approximation thanks to Poincaré's inequality 5.6. Hence a thinner grid gives better approximation.

2) Polynomial Approximation

The Bramble Hilbert lemma 5.5 shows that a polynomial approximation is a good candidate for Sobolev spaces approximation. Moreover, the polynomials are the easiest functions to work with.
On each nodes, we define a piece-wise polynomial function φ_i of degree lesser than m which is such that

$$\varphi_i(x_j) = \delta_{ij}$$

Such polynomial exists and form an orthogonal basis of functions using Averaged Taylor Polynomials ([BS08] Chap 4). Define

$$\mathbb{V}_\delta = \text{Span}\left\{(\varphi_i)_i\right\} \subset \mathbb{V}$$

We will only consider the linear approximation :

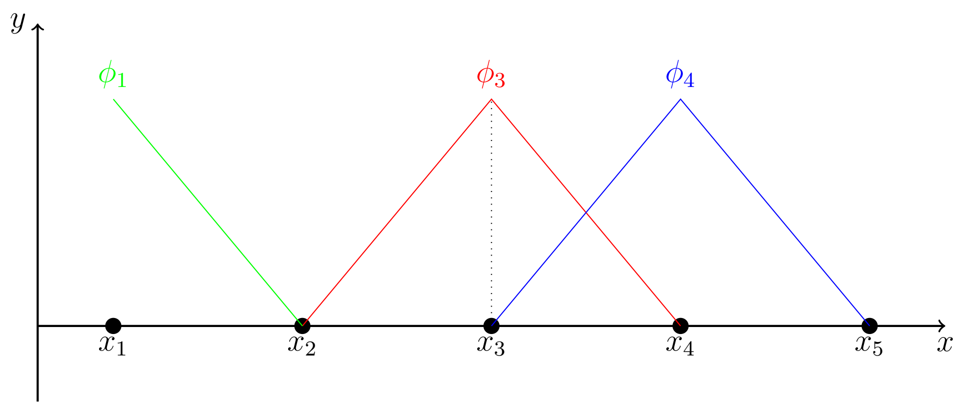

Figure 2: Some basis functions of the nodal basis of linear functions

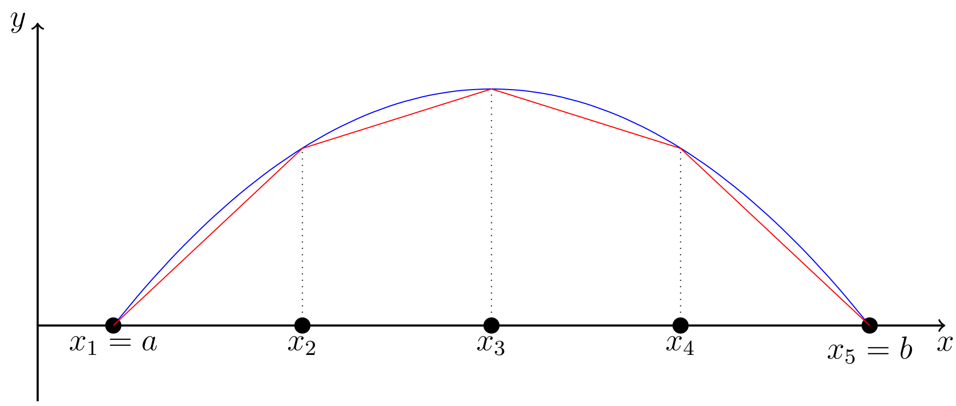

Figure 3: Finite Element approximation in 1D of the function $(x - a)(x - b)$

Part 2
Certified Reduced Basis Method

This part sums up *Certified Reduced Basis Methods for Parametrized Partial Differential Equations.* [HRS16] chapters that were most important in our research. This framework allows to do significantly faster computations in the case of FEM, see [Sta23].

I - Reduced Basis Method

The goal of the reduced basis method is to find an appropriate functional discrete space that allows accurate approximation in the smallest dimension as it is possible.

1) Solution manifold and Reduced Basis Approximation

Definition 2.1: Solution manifold

If we are able to write $u(\mu)$ in analytic form, the solution manifold is:

$$\mathcal{M} = \{u(\mu) \;/\; \mu \in \mathbb{P}\} \subset \mathbb{V}$$

If we can't, consider $\mathbb{V}_\delta$ such as in 2) Discretization

$$\mathcal{M}_\delta = \{u_\delta(\mu) \;/\; \mu \in \mathbb{P}\} \subset \mathbb{V}_\delta$$

Admits there exists $\mathbb{V}_{rb} \subset \mathbb{V}_\delta$, dim $(\mathbb{V}_{rb}) = N$ such that $N \ll N_\delta <$ dim $(\mathbb{V}) = +\infty$, there exists $\xi_1, \ \dots \ , \xi_N \in \mathbb{V}_\delta$, such that

$$\mathbb{V}_{rb} = \text{Span}\,(\xi_1, \ \dots \ , \xi_N)$$

Definition 2.2: Reduced PDE

Find $u_{rb}(\mu) \in \mathbb{V}_{rb}$ such that

$$\begin{cases} a(u_{rb}(\mu), v_\delta; \mu) = f(v_{rb}; \mu) \;\; \forall \; v_{rb} \in \mathbb{V}_{rb} \\ s_{rb}(\mu) = \ell(u_{rb}(\mu); \mu) \end{cases}$$

For a given $\mathbb{V}_{rb}$ and $\mu \in \mathbb{P}$, Céa's lemma holds with same proof as before:

$$\|u(\mu) - u_{rb}(\mu)\|_{\mathbb{V}} \leq \left(1 + \frac{\gamma(\mu)}{\alpha(\mu)}\right) \inf_{v_{rb} \in \mathbb{V}_{rb}} \|u(\mu) - v_{rb}\|_{\mathbb{V}}$$

The goal is to get $\|u_\delta(\mu) - u_{rb}(\mu)\|$ as close to 0 as possible while keeping $N = dim(\mathbb{V}_{\text{rb}})$ small.

$$\inf_{v_{rb} \in \mathbb{V}_{rb}} \|u(\mu) - v_{rb}\|_{\mathbb{V}} \leq \|u(\mu) - u_{rb}(\mu)\|_{\mathbb{V}} \leq \underbrace{\|u_\delta(\mu) - u_{rb}(\mu)\|_{\mathbb{V}}}_{\text{to be controlled}} + \underbrace{\|u(\mu) - u_\delta(\mu)\|_{\mathbb{V}}}_{\text{controlled by 1.4}}$$

For that we will define some measure of the distance between the space of δ solutions and the reduced space.

$$E(\mathcal{M}_\delta, \mathbb{V}_{rb}) = \sup_{u_\delta \in \mathcal{M}_\delta} \inf_{v_{rb} \in \mathbb{V}_{rb}} \|u_\delta - v_{rb}\|_{\mathbb{V}}$$

Definition 2.3: Kolmogorov N-Width

Assuming a reduced space exists, the Kolmogorov N-width measures the best distance we can hope with a N dimensional reduced basis and is defined as:

$$d_N(\mathcal{M}_\delta) := \inf_{\{\mathbb{V}_{rb} /\ \dim\ (\mathbb{V}_{rb}) = N\}} E(\mathcal{M}_\delta, \mathbb{V}_{rb})$$

Instead of

$$\sup_{u_\delta \in \mathcal{M}_\delta} \inf_{v_{rb} \in \mathbb{V}_{rb}} \|u_\delta - v_{rb}\|_{\mathbb{V}}$$

we can consider the least square distance which allows faster computations ;

Definition 2.4: Least square distance

$$d_{\text{LS}}(\mathcal{M}_\delta) := \sqrt{\int_{\mu \in \mathbb{P}} \inf_{v_{rb} \in \mathbb{V}_{rb}} \|u_\delta(\mu) - v_{rb}\|^2_{\mathbb{V}}}$$

Now that we know what we are looking for, we study 2 algorithm for generating such spaces:

2) Reduced basis generation by Proper Orthogonal Decomposition

Let $\mathbb{P}_h = \{\mu_1, \ \ldots \ , \mu_M\} \subset \mathbb{P}$ be a discrete and finite point-set.
Define:

$$\mathcal{M}_\delta(\mathbb{P}_h) = \{u_\delta(\mu) \ / \ \mu \in \mathbb{P}_h\}$$

of cardinality $\mathbf{M} = |\mathbb{P}_h|$.
We assume that $\mathcal{M}_\delta(\mathbb{P}_h)$ can efficiently approximate $\mathcal{M}_\delta$.
Let $\mathbb{V}_{\mathcal{M}} = \text{Span}\,\{u_\delta(\mu) \ / \ \mu \in \mathbb{P}_h\}$. The POD minimizes the least-squared distance for $\mathbb{P}_h$ on all N-dimensional subspaces of $\mathbb{V}_{\mathcal{M}}$:

$$\sqrt{\frac{1}{M} \sum_{\mu \in \mathbb{P}_h} \inf_{v_{rb} \in \mathbb{V}_{rb}} \|u_\delta(\mu) - v_{rb}\|^2_{\mathbb{V}}}$$

Let $\psi_m = u_\delta(\mu_m)$ for $m \in \{1, ..., M\}$ (ψ_m is well-defined by unicity of Lax-Milgram). We project any $v_\delta \in \mathbb{V}_{\mathcal{M}}$ on the space generated by the ψ_m:

$$C(v_\delta) = \frac{1}{M} \sum_{m=1}^{M} \langle v_\delta | \psi_m \rangle_{\mathbb{V}} \, \psi_m \in \mathbb{V}_{\mathcal{M}}$$

This operator is linear and symmetric. This operator is positive:

$$\langle C(v_\delta) | v_\delta \rangle = \frac{1}{M} \sum_{m=1}^{M} \langle v_\delta | \psi_m \rangle \langle \psi_m | v_\delta \rangle = \frac{1}{M} \sum_{m=1}^{M} \langle v_\delta | \psi_m \rangle^2 \geq 0$$

C being SPD is a consequence of an algebra point of view $C = SS^T$ where S is a snapshot of solutions, i.e. it is the SVD matrix [Vol12].

Since it is symmetric and $\mathbb{V}_{\mathcal{M}}$ is finite dimensional, there exists an orthonormal basis of eigenvectors and real eigenvalues $(\lambda_n, \xi_n) \in \mathbb{R}_+ \times \mathbb{V}_{\mathcal{M}}$ such that

$$\langle C(\xi_n) | \psi_m \rangle_{\mathbb{V}} = \lambda_n \langle \xi_n | \psi_m \rangle_{\mathbb{V}}$$

we choose the numerating (permutation matrices are orthogonals) s.t. $\lambda_1 \geq \ \ldots \ \geq \lambda_M \geq 0$.

Proposition 2.5: Proper Orthogonal Projection

$\mathbb{V}_{\text{POD}} = \text{Span}\left(\{\xi_m\}_{1 \leq m \leq N}\right) \subset \mathbb{V}$ of dimension N (or less).

$\mathcal{D}$

See the lecture notes "Proper Orthogonal Decomposition: Theory and Reduced-Order Modelling" [Vol12]. □

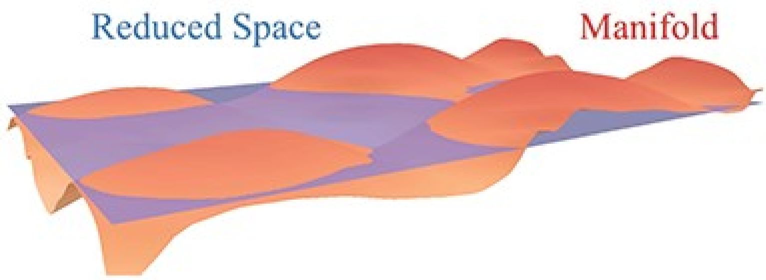

Figure 4: A manifold and a possible plan POD representation

We can define the (orthogonal) projection on the subspace

$$P_N[f] = \sum_{i=1}^{N} \langle f | \xi_i \rangle_{\mathbb{V}} \, \xi_i$$

The least square distance is such that:

$$d_{\text{LS}}^2 = \frac{1}{M} \sum_{m=1}^{M} \|\psi_m - P_N(\psi_m)\|_{\mathbb{V}}^2 = \sum_{m=N+1}^{M} \lambda_m$$

It is a classical result proven in [Vol12].

Remark :

Notice that when the projection space grows, this error estimation tends to 0.

This method has a major flaw: the complexity scales as $\mathcal{O}(N N_\delta^2)$.
Hence we seek an alternative, less precise approach that will allows faster computing with an error estimator.

3) Reduced basis generation by Greedy algorithm

Assume there exists $\eta(\mu)$ dependant of μ be an upperbound of the error approximation such that:

$$\|u_\delta(\mu) - u_{rb}(\mu)\|_\mu \leq \eta(\mu) \quad \forall \mu \in \mathbb{P}$$

At dimensionality n, choose $\psi_{n+1} = u_\delta(\mu_{n+1})$ such that:

$$\mu_{n+1} = \arg\max_{\mu \in \mathbb{P}} \eta_n(\mu)$$

i.e. we add the parametrized solution that the current space worst approximates.

Remark :

Note η_n depends on the iteration (otherwise we take the same μ each time).
It will be taken s.t. $\eta_n(\psi_i) = 0 \ \forall i$.

The reduced basis generation using a Greedy method realizes the same asymptotic rate of decay as the Kolmogorov N-width [Bin+11].
The following theorem shows that under the right conditions, a very small amount of basis functions will be enough to have an accurate reduced basis.

Theorema 2.6

Assume that $\mathcal{M}$ has exponentially small Kolmogorov N-width, i.e. $d_N(F) \leq ce^{-aN}$ with $a > log(1 + \sqrt{\frac{\gamma}{\alpha}})$.
Then there exists $\beta > 0$ such that

$$\forall \mu \in \mathbb{P}, \|u_\delta(\mu) - u_{rb}(\mu)\|_{\mathbb{V}} \leq Ce^{-\beta N}$$

$\mathcal{D}$

See paper "Apriori convergence of the greedy algorithm for the parametrized reduced basis method." [Buf+21] □

Example 1: Some Kolmogorov N-width for several PDEs

$INS(f)$,	$f \in \mathcal{K}_\gamma^{\bar{\omega},s}$,	$d_n(\mathcal{M})_{L^2} < \exp -n^{1/3}$	[Schwab and Suri 1999]
$-\mathrm{div}(\boldsymbol{\mu}\nabla u) = f$,	$\mu \in \mathbb{P} \subset \mathbb{R}^m$,	$d_n(\mathcal{M})_{L^2} < \exp -n$	[Babuška et al. 2007]
$u^3 - \nabla \cdot (\exp \mu)\nabla u = f$,	$\mu \in K \subset W^{s,\infty}(\Omega)$,	$d_n(\mathcal{M})_{L^2} < n^{-\frac{s}{d}}$	[Cohen and DeVore, 2016]
$\partial_t u - \mu\partial_x u = 0$,	$(\mu, t) \in [0,1]^2$,	$d_n(\mathcal{M})_{L^2} > n^{-\frac{1}{2}}$	[Ohlberger and Rave, 2015]
$\partial_{tt}^2 u - \mu\partial_{xx}^2 u = 0$,	$(\mu, t) \in [0,1]^2$,	$d_n(\mathcal{M})_{L^2} > n^{-\frac{1}{2}}$	[Greif and Urban, 2019]

See [Sta23] and references therein.

4) Reduced solution computation

Suppose there exists an **affine decomposition** of a,f,ℓ i.e. there exists:

$$\mathcal{Q}_a \in \mathbb{N}, (a_q(v,w))_{1\le q\le \mathcal{Q}_a} \qquad a_q : \mathbb{V}\times\mathbb{V} \to \mathbb{R}$$
$$\mathcal{Q}_f \in \mathbb{N}, (f_q)_{1\le q\le \mathcal{Q}_f} \qquad f_q : \mathbb{V} \to \mathbb{R}$$
$$\mathcal{Q}_\ell \in \mathbb{N}, (\ell_q)_{1\le q\le \mathcal{Q}_\ell} \qquad \ell_q : \mathbb{V} \to \mathbb{R}$$

such that

$$\begin{cases} a(v,w\,;\mu) &= \sum_{q=1}^{\mathcal{Q}_a} \theta_a^q(\mu) a_q(v,w) \\ f(v\,;\mu) &= \sum_{q=1}^{\mathcal{Q}_f} \theta_f^q(\mu) f_q(v) \\ \ell(v\,;\mu) &= \sum_{q=1}^{\mathcal{Q}_\ell} \theta_q^\ell(\mu) \ell_q(v) \end{cases}$$

with

$$\theta_a^q : \mathbb{P} \to \mathbb{R} \qquad \theta_f^q : \mathbb{P} \to \mathbb{R} \qquad \theta_\ell^q : \mathbb{P} \to \mathbb{R}$$

i.e. it is supposed that the equation is described by linear functions independents of μ multiplied by a scalar dependent of μ. This is called the **affine assumption**.

Example 2: Affine assumption example

The heat equation admits an affine decomposition, see 2.3.1 and 3.4.1 [HRS16]. It can also be forced through the Empirical Interpolation Method, see Part 5 of the same reference.

Compute for each $1 \le q \le \mathcal{Q}_a, \mathcal{Q}_f, \mathcal{Q}_\ell$ the quantities

$$\mathbf{A}_\delta^q \mid f_\delta^q \mid \ell_\delta^q$$

which are the representation of these functions in the basis of discretization (as for the Truth Solver 1.5). Then compute for each q

$$\begin{cases} \mathbf{A}_{rb}^q &= \mathbf{B}\mathbf{A}_\delta^q\mathbf{B}^T \\ f_{rb}^q &= \mathbf{B}^T f_\delta^q \\ \ell_{rb}^q &= \mathbf{B}^T \ell_\delta^q \end{cases}$$

where $\mathbf{B}$ is the projection matrix from $\mathrm{Span}\,(\varphi_1, \ \dots \ ,\varphi_{N_\delta})$ to $\mathrm{Span}\,(\xi_1, \ \dots \ ,\xi_N)$ which is the orthonormed reduced basis (by Gram-Schmidt) for stability.

Then for each $\mu \in \mathbf{P}$, considering the dependency in μ being only on the θ^q, we can rapidly compute the X^μ quantities such that

$$\begin{cases} \mathbf{A}_{rb}^\mu &= \sum_{q=1}^{\mathcal{Q}_a} \theta_a^q(\mu) \mathbf{A}_{rb}^q \\ f_{rb}^q &= \sum_{q=1}^{\mathcal{Q}_f} \theta_f^q(\mu) f_\delta \\ \ell_{rb}^\mu &= \sum_{q=1}^{\mathcal{Q}_\ell} \theta_\ell^q(\mu) \ell_\delta^q \end{cases}$$

We can finally solve

$$\boxed{\mathbf{A}_{rb}^\mu u_{rb}^\mu = f_{rb}^\mu}$$

II - Error estimation

Lets introduce the discrete coercivity and continuous constants such that

Definition 2.7: Discrete constants

$$\alpha_\delta(\mu) = \inf_{\substack{v_\delta \in \mathbb{V}_\delta \\ \|v_\delta\|_{\mathbb{V}} = 1}} |a(v_\delta, v_\delta\ ; \mu)|, \quad \text{and} \quad \gamma_\delta(\mu) = \sup_{\substack{v_\delta, w_\delta \in \mathbb{V}_\delta \\ \|v_\delta\|_{\mathbb{V}} = \|w_\delta\|_{\mathbb{V}} = 1}} |a(v_\delta, w_\delta\ ; \mu)|$$

Since the supremum and the infimum are taken on a subset of $\mathbb{V}$, we get $\alpha \leq \alpha_\delta$ and $\gamma_\delta \leq \gamma$

1) Expected behavior of an error estimate

Following "Error Analysis and Estimation for the Finite Volume Method With Applications to Fluid Flows" [Jas96], we expect the following behavior from an error estimate:

- Give reliable informations about the distribution of the error
- Work well on coarse mesh
- Scale corresponding to mesh refinement
- Scale corresponding to discretisation
- Based on local solution and mesh information, cell-by-cell
- Asymptotically correct
- Over-estimate of the actual error

Definition 2.8: Asymptotically correct

Let N be the number of computation points.
Let E_N the exact error of the approximation solution u_N with respect to the exact solution u for a prescribed PDE.

$$E_N = \|u_N - u_h\|$$

Let e_N be an error estimate of E_N. e_N is *asymptotically correct* if

$$\frac{e_N - E_N}{E_N} \underset{N\to\infty}{\longrightarrow} 0$$

Which is strictly equivalent to

$$\xi_N := \frac{e_N}{E_N} \underset{N\to\infty}{\longrightarrow} 1$$

where $\xi_N \geq 1$ is the effectivity of the error estimate.
The error estimate tends to the exact error faster than the estimated solution tends to the exact solution.

2) Error estimator

We define naturally the error and the residual as the difference between the discrete and reduced solutions to see how well the reduced solution verifies the PDE.

Definition 2.9: Error and classic error equation

For $\mu \in \mathbb{P}$, we define the error of the discrete space by the reduced basis such that

$$e(\mu) = u_\delta(\mu) - u_{rb}(\mu)$$

which satisfies the equation

$$a(e(\mu), v_\delta\ ; \mu) = r(v_\delta\ ; \mu) \quad \forall v_\delta \in \mathbb{V}_\delta$$

where $r(\cdot\ ; \mu) \in \mathbb{V}'_\delta$ (the topological dual),

$$r(v_\delta\ ; \mu) = f(v_\delta\ ; \mu) - a(u_{rb}, v_\delta\ ; \mu)$$

Note that $r(\cdot\ ; \mu)$ being in the dual of $\mathbb{V}_\delta$, we can apply Riesz (see Theorem 5.1) hence it exists $\hat{r}_\delta$ satisfying

$$\langle \hat{r}_\delta(\mu) | v_\delta \rangle_{\mathbb{V}} = r(v_\delta\ ; \mu)$$

We recall that

$$\|\hat{r}_\delta(\mu)\|_{\mathbb{V}} = \|r(\cdot\ ; \mu)\|_{\mathbb{V}'_\delta} = \sup_{\substack{v_\delta \in \mathbb{V}_\delta \\ \|v_\delta\|_{\mathbb{V}} = 1}} |r(v_\delta\ ; \mu)|$$

Proposition 2.10

For a compliant problem, it holds for all $\mu \in \mathbb{P}$

$$s_\delta(\mu) - s_{rb}(\mu) = \|u_\delta(\mu) - u_{rb}(\mu)\|_\mu^2$$

Hence

$$s_\delta(\mu) \geq s_{rb}(\mu)$$

Assume there is a known lower bound α_{LB} of α_δ in a way that's independent of N_δ. An efficient estimator of such lower bound will be given later.
We can use this lower bound to define a upper bound of the error independent of the dimension N.

Recall that we want $\eta(\mu)$ s.t.

$$\|u_\delta(\mu) - u_{rb}(\mu)\|_\mu \leq \eta(\mu) \quad \forall \mu \in \mathbb{P}$$

Thus we search for an energy norm $\|\cdot\|_\mu$ error estimator. It is also the most natural norm to consider since it is the one induced by the PDE.

The following error estimator is the main interest of this report.

Definition 2.11: Energy norm, output, relative output

We define computable upper bound control of the energy norm, output and relative output:

$$\eta_{en}(\mu) = \frac{\|\hat{r}_\delta(\mu)\|_{\mathbb{V}}}{\alpha_{\mathrm{LB}}(\mu)^{1/2}}$$

$$\eta_s(\mu) = \frac{\|\hat{r}_\delta(\mu)\|_{\mathbb{V}}^2}{\alpha_{\mathrm{LB}}(\mu)} = (\eta_{en}(\mu))^2$$

$$\eta_{s,rel} = \frac{\|\hat{r}_\delta(\mu)\|_{\mathbb{V}}^2}{\alpha_{\mathrm{LB}}(\mu) s_{rb}(\mu)} = \frac{\eta_s(\mu)}{s_{rb}(\mu)}$$

Remark :

η_{en} is a natural upper bound:

Recalling the definition of $\|\hat{r}_\delta(\mu)\|_{\mathbb{V}}$ p.11

$$\begin{aligned}
\|\hat{r}_\delta(\mu)\|_{\mathbb{V}}^2 &\geq \left(\frac{|r(e(\mu)\ ;\mu)|}{\|e(\mu)\|_{\mathbb{V}}}\right)^2 \\
&= \left(\frac{a(e(\mu), e(\mu)\ ;\mu)}{\|e(\mu)\|_{\mathbb{V}}}\right)^2 \\
&\geq \frac{a(e(\mu), e(\mu)\ ;\mu)}{\|e(\mu)\|_{\mathbb{V}}^2} \alpha_{\mathrm{LB}}(\mu)\, \|e(\mu)\|_{\mathbb{V}}^2 \\
&= \alpha_{\mathrm{LB}}(\mu)\, \|e(\mu)\|_{\mu}^2 \\
\text{Hence } \frac{\|\hat{r}_\delta(\mu)\|_{\mathbb{V}}}{\sqrt{\alpha_{\mathrm{LB}}(\mu)}} &\geq \|e(\mu)\|_{\mu}
\end{aligned}$$

And $\|\cdot\|_\mu$ is called the energy norm induced by the PDE (thus $a(\cdot,\cdot\ ;\mu)$) since it's the natural norm defined by the PDE.

Proposition 2.12: Upper bound control

$$\|u_\delta(\mu) - u_{rb}(\mu)\|_\mu \leq \eta_{en}(\mu)$$

$$s_\delta(\mu) - s_{rb}(\mu) \leq \eta_s(\mu)$$

Suppose $s_\delta > 0$,

$$\frac{s_\delta(\mu) - s_{rb}(\mu)}{s_\delta(\mu)} \leq \eta_{s,rel}$$

We can define the error estimator effectivity that evaluates the sharpness of the estimator. Following Definition 2.8, we will need them to be as close as possible to 1.

Definition 2.13: Effectivity

We define the effectivity of the computable estimators:

$$\begin{aligned}
\text{eff}_{en}(\mu) &= \frac{\eta_{en}(\mu)}{\|e(\mu)\|_\mu} \\
\text{eff}_s(\mu) &= \frac{\eta_s(\mu)}{s_\delta(\mu) - s_{rb}(\mu)} = \text{eff}_{en}(\mu)^2 \\
\text{eff}_{s,rel}(\mu) &= \frac{\eta_{s,rel}(\mu)}{(s_\delta(\mu) - s_{rb}(\mu))/s_\delta(\mu)}
\end{aligned}$$

These effectivities are ≥ 1 by Proposition 2.12.
One may see that these are not computable quantities. To evaluate their sharpness, we can use the following upper bounds:

Proposition 2.14: Effectivity control

For all $\mu \in \mathbb{P}$

$$1 \leq \text{eff}_{en} \leq \sqrt{\gamma_\delta/\alpha_{\text{LB}}}$$
$$1 \leq \text{eff}_s \leq \gamma_\delta/\alpha_{\text{LB}}$$
Suppose $s_\delta > 0$
$$1 \leq \text{eff}_{s,rel} \leq (1 + \eta_{s,rel})\gamma_\delta/\alpha_{\text{LB}}$$

The estimators are independent of N, we won't have to evaluate α^n_{LB} for all n.

3) Online and Offline computation

We know how to :
Compute $\alpha_{\text{LB}}(\mu)$, see [HRS16] part 4.3. or p.24.
Compute $\|\hat{r}_\delta(\mu)\|_{\mathbb{V}}$ see [HRS16] part 4.2.5. or p.24.
To use the ROM with the Greedy Algorithm we proceed as follow:

- **Offline mode**:
  Estimate $\eta_{\text{en}}(\mu) \forall \mu \in \mathbb{P}_h$. Following p.8, add the worst estimate solution to the basis. Do it until $\eta_{\text{en}}(\mu)$ is lesser than a set tolerance.
- **Online mode**:
  For a new $\mu \in \mathbb{P}$, compute all the $\theta^q_a(\mu), \theta^q_f(\mu), \theta^q_\ell(\mu)$.
  Solve the reduced basis linear system to get u_{rb}.

The hope is that the Online Mode will be significantly faster and still accurate.

Part 3
Finite Volume Method

This part is mostly written from *The Finite Volume Method in Fluid Dynamics* [MMD16]. We present the Finite Volume Method used in CFD which is cell centered. The FVM does not have an established Reduced Basis Method yet, and we want to work in that direction later.

I - Integral of Finite Volume

We consider the General Conservation Equation for a scalar quantity ϕ in a fluid

$$\partial_t(\rho\phi) + \nabla \cdot (\rho v \phi) = \nabla \cdot (\Gamma \nabla \phi) + Q$$

Suppose the steady-state

$$\nabla \cdot (\rho v \phi) = \nabla \cdot (\Gamma \nabla \phi) + Q$$

Integrate in a Control Volume

$$\int_{V_C} \nabla \cdot (\rho v \phi) = \int_{V_C} \nabla \cdot (\Gamma \nabla \phi) + \int_{V_C} Q$$

Using Green-Ostrogradsky on the gradients

$$\int_{\partial V_C} (\rho v \phi - \Gamma \nabla \phi) \cdot dS = \int_{V_C} Q$$

We then decompose the integrand over the complete border with the sum of the integrands on the faces:

$$\int_{\partial V_C} (\rho v \phi - \Gamma \nabla \phi) \cdot dS = \sum_f \int_f (\rho v \phi - \Gamma \nabla \phi) \cdot dS_f$$

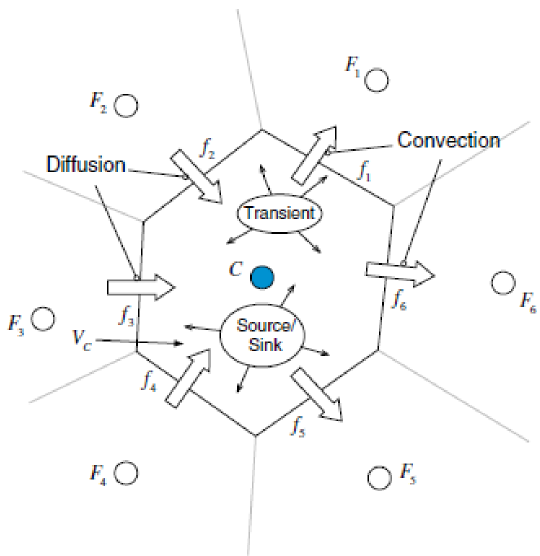

Figure 5: Conservation in a controle volume, from [MMD16]

The 1 cell centered FVM make use of this proposition:

Proposition 3.1: Centroid

Suppose f is linear and Ω convex.
Then the centroid of the considered set $c = \frac{\int_\Omega x dx}{\text{mes}(\Omega)} \in \Omega$ is such that

$$f(c) = \frac{1}{\text{mes}(\Omega)} \int_\Omega f$$

Coming back to

$$\int_{\partial V_C} (\rho v \phi - \Gamma \nabla \phi) \cdot dS = \sum_f \int_f (\rho v \phi - \Gamma \nabla \phi)_f \cdot dS_f$$

We suppose the grid thin enough to approximate linearity, hence using the centroid approximation 3.1

$$\int_{\partial V_C} (\rho v \phi - \Gamma \nabla \phi) \cdot dS \simeq \sum_f (\rho v \phi - \Gamma \nabla \phi)_f \cdot S_f$$

and similarly

$$\int_{V_C} Q \simeq Q_C V_C$$

Definition 3.2: Discretized Conservation Equation

$$\sum_{f \sim \text{faces}(C)} (\rho v \phi - \Gamma \nabla \phi)_f \cdot S_f = Q_C V_C$$

Then suppose that we can linearise the flux

$$(\rho v \phi - \Gamma \nabla \phi)_f \cdot S_f = \text{Flux}C_f \phi_C + \text{Flux}F_f \phi_f + \text{Flux}V_f$$

and the source

$$Q_C V_C = \text{Flux}C \phi_C + \text{Flux}V$$

Then it is straightforward to write the equation such that

$$a_C \phi_C + \sum_{f \sim \text{faces}(C)} a_F \phi_F = b_C$$

with a_C,a_F,b_C depending on the Flux$X_{f/C}$.

II - Linearisation of the discretised equation

1) Linearisation of the diffusion flux

In the general case, the grid and the centroids don't have any reason to have create an orthogonal mesh.

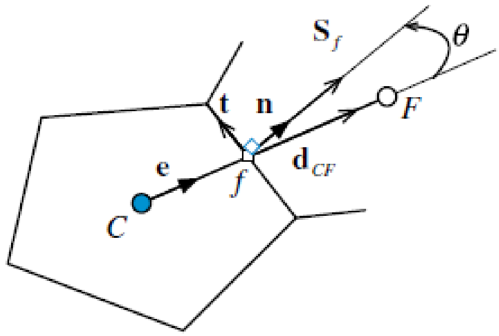

Figure 6: Non orthogonal mesh, from [MMD16]

We want to approximate $J_D = -\Gamma\nabla\phi$ as a linear function of ϕ_C and ϕ_F. The orthogonal situation would be

$$\nabla\phi = \frac{\partial\phi}{\partial n} \simeq \frac{\phi_F - \phi_C}{\|d\|}\mathbf{n}$$

and

$$(\nabla\phi)_f \cdot \mathbf{S_f} \simeq \frac{\phi_F - \phi_C}{\|d\|} S_f$$

with $S_f = S_f\mathbf{n}$. In the non-orthogonal case:

$$\nabla\phi = \frac{\partial\phi}{\partial e} \simeq \frac{\phi_F - \phi_C}{\|d\|}\mathbf{e} + ((\nabla\phi)\cdot\mathbf{t})\mathbf{t}$$

$$\mathbf{S}_f = E_f\mathbf{e} + T_f\mathbf{t} = \mathbf{E}_f + \mathbf{T}_f$$

Hence

$$(\nabla\phi)_f \cdot \mathbf{S}_f = \frac{\phi_F - \phi_C}{\|d\|} E_f + (\nabla\phi)_f \cdot \mathbf{T}_f$$

The choice of $\mathbf{E}_f$ and $\mathbf{T}_f$ is not discussed.
We need to compute $(\nabla\phi)_f$:

$$\nabla\phi_f = g_C\nabla\phi_C + g_F\nabla\phi_F$$

where $g_C + g_F = 1$ are geometric interpolation factors with respect to F and C (coefficients of the barycenter).

2) Computation of $(\nabla\phi)_f$

a) Green-Gauss gradient

$$\nabla\phi_C = \frac{1}{V_C}\sum_f \phi_f\mathbf{S}_f$$

It is still needed to compute ϕ_f. A simple and natural way is

$$\phi_f = g_c\phi_C + g_F\phi_F$$

F being the centroid of the neighbour cell that shares the face. Another more accurate way is to compute a mean based on the vertices and F.
Both way are just using convex combination of neighbour cells.

b) Gradient on faces

Once we computed the gradient on centroids, we can approximate the gradient on faces:

$$\overline{\nabla \phi_f} = g_C \nabla \phi_C + g_F \nabla \phi_F$$

and consider

$$\nabla \phi_f = \overline{\nabla \phi_f} + \underbrace{\left(\frac{\phi_F - \phi_C}{d_{CF}} - \overline{\nabla \phi_f} \cdot \mathbf{e}_{CF} \right) \mathbf{e}_{CF}}_{\text{Correction interpolated face gradient}}$$

where

$$d_{CF} = |r_F - r_C|$$
$$\mathbf{e}_{CF} = \mathbf{r}_F - \mathbf{r}_C$$

3) Convection flux and source term

We admit the linearisation process of these terms.
Convection term will be approximated by Upwind Scheme.
Source term will be admitted to be constant or at least independent of the solution.

4) Error estimates

We refer to “Error Analysis and Estimation for the Finite Volume Method With Applications to Fluid Flows” [Jas96] for details on the error estimators.

The main issue of the FVM is that there is no such thing as "basis functions" : we do not create the solution by using discrete spaces. There is not much mathematical framework other than classical approximations.
The only basis function that create the method is piecewise constant fonctions on each control volume.

The second flaw is the estimates that are not standards nor mathematically well established. That is why we try to see the FVM as a derivation of FEM with piecewise constant fonctions approximation instead of piecewise linear.

Part 4

Cell centered FVM Reduced Basis Method

The goal is to apply the well established Certified Reduced Basis Method error estimators to a Weak Finite Volumes formulation in the cell centered with two flux points.
Since FVM searches the solution in the piecewise constant functions, we want to find a bilinear form $a(\cdot,\cdot) : \mathbb{P}^0 \times \mathbb{P}^0 \to \mathbb{R}$ with $\mathbb{P}^0$ the piecewise constant functions.

I - Finite Volume Weak Formulation

1) Construction of the weak formulation

We follow the Weak Formulation from Raphaele Herbin presentation that is also described in "Analysis tools for finite volume schemes" [Eym+07]

Problem: let $b \geq 0$, $Q \in \mathbf{L}^2(\Omega)$ and $v \in \mathbb{R}^d$

$$\begin{cases} -\Delta u + \nabla\cdot(vu) + bu = Q & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega \end{cases}$$

Define $\mathcal{B}$ the set of control volumes and $\mathcal{E}$ the set of its faces. We suppose the mesh to be admissible in the sense that orthogonality conditions holds.
Recall:

$$\mathbb{P}^0(\mathcal{B}) = \left\{u \in \mathbf{L}^2(\Omega) \;/\; \forall C \in \mathcal{B}, u\big|_b \in \mathbb{P}^0(b)\right\}$$

Bilan on a control volume $C \in \mathcal{B}$ with faces f:

$$\sum_{f\in \mathrm{F}(C)} \int_f -\nabla u \cdot \mathbf{n}_f d\gamma(x) + \sum_{f\in \mathrm{F}(C)} \int_f (vu)\cdot \mathbf{n}_f d\gamma(x) + \int_{V_C} bu = \int_{V_C} Q$$

Remark :
$\gamma(x)$ is the $(d-1)$-Lesbegue measure.

We then approximate the equation with Upwind Finite Volume scheme:

$$\sum_{f\in \mathrm{F}(C)} F_{C,f} + \sum_{f\in \mathrm{F}(C)} (v_f^+ u_C + v_f^- u_F) + b_C\,|V_C|\,u_C = |V_C|\,f_C$$

where

$$v^+ := \max(0,v) \;\;\&\;\; v^- := \max(0,-v)$$

Define

$$\mathcal{E}_{\text{int}} := \mathcal{E}\cap\Omega \;\;\&\;\; \mathcal{E}_{\text{ext}} := \mathcal{E}\cap\partial\Omega$$

Then we define $F_{C,f}$ such that:

$$F_{C,f} := \begin{cases} -\dfrac{\gamma(f)}{r_{CF}}(u_F - u_C) & \text{if } f \in \mathcal{E}_{\text{int}} \\ -\dfrac{\gamma(f)}{r_{Cf}}(-u_C) & \text{if } f \in \mathcal{E}_{\text{ext}} \end{cases}$$

Note r_{Cf} is the distance between C and the border.
We do a sumation over $\mathcal{B}$:

$$\sum_{C\in\mathcal{B}}\left[\sum_{f\in \mathrm{F}(C)} F_{C,f} + \sum_{f\in \mathrm{F}(C)}(v_f^+ u_C + v_f^- u_F) + \int_{V_C} bu\right] = \sum_{C\in\mathcal{B}}\int_{V_C} Q$$

$$\iff \sum_{\substack{f\in\mathcal{E}_{\text{int}}\\ f=C|F}} -\frac{\gamma(f)}{r_{CF}}(u_F - u_C) + \sum_{f\in\mathcal{E}_{\text{ext}}}\frac{\gamma(f)}{r_{Cf}}u_C + \sum_{C\in\mathcal{B}}\left[\sum_{f\in\mathrm{F}(C)}(v_f^+ u_C + v_f^- u_F)\right] + \int_\Omega bu = \int_\Omega Q$$

We want to describe this equation only with bilinear form. Remark that:

$$\frac{\gamma(f)}{r_{CF}}(u_C - u_F) = \frac{\gamma(f)}{r_{CF}}(u_C - u_F)(1-0) = \frac{\gamma(f)}{r_{CF}}(u_C - u_F)(\mathbf{1}_C(x_C) - \mathbf{1}_C(x_F))$$

and

$$\frac{\gamma(f)}{r_{Cf}}u_C = \frac{\gamma(f)}{r_{Cf}}u_C\mathbf{1}_C(x_C)$$

Definition 4.1: Discrete inner product

$$\langle u|\phi\rangle_{\mathcal{B}} = \sum_{\substack{f\in\mathcal{E}_{\text{int}}\\ f=C|F}}\frac{\gamma(f)}{2r_{CF}}(u_F - u_C)(\phi_F - \phi_C) + \sum_{f\in\mathcal{E}_{\text{ext}}}\frac{\gamma(f)}{r_{Cf}}u_C\phi_C$$

Proposition 4.2

Let $u \in \mathbb{P}^0(\mathcal{B})$:

$$\langle u|\mathbf{1}_C\rangle_{\mathcal{B}} = \sum_{f\in\mathrm{F}(C)} F_{C,f}$$

Choosing $\phi = \mathbf{1}_C$ or $u = \mathbf{1}_C$ is equivalent to only consider the corresponding cell and its fluxes.

$\mathcal{D}$

We split the following sum between the set neighbour cells of K and the set of cells that has K as neighbour cell:

$$\sum_{\substack{f\in\mathcal{E}_{\text{int}}\\ f=C|F}}\frac{\gamma(f)}{2r_{CF}}(u_F - u_C)(\mathbf{1}_K(x_F) - \mathbf{1}_K(x_C)) = \sum_{\substack{f\in\mathcal{E}_{\text{int}}\\ f=K|F}}\frac{\gamma(f)}{2r_{KF}}(u_F - u_K)(\mathbf{1}_K(x_F) - \mathbf{1}_K(x_K))$$

$$
\begin{aligned}
&+ \sum_{\substack{f\in\mathcal{E}_{\text{int}}\\ f=C|K}} \frac{\gamma(f)}{2r_{CK}}(u_K-u_C)(\mathbf{1}_K(x_K)-\mathbf{1}_K(x_C))\\
&= \sum_{\substack{f\in\mathcal{E}_{\text{int}}\\ f=K|F}} \frac{\gamma(f)}{2r_{KF}}(u_F-u_K)(0-1)\\
&+ \sum_{\substack{f\in\mathcal{E}_{\text{int}}\\ f=C|K}} \frac{\gamma(f)}{2r_{CK}}(u_K-u_C)(1-0)\\
&= \sum_{\substack{f\in\mathcal{E}_{\text{int}}\\ f=K|F}} -\frac{\gamma(f)}{2r_{KF}}(u_F-u_K) + \sum_{\substack{f\in\mathcal{E}_{\text{int}}\\ f=C|K}} \frac{\gamma(f)}{2r_{CK}}(u_K-u_C)\\
&= 2\sum_{\substack{f\in\mathcal{E}_{\text{int}}\\ f=K|F}} -\frac{\gamma(f)}{2r_{KF}}(u_F-u_K) \quad (\star)\\
&= \sum_{\substack{f\in\mathcal{E}_{\text{int}}\\ f=K|F}} -\frac{\gamma(f)}{r_{KF}}(u_F-u_K)\\
&= \sum_{f\in(F(K))_{\text{int}}} F_{K,f}(u)
\end{aligned}
$$

($\star$) the set of Control Volumes that has K as a neighbour is exactly $(F(K))_{\text{int}}$.
and

$$\sum_{f\in\mathcal{E}_{\text{ext}}} \frac{\gamma(f)}{r_{Cf}} u_C \mathbf{1}_K(x_C) = \sum_{f\in(F(K))_{\text{ext}}} \frac{\gamma(f)}{r_{Cf}} u_K = \sum_{f\in(F(K))_{\text{ext}}} F_{K,f}(u)$$

The sum of both terms gives the result. □

Remark :

The paper does not divide by 2. We believe it is a small mistake, but we may have wrongly interpreted the sum.

The same way we want to define a bilinear form which gives the convection term of C when we apply $\mathbf{1}_C$, thus we define:

$$c_{\mathcal{B}}(u,\phi) = \sum_{C\in\mathcal{B}} \phi_C \left[\sum_{f\in \mathrm{F}(C)} (v_f^+ u_C + v_f^- u_F)\right]$$

And the weak formulation of integrals is natural Proposition 3.1:

$$b_C u_C\,|V_C| = \int_{V_C} bu = \int_\Omega bu\mathbf{1}_C$$
$$Q_C\,|V_C| = \int_{V_C} Q = \int_\Omega Q\mathbf{1}_C$$

Hence we define the following weak FVM:

$$\text{Find } u \in \mathbb{P}^0(\mathcal{B}) \text{ s.t. } \langle u|\phi\rangle_{\mathcal{B}} + c_{\mathcal{B}}(u,\phi) + \int_\Omega bu\phi = \int_\Omega Q\phi \quad \forall \phi \in \mathbb{P}^0(\mathcal{B})$$

$\mathcal{D}$: Weak FVM $\iff$ FVM

$\Longrightarrow$: $\phi = \mathbf{1}_K$
$\Longleftarrow$: Take $\phi \in \mathbb{P}^0(\mathcal{B})$, multiply the strong form on a control volume and sum over $C \in \mathcal{B}$.

□

Proposition 4.3: WFVM Poincaré inequality

Take $u \in \mathbb{P}^0(\mathcal{B})$.

$$\|u\|_{\mathbf{L}^2} \leq \operatorname{diam}(\Omega) \|u\|_{1,\mathcal{B}}$$

$\mathcal{D}$

"Finite Volume Methods" [EGH00] Lemma 9.1

□

By analogy with Poincaré inequality on $\mathbf{H}_0^1$ we can define:

Definition 4.4: Discrete $\mathrm{H}_0^1(\mathcal{B})$ norm

$$\|u\|_{1,\mathcal{B}} := (\langle u|u\rangle_{\mathcal{B}})^{1/2}$$

From here the most important point is to have the Hilbertian structure to make all the developed theory beforehand works. Thanksfully, the following property holds:

Proposition 4.5: Hilbert structure

$(\mathbb{P}^0(\mathcal{B}), \langle\cdot|\cdot\rangle_{\mathcal{B}})$ is an Hilbert.

$\mathcal{D}$

Let $\varepsilon > 0$. Let $(f_n)_n \in \mathbb{P}^0(\mathcal{B})^{\mathbb{N}}$ a Cauchy sequence:

$$\exists n_0 \text{ s.t. } \quad \|f_p - f_q\|_{1,\mathcal{B}} \leq \varepsilon \quad \forall p,q \geq n_0$$

Then by WFVM Poincaré 4.3 $\|f_p - f_q\|_{\mathbf{L}^2(\Omega)} \underset{p,q\to\infty}{\longrightarrow} 0$. Yet $\mathbf{L}^2$ is complete hence $f_n \underset{n\to\infty}{\longrightarrow} f$ in $\mathbf{L}^2(\Omega)$.

It is easy to verify that f is piecewise constant on $\mathcal{B}$ and that $f_n|_b \longrightarrow f|_b$.
Hence $F_{C,\sigma}(f_n) \longrightarrow F_{C,\sigma}(f)$. □

What we can learn from that is that we will be able to apply all the existence theorems we want.
We can hope that if $u \in \mathbf{H}^1(\Omega)$:

$$\|u\|_{1,\mathcal{B}} \sim \|\nabla u\|_{\mathbf{L}^2(\Omega)}$$

This is most likely possible regarding the jump norm equivalence proven in [BR87].
We can define the discrete $\mathbb{P}^0(\mathcal{B})$ norm:

$$\|u\|_{\mathcal{B}} := \|u\|_{\mathbf{L}^2(\Omega)} + \|u\|_{1,\mathcal{B}}$$

that is defined by analogy with the $\mathbf{H}^1(\Omega)$ norm.
Discrete Poincaré gives:

$$\|\cdot\|_{1,\mathcal{B}} \sim \|\cdot\|_{\mathcal{B}}$$

The paper shows the existence of an unique solution, the $\mathbf{L}^2$ strong convergence towards $\overline{u} \in H_0^1(\Omega)$ when the mesh tends to 0 which is solution of the weak formulation and of the strong FVM. It writes a reformulation of the classics FEM a priori estimates.

II - Elliptic case: Diffusion

This part presents our work. We apply *Certified Reduced Basis Methods for Parametrized Partial Differential Equations.* [HRS16] to the previous Weak FVM construction.

1) Model

We will consider a diffusion problem in a simple square divided in 9 smaller squares with different diffusion constants.

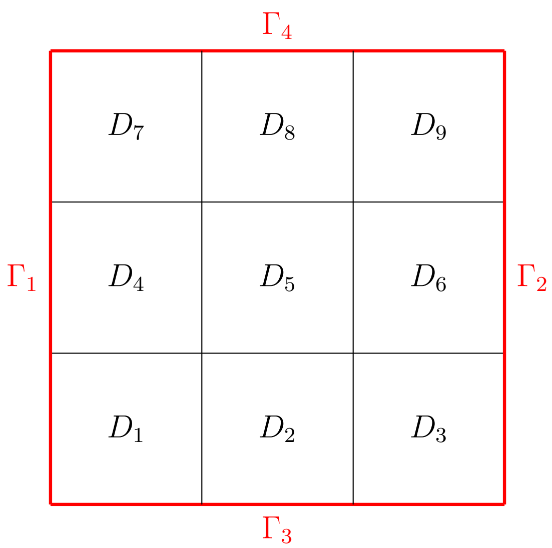

Figure 7: Parametrized diffusion problem

Let S_i be the i-th square associated to D_i. We define:

$$D(x) = \sum_{i=1}^{9} D_{[i]} \mathbf{1}_{S_i}$$

Hence the parameter $\mu = \begin{bmatrix} D_{[1]} \\ D_{[2]} \\ \vdots \\ D_{[9]} \end{bmatrix}$ lives in $\mathbb{P} =]0;1]^9 \simeq [\varepsilon;1]^9$ where $\varepsilon \simeq 0$ (to have closed set of parameters).
The FVM solve for $u \in \mathbb{P}^0(\mathcal{B})$ in each V_C :

$$-\nabla\cdot(D\nabla u) = f \iff \int_{\partial V_C} D\nabla u = D(x_C)\int_{\partial V_C} \nabla u = \int_{V_C} f$$

Hence, defining the **symmetric bilinear form**:

$$a(u,\phi\ ;\mu) = \sum_{\substack{f\in\mathcal{E}_{\text{int}} \\ f=C|F}} D(x_C)\frac{\gamma(f)}{2r_{CF}}(u_F - u_C)(\phi_F - \phi_C) + \sum_{f\in\mathcal{E}_{\text{ext}}} \frac{\gamma(f)}{r_{Cf}} D(x_C)u_C\phi_C$$

is enough to decribe the weak formulation for the FVM.
Then we will solve for u:

$$\begin{gathered} a(u,v\ ;\mu) = \langle f|v\rangle_{\mathbf{L}^2} \ \ \forall v \in \mathbb{P}^0(\mathcal{B}) \\ u = 0 \ \ \text{on } \Gamma \end{gathered}$$

2) Theoretical properties

We still have **coercivity**:

$$a(u,u) \geq \min_{i=1,\dots,9} D_i \left\|u\right\|^2_{1,\mathcal{B}}$$

Note that we also proved $\alpha \geq \min_{i=1,\dots,9} D_i$ i.e. wan can define $\alpha_{LB}(\mu) = \min_{i=1,\dots,9} D_i$.

a is **continuous**:

$$
\begin{aligned}
|a(u,\phi)| &= \left| \sum_{\substack{f\in\mathcal{E}_{\text{int}}\\ f=C|F}} D(x_C)\frac{\gamma(f)}{2r_{CF}}(u_F-u_C)(\phi_F-\phi_C) + \sum_{f\in\mathcal{E}_{\text{ext}}} \frac{\gamma(f)}{r_{Cf}} D(x_C)u_C\phi_C \right| \\
&\leq \sum_{\substack{f\in\mathcal{E}_{\text{int}}\\ f=C|F}} \left| D(x_C)\frac{\gamma(f)}{2r_{CF}}(u_F-u_C)(\phi_F-\phi_C)\right| + \sum_{f\in\mathcal{E}_{\text{ext}}} \left|\frac{\gamma(f)}{r_{Cf}} D(x_C)u_C\phi_C\right| \\
&\leq \underbrace{\max_{i=1,\dots,9} D_i}_{=C} \left(\sum_{\substack{f\in\mathcal{E}_{\text{int}}\\ f=C|F}} \sqrt{\frac{\gamma(f)}{2r_{CF}}}|u_F-u_C| \times \sqrt{\frac{\gamma(f)}{2r_{CF}}}\,|\phi_F-\phi_C| \right. \\
&\left. + \sum_{f\in\mathcal{E}_{\text{ext}}} \sqrt{\frac{\gamma(f)}{r_{CF}}}|u_C| \times \sqrt{\frac{\gamma(f)}{r_{CF}}}\,|\phi_C| \right) \\
\text{Cauchy-Schwarz} &\leq C \left(\sqrt{\sum_{\substack{f\in\mathcal{E}_{\text{int}}\\ f=C|F}} \frac{\gamma(f)}{2r_{CF}}(u_F-u_C)^2} \times \sqrt{\sum_{\substack{f\in\mathcal{E}_{\text{int}}\\ f=C|F}} \frac{\gamma(f)}{2r_{CF}}(\phi_F-\phi_C)^2} \right. \\
&\left. + \sqrt{\sum_{f\in\mathcal{E}_{\text{ext}}} \frac{\gamma(f)}{r_{CF}}u_C^2} \times \sqrt{\sum_{f\in\mathcal{E}_{\text{ext}}} \frac{\gamma(f)}{r_{CF}}\phi_C^2} \right) \\
&\leq C \left(\|u\|_{1,\mathcal{B}} \|\phi\|_{1,\mathcal{B}} + \|u\|_{1,\mathcal{B}} \|\phi\|_{1,\mathcal{B}} \right) \\
&\leq 2C \|u\|_{1,\mathcal{B}} \|\phi\|_{1,\mathcal{B}}
\end{aligned}
$$

We can also write the **affine assumption**:

$$
\begin{aligned}
a(u,\phi\,;\mu) &= \sum_{i=1}^{9} D_{[i]} \left(\sum_{\substack{f\in\mathcal{S}_{)}\cap\mathcal{E}_{\text{int}}\\ f=C|F}} \frac{\gamma(f)}{2r_{CF}}(u_F-u_C)(\phi_F-\phi_C) + \sum_{f\in S_i\cap\mathcal{E}_{\text{ext}}} \frac{\gamma(f)}{r_{Cf}} u_C\phi_C \right) \\
&= \sum_{i=1}^{9} D_{[i]} a_i(u,\phi)
\end{aligned}
$$

where

- $a_i(u,u) \geq 0$ ($= 0$ if $u=0$ on S_i) i.e. a_i is a semi-definite bilinear form.
- $D_{[i]} > 0$.

That fills the conditions for the affine assumption 4.3 [HRS16].

3) Computational methodology

Set $\mathcal{B}$ an orthogonal mesh. $\mathcal{E}$ be the set of edges of the mesh.
We will suppose that $f(\cdot\,;\mu) = f(\cdot)$.

a) Precomputation

Compute $\mathbf{M}_\delta$:

$$\langle \mathbf{1}_{V_i} | \mathbf{1}_{V_j} \rangle_{\mathcal{B}} = \begin{cases} \sum_{f \in F(V_i)} \frac{\gamma(f)}{r_{if}} & \text{if } i = j \\ -\frac{\gamma(f_{ij})}{r_{ij}} & \text{if } i,j \text{ are neighbour} \\ 0 & \text{otherwise} \end{cases}$$

Compute once for all $q = 1, ..., 9$ the matrices $\mathbf{A}_\delta^q = \left(a_q(\mathbf{1}_{V_i}, \mathbf{1}_{V_j})\right)_{i,j}$:

$$a_q(\mathbf{1}_{V_i}, \mathbf{1}_{V_j}) = \begin{cases} \sum_{f \in F(V_i)} \frac{\gamma(f)}{r_{if}} & \text{if } i = j \text{ and } i \in S_q \\ -\frac{\gamma(f_{ij})}{r_{ij}} & \text{if } i,j \text{ are neighbour and } i \in S_q \\ 0 & \text{otherwise} \end{cases}$$

Compute $\mathbf{f}_\delta = \left[(f(\mathbf{1}_{V_i}))_i\right]^T$.

b) Computation of α_{LB}

Set $\mathbb{P}_M \subset \mathbb{P}$ be a set of M arbitrary chosen parameters.
For each $\mu \in \mathbb{P}_M$, compute:

$$\mathbf{A}_\delta^\mu = \sum_{i=1}^{9} D_{[q]} \mathbf{A}_\delta^q$$

Solve for $(\lambda, w_\delta) \in \mathbb{R}^+ \times \mathbb{R}^{N_\delta}$ the eigenvalue problem:

$$\mathbf{A}_\delta^\mu w_\delta = \lambda \mathbf{M}_\delta w_\delta$$

The smallest eigenvalues gives you M coercive constant $\alpha_\delta(\mu_m)$.
Then define the function:

$$\alpha_{LB}(\mu) = \max_{m=1,\ldots,M} \left(\alpha_\delta(\mu_m) \min_{q=1,\ldots,9} \frac{D_{[q]}(\mu)}{D_{[q]}(\mu_m)} \right)$$

c) Step by step offline generation

Set $\mathbb{P}_h = \begin{bmatrix} \mu_{[1]} & \ldots & \mu_{[p]} \end{bmatrix}$ all the chosen trial parameters.
Chose any $\mu_1 \in \mathbb{P}_h$.

Loop at n:

- Compute the FOM solution $u_{\text{FVM}}(\mu_n)$ for $\mu_n \in \mathbb{P}_h$ computed in the last iteration or μ_1 if it's the first loop iteration.
  Define $\mathbf{B} = \begin{bmatrix} u_{\text{FVM}}(\mu_1) & \ldots & u_{\text{FVM}}(\mu_n) \end{bmatrix} = \begin{bmatrix} \xi_1 & \ldots & \xi_n \end{bmatrix}$.
  Compute for $q = 1, ..., 9$:

  $$\mathbf{A}_{rb}^q = \mathbf{B}^T A_\delta^q \mathbf{B}$$

  and

  $$\mathbf{f}_{rb} = \mathbf{B}^T \mathbf{f}_\delta$$

- For each $\mu \in \mathbb{P}_h$:
  Compute $\mathbf{A}_{rb}^{\mu} = \sum_{i=1}^{9} D_{[i]} A_{rb}^{i}$. Compute u_{rb}^{μ} s.t.
  $$\mathbf{A}_{rb}^{\mu} u_{rb}^{\mu} = \mathbf{f}_{rb}$$
  We then compute $\eta(\mu)$. First compute
  $$\mathbf{R} = \left(\mathbf{f}_{\delta}, A_{\delta}^{1}\mathbf{B}, \ldots, A_{\delta}^{9}\mathbf{B}\right)^{T}$$
  We then need to focus on
  $$\mathbf{G} = \mathbf{R}^{T}\mathbf{M}_{\delta}^{-1}\mathbf{R}$$
  Solve the linear system $\mathbf{M}_{\delta} y = \mathbf{R}$ then compute $\mathbf{G} = \mathbf{R}^{T} y$.
  Then compute
  $$r(\mu) = \left[1, -(u_{rb}^{\mu})^{T} D_{[1]}, \ldots, -(u_{rb}^{\mu})^{T} D_{[9]}\right]$$
  and finally compute
  $$\left\|\hat{r}_{\delta}(\mu)\right\|_{1,\mathcal{B}} = \sqrt{r(\mu)^{T}\mathbf{G}r(\mu)}$$
  Note that $\min_{i=1,\ldots 9} D_{[i]}$ is a lower bound of $\alpha(\mu)$ or compute $\alpha_{LB}(\mu)$ following p.25.
  $$\eta(\mu) = \left\|\hat{r}_{\delta}(\mu)\right\|_{1,\mathcal{B}} / \alpha_{LB}(\mu)$$
- Choose $\mu_{n+1} = \arg\max_{\mu \in \mathbb{P}_h} \eta(\mu)$.
- If $\eta(\mu_{n+1}) >$ tol (that was previously computed) then **go back** to the beginning of the loop, otherwise **terminate**.

Ensuring stability: Apply the Gram-Schmidt algorithm and redefine
$$\mathbf{B} = \text{Gram-Schmidt}(\mathbf{B})$$

d) Online procedure

Store $\mathbf{B} = \begin{bmatrix} \xi_1 & \ldots & \xi_N \end{bmatrix}$ and $A_{rb}^{q} = \mathbf{B}^{T} A_{\delta}^{q}\mathbf{B}$.

For a new $\mu = \begin{bmatrix} D_{[1]} & \ldots & D_{[9]} \end{bmatrix} \in \mathbb{P}$, compute:
$$\mathbf{A}_{rb}^{\mu} = \sum_{i=q}^{9} D_{[q]}\mathbf{B}^{T} A_{\delta}^{q}\mathbf{B}$$
Compute u_{rb}^{μ} s.t.
$$\mathbf{A}_{rb}^{\mu} u_{rb}^{\mu} = \mathbf{f}_{rb}$$

III - Parabolic case: Heat equation

1) Model

We don't change the geometry of the model. Here, we try to solve:
$$\begin{cases} \partial_t u - \nabla\cdot(D\nabla u) = g(t) f(v) & \text{in } \Omega \times \mathbb{R}_{+}^{*} \\ u(x,t) = 0 & \text{in } \partial\Omega \times \mathbb{R}_{+} \\ u(x,0) = u_0 \in \mathbf{L}^2 & \text{in } \Omega \end{cases}$$

A weak formulation would be:
Find $u \in \mathbf{L}^2(\mathbf{H}^1_0(\Omega) \times \mathbb{R}_+, \mathbb{R})$ such that $u_t \in \mathbf{L}^2(\mathbf{H}^{-1}(\Omega), \mathbb{R}_+)$ and:

$$\begin{cases} \langle \partial_t u | \varphi \rangle_{\mathbf{H}^{-1}, \mathbf{H}^1_0} + \int_\Omega D \nabla u \cdot \nabla v dx = g(t) \langle f(x) | \varphi \rangle_{\mathbf{H}^1_0} & \forall \varphi \in \mathbf{H}^1_0(\Omega) \\ u(x, 0) = u_0 \in \mathbf{L}^2 & \text{in } \Omega \end{cases}$$

Consider $T > 0$ a final time, M the number of time steps and $k = T/M$ the uniform time step.

$$\partial_t u = \frac{u^{n+1} - u^n}{k}$$

Find $(u^n)_{0 \leq n \leq M-1}$ such that $u^n \in \mathbb{P}^0(\Omega)$ and:

$$\begin{cases} \frac{1}{k} \langle u^{n+1} - u^n | \phi \rangle_{\mathbf{L}^2} + a(u^{n+1}, \phi) = g(t^{n+1}) \langle f | \phi \rangle_{\mathbf{L}^2} & \forall \phi \in \mathbb{P}^0, \; 0 \leq n \leq M-1 \\ \langle u^0 | \phi \rangle_{\mathbf{L}^2} = \langle u_0 | \phi \rangle_{\mathbf{L}^2} & \forall \phi \in \mathbb{P}^0 \end{cases}$$

where $a(u, v)$ is defined as the diffusion symmetric continuous coercive bilinear form p.**??**.

Remark :

When applying cell control, we get $\frac{1}{k} \langle u^{n+1} - u^n | \mathbf{1}_C \rangle_{\mathbf{L}^2} = V_C \frac{u_C^{n+1} - u_C^n}{\Delta t}$ which is the transient approximation in FVM.

2) Computational methodology: POD-Greedy algorithm

See the 6.1.2 [HRS16] for the general idea. We also wrote a step by step method in the longer version of this report.

IV - Results and conclusion

Numerical results involve programming knowledge that I did not have the time to learn. Giovanni is taking care of this part, but it is a time consuming part of the research and we will be able to present in September 2024.

If the numerical results look promising, we could hope to use this theory for libraries such that OpenFOAM (see ISTHACA-FV project).

If the numerical results align with our expectation, the next step is to create an estimator that takes into account the Implict part of the gradient estimation for non-orthogonal meshes and to generalize for Inf-Sup stable problems.

Part 5
Appendix

I - Representation theorems

Theorema 5.1: Riesz-Fréchet

Let $(H, \langle\cdot|\cdot\rangle_H)$ be a Hilbert space on $\mathbb{K} = \mathbb{R}$ or $\mathbb{C}$.
If $\phi \in H'$, then there exists a unique $x_0 \in H$ such as

$$\forall x \in H, \phi(x) = \langle x|x_0\rangle$$

Moreover the map

$$x_0 \in H \longmapsto \varphi_{x_0}; \left| \begin{array}{ccc} H & \to & \mathbb{K} \\ x & \mapsto & \langle x|x_0\rangle \end{array} \right. \in H'$$

is bijective, antilinear and an isometry between H and H'.

Theorema 5.2: Lax-Milgram

Let H be a Hilbert space, $a : H \times H \longrightarrow \mathbb{R}$ a continous coercive bilinear form on H.
Given any $\varphi \in H'$, there exists a unique $u \in H$ such that

$$a(u, v) = \langle\varphi|v\rangle = \varphi(v) \quad \forall v \in H$$

Moreover if a is symmetric then u is characterized by the property

$$\boxed{u \in H \text{ and } \frac{1}{2}a(u, u) - \varphi(u) = \min_{v \in H} \left\{ \frac{1}{2}a(v, v) - \varphi(v) \right\}}$$

Theorema 5.3: Banach–Nečas–Babuška

Let V, W be respectively Banach and reflexive Banach space.

$a : V \times W$ continuous bilinear form.
$f : W \to \mathbb{R}$ continuous linear form.

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

$(\star\star)$ is well-posed if and only if

$$(i) \qquad \exists C_{\text{sta}} > 0, \forall v \in V, \quad \sup_{w \in W \setminus \{0\}} \frac{a(v, w)}{\|w\|_W} \geq C_{\text{sta}} \|v\|_V$$

$$(ii) \qquad \forall w \in W, \quad (\forall v \in V, a(v, w) = 0) \Longrightarrow w = 0$$

The following control holds true :

$$\|u\|_V \leq \frac{1}{C_{\text{sta}}} \|f\|_{W'}$$

$\mathcal{D}$: Proof of Banach–Nečas–Babuška

See "Banach-Nečas-Babuška theorem and proof." [Lec24a]. □

II - Standards inequalities

Lemma 5.4: Bramble Hilbert 1D

If u has m derivates on (a, b) and $\mathbb{P}_k$ is the space of polynomials of degree lesser than $m-1$.

$$\inf_{v \in \mathbb{P}_{m-1}} \left\|u^{(k)} - v^{(k)}\right\|_{\mathbf{L}^p} \leq C(m)(b-a)^{m-k} \left\|u^{(m)}\right\|_{\mathbf{L}^p}$$

Hence for $p = \infty$ and $m = 2$ we have the linear interpolation :

$$\inf_{v \in \mathbb{P}_1} \|u - v\|_\infty \leq C(b-a)^2 \|u''\|_\infty$$

Lemma 5.5: Bramble Hilbert

If Ω is regular enough and satisfies the strong cone property, $u \in W^{m,p}(\Omega)$ and $\mathbb{P}_k$ is the space of polynomials of degree lesser than $m-1$.

$$\forall k \leq m, \quad \inf_{v \in \mathbb{P}_{m-1}} \|u - v\|_{W^{k,p}} \leq C d^{m-k} \|u\|_{W^{m,p}}$$

Proposition 5.6: Poincaré's inequality

Let K be a convex polygon, h its diameter, $\varphi \in \mathbf{H}^1(K)$.
Let $\varphi_K = \dfrac{\langle\varphi|1\rangle_K}{|K|}$ be the average estimation of φ. Then

$$\|\varphi - \varphi_K\|_K^2 \leq C h_k^2 \|\nabla \varphi_K\|_K^2$$

where C is independent of K.

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