Algunas cuestiones sobre la resolución de orden reducido de ecuaciones en derivadas parciales

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Modelización de orden reducido

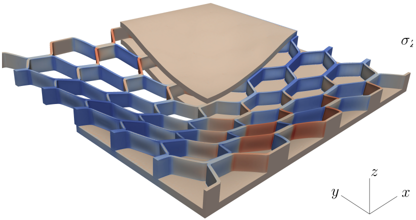
- Hoy en día muchos problemas en la ciencia y la ingeniería siguen siendo intratables, a pesar de los impresionantes avances recientes en modelado, análisis numérico, técnicas de discretización y computación.

  • Por ejemplo en química cuántica o flujo de gases enrarecidos, los modelos matemáticos están planteados en espacios de dimensión alta (D). Utilizando una malla estándar con $M \simeq 10^3$ nodos, si $D \simeq 30$ (un modelo muy simple), el número de grados de libertad es cercano a 10^{90}!!.

- La optimización de sistemas, los problemas inversos y la cuantificación de la incertidumbre son muy costosas computacionalmente, al requerir el cáculo reiterado del estado del sistema, en función de los parámetros de diseño. Esto necesita horas, días y semanas de computación. Soluciones en tiempo real o abordable para el diseño están frecuentemente fuera de alcance.

Modelización de orden reducido

- La modelización de orden reducido (ROM) se basa en la construcción de variedades de dimensión baja que aproximen bien la familia de soluciones paramétricas buscadas.
- Permite conseguir reducciones dramáticas del tiempo de cálculo.
- Las matemáticas son cruciales en la elaboración de ROMs eficaces.

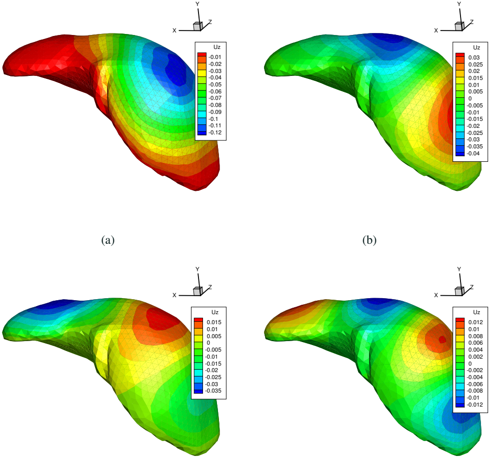


Contenidos

- Modelos reducidos de turbulencia (Modelo de Smagorinsky). Técnica de bases reducidas.
  - Aplicación al análisis del comportamiento energético de patios.
- Modelización de orden reducido de problemas elípticos paramétricos. Técnica PGD (Proper Generalized Decomposition).

Un ejemplo: Cirugía virtual del hígado

- Modos propios de vibración elástica de un hígado paramétrico.



Application to Smagorinsky turbulence model

- Ph. D. of Enrique Delgado, SINUM (2018).

Start from Navier-Stokes equations: Let $\Omega \subset \mathbb{R}^d$ bounded, with

$\partial\Omega = \Gamma = \Gamma_D \cup \Gamma_N$, where $\Gamma_D = \Gamma_{D_g} \cup \Gamma_{D_0}$

$$\left\{ \begin{array}{ll} \mathbf{u} \cdot \nabla \mathbf{u} - \dfrac{1}{\mu} \Delta \mathbf{u} + \nabla p = \mathbf{f} & \text{in } \Omega \\ \nabla \cdot \mathbf{u} = 0 & \text{in } \Omega \\ \mathbf{u} = \mathbf{g}_D & \text{on } \Gamma_{D_g} \\ \mathbf{u} = 0 & \text{on } \Gamma_{D_0} \\ -p\mathbf{n} + \left(\dfrac{1}{\mu}\right) \dfrac{\partial \mathbf{u}}{\partial \mathbf{n}} = 0 & \text{on } \Gamma_N \end{array} \right. \tag{1}$$

Smagorinsky model

$$
\begin{cases}
\mathbf{w}\cdot\nabla\mathbf{w} - \dfrac{1}{\mu}\Delta\mathbf{w} + \nabla p - \nabla\cdot(\nu_T(\mathbf{w})\nabla\mathbf{w}) = \mathbf{f} & \text{in } \Omega \\
\nabla\cdot\mathbf{w} = 0 & \text{in } \Omega \\
\mathbf{w} = \mathbf{g}_D & \text{on } \Gamma_{D_{in}} \\
\mathbf{w} = 0 & \text{on } \Gamma_{D_w} \\
-p\mathbf{n} + \left(\dfrac{1}{\mu} + \nu_T(\mathbf{w})\right)\dfrac{\partial\mathbf{w}}{\partial\mathbf{n}} = 0 & \text{on } \Gamma_{out}
\end{cases}
\tag{2}
$$

where $\nu_T(\mathbf{w})(x) = (C_S h_K)^2 |\nabla\mathbf{w}_{|_K}(x)|$.

Model intrinsically discrete, linked to a discretizaton grid.

LPS-Smagorinsky model

Finite element spaces

$$Y_h = \overline{Y}_h \oplus Y_h' \qquad M_h = \overline{M_h} \oplus M_h', \quad \sigma_h : Y_h \mapsto \overline{Y}_h : \text{ Averaging operator}$$

thus, $\mathbf{u}_h = \overline{\mathbf{u}_h} + \mathbf{u}_h'$, $\quad \mathbf{u}_h' = (Id - \sigma_h)\mathbf{u}_h = \sigma_h^* \mathbf{u}_h$, $\qquad p_h = \overline{p_h} + p_h'$

LES Closure model: Smagorinsky eddy diffusion,

$$\nu_t(\mathbf{u}_h) = (C_S h_K)^2 |\nabla(\mathbf{u}_h)| \text{ on element } K \in \mathcal{T}_h,$$

$$a_s(\mathbf{u}_h; \mathbf{u}_h, \mathbf{v}_h) = \int_\Omega \nu_t(\mathbf{u}_h')\, \nabla \mathbf{u}_h' : \nabla \mathbf{v}_h'\, d\Omega$$

Pressure stabilization:

$$s_{pres}(p, q) = \int_\Omega \tau_{K,p}(\mu)\, \sigma_h^*(\nabla p_h) \sigma_h^*(\nabla q_h)\, d\Omega,$$

with stabilization coefficients $\tau_{K,p}(\mu) = \left[c_1 \dfrac{1/\mu + \overline{\nu_T}}{h_K^2} + c_2 \dfrac{U_K}{h_K} \right]^{-1}$.

Full Order problem

LPS-Smagorinsky model

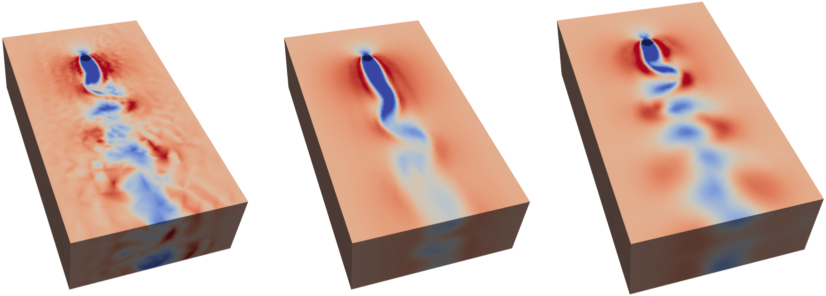
$$
\left\{
\begin{array}{ll}
\text{Find } (\mathbf{u}_h, p_h) \in X_h \text{ such that} & \\
a(\mathbf{u}_h, \mathbf{v}_h; \mu) + b(\mathbf{v}_h, p_h; \mu) + c(\mathbf{u}_h; \mathbf{u}_h, \mathbf{v}_h; \mu) & \\
+a_s(\mathbf{u}_h; \mathbf{u}_h, \mathbf{v}_h; \mu) = \langle f, \mathbf{v}_h \rangle & \forall \mathbf{v}_h \in Y_h \\
b(\mathbf{u}_h, q_h; \mu) + s_{pres}(p_h, q_h; \mu) = 0 & \forall q_h \in M_h,
\end{array}
\right. \qquad (3)
$$

where the operator terms are

a: Diffusion, b: Pressure gradient-Divergence, c: Convection,

a_s Eddy diffusion, s_{pres}: Pressure discretization stabilization.

Effect of LPS stabilization for convection: Flow past a cylinder



- Quadratic elements with 4×26.512 degrees of freedom

Magnitude of the velocity for $Re = 200$.

Convection stabilization by

- Plain Galerkin method (left): No stabilization
- Pure penalty method (center): $\sigma_h^* = Id$.
- Projection-stabilized one (right): $\sigma_h^* = Id - \sigma_h$.

Construction of Reduced Basis Space: Reduced basis problem

Given the space $X_N = Y_N \times M_N, 1 \leq N \leq N_{\max}$

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$$A(U_N(\mu), V_N; \mu) = F(V_N) \quad \forall V_N \in X_N$$

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- Choose μ_{N+1} as

$$\mu_{N+1} = \arg\max_{\mu \in \overline{\mathcal{D}}} \|U_h(\mu) - U_N(\mu)\|_X$$

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- Construct the new reduced spaces

$$Y_{N+1} = \text{span}\{\zeta_i^{\mathbf{v}} := \mathbf{u}(\mu^i), i = 1, \ldots, N+1\}$$

$$M_{N+1} = \text{span}\{\xi_i^p := p(\mu^i), i = 1, \ldots, N+1\}$$

Reduced Basis problem

Given the space $X_N = Y_N \times M_N, \quad 1 \leq N \leq N_{\max},$

$$\begin{cases} \text{Find } (\mathbf{u}_N, p_N) \in X_N \text{ such that} \\ a(\mathbf{u}_N, \mathbf{v}_N; \mu) + b(\mathbf{v}_N, p_N; \mu) + c(\mathbf{u}_N; \mathbf{u}_N, \mathbf{v}_N; \mu) \\ +a_s(\mathbf{u}_N; \mathbf{u}_N, \mathbf{v}_N; \mu) = \langle f, \mathbf{v}_N \rangle & \forall \mathbf{v}_N \in Y_N \\ b(\mathbf{u}_N, q_N; \mu) + s_{pres}(p_N, q_N; \mu) = 0 & \forall q_N \in M_N, \end{cases}$$

where we recall the operator terms:

a: Diffusion, b: Pressure gradient-Divergence, c: Convection,

a_s Eddy diffusion, s_{pres}: Pressure discretization stabilization.

- Typycally, $dim(X_M)$ is much smaller than $dim(X_h)$.

Empirical interpolation of turbulent viscosity and stabilized coefficients

- The eddy diffusion term is approximated as

$$g(x,\mu) = \nu_t(\mathbf{u}_N)(x,\mu) \simeq \sum_{j=1}^{M} \alpha_j(\mu)\, q_j(x),$$

where $\{q_1,\ldots,q_M\}$ are a linear combination of particular snapshots $g(x,\mu^1),\ldots,g(x,\mu^M)$ determined, together with the interpolation points x_i, hierarchically to improve the approximation properties of interpolation operator by incorporating iteratively the worse case.
The coefficients $\alpha_j(\mu)$ are determined to interpolate g at the x_i,

$$\sum_{j=1}^{M} \alpha_j(\mu)\, q_j(x_i) = g(x_i,\mu) \qquad i = 1,\ldots,M$$

- A similar approximation is built for the stabilized coefficients $\tau_{K,p}(\mu)$.

Role of mathematics: A-posteriori error estimator

- It holds

$$\left|\partial_1 A(U^1, V;\mu)(Z) - \partial_1 A(U^2, V;\mu)(Z)\right| \le \rho_T \|U^1 - U^2\|_X \|Z\|_X \|V\|_X.$$

Let $\beta_N(\mu) = \inf_{Z_h \in X_h} \sup_{V_h \in X_h} \frac{\partial_1 A(U_N(\mu), V_h;\mu)(Z_h)}{\|Z_h\|_X \|V_h\|_X}$, $\tau_N(\mu) = \frac{4\epsilon_N(\mu)\rho_T}{\beta_N{}^2}$,

with $\epsilon_N(\mu) = \|\mathcal{R}(\cdot;\mu)\|_{X'}$, $\mathcal{R}(V_h;\mu) = F(V_h;\mu) - A(U_N(\mu), V_h;\mu)$

Theorem

If $\beta_N > 0$ and $\tau_N(\mu) \le 1$, then there exists a unique solution $U_h(\mu)$ to (FE) such that

$$\|U_h(\mu) - U_N(\mu)\|_X \le \Delta_N(\mu),$$

where $\Delta_N(\mu) = \frac{\beta_N}{2\rho_T}\left[1 - \sqrt{1 - \tau_N(\mu)}\right].$

Reynolds range: $\mu \in [1000, 5100]$

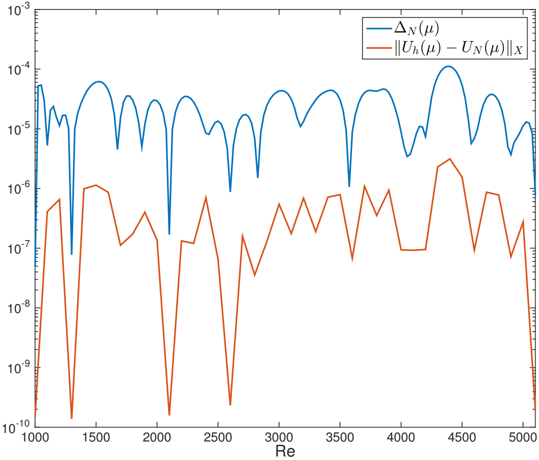


Figure: *A posteriori* error bound at N=16

FE and RB velocity solution

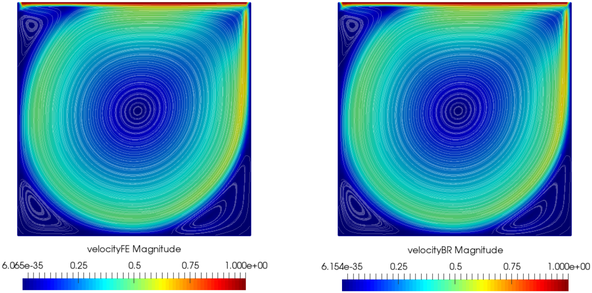


Figure: FE (left) and RB (right) velocity solution for $\mu = 4521$

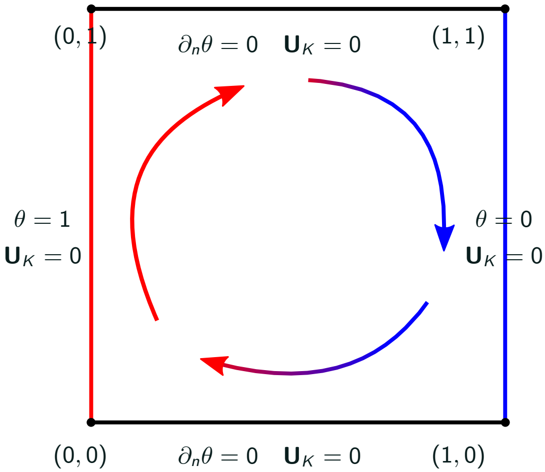
Results: Error and speed-up analysis.

FE dof: 30603
EIM dof: 25 (ν_T) + 20 ($\tau_{K,p}$), RB dof: 32

Data	$\mu = 1610$	$\mu = 2751$	$\mu = 3886$	$\mu = 4521$
T_{FE}	4083.19s	6918.53s	9278.51s	10201.7s
T_{online}	0.71s	0.69s	0.69s	0.7s
speedup	5750	10026	13280	14459
$\|\mathbf{u}_h - \mathbf{u}_N\|_T$	$2.4 \cdot 10^{-5}$	$4.129 \cdot 10^{-6}$	$3.14 \cdot 10^{-5}$	$3.23 \cdot 10^{-5}$
$\|p_h - p_N\|_0$	$2.17 \cdot 10^{-7}$	$1.99 \cdot 10^{-8}$	$5.38 \cdot 10^{-8}$	$6.36 \cdot 10^{-8}$

Table: Data summary

Boussinesq-Smagorinsky model. Problem description



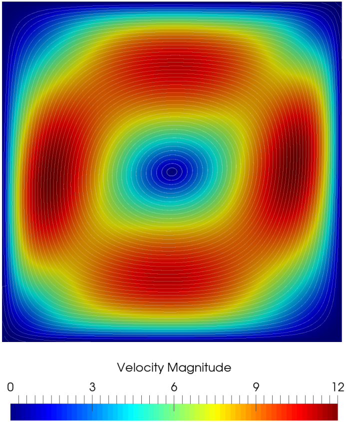
Boussinesq-Smagorinsky model

$$
\begin{cases}
\mathbf{U}_K \cdot \nabla \mathbf{U}_K - Pr\Delta \mathbf{U}_K + \nabla p - \nabla \cdot (\nu_T(\mathbf{U}_K)\nabla \mathbf{U}_K) = \mathbf{f} + Pr\, Ra\, \theta\, \mathbf{e}_2 & \text{in } \Omega \\
\nabla \cdot \mathbf{U}_K = 0 & \text{in } \Omega \\
\mathbf{U}_K \cdot \nabla \theta - \Delta \theta - \dfrac{1}{Pr} \nabla \cdot (\nu_T(\mathbf{U}_K)\nabla \theta) = Q & \text{in } \Omega \\
\mathbf{U}_K = 0 & \text{on } \Gamma \\
\theta = \theta_D & \text{on } \Gamma_D \\
\theta = 0 & \text{on } \Gamma_0 \\
\partial_n \theta = 0 & \text{on } \Gamma_N
\end{cases}
$$

where, $\nu_T(\mathbf{U}_K)(x) = (C_S h_K)^2 |\nabla(\Pi_h \mathbf{U}_K)_{|K}(x)|$

FE velocity-temperature solution

- Rayleigh range: $Ra \in [10^3, 10^5]$.
- Taylor-Hood Finite Element, $(\mathbb{P}2 - \mathbb{P}2 - \mathbb{P}1)$, Regular mesh (2601 nodes and 5000 triangles).



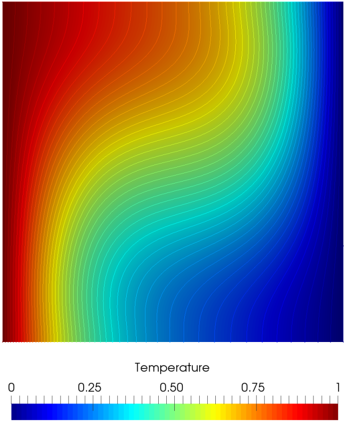
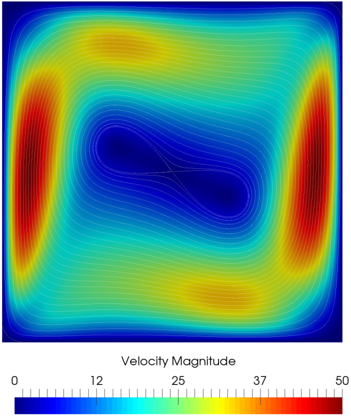


Figure: FE velocity and temperature solution for $Ra = 4363$

FE velocity-temperature solution



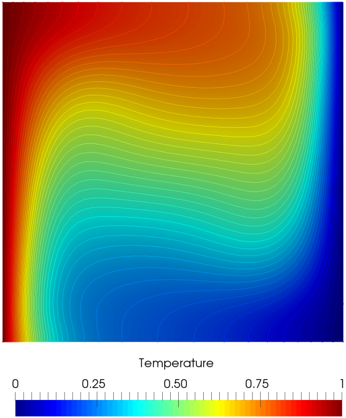


Figure: FE velocity and temperature solution for $Ra = 53778$

FE velocity-temperature solution. Large Rayleigh range: $Ra \in [10^5, 10^6]$

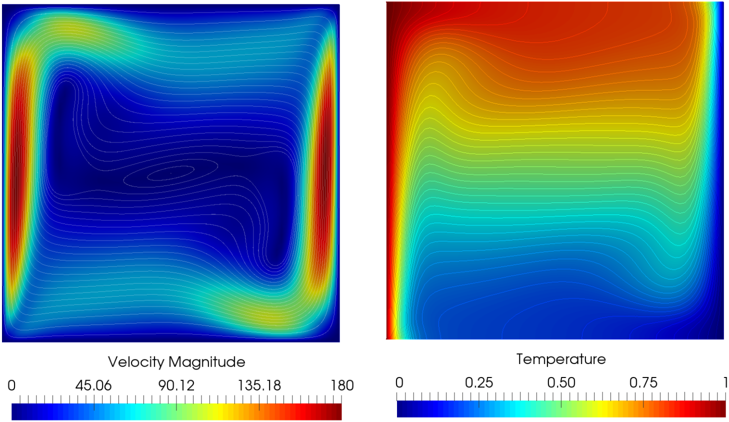


Figure: FE velocity and temperature solution for $Ra = 667746$

Results: Error and speed-up analysis.

- Moderate Rayleigh number range, $Ra \in [10^3, 10^5]$:
  FE dof: 33204, EIM dof: 42, RB dof: 88.

Data	$Ra = 4060$	$Ra = 17808$	$Ra = 53778$	$Ra = 93692$
T_{FE}	633.65s	585.83s	553.25s	677.86s
T_{online}	0.55s	0.5s	0.46s	0.49s
speedup	1133	1151	1189	1367

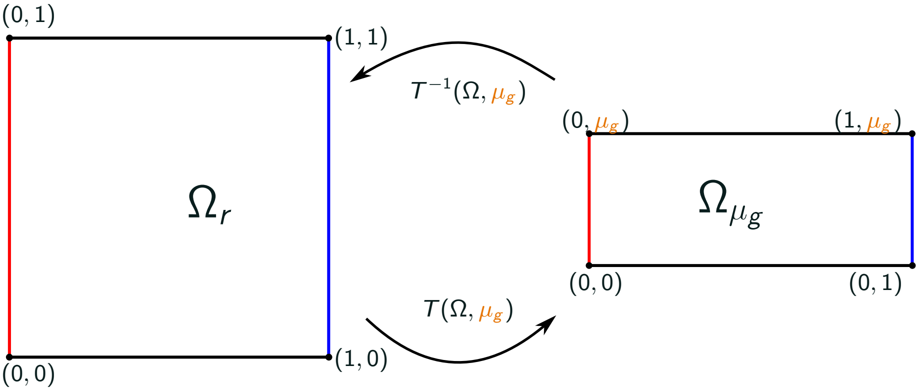
- Large Rayleigh number range, $Ra \in [10^5, 10^6]$:
  FE dof: 64684, EIM dof: 150, RB dof: 256

Data	$\mu = 16941$	$\mu = 355402$	$\mu = 667746$	$\mu = 921441$
T_{FE}	3563.11s	3675.01s	4354.26s	4928.37s
T_{online}	9.28s	11.34s	15.22s	16.8s
speedup	383	324	285	293

- Errors in H^1 norm below 10^{-5} in all cases.

Geometrical parameters

- Change of variable from reference domain.



$$DT(\Omega; \mu_g) = \begin{pmatrix} 1 & 0 \\ 0 & \mu_g \end{pmatrix}.$$

Variational formulation

Boussinesq-Smagorinsky F.E. with geometrical parametrization

$$\left\{\begin{array}{l} \text{Given } \boldsymbol{\mu} = (\mu_g, Ra) \in \mathcal{D} = \mathcal{D}_g \times \mathcal{D}_{Ra}, \\ \text{find } U_h(\boldsymbol{\mu}) = (\mathbf{u}_h, p_h, \theta_h) \in X_h \text{ s.t.} \\ A(U_h(\mu), V_h; \mu_g) = F(V_h; Ra) \qquad \forall V_h \in X_h \end{array}\right. \tag{4}$$

- Same finite element spaces for all parameters.

FE velocity solutions. Parameter range: $Ra = 10^5, \mu_g \in [0.5, 2]$.

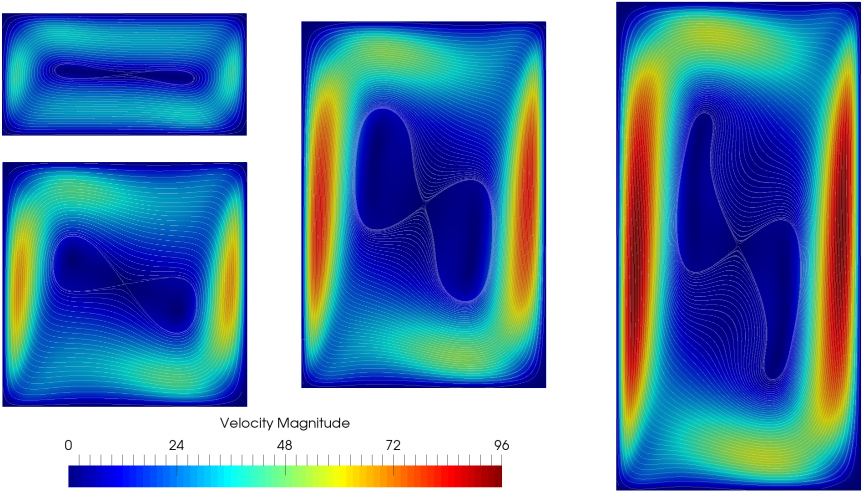
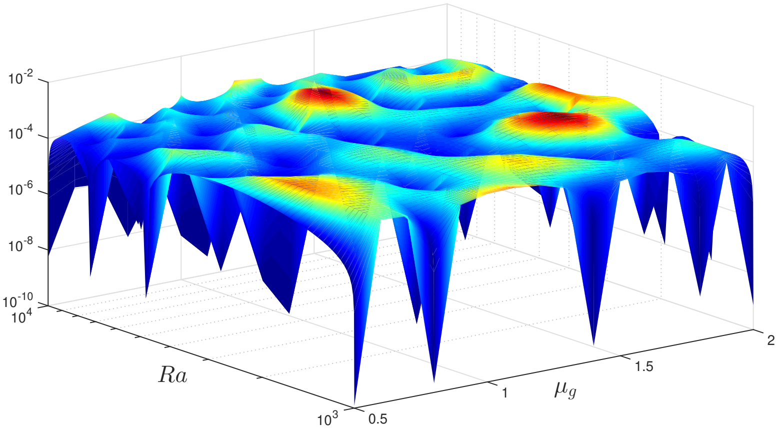


Figure: FE velocities for different values of μ_g. ($Ra = 10^5$)

A posteriori error bound at $N = N_{\max}$



Results: Error and speed-up analysis.

- Geometric parameter, $\mu \in [0.5, 2]$, $Ra = 10^5$

FE dof: 33204, EIM dof: 73, RB dof: 128 $\mu \in [0.5, 2]$

Data	$\mu_g = 0.64$	$\mu_g = 1.08$	$\mu_g = 1.44$	$\mu_g = 1.87$
T_{FE}	808.91s	810.16s	866.1s	851.82s
T_{online}	2.68s	2.55s	2.61s	2.52s
speedup	301	317	331	337

- Geometric and physical parameter, $\mu \in [0.5, 2]$, $Ra \in [10^3, 10^4]$ FE dof: 33204, EIM dof: 138, RB dof: 216

Data	$Ra = 2143$ $\mu_g = 1.95$	$Ra = 3506$ $\mu_g = 0.71$	$Ra = 5922$ $\mu_g = 1.13$	$Ra = 9618$ $\mu_g = 1.63$
T_{FE}	600.96s	914.18s	684.95s	630.94s
T_{online}	11.08s	15.73s	14.52s	11.46s
speedup	54	58	47	55

Present and future work

- Turbulence modeling:
  - Extension to transient and 3D flows.
  - Application to more complex turbulence models (VMS).
  - Applications to energy-efficient design of buildings.
- Numerical Analysis:
  - Take advantage of VMS formulation: Use the modeled u' as error indicator.
  - Further analysis of inf-sup conditions for RBM.
  - Error estimates for EIM of eddy viscosity.

Parametric elliptic problems

Let

- A separable Hilbert space $(H, (\cdot,\cdot))$.
- A measure space $(\Gamma, \mathcal{B}, \mu)$, with standard notations, so that μ is σ-finite.
- A form $a \in L^\infty(\Gamma, B_s(H); d\mu)$ uniformly elliptic and coercive on H w. r. t. γ.
- A data function $f \in L^2(\Gamma, H'; d\mu)$

We are interested in solving the variational problem:

Find $u(\gamma) \in H$ such that

$$a(u(\gamma), v; \gamma) = \langle f(\gamma), v\rangle_{H'-H}, \quad \forall v \in H, \; d\mu\text{-a.e. } \gamma \in \Gamma, \tag{5}$$

This is a common situation in many engineering problems when the properties of the media are parameter-depending.

Proper Orthogonal Decomposition

Objective: Approximate

$$u(\gamma) \simeq \sum_{k\geq 1} \Phi_k(\gamma)\, w_k, \;\; w_k \in H.$$

The POD searches for $w_1, w_2, \cdots$ such that for each $n = 1, 2, \cdots$ the space $S_n = Span\{w_1, \cdots, w_n\}$ minimizes

$$\int_\Gamma \|u(\gamma) - u_Z(\gamma)\|_H^2 \, d\mu(\gamma)$$

among all sub-spaces Z of H of dimension n, where $u_Z(\gamma) \in Z$ solves

$$a(u_Z(\gamma), z; \gamma) = \langle f(\gamma), z\rangle, \quad \forall z \in Z, \;\; d\mu\text{-a.e. } \gamma \in \Gamma, \tag{6}$$

Proper Orthogonal Decomposition

The $w_1, w_2, \cdots$ turn out to be the eigenfunctions of the POD operator $\mathcal{R} : H \mapsto H$, given by

$$\mathcal{R}(v) = \int_\Gamma (v, u(\gamma))_H \, u(\gamma) \, d\mu(\gamma), \text{ for } v \in H.$$

This operator is self-adjoint, positive and compact, what gives the existence (and uniqueness) of the optimal sub-spaces.

- The POD is a generalization of the Singular Values Decomposition of matrices. Also called Principal Component Analysis, Karhunen-Loève decomposition,
- Needs to know the inner products $(v, u(\gamma))_H$ to compute $\mathcal{R}$. In practice a quadrature formula is applied and only a certain number of $u(\gamma_i)$ ("snapshots") need to be computed.
- Then the targeted PDE needs to be a-priori solved to compute the POD expansion of its parametric solution.

Proper Generalized Decomposition

The PGD searches also for a similar tensorized decomposition

$$u(\gamma) \simeq \sum_{k\geq 1} \Phi_k(\gamma)\, w_k, \;\; u_k \in H.$$

but the w_k are computed online, iteratively.

- This is done by partial Galerkin problems.
- For instance, the first summand $u_1(\gamma) = \Phi_1(\gamma)\, w_1$, with $\Phi_1(\gamma) \in L^2(\Gamma, d\mu)$ and $w_1 \in H$ is a solution of

$$\begin{aligned} a(\Phi_1(\gamma)\, w_1, \Phi_1(\gamma)\, v) &= \langle f(\gamma), \Phi_1(\gamma)\, v\rangle, \;\; \forall v \in H, d\mu\text{-a.e. } \gamma \in \Gamma; \\ \int_\Gamma a(\Phi_1(\gamma)\, w_1, w_1)\, s(\gamma) d\mu(\gamma) &= \int_\Gamma \langle f(\gamma), w_1\rangle\, s(\gamma) d\mu(\gamma), \;\; \forall s \in L^2(\Gamma, d\mu). \end{aligned}$$

- These problems are solved by a power-iteration algorithm

Proper Generalized Decomposition

The following term

$$u_k(\gamma) = \sum_{k=1}^{n} \Phi_k(\gamma)\, w_k, = u_{k-1} + \Phi_{k-1}(\gamma)\, w_{k-1} \;\; w_{k-1} \in H.$$

is computed by a deflation algorithm, i. e., the same but replacing f by the current residual, $r_{k-1}(\gamma) = f(\gamma) - A(\gamma)u_{k-1}$.

- The PGD has been characterized by a non-optimal descent method for elliptic problems (Falcó and Nouy, 2016).

Optimal sub-spaces of finite dimension

Problem targeted: Find the best subspace W of H of dimension $\leq k$ that minimizes the mean quadratic error between $u(\gamma)$ and $u_W(\gamma)$ with respect to the norm generated by the form $a(\cdot,\cdot;\gamma)$.
That is, W solves

$$(\mathrm{P}) \qquad \min_{Z\in\mathcal{S}_k} \int_\Gamma a(u(\gamma)-u_Z(\gamma), u(\gamma)-u_Z(\gamma);\gamma)\, d\mu(\gamma), \tag{7}$$

where $\mathcal{S}_k$ is the family of subspaces of H of dimension $\leq k$ and $u_Z(\gamma)\in Z$ is the solution of the Galerkin approximation of problem (6) on Z,

$$a(u_Z(\gamma), z;\gamma) = \langle f(\gamma), z\rangle, \quad \forall z\in Z,\ d\mu\text{-a.e. } \gamma\in\Gamma,$$

.

A look at the 1D case

When $k = 1$, problem (P) can be written as

$$\min_{v \in H, \varphi \in L^2(\Gamma; d\mu)} \int_\Gamma a(u(\gamma) - \varphi(\gamma)v, u(\gamma) - \varphi(\gamma)v; \gamma) d\mu(\gamma).$$

So, taking the derivative of the functional

$$(v, \varphi) \in H \times L^2(\Gamma; d\mu) \mapsto J(v, \varphi) = \int_\Gamma a(u(\gamma) - \varphi(\gamma)v, u(\gamma) - \varphi(\gamma)v; \gamma) d\mu(\gamma),$$

we deduce that w is a solution of the non-linear variational problem

$$\int_\Gamma \frac{a(u(\gamma), w; \gamma)}{a(w, w, \gamma)} a(u(\gamma), v; \gamma) d\mu(\gamma) = \int_\Gamma \frac{a(u(\gamma), w; \gamma)^2}{a(w, w, \gamma)^2} a(w, v; \gamma) d\mu(\gamma), \tag{8}$$

$\forall\, v \in H.$

A look at the 1D case

- If a does not depend on γ, statement (8) is equivalent to

$$\mathcal{R}w = \int_\Gamma a(u(\gamma), w)u(\gamma)d\mu(\gamma) = \lambda\, w,$$

where

$$\lambda = \frac{\displaystyle\int_\Gamma a(u(\gamma), w)^2 d\mu(\gamma)}{a(w,w)}.$$

i.e. w is an eigenvector of the POD operator $\mathcal{R}$ when the inner product in H is the form $a(\cdot,\cdot)$.

- However, when a depends on γ problem (8) does not correspond to a proper eigenvalue equation: It is a non-linear eigenfunction problem, where no eigenvalues appear.

Then, we are considering a genuine extension of the POD.

Optimal sub-spaces

Theorem

There exists at least a sub-space $Z \in S_k$ that solves problem (P)

• Proof by direct method of the Calculus of Variations + compactness argument.

• Special proof for the 1D case. This problem is equivalent to

$$\text{(P')} \qquad \max_{\substack{\Psi \in H \\ \|\Psi\|=1}} \int_\Gamma \frac{\langle f(\gamma), \Psi\rangle^2}{a(\Psi, \Psi; \gamma)}\, d\mu(\gamma).$$

Theorem

Problem (P') admits at least one solution.

• Proof by combination of direct method of the Calculos of Variations, compactness in Hilbert spaces, uniform boundedness and ellipticity of forms $a(\cdot, \cdot; \gamma)$ and Fatou's Lemma.

Characterization of PGD algorithm

- The problem to compute the PGD modes,

$$\begin{aligned} a(\Phi_1(\gamma)\, w_1, \Phi_1(\gamma)\, v) &= \langle f(\gamma), \Phi_1(\gamma)\, v \rangle, \ \forall v \in H, d\mu\text{-a.e. } \gamma \in \Gamma; \\ \int_\Gamma a(\Phi_1(\gamma)\, w_1, w_1)\, s(\gamma) d\mu(\gamma) &= \int_\Gamma \langle f(\gamma), w_1 \rangle\, s(\gamma) d\mu(\gamma), \ \forall s \in L^2(\Gamma, d\mu). \end{aligned}$$

turns out to be the first-order optimality conditions of the critical points of the functional $J(v, \varphi)$.

Tensor approximation

Similarly to the PGD, we expand $u(\gamma)$ by the tensor approximation

$$u(\gamma) = \sum_{k\geq 1} \Phi_k(\gamma)\, w_k, \;\; w_k \in H.$$

where the w_k are obtained by a deflation algorithm similar to the one followed by PGD:

- Initialization:

$$w_1 = \operatorname{argmin}_{\Psi\in H} \int_\Gamma a(u(\gamma) - u_\Psi(\gamma), u(\gamma) - u_\Psi(\gamma); \gamma)\, d\mu(\gamma),$$

  where u_Ψ is the Galerkin solution of the targeted elliptic problem on $span\{\Psi\}$.

- Iteration: Known $u_{k-1}(\gamma) = \sum_{i=1}^{k-1} \Phi_i(\gamma)\, w_i,$, let $e_{k-1} = u - u_{k-1}$.

$$w_k = \operatorname{argmin}_{\Psi\in H} \int_\Gamma a(e_{k-1}(\gamma) - u_\Psi(\gamma), e_{k-1}(\gamma) - u_\Psi(\gamma); \gamma)\, d\mu(\gamma),$$

Tensor approximation

- It holds that $w_k = (e_{k-1})_W$, with W a solution of

$$\max_{\Psi \in H} \left\{ \int_\Gamma \langle f(\gamma), (e_{k-1})_\Psi(\gamma) \rangle \, d\mu(\gamma) - \bar{a}(u_{k-1}, (e_{k-1})_\Psi) \right\},$$

and $(e_{k-1})_\Psi \in L^2(\Gamma, Z; d\mu)$ the solution of

$$\bar{a}((e_{k-1})_\Psi, z) = \int_\Gamma \langle f(\gamma), z(\gamma) \rangle \, d\mu(\gamma) - \bar{a}(u_{k-1}, z), \quad \forall \, z \in L^2(\Gamma, Z; d\mu).$$

- This allows us to carry out the different iterations without needing to know the function u.

Theorem

The approximations u_n provided by the deflation algorithm strongly converge to the solution u of problem (P).

- Proof by orthogonality properties of residuals, consequence of the symmetry of forms a.

Test case

- Consider the elliptic problem with variable diffusion

$$\left\{ \begin{array}{rcll} -\nabla \cdot (\mu(\gamma)\, \nabla u) & = & f & \text{in} \quad \Omega, \\ u & = & 0 & \text{on} \quad \partial\Omega; \end{array} \right.$$

where $\Omega = (0,1)^2$ and

$$\mu(\gamma)(x,y) = \left\{ \begin{array}{lll} \gamma + \sigma & \text{if} & 0 \le x \le 1/4, \\ 1 + \sigma & \text{if} & 1/4 \le x \le 1. \end{array} \right. \quad \text{for all } (x,y) \in \overline{\Omega}.$$

σ is a real number to be selected to vary the minimum α of $\mu(\gamma)$.

Computation of PGD modes

• The PGD modes are solved by the Power Iteration Algorithm with normalization to solve for the critical points of the functional to be minimized $J(v,\varphi)$:

(a) $\tilde{w}^{n+1} \in H$ satisfying, $\forall v \in H, d\mu$-a.e. $\gamma \in \Gamma$,

$$\int_\Gamma a(\Phi^n(\gamma)\,\tilde{w}^{n+1}, \Phi^n(\gamma)\,v)d\mu(\gamma) \quad = \quad \int_\Gamma \langle f(\gamma), \Phi^n(\gamma)\,v\rangle,\ d\mu(\gamma)\,;$$

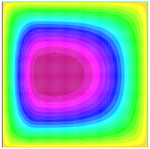
(b) $w^{n+1} = \dfrac{\tilde{w}^{n+1}}{\|\tilde{w}^{n+1}\|_H}$;

(c) $\Phi^{n+1} \in L^2(\Gamma, d\mu)$ satisfying, $\forall s \in L^2(\Gamma, d\mu)$,

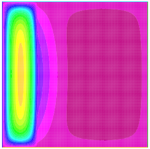
$$\int_\Gamma a(\Phi^{n+1}(\gamma)\,w^{n+1}, w^{n+1})\,s(\gamma)d\mu(\gamma) \quad = \quad \int_\Gamma \langle f(\gamma), w^{n+1}\rangle\,s(\gamma)d\mu(\gamma),\ .$$

• This algorithm converges with linear rate if f/α is small enough.

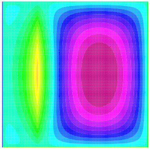
Computed modes



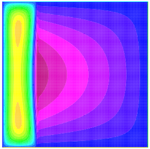
(a) Mode 1



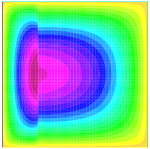
(b) Mode 2



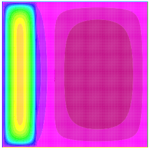
(c) Mode 3



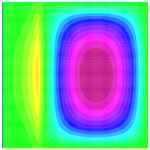
(d) Mode 4



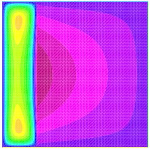
(e) Mode 5



(f) Mode 6



(g) Mode 7

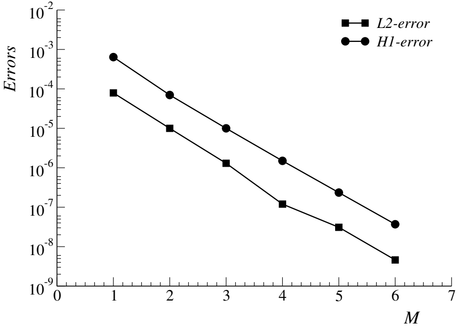


(h) Mode 8

Convergence history

The next figure displays $\|u(\gamma) - \Sigma_{i=1}^{M} \Phi_i(\gamma) w_i\|_X$

with $X = L^2(\Gamma, L^2(\Omega); d\mu)$ and $X = L^2(\Gamma, H^1(\Omega); d\mu)$.



(i) CV

- The expansion converges with *spectral* rate, like ρ^{-M} for $\rho > 1$.

Concluding remarks

- We have constructed an on-line tensorized approximation of parameterized elliptic equations (similar to PGD) with optimal approximation of each summand and orthogonality between summands (similar to POD).
- Optimization algorithms to compute the modes.
- Extensions to evolution and non-linear problems.
- Extension to more complex basic approximation structures (tensor trees).