PGD: algorithms and applications to several stochastic PDEs

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Numerical Methods for HighDim Pbs, Ecole des Ponts

Content :

Parametric model uncertainty :

- A model $\mathcal{M}$ involving uncertain input parameters D
- Treat uncertainty in a probabilistic framework : $D(\theta) \in (\Theta, \Sigma, d\mu)$
- Assume $D = D(\boldsymbol{\xi}(\theta))$, where $\boldsymbol{\xi} \in \mathbb{R}^{\mathrm{N}}$ with known probability law

The model solution is stochastic and solves :

$$\mathcal{M}(U(\xi); D(\xi)) = 0 \quad \text{a.s.}$$

Uncertainty in the model solution :

- $U(\xi)$ can be high-dimensional
- $U(\xi)$ can be analyzed by sampling techniques, solving multiple deterministic problems (*e.g.* MC)
- We would like to construct a functional approximation of $U(\xi)$

$$U(\xi) \approx \sum_k u_k \Psi_k(\xi)$$

An example

Consider the deterministic linear scalar elliptic problem (in Ω)

$$\text{Find } u \in \mathbb{V} \text{ s.t. :} \qquad a(u,v) = b(v), \ \forall v \in \mathbb{V}$$

where

$$a(u,v) \equiv \int_\Omega k(\boldsymbol{x}) \nabla u(\boldsymbol{x}) \cdot \nabla v(\boldsymbol{x}) \mathrm{d}\boldsymbol{x} \qquad \text{(bilinear form)}$$

$$b(v) \equiv \int_\Omega f(\boldsymbol{x}) v(\boldsymbol{x}) \mathrm{d}\boldsymbol{x} \ (+ \text{ BC terms}) \qquad \text{(linear form)}$$

$$\epsilon < k(\boldsymbol{x}) \text{ and } f(\boldsymbol{x}) \text{ given} \qquad \text{(problem data)}$$

$$\mathbb{V} \ (= H_0^1(\Omega)) \text{ deterministic space} \qquad \text{(vector space).}$$

Stochastic elliptic problem

- Conductivity k, source field f (and BCs) uncertain
- Considered as random :
- Probability space $(\Theta, \Sigma, d\mu)$:

$$\mathbb{E}[h] \equiv \int_{\Theta} h(\theta)\mathrm{d}\mu(\theta), \quad h \in \mathrm{L}^2(\Theta, \mathrm{d}\mu) \implies \mathbb{E}\left[h^2\right] < \infty.$$

- Assume $0 < \epsilon_0 \leq k$ a.e. in $\Theta \times \Omega$, $k(\boldsymbol{x}, \cdot) \in \mathrm{L}^2(\Theta, \mathrm{d}\mu)$ a.e. in Ω and $f \in \mathrm{L}^2(\Omega, \Theta, \mathrm{d}\mu)$

Variational formulation : Find $U \in \mathbb{V} \otimes \mathrm{L}^2(\Theta, \mathrm{d}\mu)$ s.t.

$$A(U, V) = B(V) \quad \forall V \in \mathbb{V} \otimes \mathrm{L}^2(\Theta, \mathrm{d}\mu),$$

where $A(U, V) \doteq \mathbb{E}[a(U, V)]$ and $B(V) \doteq \mathbb{E}[b(V)]$.

Stochastic Galerkin problem

Stochastic expansion :

- Let $\{\Psi_0, \Psi_1, \Psi_2, \dots\}$ be an orthonormal basis of $\mathrm{L}^2(\Theta, \mathrm{d}\mu)$
- $W \in \mathbb{V} \otimes \mathrm{L}^2(\Theta, \mathrm{d}\mu)$ has for expansion

$$W(\boldsymbol{x}, \theta) = \sum_{\alpha=0}^{+\infty} w_\alpha(\boldsymbol{x}) \Psi_\alpha(\theta), \quad w_\alpha(\boldsymbol{x}) \in \mathbb{V}$$

- Galerkin problem : (truncated)

Find $\{u_0, \dots, u_{\mathrm{P}}\}$ s.t. for $\beta = 0, \dots, \mathrm{P}$

$$\sum_\alpha a_{\alpha,\beta}(u_\alpha, v_\beta) = b_\beta(v_\beta), \quad \forall v_\beta \in \mathbb{V}$$

with $a_{\alpha,\beta}(u, v) := \int_\Omega \mathbb{E}\left[k \Psi_\alpha \Psi_\beta\right] \nabla u \cdot \nabla v \mathrm{d}\boldsymbol{x}$, $b_\beta(v) := \int_\Omega \mathbb{E}\left[f \Psi_\beta\right] v(\boldsymbol{x}) \mathrm{d}\boldsymbol{x}$.

Large system of coupled linear problem, globally SPD.

Stochastic parametrization

- Parameterization using N independent $\mathbb{R}$-valued r.v. $\boldsymbol{\xi}(\theta) = (\xi_1 \cdots \xi_{\mathrm{N}})$
- Let $\Xi \subseteq \mathbb{R}^{\mathrm{N}}$ be the range of $\boldsymbol{\xi}(\theta)$ and p_{ξ} its pdf
- The problem is solved in the image space $(\Xi, \mathcal{B}(\Xi), p_{\xi})$

$$U(\theta) \equiv U(\boldsymbol{\xi}(\theta)) \text{ Stochastic basis : } \Psi_{\alpha}(\boldsymbol{\xi})$$

- Spectral polynomials (Hermite, Legendre, Askey scheme, ...) [Ghanem and Spanos, 1991], [Xiu and Karniadakis 2001]
- Piecewise continuous polynomials (Stochastic elements, multiwavelets, ...) [Deb *et al*, 2001], [olm *et al*, 2004]
- Truncature w.r.t. polynomial order : advanced selection strategy [Nobile *et al*, 2010]

Size of $\dim \mathbb{S}^{\mathrm{P}}$ - Curse of dimensionality

Stochastic Galerkin solution

$U(\boldsymbol{x}, \xi) \approx \sum_{\alpha=0}^{\mathrm{P}} u_\alpha(\boldsymbol{x}) \Psi_\alpha(\xi)$

Find $\{u_0, \ldots u_{\mathrm{P}}\}$ s.t. $\sum_\alpha a_{\alpha,\beta}(u_\alpha, v_\beta) = b_\beta(v_\beta), \ \forall v_{\beta=0,\ldots \mathrm{P}} \in \mathbb{V}$

- A priori selection of the subspace $\mathbb{S}^{\mathrm{P}}$
- Is the truncature / selection of the basis well suited ?
- Size of the Galerkin problem scales with $\mathrm{P}+1$: iterative solver
- Memory requirements may be an issue for large bases

Paradigm :

- Decouple the modes computation (smaller size problems, complexity reduction)
- Use reduced basis representation : find important components in U (reduce complexity and memory requirements)

Proper Generalized Decomposition *

*. Also GSD : Generalized Spectral Decomposition

Content :

Separated representation

The rank-m PGD approximation of U is [Nouy, 2007, 2008, 2010]

$$U(\boldsymbol{x}, \theta) \approx U^m(\boldsymbol{x}, \theta) = \sum_{\alpha=1}^{m<\mathrm{P}} u_\alpha(\boldsymbol{x}) \lambda_\alpha(\theta), \quad \lambda_\alpha \in \mathbb{S}^\mathrm{P}, \; u_\alpha \in \mathbb{V}.$$

Interpretation : U is approximated on

- the stochastic reduced basis $\{\lambda_1, \dots, \lambda_m\}$ of $\mathbb{S}^\mathrm{P}$
- the deterministic reduced basis $\{u_1, \dots, u_m\}$ of $\mathbb{V}$

none of which is selected *a priori*

The questions are then :

- how to define the (deterministic or stochastic) reduced basis ?
- how to compute the reduced basis and the m-terms PGD of U ?

Optimal L_2-spectral decomposition

POD, KL decomposition

$$U^m(\boldsymbol{x},\theta) = \sum_{\alpha=1}^{m} u_\alpha(\boldsymbol{x})\lambda_\alpha(\theta) \text{ minimizes } \mathbb{E}\left[\|U^m - U\|^2_{\mathrm{L}^2(\Omega)}\right]$$

The modes u_α are the m dominant eigenvectors of the kernel $\mathbb{E}\left[U(\boldsymbol{x},\cdot)U(\boldsymbol{y},\cdot)\right]$:

$$\int_\Omega \mathbb{E}\left[U(\boldsymbol{x},\cdot)U(\boldsymbol{y},\cdot)\right] u_\alpha(\boldsymbol{y})\mathrm{d}\boldsymbol{y} = \beta u_\alpha(\boldsymbol{x}), \quad \|u_\alpha\|_{\mathrm{L}^2(\Omega)} = 1.$$

The modes are orthonormal :

$$\lambda_\alpha(\theta) = \int_\Omega U(\boldsymbol{x},\theta)u_\alpha(\boldsymbol{x})\mathrm{d}\boldsymbol{x}$$

However $U(\boldsymbol{x},\theta)$, so $\mathbb{E}\left[u(\boldsymbol{x},\cdot)u(\boldsymbol{y},\cdot)\right]$ is not known !

- Solve the Galerkin problem in $\mathbb{V}^h \otimes \mathbb{S}^{\mathrm{P}'<\mathrm{P}}$ to construct $\{u_\alpha\}$, and then solve for the $\{\lambda_\alpha \in \mathbb{S}^{\mathrm{P}}\}$.
- Solve the Galerkin problem in $\mathbb{V}^H \otimes \mathbb{S}^{\mathrm{P}}$ to construct $\{\lambda_\alpha\}$, and then solve for the $\{u_\alpha \in \mathbb{V}^h\}$ with $\dim \mathbb{V}^H \ll \dim \mathbb{V}^h$.

See works by groups of Ghanem and Matthies.

Alternative definition of optimality

$A(\cdot,\cdot)$ is symmetric positive definite, so U minimizes the energy functional

$$\mathcal{J}(V) \equiv \frac{1}{2}A(V,V) - B(V)$$

We define U^m through

$$\mathcal{J}(U^m) = \min_{\{u_\alpha\},\{\lambda_\alpha\}} \mathcal{J}\left(\sum_{\alpha=1}^{m} u_\alpha \lambda_\alpha\right).$$

- Equivalent to minimizing a Rayleigh quotient
- Optimality w.r.t the A-norm (change of metric) :

$$\|V\|_A^2 = \mathbb{E}\left[a(V,V)\right] = A(V,V)$$

Sequential construction :

For $i = 1, 2, 3 \dots$

$$\mathcal{J}(\lambda_i u_i) = \min_{v \in \mathbb{V}, \beta \in \mathbb{S}^{\mathrm{P}}} \mathcal{J}\left(\beta v + \sum_{j=1}^{i-1} \lambda_j u_j\right) = \min_{v \in \mathbb{V}, \beta \in \mathbb{S}^{\mathrm{P}}} \mathcal{J}\left(\beta v + U^{i-1}\right)$$

The optimal couple (λ_i, u_i) solves simultaneously

- a) deterministic problem $u_i = \mathcal{D}(\lambda_i, U^{i-1})$

$$A(\lambda_i u_i, \lambda_i v) = B(\lambda_i v) - A\left(U^{i-1}, \lambda_i v\right), \quad \forall v \in \mathbb{V}$$

- b) stochastic problem $\lambda_i = \mathcal{S}(u_i, U^{i-1})$

$$A(\lambda_i u_i, \beta u_i) = B(\beta u_i) - A\left(U^{i-1}, \beta u_i\right), \quad \forall \beta \in \mathbb{S}^{\mathrm{P}}$$

Sequential construction :

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The optimal couple (λ_i, u_i) solves simultaneously

- a) deterministic problem $\quad u_i = \mathcal{D}(\lambda_i, U^{i-1})$

$$\int_\Omega \mathbb{E}\left[\lambda_i^2 k\right] \boldsymbol{\nabla} u_i \cdot \boldsymbol{\nabla} v \mathrm{d}\boldsymbol{x} = \mathbb{E}\left[-\int_\Omega \lambda_i k \boldsymbol{\nabla} U^{i-1} \cdot \boldsymbol{\nabla} v \mathrm{d}\boldsymbol{x} + \int_\Omega \lambda_i f v \mathrm{d}\boldsymbol{x}\right], \quad \forall v.$$

- b) stochastic problem $\quad \lambda_i = \mathcal{S}(u_i, U^{i-1})$

$$\mathbb{E}\left[\lambda_i \beta \int_\Omega k \boldsymbol{\nabla} u_i \cdot \boldsymbol{\nabla} u_i \mathrm{d}\boldsymbol{x}\right] = \mathbb{E}\left[-\beta \left(\int_\Omega k \boldsymbol{\nabla} U^{i-1} \cdot \boldsymbol{\nabla} u_i \mathrm{d}\boldsymbol{x} + \int_\Omega f u_i \mathrm{d}\boldsymbol{x}\right)\right], \quad \forall \beta.$$

Sequential construction :

For $i = 1, 2, 3 \ldots$

$$\mathcal{J}(\lambda_i u_i) = \min_{v \in \mathbb{V}, \beta \in \mathbb{S}^{\mathrm{P}}} \mathcal{J}\left(\beta v + \sum_{j=1}^{i-1} \lambda_j u_j\right) = \min_{v \in \mathbb{V}, \beta \in \mathbb{S}^{\mathrm{P}}} \mathcal{J}\left(\beta v + U^{i-1}\right)$$

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- a) deterministic problem $\quad u_i = \mathcal{D}(\lambda_i, U^{i-1})$

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- b) stochastic problem $\quad \lambda_i = \mathcal{S}(u_i, U^{i-1})$

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- The couple (λ_i, u_i) is a fixed-point of :

$$\lambda_i = \mathcal{S} \circ \mathcal{D}(\lambda_i, \cdot), \quad u_i = \mathcal{D} \circ \mathcal{S}(u_i, \cdot)$$

$\Rightarrow$ arbitrary normalization of one of the two elements.

Algorithms inspired from dominant subspace methods
Power-type, Krylov/Arnoldi, ...

Power Iterations

1. Set $l = 1$
2. initialize λ (*e.g.* randomly)
3. While not converged, repeat (power iterations)
   - **a)** Solve : $u = \mathcal{D}(\lambda, U^{l-1})$
   - **b)** Normalize u
   - **c)** Solve : $\lambda = \mathcal{S}(u, U^{l-1})$
4. Set $u_l = u$, $\lambda_l = \lambda$
5. $l \leftarrow l + 1$, if $l < m$ repeat from step 2

Comments :

- Convergence criteria for the power iterations (subspace with dim > 1 or clustered eigenvalues) [Nouy, 2007,2008]
- Usually few (4 to 5) inner iterations are sufficient

Power Iterations with Update

1. Same as Power Iterations, but after (u_l, λ_l) is obtained (step 4) update of the stochastic coefficients :
   - Orthonormalyze $\{u_1, \ldots, u_l\}$ (optional)
   - Find $\{\lambda_1, \ldots, \lambda_l\}$ s.t.

$$A\left(\sum_{i=1}^{l} u_i\lambda_i, \sum_{i=1}^{l} u_i\beta_i\right) = B\left(\sum_{i=1}^{l} u_i\beta_i\right), \quad \forall \beta_{i=1,\ldots,l} \in \times\mathbb{S}^{\mathrm{P}}$$

2. Continue for next couple

Comments :

- Improves the convergence
- Low dimensional stochastic linear system $(l \times l)$
- Cost of update increases linearly with the order l of the reduced representation

Arnoldi, Full Update version

1. Set $l = 0$
2. Initialize $\lambda \in \mathbb{S}^{\mathrm{P}}$
3. For $l' = 1, 2, \ldots$ (Arnoldi iterations)
   - Solve deterministic problem $u' = \mathcal{D}(\lambda, U^l)$
   - Orthogonalize : $u_{l+l'} = u' - \sum_{j=1}^{l+l'-1} (u', u_j)_\Omega$
   - If $\|u_{l+l'}\|_{\mathrm{L}^2(\Omega)} \leq \epsilon$ or $l + l' = m$ then break
   - Normalize $u_{l+l'}$
   - Solve $\lambda = \mathcal{S}(u_{l'}, U^l)$
4. $l \leftarrow l + l'$
5. Find $\{\lambda_1, \ldots, \lambda_l\}$ s.t. (Update)

$$A\left(\sum_{i=1}^{l} u_i \lambda_i, \sum_{i=1}^{l} u_i \beta_i\right) = B\left(\sum_{i=1}^{l} u_i \beta_i\right), \quad \forall \beta_{i=1,\ldots,l} \in \mathbb{S}^{\mathrm{P}}$$

6. If $l < m$ return to step 2.

Summary

- Resolution of a sequence of deterministic elliptic problems, with elliptic coefficients $\mathbb{E}\left[\lambda^2 k\right]$ and modified (deflated) rhs

  dimension is $\dim \mathbb{V}^h$

- Resolution of a sequence of linear stochastic equations

  dimension is $\dim \mathbb{S}^{\mathrm{P}}$

- Update problems : system of linear equations for stochastic random variables

  dimension is $m \times \dim \mathbb{S}^{\mathrm{P}}$

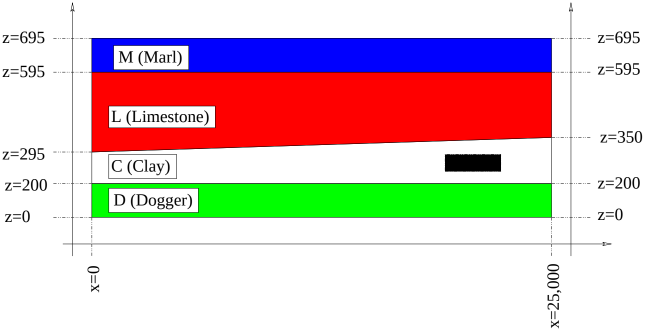
- To be compared with the Galerkin problem dimension

  $\dim \mathbb{V}^h \times \dim \mathbb{S}^{\mathrm{P}}$

Weak modification of existing (FE/FV) codes
(weakly intrusive)

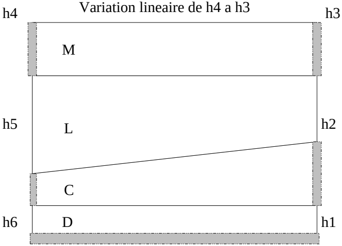
Content :

Example definition



- Rectangular domain 25,000$\times$695 (m)
- 4 Geological layers : D (Dogger), C (Clay), L (Limestone) and M (Marl)

Test case definition (cont.) : uncertain Dirichlet boundary conditions



Δ Head (m)	Expectation	Range	distribution
$\Delta h_{1,2}$	+51	± 10	Uniform
$\Delta h_{1,3}$	+21	± 5	Uniform
$\Delta h_{1,6}$	-3	± 2	Uniform
$\Delta h_{2,5}$	-110	± 10	Uniform
$\Delta h_{3,4}$	-160	± 20	Uniform

Heads at boundaries are taken independent

Example definition (cont.) : Uncertain conductivities

Layer	k_i median	k_i min	k_i max	distribution
Dogger	25	5	125	LogUniform
Clay	$3\ 10^{-6}$	$3\ 10^{-7}$	$3\ 10^{-5}$	LogUniform
Limestone	6	1.2	30	LogUniform
Marl	$3\ 10^{-5}$	$1\ 10^{-5}$	$1\ 10^{-4}$	LogUniform

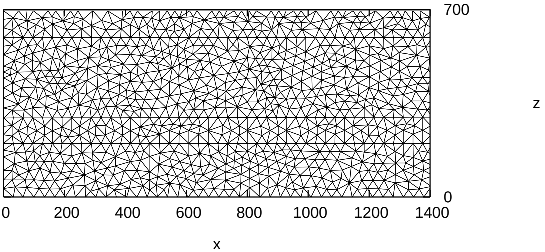
Conductivities are taken independent

Parameterization

- 9 independent r.v. $\{\xi_1, \dots, \xi_9\} \sim U[0,1]^9$
- Stochastic space $\mathbb{S}^{\mathrm{P}}$: Legendre polynomial up to order No
- $\dim \mathbb{S}^{\mathrm{P}} = \mathrm{P} + 1 = (9 + \mathrm{No})!/(9!\mathrm{No}!)$

Deterministic discretization :

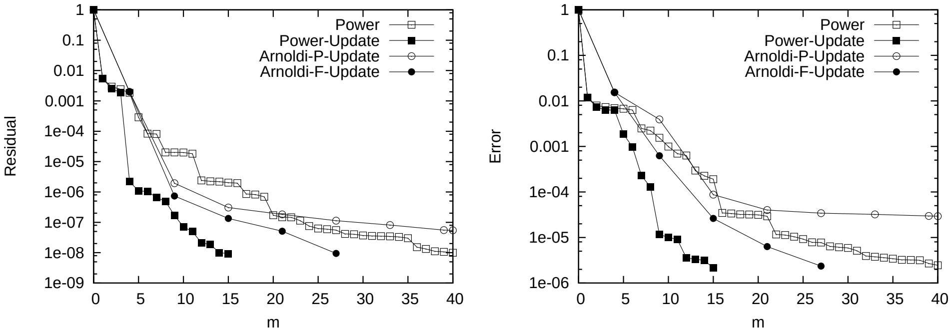
- $\mathbb{P}-1$ finite-element
- Mesh conforming with the geological layers



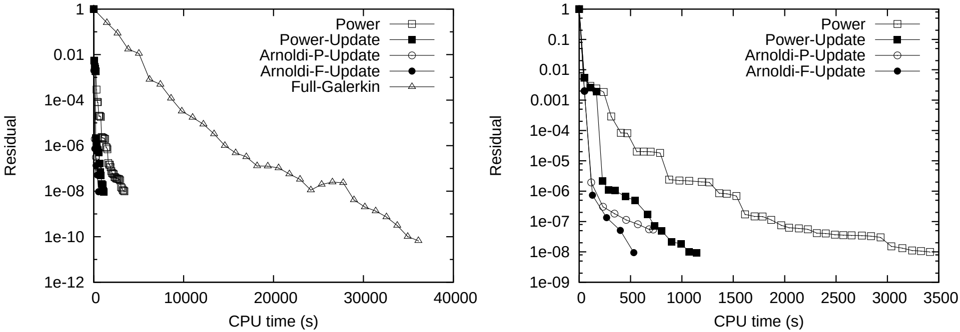
- $N_e \approx 30,000$ finite elements
- $\dim(\mathbb{V}^h) \approx 15,000$
- Dimension of Galerkin problem : 8.2 10^5 $(\mathrm{No}=2)$, 3.3 10^6 $(\mathrm{No}=3)$

Convergence

Galerkin residual (left) and error (right) norms as a function of m ($\text{No} = 3$)



CPU times (No $= 3$)



Full separation

So far, deterministic / stochastic separation :

$$U^m(\boldsymbol{x}, \boldsymbol{\xi}) = U^m(\boldsymbol{x}, \xi_1, \dots, \xi_{\mathrm{N}}) = \sum_{r=1}^{m} u_r(\boldsymbol{x}) \lambda_r(\xi_1, \dots, \xi_{\mathrm{N}}),$$

where $\lambda_r(\boldsymbol{\xi}) \in \mathbb{S}$.
Does not address high-dimensionality issue whenever N is large.

However, if the ξ_i are independent, $\mathbb{S}$ has a tensor product structure,

$$\mathbb{S} = \mathbb{S}_1 \otimes \cdots \otimes \mathbb{S}_{\mathrm{N}},$$

we can think of a decomposition of the form

$$U^m(\boldsymbol{x}, \boldsymbol{\xi}) = \sum_{r=1}^{m} u_r(\boldsymbol{x}) \lambda_r^1(\xi_1) \dots \lambda_r^{\mathrm{N}}(\xi_{\mathrm{N}}),$$

where now $\lambda_r^i(\xi_i) \in \mathbb{S}_i$.

Full separation

Extension of the previous algorithms for the computation of

$$U^m(\boldsymbol{x}, \xi) = \sum_{r=1}^{m} u_r(\boldsymbol{x}) \lambda_r^1(\xi_1) \ldots \lambda_r^{\mathrm{N}}(\xi_{\mathrm{N}}),$$

is straightforward :

- same deterministic problems
- stochastic and update problems for the (separated) λ_r are substituted with alternated direction resolutions : iterations over sequence of one-dimensional problems.

For instance, stochastic problem(s) in direction i : find $\lambda \in \mathbb{S}_i$ such that

$$\mathbb{E}\left[\left(\lambda_r^1 \ldots \lambda \ldots \lambda_r^{\mathrm{N}}\right)\left(\lambda_r^1 \ldots \beta \ldots \lambda_r^{\mathrm{N}}\right)\int_\Omega k \boldsymbol{\nabla} u_r \cdot \boldsymbol{\nabla} u_r \mathrm{d}\boldsymbol{x}\right]$$

$$= \mathbb{E}\left[-\left(\lambda_r^1 \ldots \beta \ldots \lambda_r^{\mathrm{N}}\right)\left(\int_\Omega k \boldsymbol{\nabla} U^{r-1} \cdot \boldsymbol{\nabla} u_r \mathrm{d}\boldsymbol{x} + \int_\Omega f u_r \mathrm{d}\boldsymbol{x}\right)\right], \quad \forall \beta \in \mathbb{S}_i.$$

Full separation

Clearly, using

$$U^m(\boldsymbol{x},\xi) = \sum_{r=1}^{m} u_r(\boldsymbol{x}) \lambda_r^1(\xi_1)\dots\lambda_r^{\mathrm{N}}(\xi_{\mathrm{N}}),$$

we trade convergence with complexity reduction.

This can be mitigated using using a R_λ-rank approximation of the stochastic coefficients :

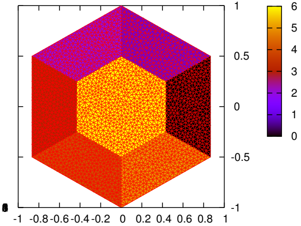
$$U^m(\boldsymbol{x},\xi) = \sum_{r=1}^{m} u_r(\boldsymbol{x}) \left(\sum_{r'=1}^{R_\lambda} \lambda_{r,r'}^1(\xi_1)\dots\lambda_{r,r'}^{\mathrm{N}}(\xi_{\mathrm{N}}) \right),$$

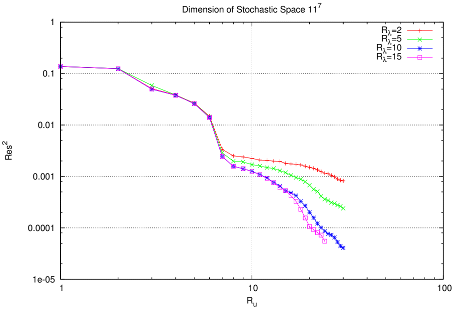
with a greedy-type approximation of low rank approximation of λ_r.

- Extension of the algorithms is immediate
- R_λ can be made rank dependent
- Efficient implementation requires separated representation of the operator.

An example : diffusion

- Independent random conductivities over 7 sub-domains, with same distribution (log-normal) : $\mathrm{N} = 7$
- $\mathbb{S}_{i=1,7} = \Pi_{10}(\mathbb{R})$, so $\dim \mathbb{S} = 11^7$





Wave equation (Deterministic)

Consider the deterministic wave equation,

$$-\omega^2 \rho u(\boldsymbol{x}) - \boldsymbol{\nabla} \cdot (\tilde{\kappa} \boldsymbol{\nabla} u(\boldsymbol{x})) = f(\boldsymbol{x}), \qquad \text{in} \Omega$$
$$u(\boldsymbol{x} \in \partial\Omega) = 0$$

- ω is the frequency
- ρ the density
- $\tilde{\kappa} \doteq \kappa(1 - i\beta\omega) \in \mathbb{C}$ the wave velocity with $\kappa, \beta > 0$

Let $L_2(\Omega) = L_2(\Omega, \mathbb{C})$ with inner product and norm

$$(u, v)_\Omega = \mathrm{Re}\left(\int_\Omega u^*(\boldsymbol{x}) v(\boldsymbol{x}) d\Omega \right), \quad \|u\|^2_{L_2(\Omega)} = (u, u)_\Omega,$$

The weak formulation : Find $u \in H^1_0(\Omega, \mathbb{C})$ such that

$$a(u, v) - b(v) = 0 \quad \forall v \in H^1_0(\Omega),$$

with the bilinear and linear forms

$$a(u, v) = \mathrm{Re}\left[-\omega^2 \int_\Omega u^* v d\Omega + \int_\Omega \tilde{\kappa} \boldsymbol{\nabla} u^* \cdot \boldsymbol{\nabla} v \, d\Omega \right], \quad b(v) = \mathrm{Re}\left[\int_\Omega f^* v \, d\Omega \right].$$

Wave equation (Stochastic version)

Take now ω, ρ and κ as second order random variable defined on a probability space $\mathcal{P} = (\Theta, \Sigma_\Theta, \mu)$.
We extend $L_2(\Omega)$ and $H_0^1(\Omega)$ to $L_2(\Omega, \Theta)$ and $H_0^1(\Omega, \Theta)$ by tensorization, and we assume

$$U(\boldsymbol{x}, \theta) \in L_2(\Omega, \Theta) \Leftrightarrow \mathbb{E}\left\{(U(\cdot), U(\cdot))_\Omega\right\} < \infty.$$

Variational form of the stochastic wave equation
Find $U \in H_0^1(\Omega, \Theta)$ such that

$$A(U, V) - B(V) = 0, \quad \forall V \in H_0^1(\Omega, \Theta),$$

where

$$A(U, V) = \mathbb{E}\left\{\mathrm{Re}\left[-\omega^2(\theta)\int_\Omega U^*(\theta) V(\Theta) d\Omega + \int_\Omega \kappa(\theta) \boldsymbol{\nabla} U^*(\theta) \cdot \boldsymbol{\nabla} V(\theta)\, d\Omega\right]\right\},$$

and

$$B(V) = \mathbb{E}\left\{\mathrm{Re}\left[\int_\Omega f^* V(\theta)\, d\Omega\right]\right\}.$$

PGD approximation

We seek for $U \in H_0^1(\Omega, \Theta) = H_0^1(\Omega) \otimes L_2(\Theta)$ has the separated form

$$U(\boldsymbol{x}, \theta) = \sum_{r=0}^{r=\infty} u_r(\boldsymbol{x}) \lambda_r(\theta), \quad u_r \in H_0^1(\Omega), \ \lambda_r \in L_2(\Theta),$$

following the PGD approach based on the deterministic and stochastic problems

$$u_R = D(U^{R-1}, \lambda_R) : \quad A(U^{R-1} + u_R \lambda_R, v \lambda_R) - B(v \lambda_R) = 0, \forall v \in H_0^1(\Omega) \qquad \text{Deter. problem}$$

$$\lambda_R = S(U^{R-1}, u_R) : \quad A(U^{R-1} + u_R \lambda_R, u_R \beta) - B(u_R \beta) = 0, \forall \beta \in L_2(\Theta) \qquad \text{Stoch. problem}$$

and update problem :
given $u_{r=1,\ldots,R}$ compute $\lambda_{r=1,\ldots,R}$ such that

$$A\left(\sum_{r=0}^{R} u_r \lambda_r, u_{r'} \beta\right) - B(u_{r'} \beta) = 0, \quad \forall \beta \in L_2(\Theta) \text{ and } r' = 1, \ldots, R.$$

PGD-Arnoldi algorithm

Assume rank-R approximation has been obtained.

1. **Initialization :** set $\lambda \in L_2(\Theta)$, $l = 0$
2. **Arnoldi subspace generation :**
   - Set $w = D(U^R, \lambda)$
   - For $r = 1, \dots, R + l$ $w \leftarrow (w, u_r)_\Omega$
   - If $h = (w, w)_\Omega < \varepsilon$ break
   - Set $l \leftarrow l + 1$, $u_{R+l} = w/h$
   - Set $\lambda = S(U^R, u_{R+l})$
   - Repeat for next Arnoldi vector
3. **Update solution :** set $R \leftarrow R + l$ and solve

$$A\left(\sum_{r=0}^{R} u_r \lambda_r, u_{r'} \beta\right) - B(u_{r'} \beta) = 0, \quad \forall \beta \in L_2(\Theta) \text{ and } r' = 1, \dots, R.$$

4. **Check residual to restart at step 1 or stop**

Advantage : limited number of deterministic problem solves to generate the deterministic basis.

Stochastic parametrization

We introduce a finite set of N independndt real-valued r.v. $\boldsymbol{\xi} \doteq (\xi_1 \ldots \xi_{\mathrm{N}})$ with uniform distribution on $\Xi \doteq \mathbb{1}_N$. The random frequency, density and stiffness are parametrized using $\boldsymbol{\xi}$,

$$(\omega, \kappa, \rho)(\theta) \longrightarrow (\omega, \kappa, \rho)(\boldsymbol{\xi}(\theta)),$$

and U is sought in the image probability space :

$$H_0^1(\Omega, \Xi) \ni U(\boldsymbol{x}, \boldsymbol{\xi}(\theta)) \approx \sum_{r=1}^{R} u_r(\boldsymbol{x}) \lambda_r(\boldsymbol{\xi}(\theta)).$$

- $U(\boldsymbol{x}, \dot{)}$ is expected to be smooth a.s. : need for a limited number of spatial modes to span the stochastic solution space,
- $U(\cdot, \boldsymbol{\xi})$ can exhibit steep and complex dependences with respect to the input parameters.

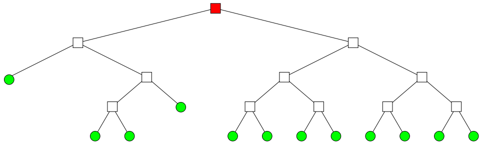
The complexity of the mapping $\boldsymbol{\xi} \in \Xi \mapsto U(\cdot, \boldsymbol{\xi}) \in H_0^1(\Omega)$ reflects in the stochastic coefficients $\lambda_r(\boldsymbol{\xi})$ and calls for appropriate discretization at the stochastic level.

stochastic multi-resolution framework

Presently, we use piecewise polynomial approximations at the stochastic level :

- Ξ is adaptively decomposed into sub-domains through a sequence a dyadic (1d) partitions
- A tree structure is used to manage the resulting stochastic space
- Multi-resolution analysis is used to control the local adaptation (anisotropic refinement of the partition of Ξ)
- Stochastic and update problems are solved independently over the sub-domains (efficient parallelization)

(see [Tryoen, LM and Ern, SISC 2012])



PGD-Arnoldi with Adaptation at the Stochastic level

Given the approximation U^r and a stochastic space $\mathbb{S}^r$

1. Arnoldi iterations to generate orthonormal $u_{r+1}, \ldots u_{r+l}$, using $\lambda \in \mathbb{S}^r$
2. set $r \leftarrow r + l$
3. While not satisfying accuracy criterion, repeat
   - Solve the update problem for $\{\lambda_1, \ldots, \lambda_r\}$ in $\mathbb{S}^r$
   - Enrich adaptively $\mathbb{S}^r$
4. Compute residual norm
5. If not converge restart at step 1.

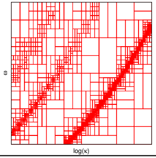
Observe :

- Same approximation space for all stochastic coefficients (ease implementation and favor parallelization)
- Continuous enrichment, no coarsening
- Successive Arnoldi spaces generated using an coarse stochastic space ! (in fact robust)
- Accuracy requirement should balance stochastic discretization and reduced space errors.

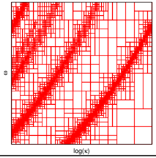
Example

- $\log(\kappa) \sim U[-4 : -2]$
- $\omega \sim U[0.5, 1]$
- $\rho = 1$ and $\beta = 0.05$
- Third order (Legendre) expansion.

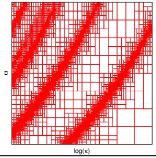
$r = 8$



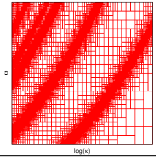
$r = 13$



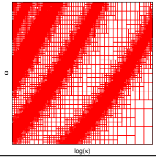
$r = 19$



$r = 26$



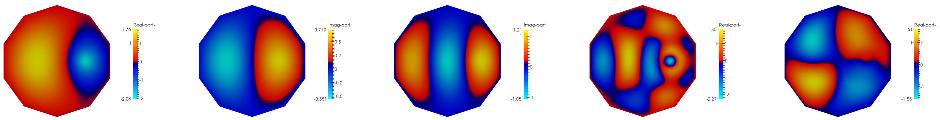
$r = 30$



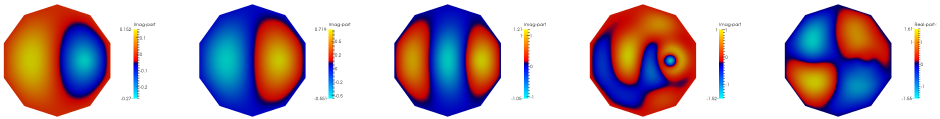
Example

Selected Arnoldi modes : real part (top) and imaginary part (bottom)

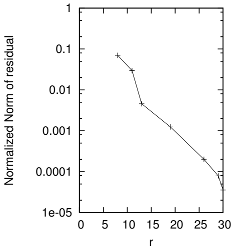
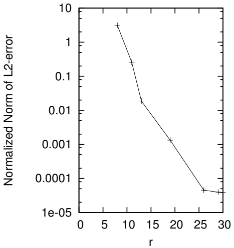
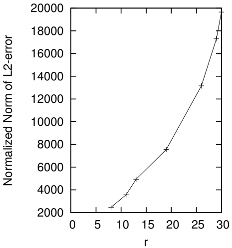
$r = 1$	$r = 3$	$r = 5$	$r = 15$	$r = 25$



$r = 1$	$r = 3$	$r = 5$	$r = 15$	$r = 25$



Example

Residual	Error	# of sub-domains
		

Content :

Stochastic Navier-Stokes equations

Consider the steady, incompressible Navier-Stokes equations

$$\begin{aligned} &\boldsymbol{U}(\theta)\boldsymbol{\nabla}\boldsymbol{U}(\theta) = -\boldsymbol{\nabla}P(\theta) + \nu(\theta)\nabla^2\boldsymbol{U}(\theta) + \boldsymbol{f}(\theta) && \text{in } \Omega, \\ &\boldsymbol{\nabla}\cdot\boldsymbol{U}(\theta) = 0 && \text{in } \Omega, \\ &\boldsymbol{U}(\theta) = 0 && \text{on } \partial\Omega. \end{aligned}$$

in a bounded (2d) domain Ω.
In view of PGD of the solution, we need to consider (mainly)

1. non-linear character (increases when $\nu \downarrow 0$)
2. enforcement of the divergence free constraint
3. stabilization (upwinding) due to the convective term

None of these will be really address here, simply numerical experiments !
[Tamellini, LM, Nouy, SISC, 2014]

Weak form

Deterministic space $\mathbb{V} = H^1_{0,div}(\Omega)$.
Weak formulation : Find $U \in \mathbb{X} \doteq \mathbb{V} \otimes \mathbb{S}$ such that

$$\mathbb{E}\left\{\int_\Omega [(U(\theta)\nabla U(\theta)) \cdot V(\theta) + \nu(\theta)\nabla U(\theta)\ \nabla V(\theta) - F(\theta) \cdot V(\theta)]\, dx\right\} \quad \forall V \in \mathbb{X}.$$

The deterministic problem $u = D(\lambda, U^m)$ writes : $\forall v \in \mathbb{V}$

$$\int_\Omega \left(\mathbb{E}\left\{\lambda^3\right\} u\nabla u + u\nabla \bar{u}_m(\lambda) + \bar{u}_m(\lambda)\nabla u\right) \cdot v dx + \int_\Omega \mathbb{E}\left\{\nu\lambda^2\right\} \nabla u \nabla v dx$$
$$= \int_\Omega \mathbb{E}\left\{\lambda(F - U^m\nabla U^m)\right\} \cdot v dx - \int_\Omega \mathbb{E}\left\{\nu\lambda\nabla U^m\right\} \nabla v dx.$$

where $\bar{u}_m(\lambda) = \mathbb{E}\left\{\lambda^2 U^m\right\}$.
Stochastic problem $\lambda = S(u, U^m)$ writes : $\forall \beta \in \mathbb{S}$

$$\mathbb{E}\left\{\lambda^2\beta\right\} \int_\Omega (u\nabla u \cdot u) dx + \mathbb{E}\left\{\lambda\beta \int_\Omega (u\nabla U^m + U^m \nabla u) \cdot u dx\right\} + \int_\Omega \mathbb{E}\left\{\nu\lambda\beta\right\} \nabla u \nabla u dx$$
$$= \mathbb{E}\left\{\beta \int_\Omega (F - U^m\nabla U^m) \cdot u dx\right\} - \mathbb{E}\left\{\beta \int_\Omega \nu\nabla U^m \nabla u dx\right\}.$$

Complexity

- Resolution of a sequence of deterministic problems, NS + Lin. term and deflated rhs

  dimension is $\dim \mathbb{V}^h$
- Resolution of a sequence of quadratic stochastic equations

  dimension is $\dim \mathbb{S}$
- Update problems : system of quadratique equations for stochastic random variables

  dimension is $m \times \dim \mathbb{S}$
- To be compared with the Galerkin problem dimension

  $\dim \mathbb{V}^h \times \dim \mathbb{S}$

Weak modification of existing (FE/FV) codes
(weakly intrusive)

Stochastic discretization :

- Parametrization of $\nu(\theta)$ and $\boldsymbol{F}(\theta)$ using N i.i.d. random variables :

$$\boldsymbol{\xi} = \{\xi_1, \dots, \xi_\mathrm{N}\} \sim N(0, I^2).$$

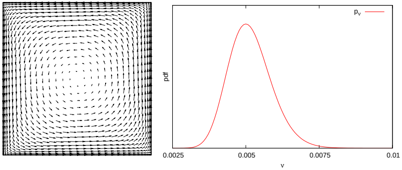
- Wiener-Hermite polynomials for the basis for $\mathbb{S}$

$$\lambda(\theta) = \sum_\alpha \lambda_\alpha \Psi_\alpha(\boldsymbol{\xi}(\theta)),$$

- Truncature to (total) polynomial degree No :

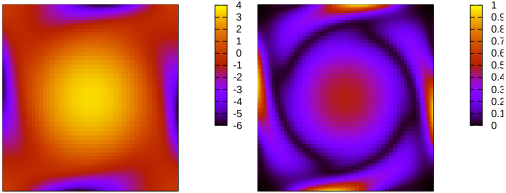
$$\dim \mathbb{S} = \frac{(\mathrm{No} + \mathrm{N})!}{\mathrm{No}!\mathrm{N}!}.$$

Case of a deterministic forcing and a random (Log-normal) viscosity :



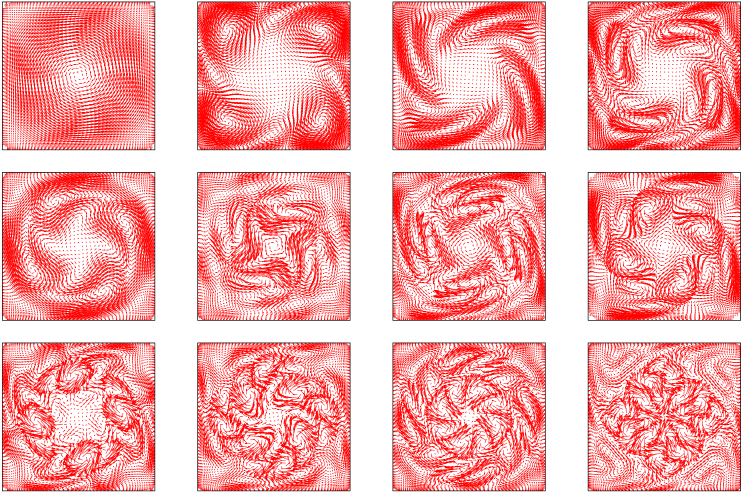
$$\nu(\theta) = \frac{1}{200} \exp\left(\frac{\sigma_\nu}{\sqrt{\mathrm{N}}} \sum_{i=1}^{\mathrm{N}} \xi_i(\theta)\right) \quad (+10^{-4}), \quad \xi_i \sim N(0,1) \ i.i.d.$$

Same problem but for parametrization involving N Gaussian R.V.
Galerkin solution for $\mathrm{N} = 1$ and $\mathrm{No} = 10$ (Wiener-Hermite expansion)

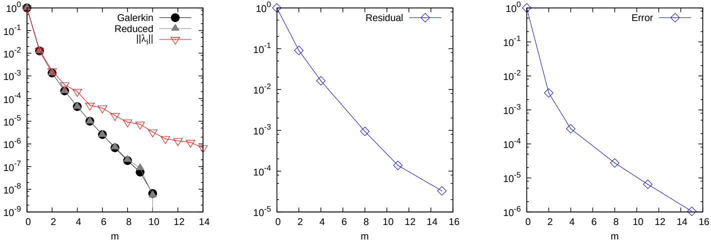


Mean and standard deviation of U^G rotational.

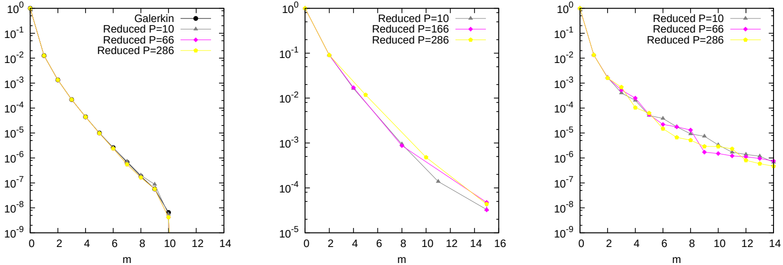
First PGD-Arnoldi modes for $\mathrm{N} = 1$ and $\mathrm{No} = 10$



Convergence of PGD solution $\mathrm{N} = 1$ and $\mathrm{No} = 10$



Convergence with rank of resiudal and error norms ; POD coefficients at $m = 15$ (right)

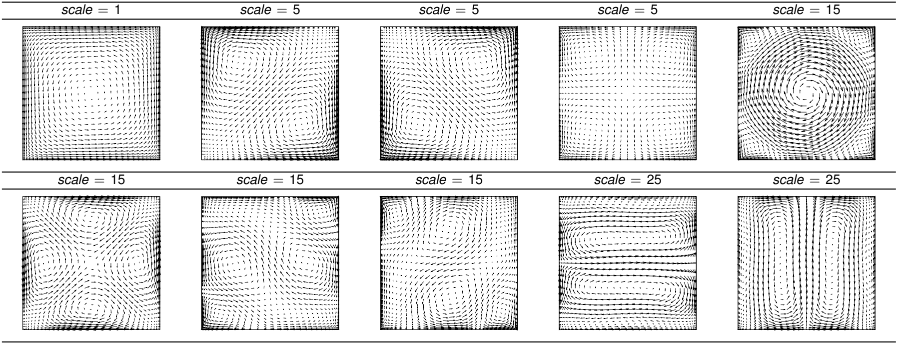


Norms of the POD coefficients at $m = 15$ (left), residual norm (center), $\|\lambda\|$'s norm

Stochastic forcing $\boldsymbol{F}$: Hodge's decomposition

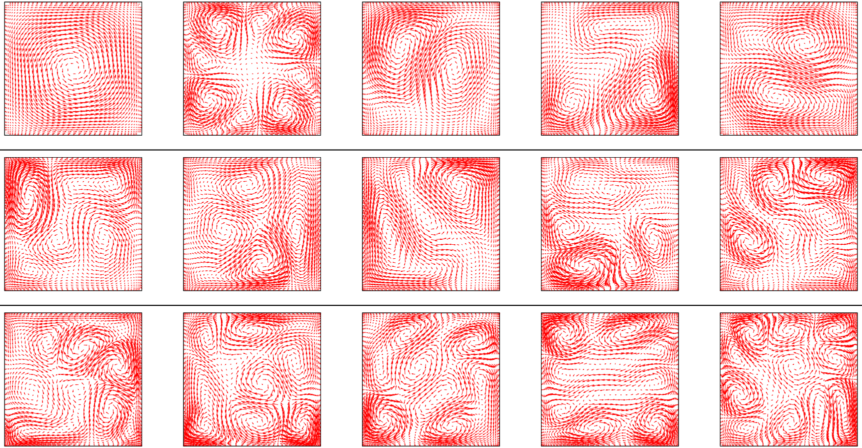
$$\boldsymbol{F}(\boldsymbol{x},\theta) \approx \boldsymbol{F}^{\mathrm{N}}(\boldsymbol{x},\boldsymbol{\xi}(\theta)) = \boldsymbol{f}^0 + \sum_{k=0}^{\mathrm{N}} \sqrt{\gamma_k}\,\boldsymbol{f}^k(\boldsymbol{x})\xi_k(\theta).$$

KL modes of the forcing :

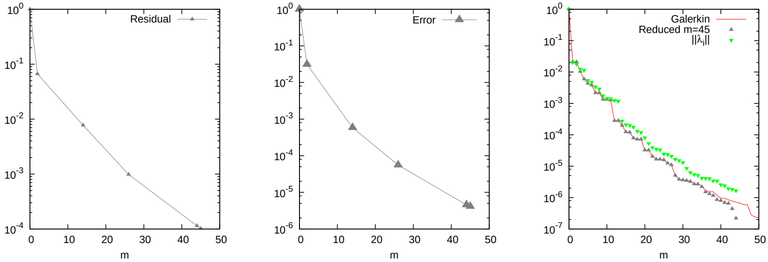


Forcing modes for $L = 1$, $\sigma / f^0_\omega = 0.2$

First PGD-Arnoldi modes



Results at $\overline{\nu} = 1/50$: $\mathrm{No} = 3$, $\mathrm{N} = 11$, $\mathrm{P} = 364$

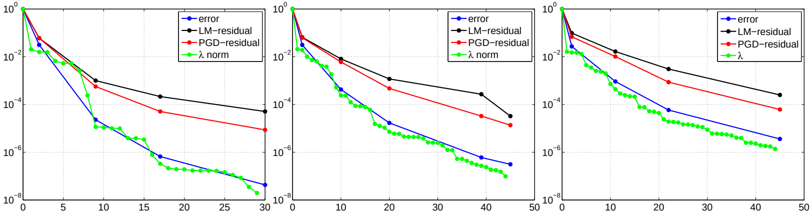


Residual (left), $\|U^m - U^G\|$ (center) and norm of POD modes for $m = 45$ (right).

Essentially < 50 Navier-Stokes solves !

Residual computation :

- computation of the residual in $H^1_{0,div}(\Omega)$
- need to reconstruct the pressure
- 2 alternatives : apply PGD to the pressure unknown, given the reduced velocity approximation, or recycle the pressure fields associated to the enforcement of the divergence-free constraint during the Arnoldi process as a reduced pressure basis.



Comparison of different error measures of the PGD solution at $\overline{\nu} = 1/10$, $1/50$ and $1/100$ (from left to right).

Thanks for your attention
(and to the organizers !)