# Proper Generalized Decomposition for Linear and Non-Linear Stochastic Models

**Olivier Le Maître** [1]
Lorenzo Tamellini [2] and Anthony Nouy [3]

[1] LIMSI-CNRS, Orsay, France
[2] MOX, Politecnico Milano, Italy
[3] GeM, Ecole Centrale Nantes, France

Radon Special Semester, WS on Multiscale Simulation & Analysis in Energy and the Environment, Linz - (12-16)/12/2011

## 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 :

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

## Uncertainty in the model solution :

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

$$U(\boldsymbol{\xi}) \approx \sum_k u_k \Psi_k(\boldsymbol{\xi})$$

Consider the deterministic linear scalar elliptic problem (in $\Omega$)

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

where

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

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

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

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

## 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 $\Omega$ and $f \in \mathrm{L}^2(\Omega, \Theta, \mathrm{d}\mu)$

## Variational formulation :

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

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

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

## Stochastic expansion :

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

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

- Truncated expansion :

$$\text{span}\,\{\Psi_0, \ldots, \Psi_\mathrm{P}\} = \mathrm{S}^\mathrm{P} \subset \mathrm{L}^2(\Theta, \mathrm{d}\mu)$$

- Galerkin problem :

Find $U \in \mathrm{V} \otimes \mathrm{S}^\mathrm{P}$ s.t.

$$A(U, V) = B(V) \quad \forall V \in \mathrm{V} \otimes \mathrm{S}^\mathrm{P},$$

with $U = \sum_{\alpha=0}^{\mathrm{P}} u_\alpha \Psi_\alpha$ and $V = \sum_{\alpha=0}^{\mathrm{P}} v_\alpha \Psi_\alpha$

## Stochastic expansion :

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

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

- Truncated expansion :

$$\text{span}\,\{\Psi_0, \ldots, \Psi_\mathrm{P}\} = \mathrm{S}^\mathrm{P} \subset \mathrm{L}^2(\Theta, \mathrm{d}\mu)$$

- Galerkin problem :

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

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

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

## Stochastic expansion :

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

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

- Truncated expansion :

$$\text{span}\,\{\Psi_0, \ldots, \Psi_\mathrm{P}\} = \mathrm{S}^\mathrm{P} \subset \mathrm{L}^2(\Theta, \mathrm{d}\mu)$$

- Galerkin problem :

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

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

Large system of coupled linear problem, globally SDP.

## Stochastic parametrization

- Parameterization using $\mathrm{N}$ 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 $p_\xi$ 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** $\dim \mathrm{S}^{\mathrm{P}}$ **- Curse of dimensionality**

## Stochastic Galerkin solution

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

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

- A priori selection of the subspace $\mathrm{S}^{\mathrm{P}}$
- 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

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

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

separated representation

Interpretation : $U$ is approximated on

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

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 $u_\alpha$ 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 !

## Optimal $L_2$-spectral decomposition : POD, KL decomposition

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

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

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 $i = 1, 2, 3 \ldots$

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

The optimal couple $(\lambda_i, u_i)$ solves simultaneously

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

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

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

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

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

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

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

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

## Properties :

- The couple $(\lambda_i, u_i)$ is a fixed-point of :

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

- Homogeneity property :

$$\frac{\lambda_i}{c} = \mathcal{S}(cu_i, \cdot), \quad \frac{u_i}{c} = \mathcal{D}(c\lambda_i, \cdot), \quad \forall c \in \mathbb{R} \setminus \{0\}.$$

$\Rightarrow$ 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 $\lambda$ (*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 $(u_l, \lambda_l)$ is obtained (step 4) update of the stochastic coefficients :
   - Orthonormalyze $\{u_1, \ldots, u_l\}$ (optional)
   - Find $\{\lambda_1, \ldots, \lambda_l\}$ s.t.

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

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 $\lambda \in \mathrm{S}^{\mathrm{P}}$
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)

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

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 $\dim \mathrm{V}^h$

- Resolution of a sequence of linear stochastic equations

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

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

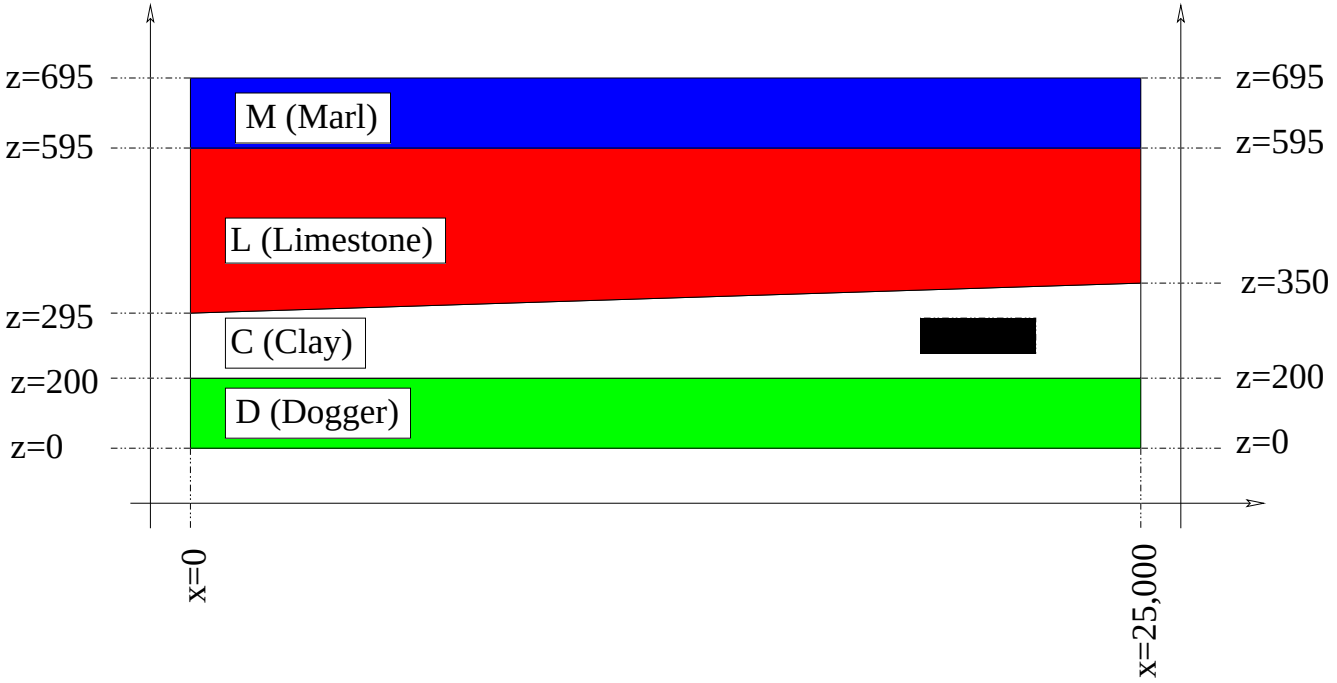
  dimension is $m \times \dim \mathrm{S}^{\mathrm{P}}$

- To be compared with the Galerkin problem dimension

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

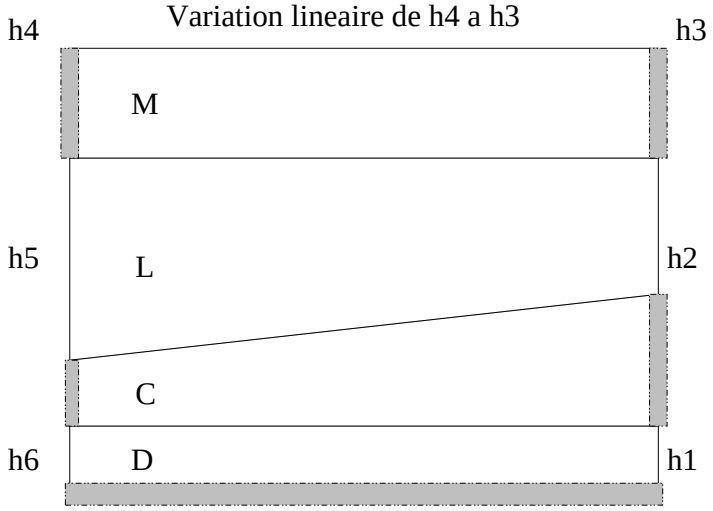
Weak modification of existing (FE/FV) codes
(weakly intrusive)

## 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




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

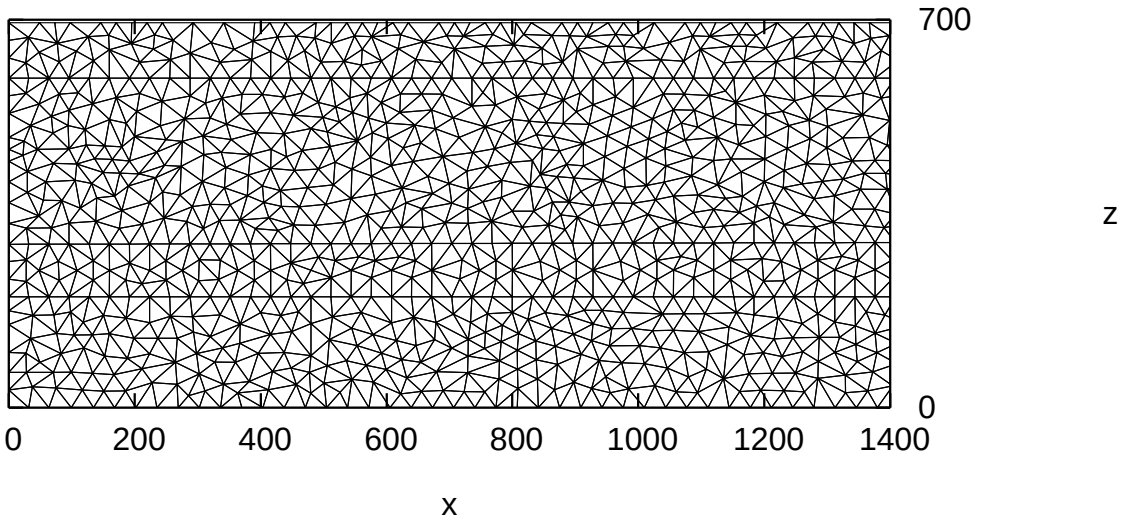
Conductivities are taken independent

## Parameterization

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

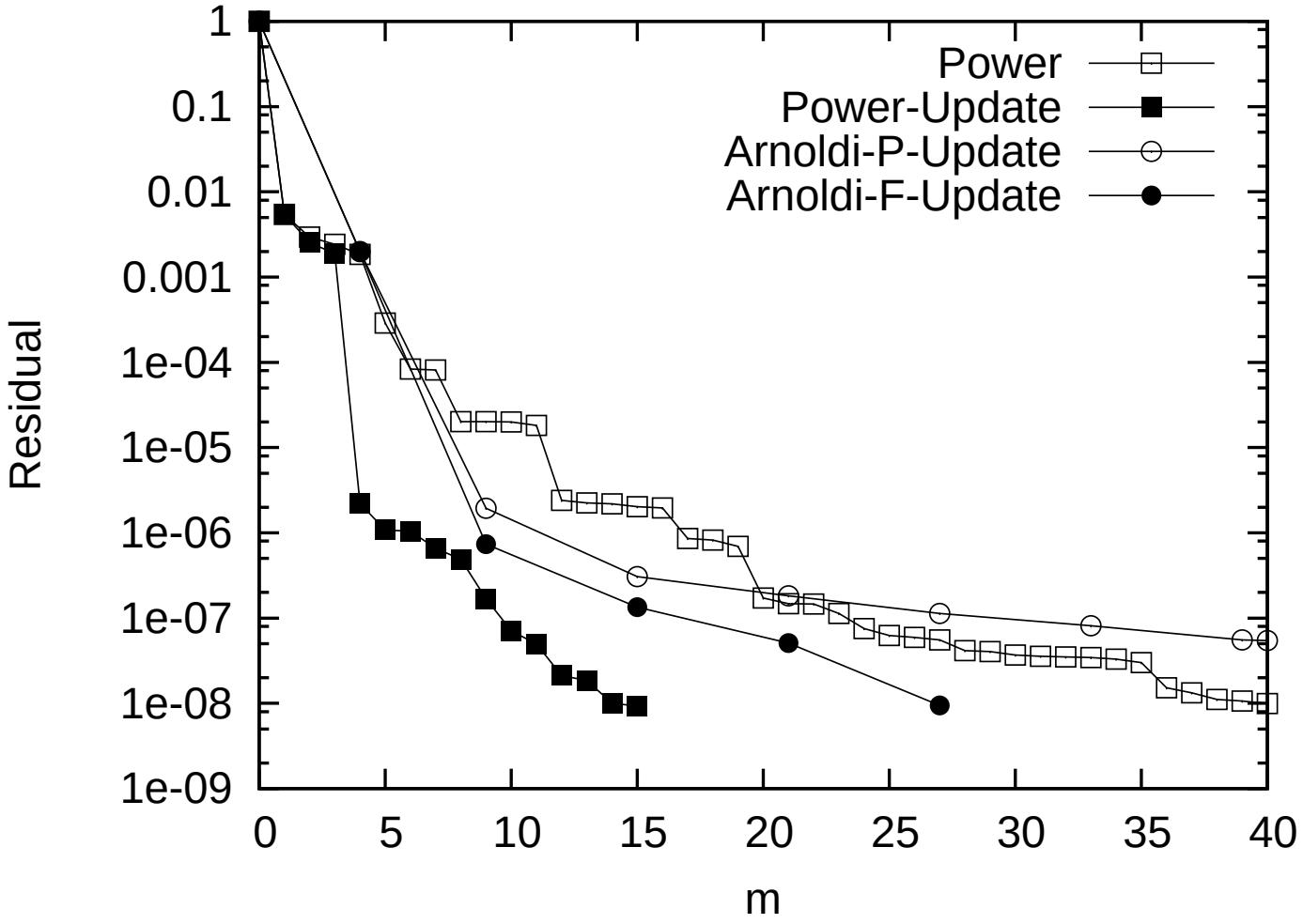
## Deterministic discretization :

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

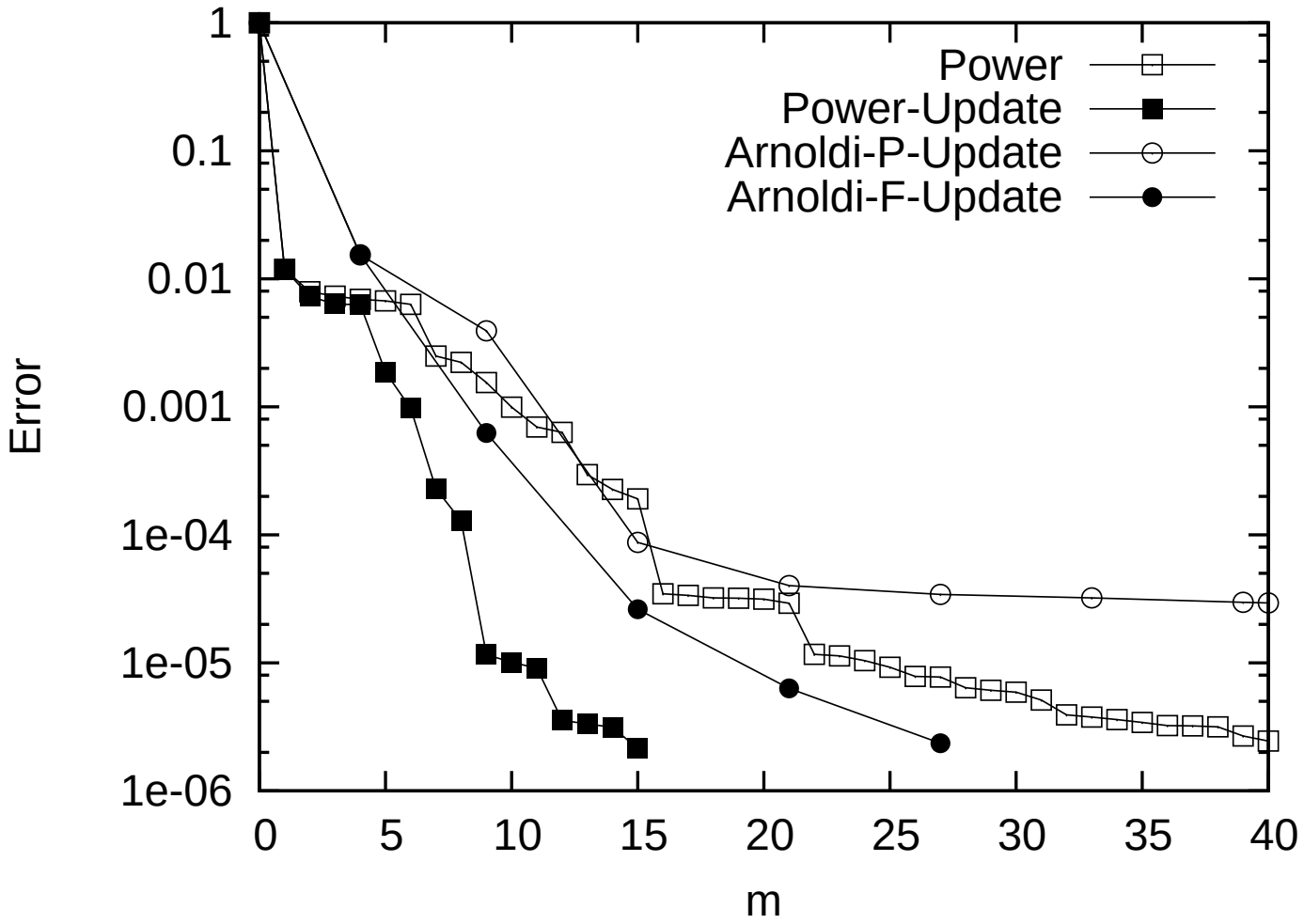



- $N_e \approx 30,000$ finite elements
- $\dim(\mathrm{V}^h) \approx 15,000$
- Dimension of Galerkin problem : $8.2\ 10^5$ $(\mathrm{No} = 2)$, $3.3\ 10^6$ $(\mathrm{No} = 3)$

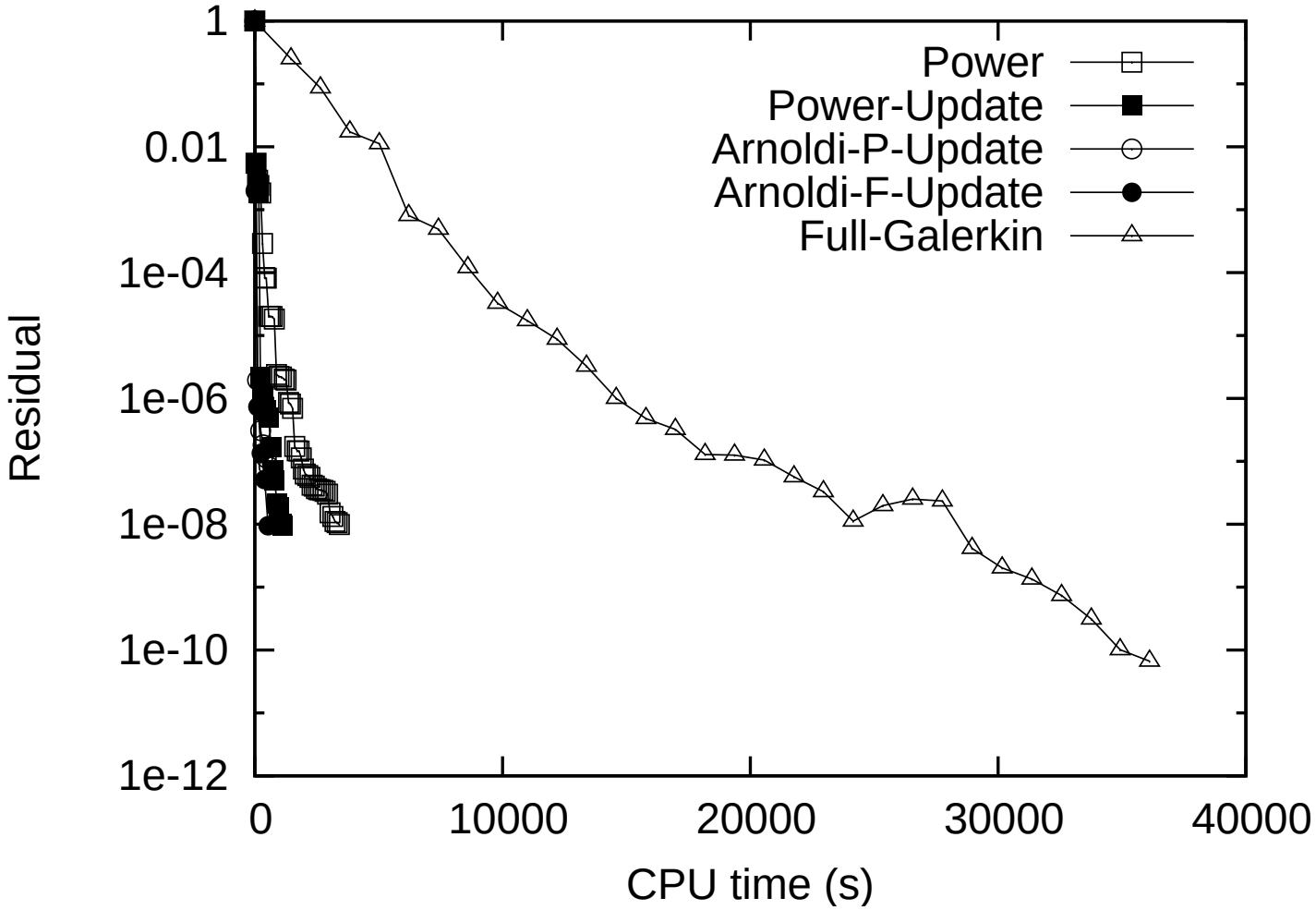
## Norm of Galerkin residual as a function of $m$ ($\mathrm{No} = 3$)



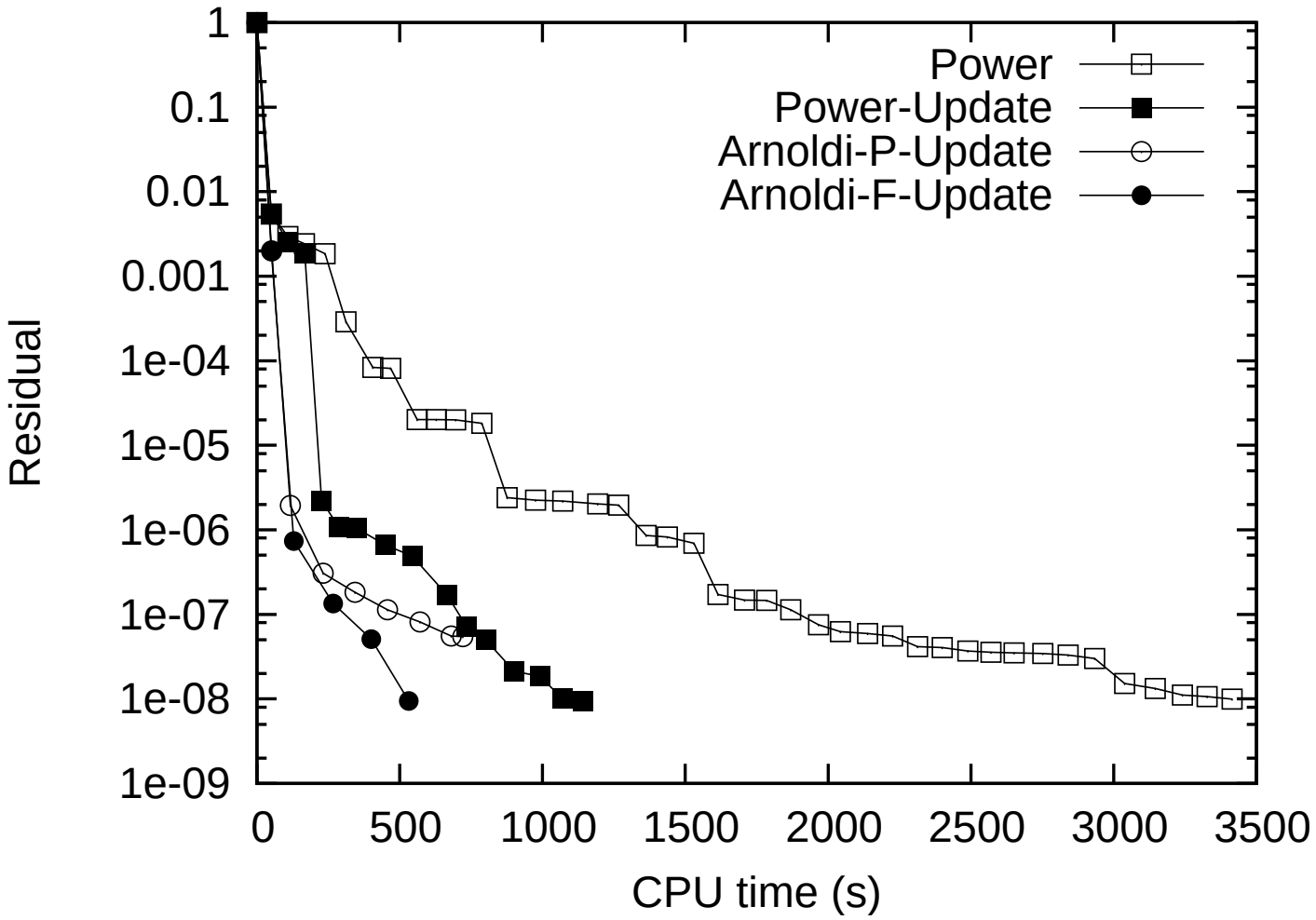
# Norm of error (vs Galerkin) as a function of $m$ ($\mathrm{No} = 3$)



## CPU times ($\mathrm{No} = 3$)



# CPU times of PGD algorithms ($\mathrm{No} = 3$)



## Extension to general problems

- Non-definite / non symmetric linear and nonlinear problems : no optimality results

  [Nouy, 2008]

- Algorithms : from numerical experiments methods & algorithms can be safely applied [Nouy & olm, 2009]
- Illustration on the Incompressible Navier-Stokes equations

Test problem : steady, two dimensional, Newtonian fluid in a square domain $\Omega$ :

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

- $\boldsymbol{U}$ the velocity field,
- $P$ the pressure field,
- uncertainty in the viscosity $\nu = \nu(\theta)$ and forcing $\boldsymbol{F} = \boldsymbol{F}(\boldsymbol{x}, \theta)$.

## Functional spaces :

$\mathrm{L}^2(\Omega)$ the space of functions that are square integrable over $\Omega$, equipped with the inner product and norm

$$(p, q)_\Omega := \int_\Omega pq \, \mathrm{d}\Omega, \qquad \|q\|_{\mathrm{L}^2(\Omega)} = (q, q)_\Omega^{1/2}.$$

Extended to vector valued functions by summation over vectors components, and to the constrained space

$$\mathrm{L}_0^2(\Omega) = \left\{ q \in \mathrm{L}^2(\Omega) : \int_\Omega q \, \mathrm{d}\Omega = 0 \right\}.$$

$\mathbf{H}^1(\Omega)$, Sobolev space of vector valued functions with all components and their first derivatives being square integrable over $\Omega$, and $\mathbf{H}_0^1(\Omega)$ the constrained space of such vector functions vanishing on $\partial\Omega$,

$$\mathbf{H}_0^1(\Omega) = \left\{ \boldsymbol{v} \in \mathbf{H}^1(\Omega), \ \boldsymbol{v} = 0 \text{ on } \partial\Omega \right\}.$$

## Weak formulation :

Find $\boldsymbol{U} \in \mathbf{H}_0^1(\Omega) \otimes \mathrm{S}$ and $P \in \mathrm{L}_0^2(\Omega) \otimes \mathrm{S}$, such that

$$\begin{aligned} &C(\boldsymbol{U}, \boldsymbol{U}, \boldsymbol{V}) + D(\boldsymbol{V}, P) + A(\boldsymbol{U}, \boldsymbol{V}) = \mathbb{E}\left[(\boldsymbol{F}, \boldsymbol{V})_\Omega\right] && \forall \boldsymbol{V} \in \mathbf{H}_0^1(\Omega) \otimes \mathrm{S}, \\ &D(\boldsymbol{U}, Q) = 0 && \forall Q \in \mathrm{L}_0^2(\Omega) \otimes \mathrm{S}. \end{aligned}$$

where :

- $C(\boldsymbol{U}, \boldsymbol{V}, \boldsymbol{W}) \doteq \mathbb{E}\left[c(\boldsymbol{U}, \boldsymbol{V}, \boldsymbol{W})\right] = \mathbb{E}\left[\int_\Omega (\boldsymbol{U}\nabla \boldsymbol{V}) \cdot \boldsymbol{W} d\boldsymbol{x}\right]$
- $D(\boldsymbol{V}, Q) \doteq \mathbb{E}\left[d(\boldsymbol{V}, Q)\right] = \mathbb{E}\left[\int_\Omega Q \nabla \boldsymbol{V} d\boldsymbol{x}\right]$
- $A(\boldsymbol{U}, \boldsymbol{V}) \doteq \mathbb{E}\left[\nu a(\boldsymbol{U}, \boldsymbol{V})\right] = \mathbb{E}\left[\nu \int_\Omega \nabla \boldsymbol{V} : \nabla \boldsymbol{V} d\boldsymbol{x}\right]$

Weak formulation in (weakly) Divergence Free space : Let $\mathbf{H}^1_{0;\mathrm{div}}(\Omega)$

$$\mathbf{H}^1_{0;\mathrm{div}}(\Omega) = \left\{ \boldsymbol{v} \in \mathbf{H}^1_0(\Omega),\ d(\boldsymbol{v}, q) = 0\ \forall q \in \mathrm{L}^2_0(\Omega) \right\}.$$

The problem becomes :
Find $\boldsymbol{U} \in \mathbf{H}^1_{0;\mathrm{div}}(\Omega) \otimes \mathrm{S}$ such that

$$C(\boldsymbol{U}, \boldsymbol{U}, \boldsymbol{V}) + A(\boldsymbol{U}, \boldsymbol{V}) = \mathbb{E}\left[(\boldsymbol{F}, \boldsymbol{V})_\Omega\right] \qquad \forall \boldsymbol{V} \in \mathbf{H}^1_{0;\mathrm{div}}(\Omega) \otimes \mathrm{S}.$$

- Remove the pressure
- Difficulties in the discretization of $\mathbf{H}^1_{0;\mathrm{div}}(\Omega)$

## PGD approximation in $\mathbf{H}^1_{0;\mathrm{div}}(\Omega)$ :

$$\boldsymbol{U}(\boldsymbol{x},\theta) \approx \boldsymbol{U}^m(\boldsymbol{x},\theta) = \sum_{k=1}^{m} \boldsymbol{u}_k(\boldsymbol{x})\lambda_k(\theta),$$

- The deterministic functions $\boldsymbol{u}_k \in \mathbf{H}^1_{0;\mathrm{div}}(\Omega)$ form a reduced basis of $\mathbf{H}^1_{0;\mathrm{div}}(\Omega)$
- The stochastic coefficients $\lambda_k \in \mathrm{S}$ form a reduced basis of $\mathrm{S}$
- None of the two reduced bases are selected *a priori*
- Sequential construction of the approximation $\boldsymbol{U}^0 \to \boldsymbol{U}^1 \to \boldsymbol{U}^2 \to \cdots$ with Arnoldi algorithm
- $\boldsymbol{U}^{m+1} = \boldsymbol{U}^m + \lambda \boldsymbol{u}$ : successive couples $(\lambda, \boldsymbol{u})$ are defined as previously

The couple $(\lambda_{m+1}, \boldsymbol{u}_{m+1})$ is sought as the fixed point of

$$\lambda = \mathcal{S} \circ \mathcal{D}(\lambda; \boldsymbol{U}^m), \quad \boldsymbol{u} = \mathcal{D} \circ \mathcal{S}(\boldsymbol{u}; \boldsymbol{U}^m),$$

where

Determinisic problem : $\boldsymbol{u} = \mathcal{D}(\lambda; \boldsymbol{U}^m) \in \mathbf{H}^1_{0;\mathrm{div}}(\Omega)$ is the solution of

$$\begin{aligned} &C(\lambda\boldsymbol{u}, \lambda\boldsymbol{u}, \lambda\boldsymbol{v}) + C(\lambda\boldsymbol{u}, \boldsymbol{U}^m, \lambda\boldsymbol{v}) + C(\boldsymbol{U}^m, \lambda\boldsymbol{u}, \lambda\boldsymbol{v}) + A(\lambda\boldsymbol{u}, \lambda\boldsymbol{v}) \\ &= \mathbb{E}\left[(\boldsymbol{F}, \lambda\boldsymbol{v})_\Omega\right] - C(\boldsymbol{U}^m, \boldsymbol{U}^m, \lambda\boldsymbol{v}) - A(\boldsymbol{U}^m, \lambda\boldsymbol{v}), \quad \forall \boldsymbol{v} \in \mathbf{H}^1_{0;\mathrm{div}}(\Omega). \end{aligned}$$

Stochastic problem : $\lambda = \mathcal{S}(\boldsymbol{u}; \boldsymbol{U}^m) \in \mathrm{S}$ is the solution of

$$\begin{aligned} &C(\lambda\boldsymbol{u}, \lambda\boldsymbol{u}, \beta\boldsymbol{u}) + C(\lambda\boldsymbol{u}, \boldsymbol{U}^m, \beta\boldsymbol{u}) + C(\boldsymbol{U}^m, \lambda\boldsymbol{u}, \beta\boldsymbol{u}) + A(\lambda\boldsymbol{u}, \beta\boldsymbol{u}) \\ &= \mathbb{E}\left[(\boldsymbol{F}, \beta\boldsymbol{u})_\Omega\right] - C(\boldsymbol{U}^m, \boldsymbol{U}^m, \beta\boldsymbol{u}) - A(\boldsymbol{U}^m, \beta\boldsymbol{u}), \quad \forall \beta \in \mathrm{S}. \end{aligned}$$

The couple $(\lambda_{m+1}, \boldsymbol{u}_{m+1})$ is sought as the fixed point of

$$\lambda = \mathcal{S} \circ \mathcal{D}(\lambda; \boldsymbol{U}^m), \quad \boldsymbol{u} = \mathcal{D} \circ \mathcal{S}(\boldsymbol{u}; \boldsymbol{U}^m),$$

where

Determinisic problem : $\boldsymbol{u} = \mathcal{D}(\lambda; \boldsymbol{U}^m) \in \mathbf{H}^1_{0;\mathrm{div}}(\Omega)$ is the solution of

$$\mathbb{E}\left[\lambda^3\right] c(\boldsymbol{u}, \boldsymbol{u}, \boldsymbol{v}) + \mathbb{E}\left[\lambda^2 \nu\right] a(\boldsymbol{u}, \boldsymbol{v}) + c(\boldsymbol{u}, \tilde{\boldsymbol{u}}, \boldsymbol{v}) + c(\tilde{\boldsymbol{u}}, \boldsymbol{u}, \boldsymbol{v}) = (\tilde{\boldsymbol{f}}, \boldsymbol{v})_\Omega, \quad \forall \boldsymbol{v} \in \mathbf{H}^1_{0;\mathrm{div}}(\Omega),$$

with $\tilde{\boldsymbol{u}} = \mathbb{E}\left[\lambda^2 \boldsymbol{U}^m\right]$

Stochastic problem : $\lambda = \mathcal{S}(\boldsymbol{u}; \boldsymbol{U}^m) \in \mathrm{S}$ is the solution of

$$\lambda = \mathcal{S}(\boldsymbol{u}; \boldsymbol{U}^m) \Leftrightarrow \mathbb{E}\left[(\tilde{c}\lambda^2 + G\lambda + R)\beta\right] = 0, \quad \forall \beta \in \mathrm{S},$$

with $\tilde{c} \in \mathbb{R}$ and $G$, $R \in \mathrm{S}$.

Update problem : fix one of the two reduced bases and solve the Galerkin problem for the other component.

Updating of the stochastic coefficients :

Find $\{\lambda_k \in \mathrm{S}\}_{k=1}^{m}$ such that

$$C\left(\sum_i \lambda_i \boldsymbol{u}_i, \sum_j \lambda_j \boldsymbol{u}_j, \beta \boldsymbol{u}_k\right) + A\left(\sum_i \lambda_i \boldsymbol{u}_i, \beta \boldsymbol{u}_k\right) = \mathbb{E}\left[(\boldsymbol{F}, \beta \boldsymbol{u}_k)\right],$$

$\forall \beta \in \mathrm{S}$ and $k = 1, \ldots, m$.

System of $m$ quadratic stochastic equations :

$$\mathbb{E}\left[\left(\sum_{i,j=1}^{m} \tilde{q}_{k,i,j}\, \lambda_i \lambda_j + \sum_{i=1}^{m} G_{k,i} \lambda_i - R_k\right) \beta_k\right] = 0, \quad \forall \beta_k \in \mathrm{S}.$$

## Stochastic discretization :

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

$$\boldsymbol{\xi} = \{\xi_1, \ldots, \xi_{\mathrm{N}}\}$$

- Stochastic basis : Polynomial Chaos

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

where the $\Psi$s are orthonormal polynomials

$$\mathbb{E}\left[\Psi_\alpha(\boldsymbol{\xi})\Psi_\beta(\boldsymbol{\xi})\right] = \delta_{\alpha,\beta}.$$

- Truncature to (total) polynomial degree $\mathrm{No}$ :

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

## Spatial discretization

- $\mathbb{P}_n$-$\mathbb{P}_{n-2}$ Spectral Element Method

$$\mathbf{H}^1(\Omega) \ni u(\boldsymbol{x}) \approx \boldsymbol{u}^h(\boldsymbol{x}) = \sum_{i,j=1}^{n} \boldsymbol{u}_{i,j}\phi^u_{i,j}(\boldsymbol{x}) \in \mathrm{V}^h,$$

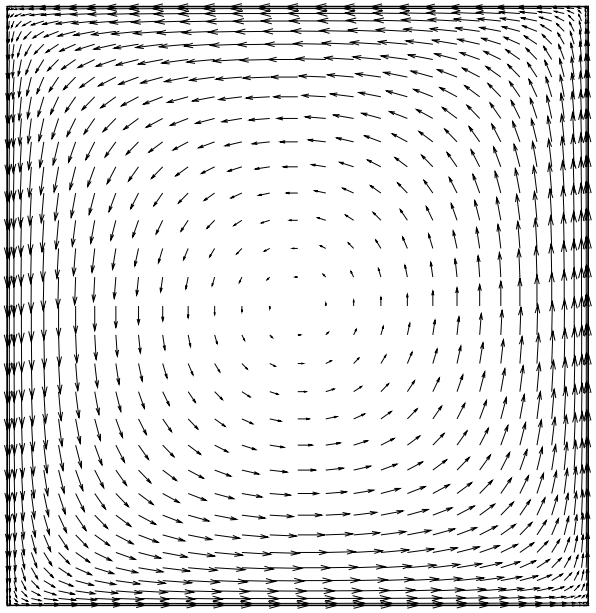
$$\mathrm{L}^2(\Omega) \ni p(\boldsymbol{x}) \approx p^h(\boldsymbol{x}) = \sum_{i,j=1}^{n-2} p_{i,j}\phi^p_{i,j}(\boldsymbol{x}) \in \Pi^h.$$

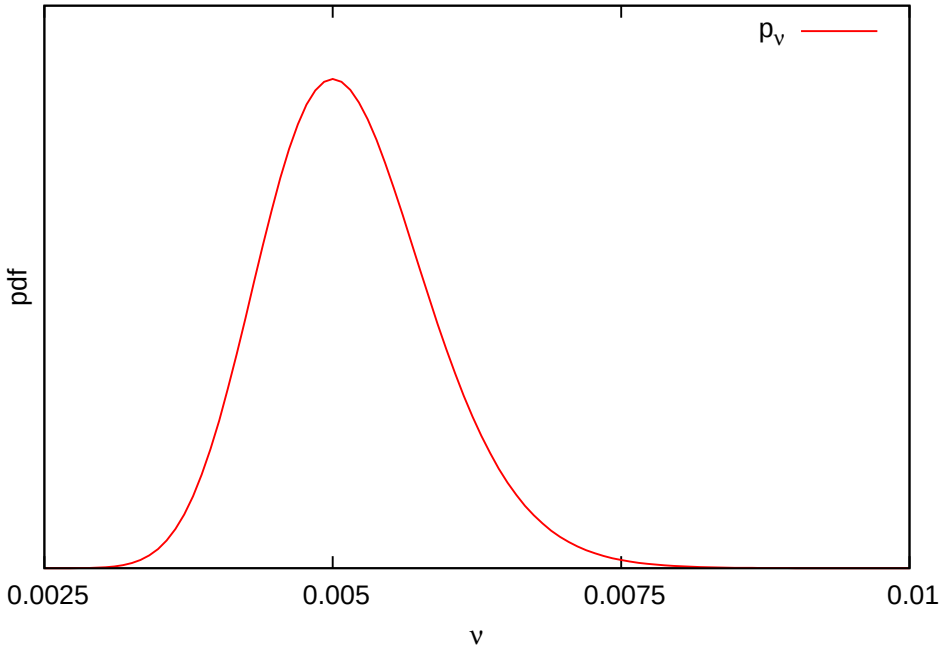
(Nodal basis on tenzorized Gauss-Lobatto grid)

- Resolution of the deterministic problem
$\boldsymbol{u} = \mathcal{D}(\lambda; U^{(i)}) \in \mathbf{H}^1_{0;\mathrm{div}}(\Omega)$ achieved by solving in $\mathrm{V}^h_0$ the constrained problem

$$\begin{aligned}
&\mathbb{E}\left[\lambda^3\right] c(\boldsymbol{u}^h, \boldsymbol{u}^h, \boldsymbol{v}^h) + \mathbb{E}\left[\lambda^2\nu\right] a(\boldsymbol{u}^h, \boldsymbol{v}^h) + c(\boldsymbol{u}^h, \tilde{\boldsymbol{u}}^h, \boldsymbol{v}^h) \\
&\quad + c(\tilde{\boldsymbol{u}}^h, \boldsymbol{u}^h, \boldsymbol{v}^h) + d(\boldsymbol{v}^h, p^h) = (\tilde{\boldsymbol{f}}, \boldsymbol{v}^h)_\Omega && \forall \boldsymbol{v}^h \in \mathrm{V}^h_0, \\
&d(\boldsymbol{u}^h, q^h) = 0 && \forall q \in \Pi^h.
\end{aligned}$$

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

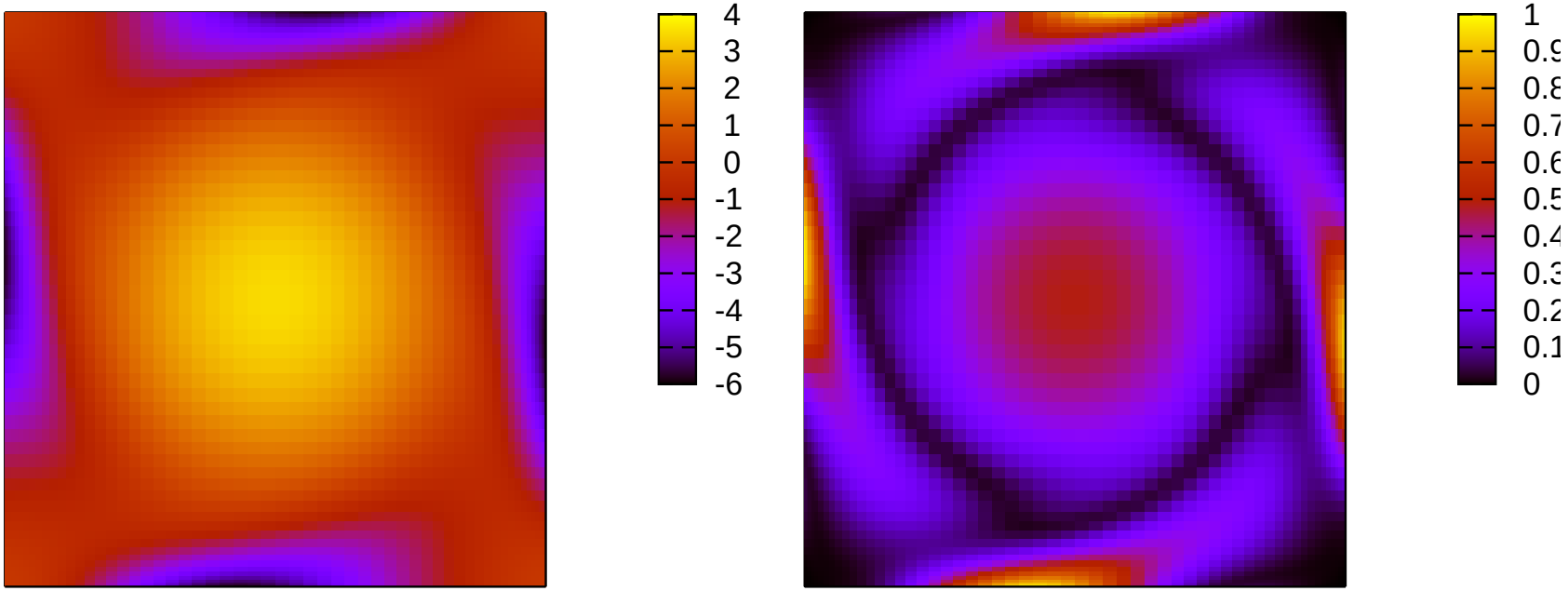





$$\nu(\theta) = \frac{1}{200} \exp\left( \frac{\sigma_\nu}{\sqrt{\mathrm{N}}} \sum_{i=1}^{\mathrm{N}} \xi_i(\theta) \right) \quad (+10^{-4}), \quad \xi_i \sim N(0,1)\ i.i.d.$$

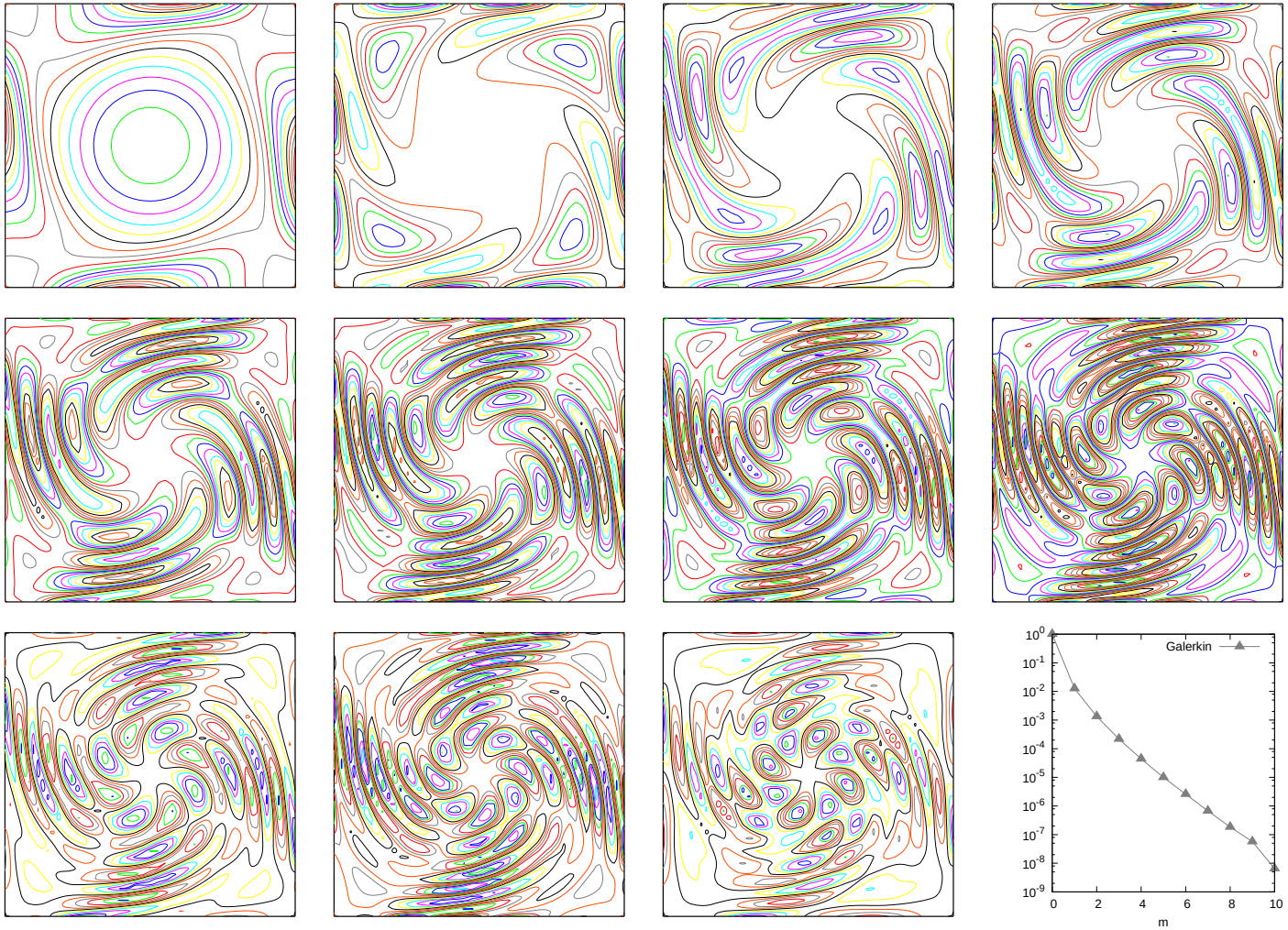
Same problem but for parametrization involving $\mathrm{N}$ Gaussian R.V.

Galerkin solution for $\mathrm{N} = 1$ and $\mathrm{No} = 10$ (Wiener-Hermite expansion)



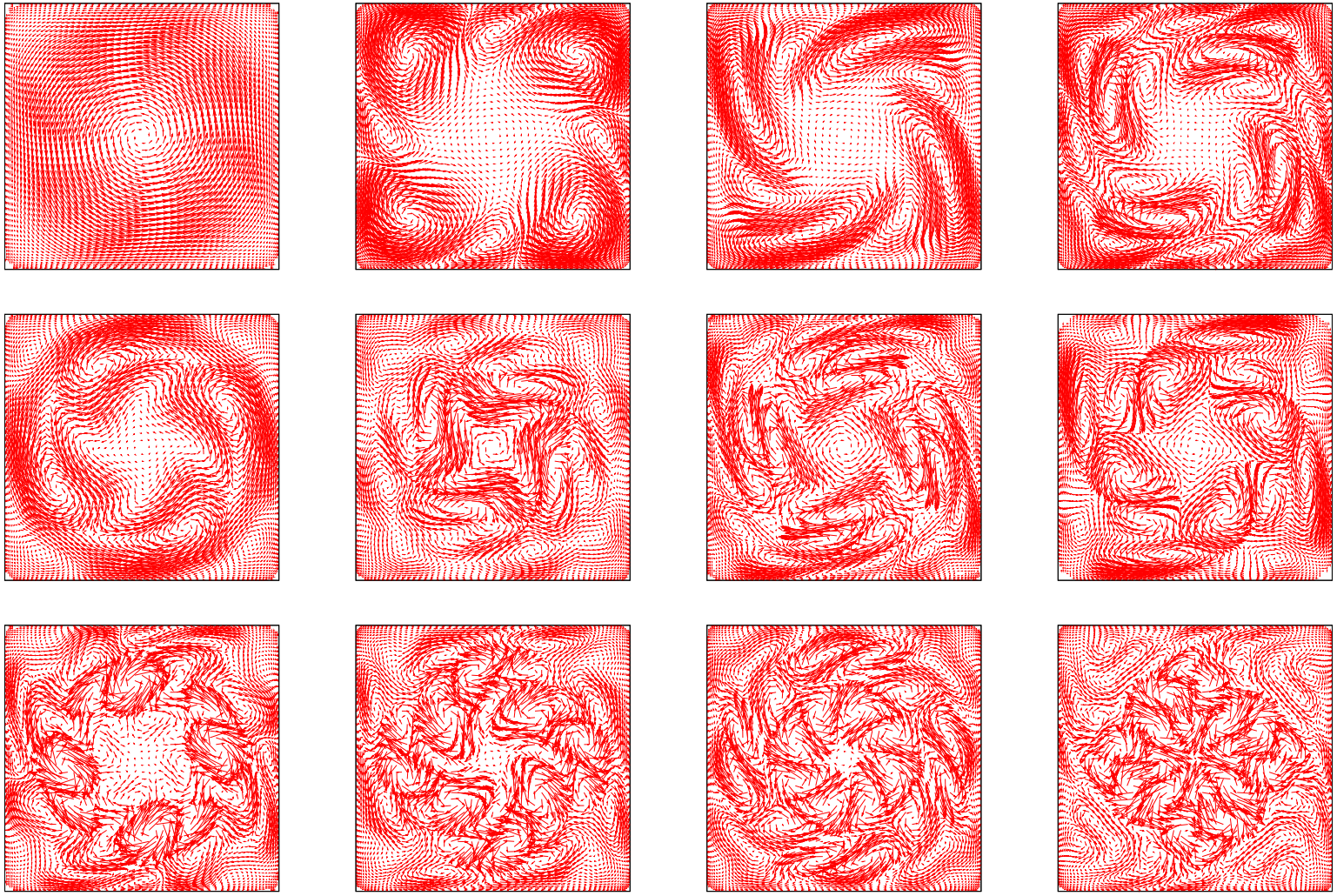

Mean and standard deviation of $U^G$ rotational.

# POD modes of the Galerkin solution for $\mathrm{N} = 1$ and $\mathrm{No} = 10$

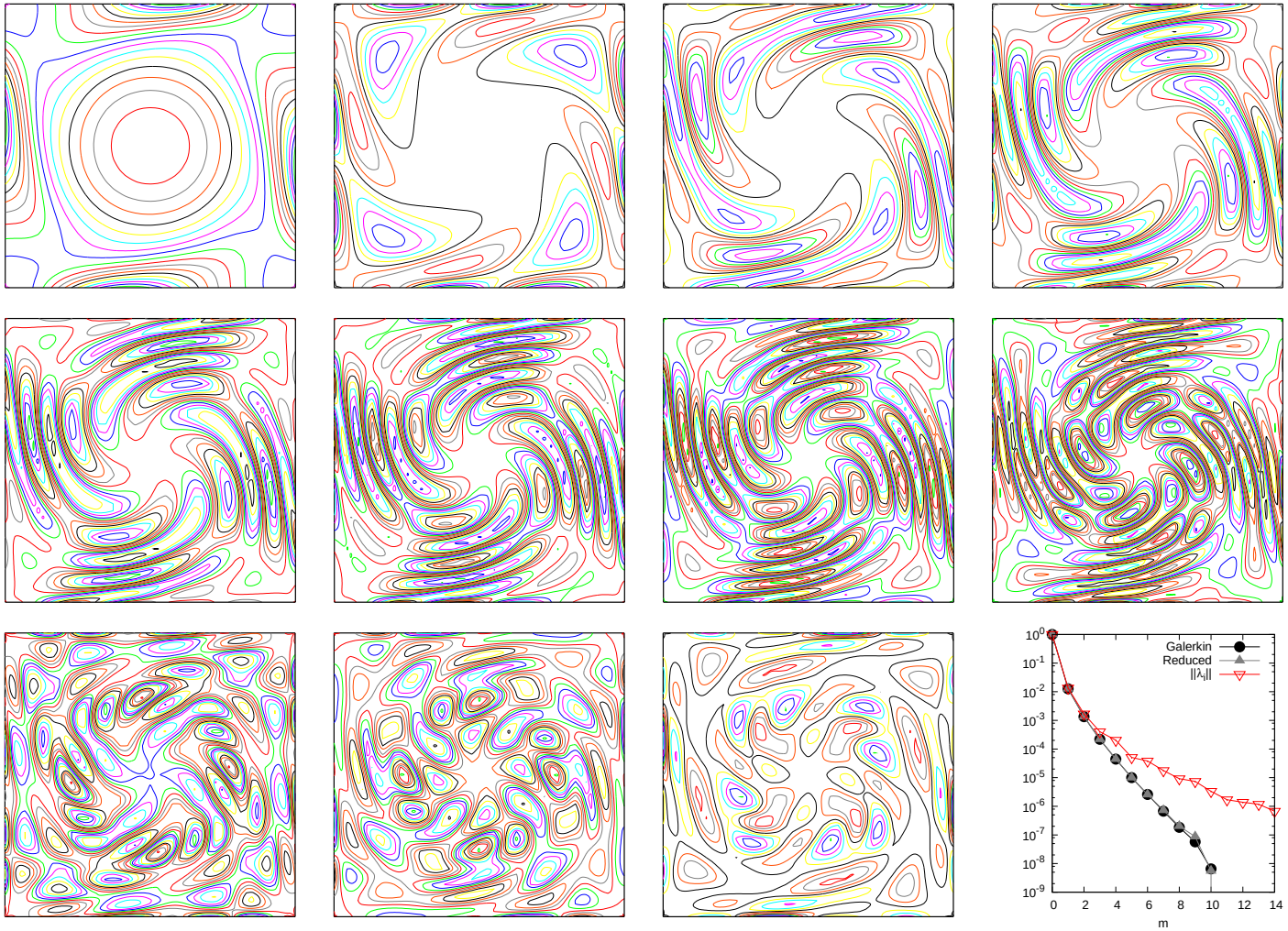



Rotational of the spatial POD modes of $U^G$.

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

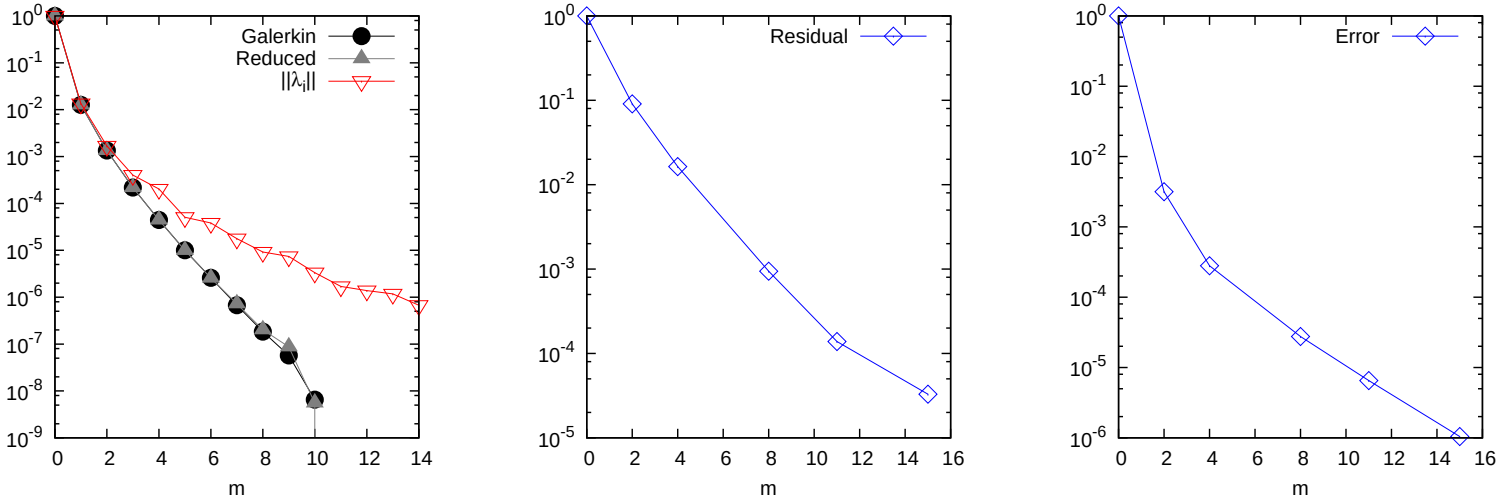


## POD modes of the PGD solution for $m = 15$, $\mathrm{N} = 1$ and $\mathrm{No} = 10$



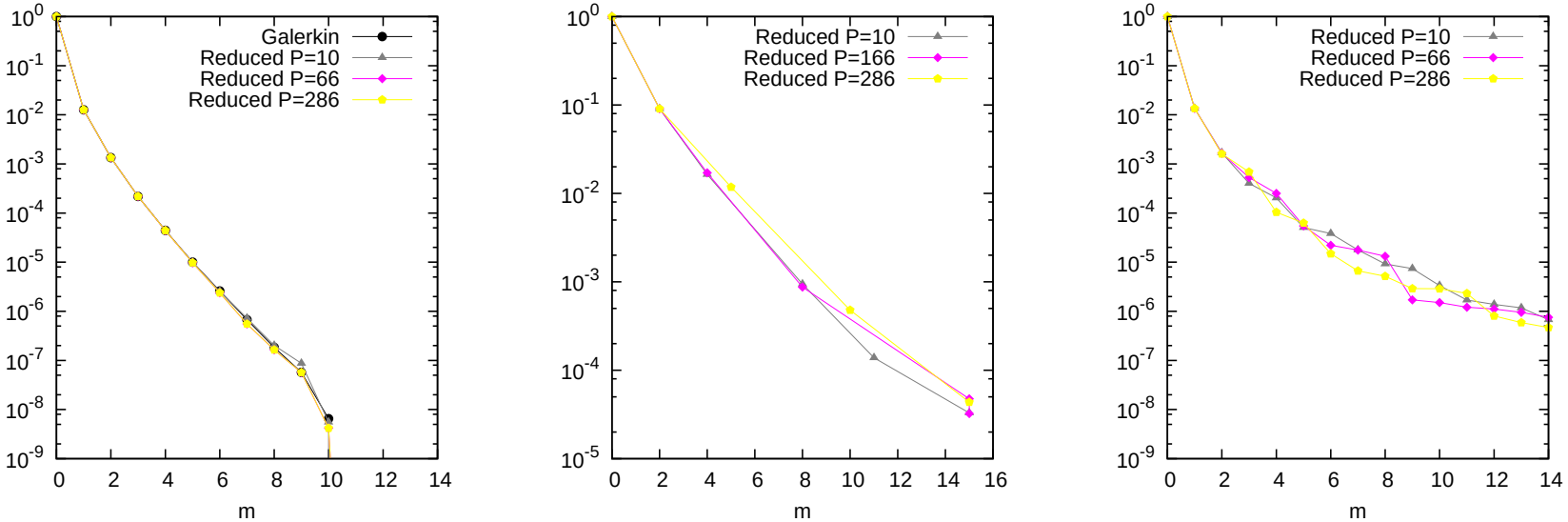

Rotational of the spatial POD modes of $U^{m=15}$.

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




Comparison of the norms of the POD coefficients at $m = 15$ (left), residual norm (center), error norm (right).

## Convergence of PGD solutions $\mathrm{N} = 1$, 2 and 3 at $\mathrm{No} = 10$




Comparison of the norms of the POD coefficients at $m = 15$ (left), residual norm (center), error norm (right).

PGD captures the essential features of the stochastic solution

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

$$\boldsymbol{F}(\boldsymbol{x},\theta) = \boldsymbol{\nabla}\Phi(\boldsymbol{x},\theta) + \boldsymbol{\nabla}\wedge\boldsymbol{\Psi}(\boldsymbol{x},\theta) = \boldsymbol{\nabla}\wedge\Psi(\boldsymbol{x},\theta)\boldsymbol{k}$$

Define $F_\omega \doteq (\boldsymbol{\nabla}\wedge\boldsymbol{F})\cdot\boldsymbol{k} = -\triangle\Psi$ and assume :

$$F_\omega(\boldsymbol{x},\theta) = f_\omega^0 + F'_\omega(\boldsymbol{x},\theta), \quad \mathbb{E}\left[F'_\omega(\boldsymbol{x},\cdot)\right] = 0, \quad F'_\omega(\boldsymbol{x},\cdot) \sim N(0,\sigma^2),$$
$$\mathbb{E}\left[F'_\omega(\boldsymbol{x},\cdot)F'_\omega(\boldsymbol{x}',\cdot)\right] = \sigma^2\exp(-|\boldsymbol{x}-\boldsymbol{x}'|/L).$$

KL expansion of $F_\omega$ :

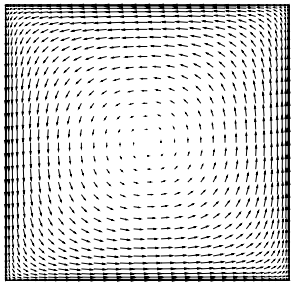
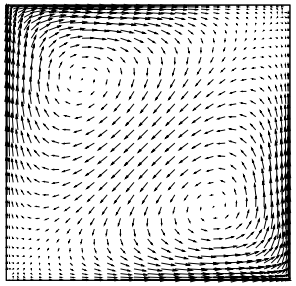
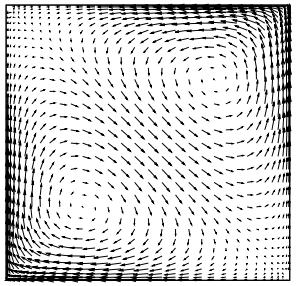
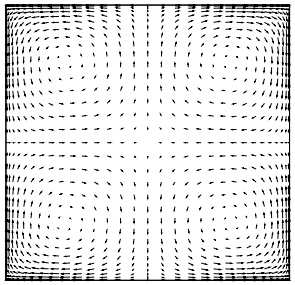
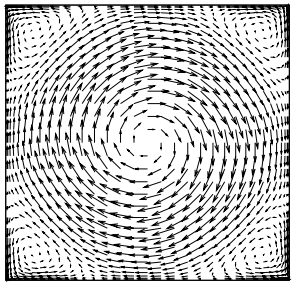
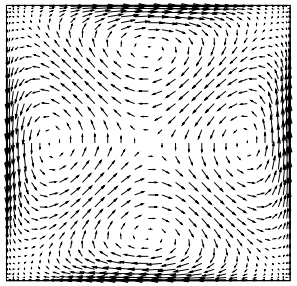
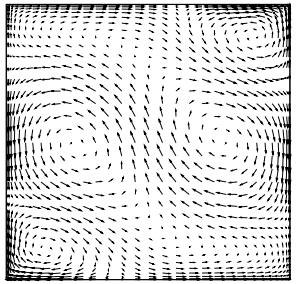
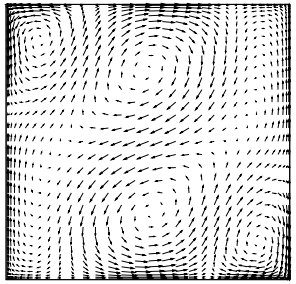
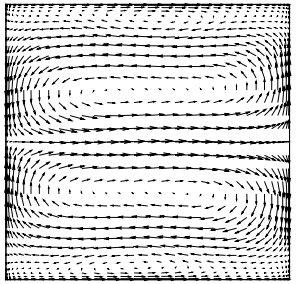
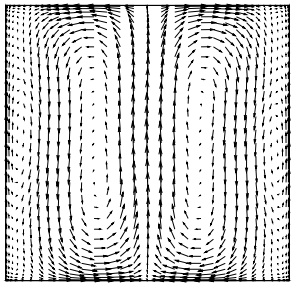
$$F_\omega(\boldsymbol{x},\theta) \approx F_\omega^{\mathrm{N}}(\boldsymbol{x},\boldsymbol{\xi}(\theta)) = f_\omega^0 + \sum_{k=0}^{\mathrm{N}}\sqrt{\gamma_k}f_\omega^k(\boldsymbol{x})\xi_k(\theta)$$

It comes

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

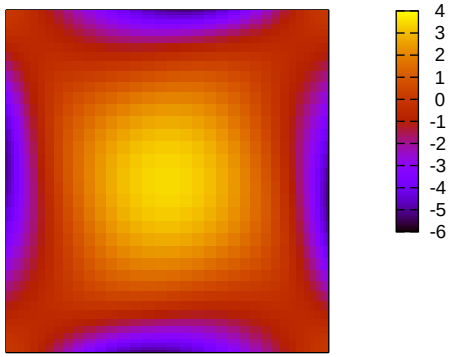
with $\boldsymbol{f}^i = \boldsymbol{\nabla}\wedge\left(\triangle^{-1}f_\omega^i\right)\boldsymbol{k}$.

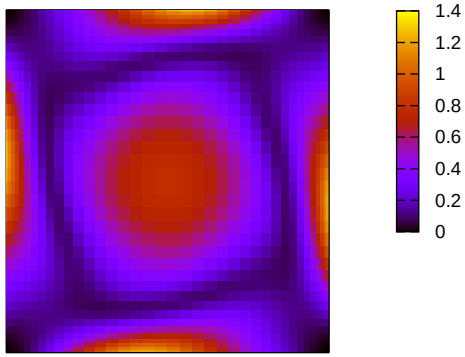
## KL modes of the forcing :

| $scale = 1$ | $scale = 5$ | $scale = 5$ | $scale = 5$ | $scale = 15$ |
|---|---|---|---|---|
|  |  |  |  |  |
| $scale = 15$ | $scale = 15$ | $scale = 15$ | $scale = 25$ | $scale = 25$ |
|  |  |  |  |  |

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

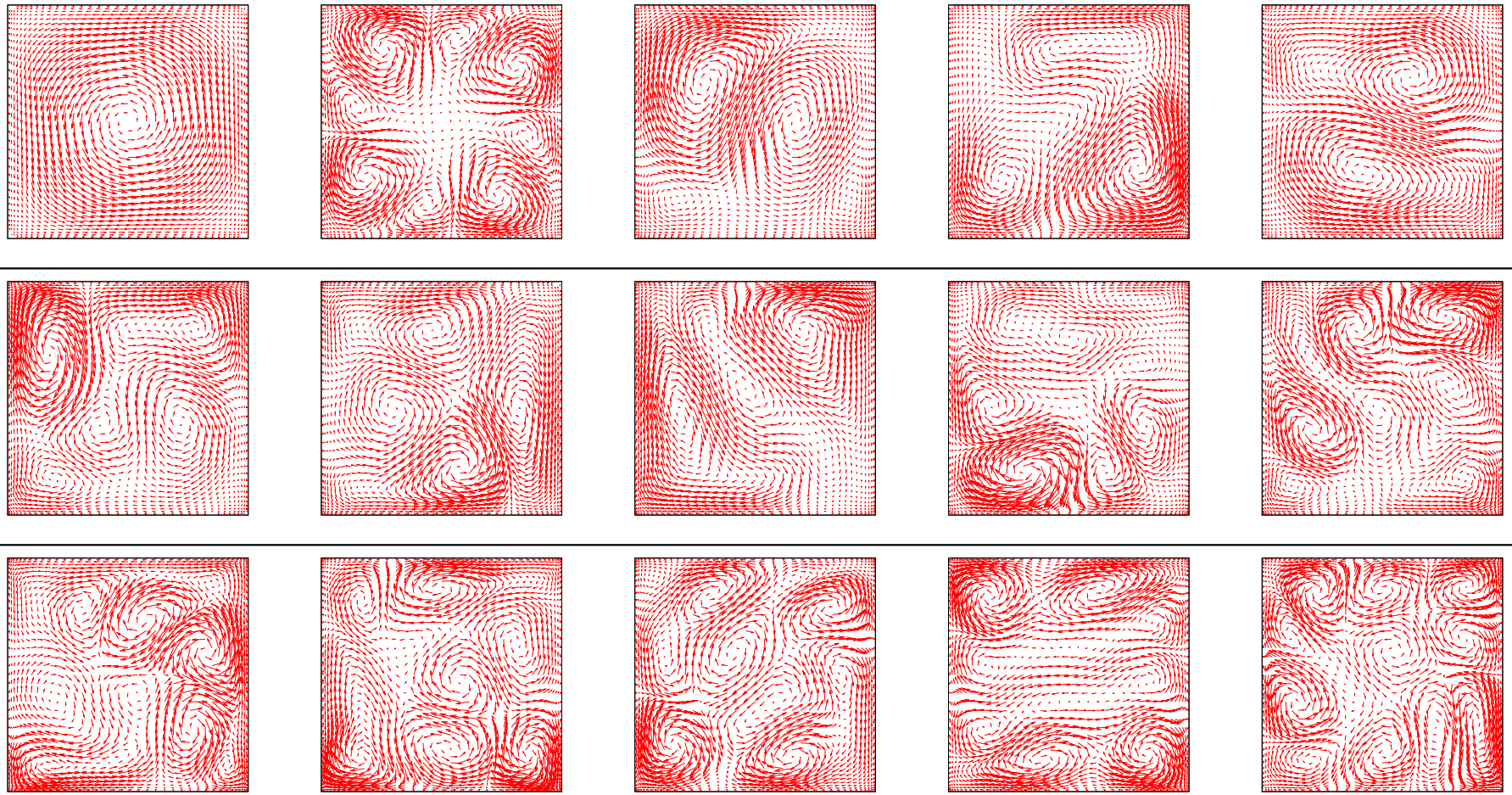
PGD solution for $\overline{\nu} = 1/50$, $\mathrm{N} = 11$, $\mathrm{No} = 3$ and $m = 45$



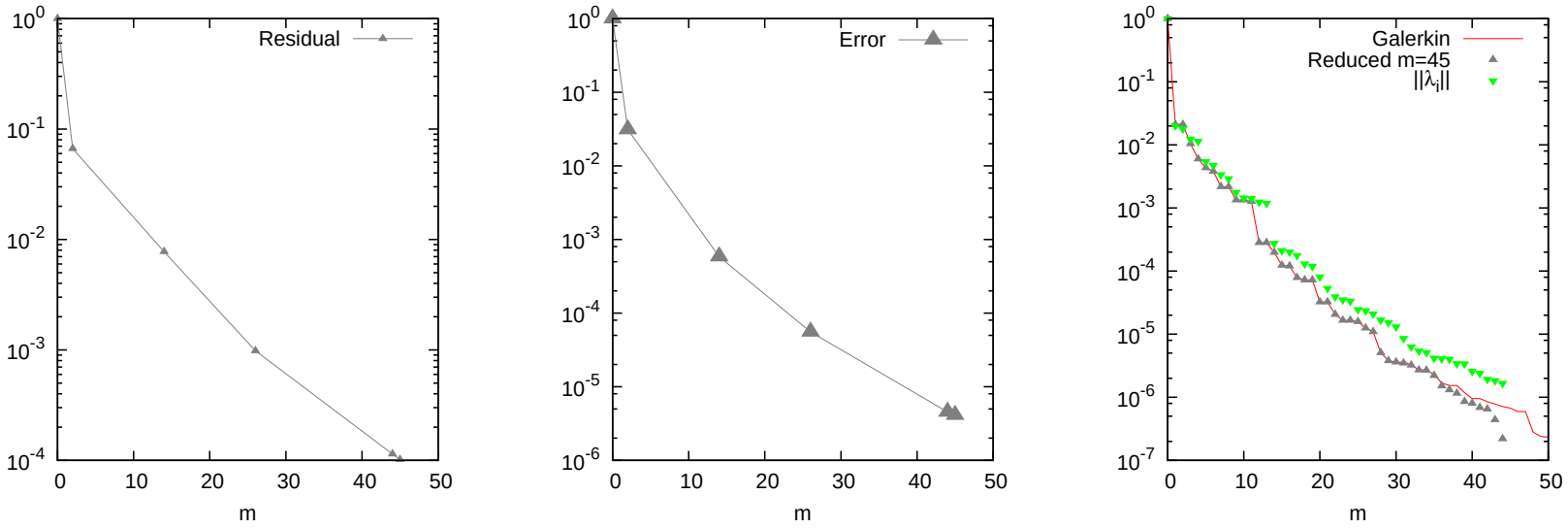




Mean and standard deviation of $\boldsymbol{\nabla} \wedge \boldsymbol{U}^{m=45}$

# First PGD-Arnoldi modes



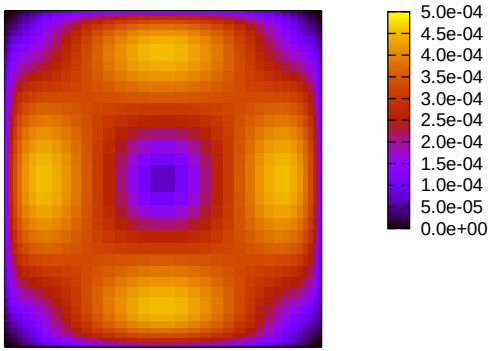
## Results at $\overline{\nu} = 1/50$ : $\mathrm{No} = 3$, $\mathrm{N} = 11$, $\mathrm{P} = 364$

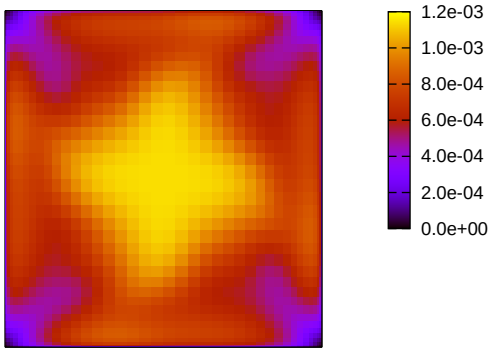


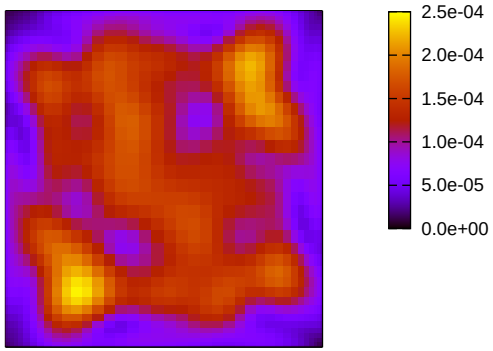

Residual (left), $\|U^m - U^G\|$ (center) and norm of POD modes for $m = 45$ (right).

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

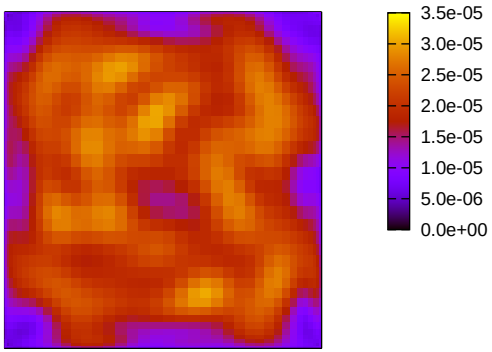
| $m = 0$ | $m = 2$ | $m = 14$ |
|---|---|---|

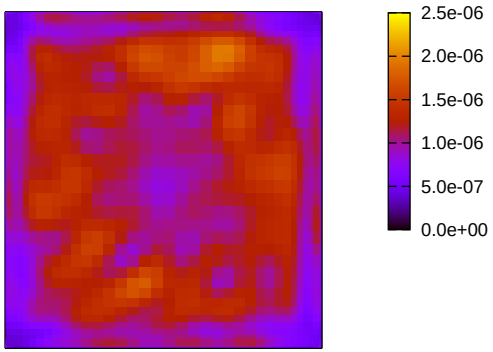


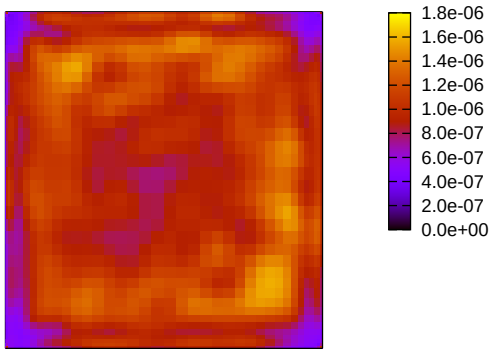




| $m = 26$ | $m = 43$ | $m = 45$ |
|---|---|---|



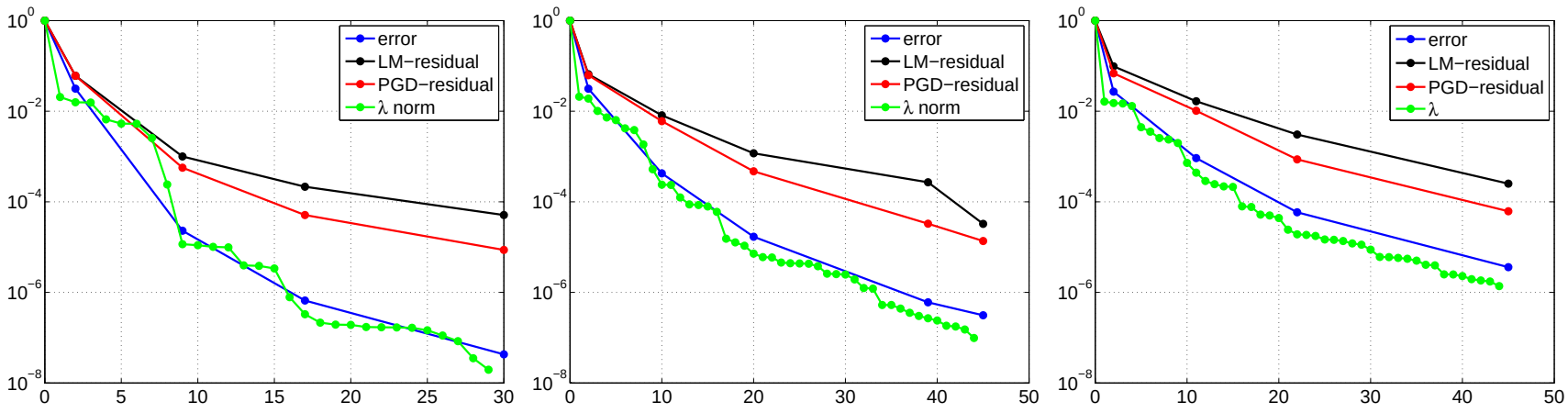




Spatial distribution of the stochastic residual.

## Residual computation :

- Residual computation in $\mathbf{H}^1_{0;\mathrm{div}}(\Omega)$ is difficult
- Projection of the $\mathbf{H}^1_0(\Omega)$-residual into $\mathbf{H}^1_{0;\mathrm{div}}(\Omega)$ amount to solving a stochastic linear equation for $P^m$
- PGD can be used for the approximation of $P^m$
- Re-use of the reduced basis of Arnoldi Lagrange multipliers $\{p_i\}$ associated to $\{\boldsymbol{u}_i\}$ was found a effective approach
- However, monitoring convergence using the decay of $\|\lambda_i\|$ appears effective

## Residual computation :




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

## On-going work :

- Evolution problems : PGD on each time step or global PGD with possibly alternative separated forms

$$u(\boldsymbol{x}, t, \theta) \approx \sum_{\alpha} u_{\alpha}(\boldsymbol{x}, t)\lambda_{\alpha}(\theta) \approx \sum_{\alpha} \widetilde{u}_{\alpha}(\boldsymbol{x})\beta_{\alpha}(t, \theta)$$
$$\approx \sum_{\alpha} \hat{u}_{\alpha}(\boldsymbol{x})\tau_{\alpha}(t)\gamma_{\alpha}(\theta)$$

- Nested separation ?
- Other definition of optimality for non definite linear operators (least square residual minimization).

Thanks for your attention

Fundings :

- ANR-TYCHE project [2010-2013]
- ANR-ASRMEI project [2008-2011]
- MoMaS (Andra, Brgm, Cea, EdF, Irsn) [2010-2011]