Examples of Applications

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PhD course on UQ - DTU

Objectives of the lecture

- Show concrete and detailed application on a basic example
- Present examples of applications involving more complex models
- Highlight efficiency and limitations.

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Heat equation

Consider the linear steady heat equation in an isotropic two-dimensional domain Ω, with boundary $\partial\Omega$.

$\boldsymbol{x} \in \Omega \mapsto u(x) \in \mathbb{R}$ is the temperature field satisfying:

$$\boldsymbol{\nabla} \cdot (\nu(\boldsymbol{x}) \boldsymbol{\nabla} u(\boldsymbol{x})) = -f(\boldsymbol{x}) \quad + BC$$

where $\nu > 0$ is the thermal conductivity and $f \in L_2(\Omega)$ is a source term.
We consider homogeneous Dirichlet and Neumann conditions over the respective portions Γ_d and Γ_n of the domain boundary $\partial\Omega = \Gamma_d \cup \Gamma_n$, i.e.

$$u(\boldsymbol{x}) = 0, \qquad \boldsymbol{x} \in \Gamma_d \quad \frac{\partial u}{\partial n} = 0, \qquad \boldsymbol{x} \in \Gamma_n.$$

Weak formulation

Let $\mathcal{V}$ be the functionals space on Ω such that:

$$\mathcal{V} = \{u \in H^1(\Omega) : u = 0 \text{ on } \Gamma_d\},$$

where $H^1(\Omega)$ is the Sobolev space of square integrable functionals whose first order derivatives are also square integrable.
The variational problem is:
Find $u \in \mathcal{V}$ such that

$$a(u, v) = b(v) \qquad \forall v \in \mathcal{V},$$

where $a(u, v)$ and $b(v)$ are bilinear and linear forms respectively defined as:

$$a(u, v) \equiv \int_\Omega \nu(\boldsymbol{x}) \boldsymbol{\nabla} u(\boldsymbol{x}) \cdot \boldsymbol{\nabla} v(\boldsymbol{x}) \mathrm{d}\boldsymbol{x}, \quad b(v) \equiv \int_\Omega f(\boldsymbol{x}) v(\boldsymbol{x}) \mathrm{d}\boldsymbol{x}.$$

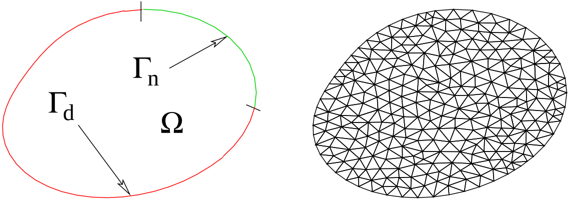
$P-1$ Finite Element discretization

Let $\mathcal{T} = \{\Sigma_1, \ldots, \Sigma_{ne}\}$ be a triangulation of Ω with *ne* non-overlapping triangular elements Σ_i.
The $P-1$ finite element space $\mathcal{V}^h$ consists in linear functions in each Σ_l, that are continuous across inter-element boundaries. A function $v \in \mathcal{V}^h$ is completely defined by its values at the mesh nodes, and v can be expressed as

$$v^h(\boldsymbol{x}) = \sum_{i \in \mathcal{N}} v_i^h \Phi_i(\boldsymbol{x}),$$

where $\mathcal{N}$ is the set of nodes which are not lying on Γ_d and $\Phi_i(\boldsymbol{x})$ are the shape functions associated to these nodes.

$$\mathcal{V}^h = span\,\{\Phi_i\}_{i \in \mathcal{N}}\,.$$



Left: sketch of the domain Ω and decomposition of the boundary $\partial\Omega$ into Dirichlet Γ_d and Neumann Γ_n regions. Right: example of a finite-element mesh with 508 elements and 284 nodes.

Discrete equations

The Galerkin formulation in $\mathcal{V}^h$ is:

Find u_i, $i \in \mathcal{N}$ such that

$$\sum_{i\in\mathcal{N}} \sum_{j\in\mathcal{N}} a_{i,j} u_i v_j = \sum_{j\in\mathcal{N}} b_j v_j,$$

where

$$a_{i,j} = \int_\Omega \nu(\boldsymbol{x}) \boldsymbol{\nabla}\Phi_i(\boldsymbol{x}) \cdot \boldsymbol{\nabla}\Phi_j(\boldsymbol{x}) \mathrm{d}\boldsymbol{x}, \quad b_i = \int_\Omega f(\boldsymbol{x})\Phi_i(\boldsymbol{x})\mathrm{d}\boldsymbol{x}.$$

The problem can be recast as a system of linear equations

$$\begin{pmatrix} a_{1,1} & \dots & a_{1,n} \\ \vdots & \ddots & \vdots \\ a_{n,1} & \dots & a_{n,n} \end{pmatrix} \begin{pmatrix} u_1 \\ \vdots \\ u_n \end{pmatrix} = \begin{pmatrix} b_1 \\ \vdots \\ b_n \end{pmatrix},$$

where $n = \mathrm{Card}(\mathcal{N})$. $[a]$ is a (sparse) symmetric positive definite matrix.

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Stochastic problem

Consider the case of random conductivity and source term, defined on an abstract probability space (Θ, Σ, P):

$$\nu \to \nu(\boldsymbol{x}, \theta), \qquad f \to F(\boldsymbol{x}, \theta).$$

Then, $u \to U(\boldsymbol{x}, \theta)$ satisfies almost surely the stochastic problem

$$\begin{cases} \nabla \cdot (\nu(\boldsymbol{x}, \theta) \nabla U(\boldsymbol{x}, \theta)) = -F(\boldsymbol{x}, \theta) & \boldsymbol{x} \in \Omega \\ U(\boldsymbol{x}, \theta) = 0 & \boldsymbol{x} \in \Gamma_d, \\ \dfrac{\partial U(\boldsymbol{x}, \theta)}{\partial n} = 0 & \boldsymbol{x} \in \Gamma_n. \end{cases}$$

Weak form of the stochastic problem

The functional space for $U(\boldsymbol{x}, \theta)$ will be $\mathcal{V} \otimes L_2(\Theta, P)$. In other words,

$$U(\cdot, \theta) \in \mathcal{V}, \quad U(\boldsymbol{x}, \cdot) \in L_2(\Theta, P),$$

The variational form of the stochastic problem is:
Find $U \in \mathcal{V} \otimes L_2(\Theta, P)$ such that

$$A(U, V) = B(V) \qquad \forall V \in \mathcal{V} \otimes L_2(\Theta, P),$$

where

$$A(U, V) \equiv \mathbb{E}\left[a(U, V)\right] = \int_\Theta \left[\int_\Omega \nu(\boldsymbol{x}, \theta) \boldsymbol{\nabla} U(\boldsymbol{x}, \theta) \cdot \boldsymbol{\nabla} V(\boldsymbol{x}, \theta) \mathrm{d}\boldsymbol{x}\right] \mathrm{d}P(\theta),$$

and

$$B(V) \equiv \mathbb{E}\left[b(V)\right] = \int_\Theta \left[\int_\Omega F(\boldsymbol{x}, \theta) V(\boldsymbol{x}, \theta) \mathrm{d}\boldsymbol{x}\right] \mathrm{d}P(\theta).$$

Semi-discrete form

introducing the deterministic discretization in $\mathcal{V}^h$ it comes

$$U^h(\boldsymbol{x},\theta) = \sum_{i \in \mathcal{N}} U_i(\theta)\Phi_i(\boldsymbol{x}) \in \left(\mathcal{V}^h \otimes L_2(\Theta, P)\right).$$

It shows that the semi-discrete solution consists in $n = \mathrm{Card}(\mathcal{N})$ random variables $U_i(\theta)$. They satisfy

$$\sum_{i \in \mathcal{N}} \sum_{j \in \mathcal{N}} \mathbb{E}\left[A_{i,j}(\theta) U_i(\theta) V_j(\theta)\right] = \sum_{i \in \mathcal{N}} \mathbb{E}\left[B_i(\theta) V_i(\theta)\right], \; \forall V_i(\theta) \in L_2(\Theta, P), \; i \in \mathcal{N},$$

where

$$A_{i,j}(\theta) = \int_\Omega \nu(\boldsymbol{x},\theta) \boldsymbol{\nabla}\Phi_i(\boldsymbol{x}) \cdot \boldsymbol{\nabla}\Phi_j(\boldsymbol{x}) \mathrm{d}\boldsymbol{x},$$

and

$$B_i(\theta) = \int_\Omega f(\boldsymbol{x},\theta)\Phi_i(\boldsymbol{x}) \mathrm{d}\boldsymbol{x}.$$

Stochastic discretization

We assume ν and F parameterized with N independent r.v. $\boldsymbol{\xi} = \{\xi_1 \cdots \xi_\mathrm{N}\}$ defined on (Θ, Σ, P):

$$\nu(\boldsymbol{x}, \theta) = \nu(\boldsymbol{x}, \boldsymbol{\xi}(\theta)), \qquad F(\boldsymbol{x}, \theta) = F(\boldsymbol{x}, \boldsymbol{\xi}(\theta)).$$

Examples of parameterization will be shown later. The space of second-order random functionals in $\boldsymbol{\xi}$ is spanned by the Polynomial Chaos basis:

$$\mathcal{S} = span\{\Psi_k(\boldsymbol{\xi})\}_{k=0}^{k=\infty} = L_2(\mathbb{R}^2, p_\xi),$$

where the Ψ_i's form a set of orthogonal multidimensional polynomials in $\boldsymbol{\xi}$:

$$\left\langle \Psi_i, \Psi_j \right\rangle = \int_\Xi \Psi_i(\boldsymbol{\eta})\Psi_j(\boldsymbol{\eta}) p_\xi(\boldsymbol{\eta}) \mathrm{d}\boldsymbol{\eta} = \delta_{ij} \left\langle \Psi_i^2 \right\rangle.$$

Provided that ν and F are second-order quantities, they have orthogonal representations:

$$\nu(\boldsymbol{x}, \boldsymbol{\xi}) = \sum_{k=0}^{\infty} \nu_k(\boldsymbol{x})\Psi_k(\boldsymbol{\xi}), \qquad F(\boldsymbol{x}, \boldsymbol{\xi}) = \sum_{k=0}^{\infty} f_k(\boldsymbol{x})\Psi_k(\boldsymbol{\xi}).$$

Stochastic discretization

Similarly, the expansion of the discrete solution U^h is

$$U^h(\boldsymbol{x},\xi) = \sum_{i\in\mathcal{N}} \left(\sum_{k=0}^{\infty} u_{i,k}\Psi_k(\xi) \right) \Phi_i(\boldsymbol{x}).$$

The stochastic expansions are truncated to a finite polynomial order No.
Different orders of truncation may be considered for the conductivity, source and solution.
For simplicity, we use the same truncation order No. It corresponds to a stochastic approximation space

$$\mathcal{S}^{\mathrm{P}} \equiv span\{\Psi_0,\dots,\Psi_{\mathrm{P}}\} \subset \mathcal{S}, \quad \mathrm{P}+1 = \frac{(\mathrm{No}+\mathrm{N})!}{\mathrm{No}!\mathrm{N}!}.$$

Stochastic Galerkin problem

The Galerkin problem is obtained by inserting the expansions of ν, F, U^h and test functions $V \in \mathcal{V}^h \otimes \mathcal{S}^{\mathrm{P}}$ into the variational form of the semi discrete stochastic problem. This results in:
Find $u_{i,k}$, $i \in \mathcal{N}$ and $k = 0, \ldots, \mathrm{P}$, such that

$$\sum_{i,j \in \mathcal{N}} \sum_{k,l,m=0}^{\mathrm{P}} \langle \Psi_k \Psi_l \Psi_m \rangle A^k_{i,j} u_{i,l} v_{j,m} = \sum_{i \in \mathcal{N}} \sum_{k=0}^{\mathrm{P}} b^k_i v_{i,k}, \quad \forall v_{i,k},\ i \in \mathcal{N},\ k = 0, \ldots, \mathrm{P}$$

where

$$A^k_{i,j} \equiv \int_\Omega \nu_k(\boldsymbol{x}) \nabla \Phi_i(\boldsymbol{x}) \cdot \nabla \Phi_j(\boldsymbol{x}) \mathrm{d}\boldsymbol{x}, \quad b^k_i \equiv \left\langle \Psi_k^2 \right\rangle \int_\Omega f_k(\boldsymbol{x}) \Phi_i(\boldsymbol{x}) \mathrm{d}\boldsymbol{x}.$$

It involves $n \times (\mathrm{P} + 1)$ deterministic quantities

Stochastic Galerkin problem

Denote $\boldsymbol{u}_k := \left(u_{1,k} \dots u_{n,k}\right)^t \in \mathbb{R}^n$ the vector of nodal values of the k-th stochastic mode of the solution.
With this notation, the Galerkin problem becomes:
Find $\boldsymbol{u}_0, \dots, \boldsymbol{u}_\mathrm{P}$ such that for all $k = 0, \dots, \mathrm{P}$

$$\sum_{l=0}^{\mathrm{P}} \sum_{m=0}^{\mathrm{P}} \langle \Psi_k \Psi_l \Psi_m \rangle \left[A^l\right] \boldsymbol{u}_m = \boldsymbol{b}_k,$$

where the matrix $\left[A^l\right]$ has for coefficients $A^l_{i,j}$ and the vector $\boldsymbol{b}_k = \left(b^k_1 \dots b^k_n\right)^t$.

Stochastic Galerkin problem

Denote $\boldsymbol{u}_k := \left(u_{1,k} \dots u_{n,k}\right)^t \in \mathbb{R}^n$ the vector of nodal values of the k-th stochastic mode of the solution.
This set of systems can be formally expressed as a single system $[\boldsymbol{A}]\boldsymbol{u} = \boldsymbol{B}$ where the global system matrix $[\boldsymbol{A}]$ has the block structure, corresponding to:

$$\begin{pmatrix} \boldsymbol{A}_{0,0} & \dots & \boldsymbol{A}_{0,\mathrm{P}} \\ \vdots & \ddots & \vdots \\ \boldsymbol{A}_{\mathrm{P},0} & \dots & \boldsymbol{A}_{\mathrm{P},\mathrm{P}} \end{pmatrix} \begin{pmatrix} \boldsymbol{u}_0 \\ \vdots \\ \boldsymbol{u}_{\mathrm{P}} \end{pmatrix} = \begin{pmatrix} \boldsymbol{b}_0 \\ \vdots \\ \boldsymbol{b}_{\mathrm{P}} \end{pmatrix}.$$

The matrix blocks are given by:

$$\boldsymbol{A}_{i,j} = \sum_{m=0}^{\mathrm{P}} [A^m] \langle \Psi_i \Psi_j \Psi_m \rangle \qquad 0 \leq i,j \leq P.$$

The system $[\boldsymbol{A}]\boldsymbol{u} = \boldsymbol{B}$ is called the spectral or Galerkin problem.

Solution of Stochastic Galerkin problem

Solution method:

- The matrix $[\boldsymbol{A}]$ of the Galerkin problem has a block symmetric structure, $\boldsymbol{A}_{i,j} = \boldsymbol{A}_{j,i}$, since $\langle \Psi_i \Psi_j \Psi_m \rangle = \langle \Psi_j \Psi_i \Psi_m \rangle$.
- The blocks are in fact symmetric because $A^k_{i,j} = A^k_{j,i}$, so the matrix $[\boldsymbol{A}]$ is symmetric.
- Standard solution techniques for (large) symmetric linear systems can be reused.
- Due to the size of the system, sparse storage is mandatory, even-though many blocks are zero.

Theoretical comments

Existence and uniqueness of the solution:
Properties of the Galerkin system have been the focus of many works. *e.g.* [Babuska,2002], [Babuska, 2005], [Frauenfelder, 2005], [Matthies, 2005]

- For Dirichlet boundary conditions, the Galerkin system for stochastic elliptic problems has a unique solution provided that the random conductivity field satisfies some probabilistic (sufficient) conditions.
- For the deterministic discretization with $P-1$ finite-elements, these probabilistic conditions reduce to
$$\frac{1}{\nu(\boldsymbol{x}, \xi)} \in L_2(\Xi, P_\Xi), \forall \boldsymbol{x} \in \Omega$$
- For Neumann boundary conditions only, $U(\boldsymbol{x}, \xi)$ is defined up to an arbitrary random variable and an integral constraint on the source term is necessary for homogeneous conditions,
$$\int_\Omega F(\boldsymbol{x}, \xi) \mathrm{d}\boldsymbol{x} = 0 \qquad a.s.$$

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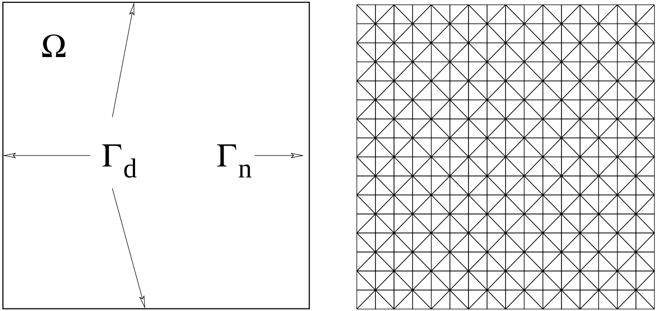
Example 1: uniform conductivity

We consider $\Omega = [0,1]^2$, with Dirichlet boundary conditions over 3 edges and a Neumann condition over the left edge $x = 1$.



Left: computational domain Ω and decomposition of the boundary $\partial\Omega$ into Dirichlet Γ_d and Neumann Γ_n parts. Right: typical finite-element triangulation of Ω using 512 elements and 289 nodes.

Consider first the case of a uniform deterministic source term and constant random conductivity

$$F(\boldsymbol{x}, \theta) = f(\boldsymbol{x}) = 1, \qquad \nu(\boldsymbol{x}, \theta) = \beta(\theta).$$

- The random conductivity β is assumed to be log-normal, with unit median value $\overline{\beta} = 1$ and coefficient of variation $C \geq 1$.
- β is parametrized with a unique normalized Gaussian variable $\xi_1(\theta)$ so $\mathrm{N} = 1$, and the PC basis is made of the one-dimensional Hermite polynomials.

$$\beta(\xi_1) = \exp\left(\mu_\beta + \sigma_\beta \xi_1\right), \qquad \mu_\beta = \log\left(\overline{\beta}\right) \text{ and } \sigma_\beta = \frac{\log C}{2.85}.$$

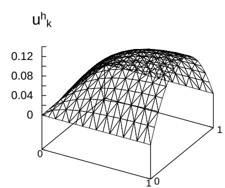
- The PC coefficients β_k have closed form expressions [Ghanem, 1999]:

$$\beta(\xi_1) = \sum_{k=0}^{\infty} \beta_k \Psi_k(\xi_1), \qquad \beta_k = \exp\left(\mu_\beta + \sigma_\beta^2/2\right) \frac{\sigma_\beta^k}{\langle \Psi_k^2 \rangle}.$$

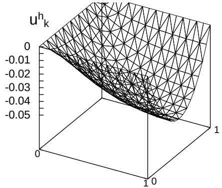
Example 1: uniform conductivity

Stochastic modes of the solution for $\mathrm{No} = 4$

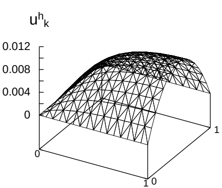
U_0^h



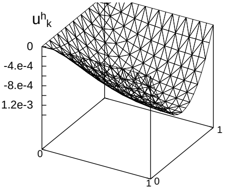
U_1^h



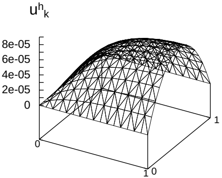
U_2^h



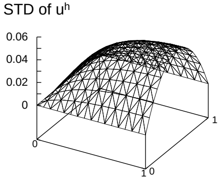
U_3^h



U_4^h



Standard deviation

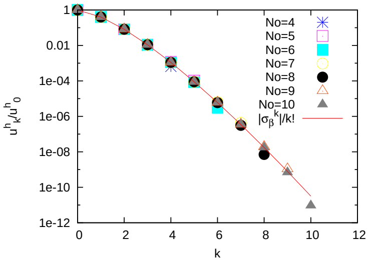


Convergence with the expansion order

β being log-normal, so is its inverse, and the expansion of $1/\beta$ is consequently given by:

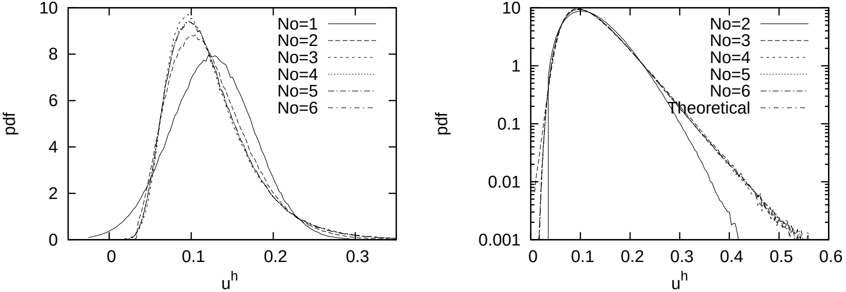
$$\left(\frac{1}{\beta}\right)_k = \exp\left(-\mu_\beta + \sigma_\beta^2/2\right) \frac{(-\sigma_\beta)^k}{\langle \Psi_k^2 \rangle}.$$

The spectrum of the numerical solution should decay as $|\sigma_\beta|^k/k!$.



Normalized spectra of the random solution u^h_k at node $\boldsymbol{x} = (1, 0.5)$ as computed using different expansion orders.

Convergence of pdf



Computed probability density functions of U^h at $\boldsymbol{x} = (1, 0.5)$ for different expansion orders No as indicated. Top plot: $\mathrm{No} = 1, \ldots, 6$. Bottom plot: same pdfs in log scale for $\mathrm{No} = 2, \ldots, 6$ together with the theoretical pdf.

Consider the random conductivity field defined as:

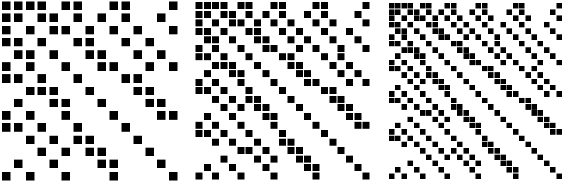
$$\nu(\boldsymbol{x},\theta) = \begin{cases} \nu^1(\theta), & x \leq 0.5 \\ \nu^2(\theta), & x > 0.5 \end{cases}$$

- ν^1 and ν^2 are two independent log-normal random variables with respective medians $\overline{\nu}^1$ and $\overline{\nu}^2$, and coefficients of variation C^1 and C^2.
- Two normalized Gaussian variables ξ_1 and ξ_2 are used to parametrize the conductivity field.
- The stochastic dimension is $\mathrm{N} = 2$, and the stochastic basis consists of two-dimensional Hermite polynomials.

The expansion on $\mathcal{S}^{\mathrm{P}}$ of the random conductivity field,

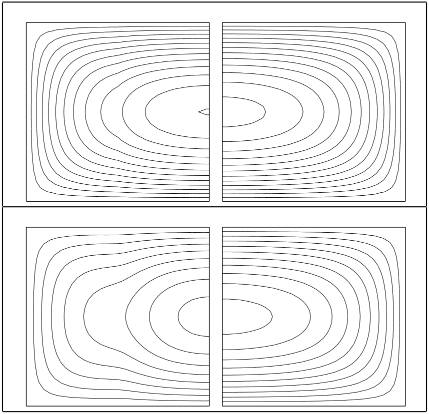
$$\nu(\boldsymbol{x}, \boldsymbol{\xi}) = \sum_{k=0}^{\mathrm{P}} \nu_k(\boldsymbol{x}) \Psi_k(\boldsymbol{\xi}), \qquad (1)$$

has many zero modes $\nu_k(\boldsymbol{x})$ (due to the independence over distinct sub-domain). Consequently, some elementary matrices $\left[A^l\right]$ are zero, resulting in a sparse block structure for the Galerkin system.



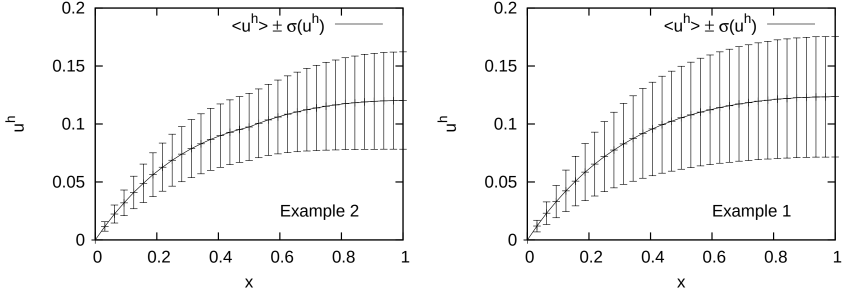
The sparsity of the full Galerkin matrix system $[\boldsymbol{A}]$ for $\mathrm{No} = 4, \ldots, 6$ (dim $\mathcal{S} = \mathrm{P} + 1 = 15, 21$ and 28).

Example 2: nonuniform conductivity



Expectations (top) and standard deviations (bottom) of U^h for $\mathrm{No} = 5$. Left: two random conductivities ($\mathrm{N} = 2$, $\mathrm{P} = 20$). Right: single random conductivity ($\mathrm{N} = 1$, $\mathrm{P} = 5$).

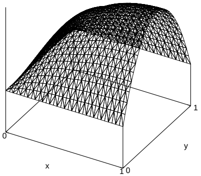
Example 2: nonuniform conductivity



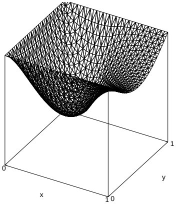
Uncertainty in U^h along the line $y = 0.5$. Left: two random conductivities ($\mathrm{N} = 2$, $\mathrm{P} = 20$). Right: single random conductivity ($\mathrm{N} = 1$, $\mathrm{P} = 5$).

Stochastic modes

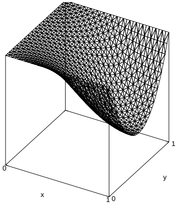
$$\Psi_0 = \psi_0(\xi_1)\psi_0(\xi_2)$$



$$\Psi_1 = \psi_1(\xi_1)\psi_0(\xi_2)$$

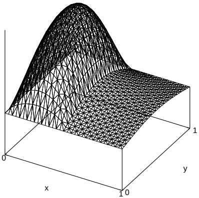


$$\Psi_2 = \psi_0(\xi_1)\psi_1(\xi_2)$$

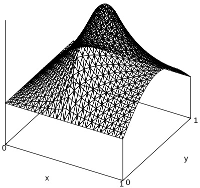


Example 2: nonuniform conductivity

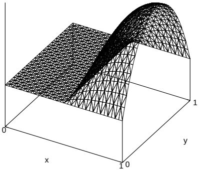
$\Psi_3 = \psi_2(\xi_1)\psi_0(\xi_2)$



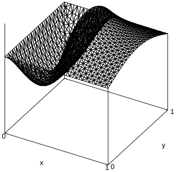
$\Psi_4 = \psi_1(\xi_1)\psi_1(\xi_2)$



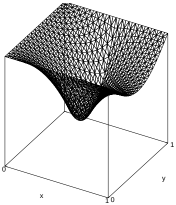
$\Psi_5 = \psi_0(\xi_1)\psi_2(\xi_2)$



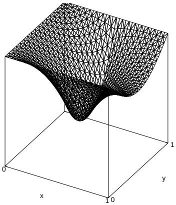
$\Psi_6 = \psi_3(\xi_1)\psi_0(\xi_2)$



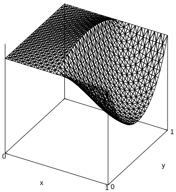
$\Psi_7 = \psi_2(\xi_1)\psi_1(\xi_2)$



$\Psi_8 = \psi_1(\xi_1)\psi_2(\xi_2)$



$\Psi_9 = \psi_0(\xi_1)\psi_3(\xi_2)$



Modes $u_k(\boldsymbol{x})$ of the stochastic solution for the nonuniform conductivity problem.

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Stochastic Galerkin Method

Flow and transport in porous media

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- Convection Dispersion Equation: ▸ Example

Navier-Stokes and Multiphysics flows

- Incompressible Navier-Stokes eq.: ▸ Boussinesq ▸ More on solvers
- Complex flows: ▸ Low-Mach ▸ Electrophoresis

Lagrangian Models

- Navier-Stokes equations: ▸ Example
- Convection dispersion equations: ▸ Example

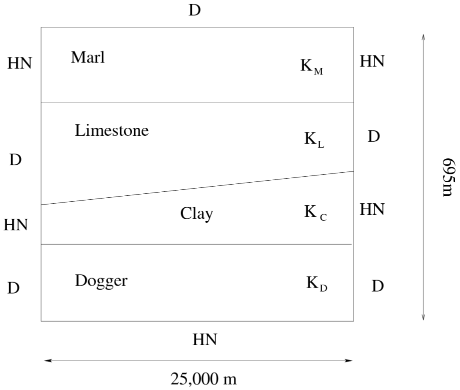
Questions & Discussion

Darcy Equation with uncertain conductivities

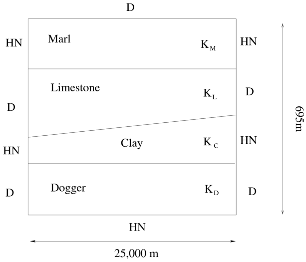
With: A. Ern (CERMICS, ENPC) and J.-M. Martinez (CEA/DEN/DM2S/LGLS).

Couplex-1 Problem (MoMaS) — Darcy flow

2D layered medium with highly contrasted permeabilities.



Couplex-1 Problem (MoMaS) — Darcy flow



Darcy velocity: $\mathbf{u} = -K\nabla H.$
Hydrodynamic load (m): $H = P/\rho g + z.$
Homogeneous Neumann (HN)
Dirichlet (D) BCs.

$$\boxed{\nabla \cdot (K\nabla H) = 0}$$

- **Uncertain** but isotropic permeability tensor K (m/year).
- K **constant** in each layer $\rightarrow$ uncertainty model with 4 RVs.
- Permeabilities are **independent**.

Uncertainty model for Permeabilities (in m/year):

Layer	Median value	Distribution	uncertainty level
Dogger	25.23	Uniform	$\pm 50\%$
Clay	$3.15\ 10^{-6}$	Log-uniform	1 decade
Limestone	6.31	Uniform	$\pm 50\%$
Marl	$3.15\ 10^{-5}$	Log-uniform	1 decade

Parameterization:
$K_D(\xi_1)$, $K_C(\xi_2)$, $K_L(\xi_3)$ and $K_M(\xi_4)$ with $(\xi_1, \ldots, \xi_4) \sim U[-1, 1]^4$.

- $N = 4$ dimensional polynomial chaos.
- Wiener-Legendre expansion of K and solution H.

Discretizations

- **Finite element** approximation in space (non-conform P1 element -A. Ern-).
- Mesh involves **25,390 elements**.
- Deterministic problem: $[k]h = f,$
  $[k] \in \mathbb{R}^{m\times m}$ SPD matrix; h (pressure) and f (rhs) $\in \mathbb{R}^m$.
- **Stochastic problem:** $[K](\xi)U(\xi) = f,$
- Truncated Wiener-Legendre expansion of $[K]$ and H:

$$[K](\xi) \approx \sum_{k=0}^{\mathrm{P}} [K_k]\Psi_k(\xi), \quad H(\xi) \approx \sum_{k=0}^{\mathrm{P}} H_k\Psi_k(\xi), \quad \mathcal{S}^{\mathrm{P}} = \mathrm{span}\{\Psi_0, \dots, \Psi_{\mathrm{P}}\}.$$

- **Galerkin Projection:**

$$\left\langle \left(\sum_{k=0}^{\mathrm{P}} [K_k]\Psi_k(\xi)\right)\left(\sum_{k=0}^{\mathrm{P}} H_k\Psi_k(\xi)\right), V(\xi)\right\rangle = \langle f, V(\xi)\rangle \quad \forall V(\xi) \in \mathbb{R}^m \times \mathcal{S}^{\mathrm{P}}.$$

- Spectral problem: **Large!**

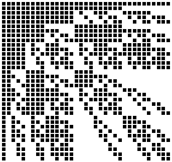
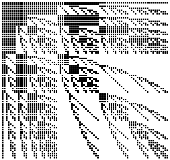
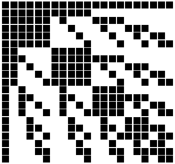
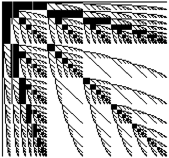
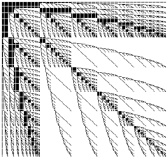
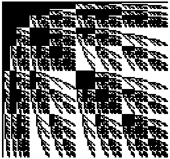
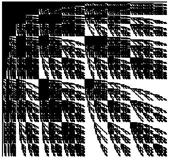
$$\sum_{i=0}^{\mathrm{P}} \sum_{j=0}^{\mathrm{P}} \langle \Psi_i \Psi_j, \Psi_k \rangle [K_i] H_j = \langle f, \Psi_k \rangle = f \delta_{k,0}, \quad k = 0, 1, \dots, \mathrm{P}$$

Large linear system of $m \times (\mathrm{P}+1)$ equations.

- Sparse multiplication tensor $\mathcal{M} = \langle \Psi_i \Psi_j, \Psi_k \rangle / \langle \Psi_k, \Psi_k \rangle$
- Galerkin system has a **(sparse) block structure**, where each block has same non-zero pattern as the deterministic matrix $[k]$.

Structure of Galerkin system:

(examples for $\mathrm{No} = 3$ -left- and $\mathrm{N} = 5$ -right-)

$\mathrm{N} = 4$-$\mathrm{P} = 35$	$\mathrm{N} = 6$-$\mathrm{P} = 84$	$\mathrm{No} = 2$-$\mathrm{P} = 20$	$\mathrm{No} = 3$-$\mathrm{P} = 55$
			
$\mathrm{N} = 8$-$\mathrm{P} = 164$	$\mathrm{N} = 10$-$\mathrm{P} = 285$	$\mathrm{No} = 4$-$\mathrm{P} = 126$	$\mathrm{No} = 5$-$\mathrm{P} = 251$
			

Iterative resolution

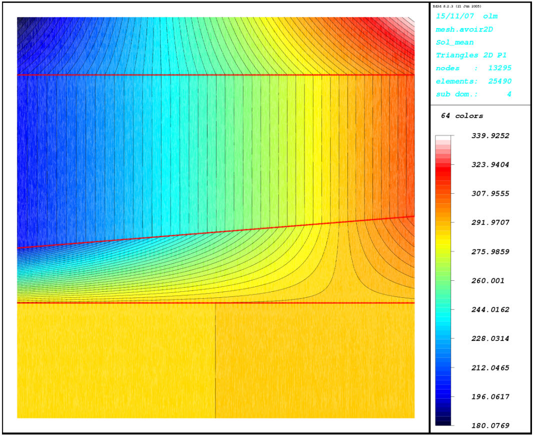
- Exploit orthogonality of the basis: $\langle \Psi_0 \Psi_j, \Psi_k \rangle = \langle \Psi_k, \Psi_k \rangle \delta_{j,k}$

$$H_k = [K_0]^{-1} \left[f\delta_{k0} - \sum_{i=1}^{\mathrm{P}} \sum_{j=0}^{\mathrm{P}} \frac{\langle \Psi_k \Psi_i \Psi_j \rangle}{\langle \Psi_k \Psi_k \rangle} [K_i] H_j \right].$$

- Jacobi type iterations on modes (mean preconditionner).
- $[K_0]$ corresponds to deterministic $[k]$ for mean properties: **re-use deterministic solver** (PCG).
- Factorize $[K_0]$ only once.
- Parallel evaluation of the rhs.
- Convergence decreases with variability in $[K]$.
- Improved preconditionners for stochastic elliptic problems (including mixed formulations) `[Powell et al., 08-10]`.

$\mathrm{No} = 4 \;\rightarrow \mathrm{P} + 1 = 69$ stochastic modes

Mean pressure field:

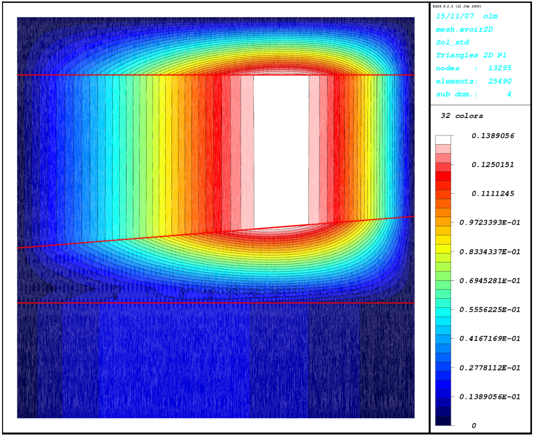


$$\mathbb{E}\left[H\right] = \langle H(\xi), 1 \rangle = H_0$$

Couplex-1 — Results

$\mathrm{No} = 4 \;\rightarrow \mathrm{P} + 1 = 69$ stochastic modes

Standard-deviation in pressure field:



$$\sigma_H^2 = \mathbb{E}\left[(H - H_0)^2\right] = \mathbb{E}\left[(\sum_{k=1}^{\mathrm{P}} H_k)(\sum_{l=1}^{\mathrm{P}} H_l)\right] = \sum_{k=1}^{\mathrm{P}} H_k^2 \langle \Psi_k, \Psi_k \rangle$$

Return

Convection dispersion equation

With: J.-M. Martinez (CEA/DEN/DM2S/LGLS) and A. Cartalade (CEA/DEN/DM2S).

1-D Convection dispersion

Model equation — A. Cartalade (CEA)

- Concentration $C(x,t)$

$$\phi \frac{\partial C}{\partial t} = -\frac{\partial}{\partial x}\left[qy - (\phi D_0 + \lambda |q|)\frac{\partial C}{\partial x}\right].$$

- IC and BC: $C(x, t=0) = 0,\ C(x=0, t) = 1.$
- Model **parameters**:
  - $q > 0$: Darcy velocity (1m/day),
  - ϕ : fluid fraction (given in $]0,1[$),
  - D_0 : molecular diffusivity ($<< 1$),
  - λ : **uncertain** hydrodynamic dispersion coefficient.

Uncertainty model

Solution method

1-D Convection dispersion

Model equation

Uncertainty model

- λ follows an **uncertain power-law**: $\boxed{\lambda = a\phi^b}$.

Solution method

1-D Convection dispersion

Model equation

Uncertainty model

- λ follows an **uncertain power-law**: $\boxed{\lambda = a\phi^b}$.
- a and b **independent** random variables.
- $\log_{10}(a) \sim U[-4, -2]$ and $b \sim U[-3.5, -1]$.

$$a(\xi_1) = \exp(\mu_1 + \sigma_1 \xi_1), \; b = \mu_2 + \sigma_2 \xi_2, \xi_1, \xi_2 \simeq U[-1, 1].$$

$$\boxed{\lambda(x, \xi_1, \xi_2) \approx \sum_k \lambda_k(x) \Psi_k(\xi_1, \xi_2)}$$

[Debusschere *et al*, J. Sci. Comp., 2004]

Solution method

1-D Convection dispersion

Model equation

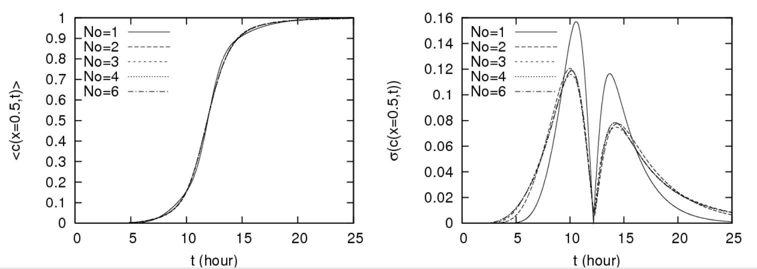
Uncertainty model

Solution method

- Wiener-Legendre expansion and Galerkin projection: $C(x,t,\xi_1,\xi_2) = \sum_{k=0}^{\mathrm{P}} C_k(x,t)\Psi_k(\xi_1,\xi_2)$.
- Spectral convergence in the stochastic space with No.
- Finite volume deterministic discretization $\mathcal{O}(\Delta x^2)$.
- Implicit time scheme $\mathcal{O}(\Delta t^2)$ (block tri-diagonal system, mean operator preconditionner).
- upwind stabilization of convection term (velocity is certain).

Convection dispersion equation — results

Expectation & standard deviation at $x = 0.5$

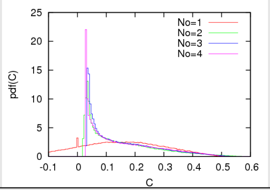
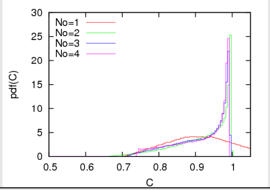
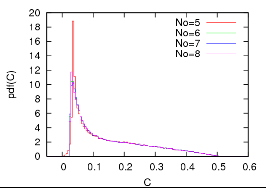
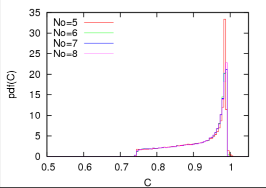


$\mathrm{No} = 1 \to \mathrm{P} + 1 = 3$, $\mathrm{No} = 6 \to \mathrm{P} + 1 = 145$.

Convergence with polynomial order No.

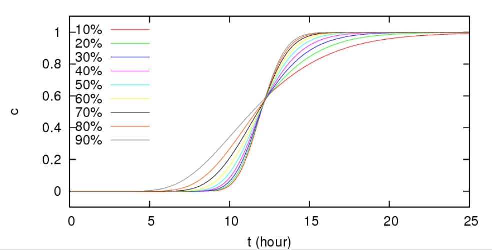
Convection dispersion equation — results

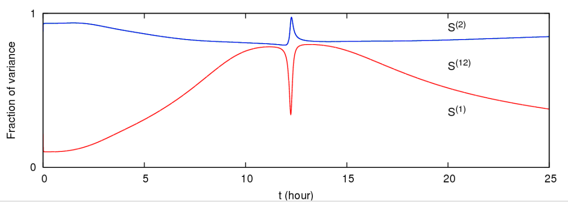
Convergence of pdfs at $x = 0.5$

$t = 10h.$	$t = 15h.$
	
	

Convection dispersion equation results

Further uncertainty analysis : quartiles & ANOVA (Sobol)





Application to the Navier-Stokes equations

Boussinesq model

With: O. Knio (JHU, Baltimore), H. Najm & B. Debusschere (SANDIA, Livermore) and R. Ghanem (USC, Los Angeles).

Natural convection — Boussinesq approximation

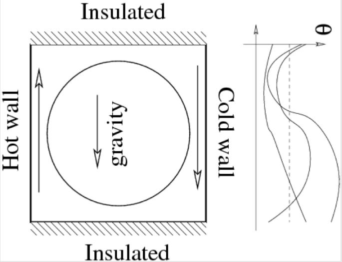
Governing equations

- **Momentum:** $$\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} \boldsymbol{u} = -\boldsymbol{\nabla} p + \frac{\mathrm{Pr}}{\sqrt{\mathrm{Ra}}} \boldsymbol{\nabla}^2 \boldsymbol{u} + \mathrm{Pr}\theta \boldsymbol{y}$$
- **Mass:** $$\boldsymbol{\nabla} \cdot \boldsymbol{u} = 0$$
- **Energy:** $$\frac{\partial \theta}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} \theta = \frac{1}{\sqrt{\mathrm{Ra}}} \nabla^2 \theta$$

Uncertain boundary conditions

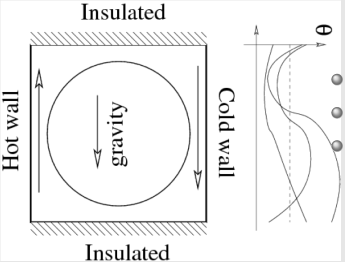
Governing equations

Uncertain boundary conditions



Governing equations

Uncertain boundary conditions

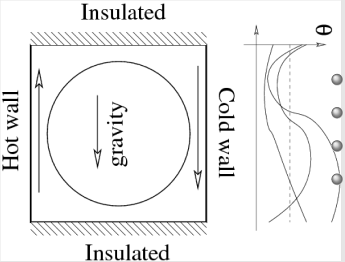


- $\boldsymbol{u} = 0$ on Γ.
- $\partial\theta(x, y = 0, 1)/\partial y = 0$.
- $\theta(x = 0, y) = 1/2$.

Natural convection — Boussinesq approximation

Governing equations

Uncertain boundary conditions

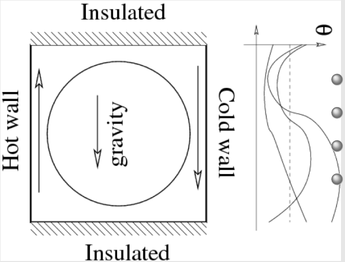


- $\boldsymbol{u} = 0$ on Γ.
- $\partial\theta(x, y = 0, 1)/\partial y = 0$.
- $\theta(x = 0, y) = 1/2$.
- $\theta(x = 1, y, \omega) = -1/2 + \theta'(y, \omega)$.

Natural convection — Boussinesq approximation

Governing equations

Uncertain boundary conditions



- $\boldsymbol{u} = 0$ on Γ.
- $\partial\theta(x, y = 0, 1)/\partial y = 0$.
- $\theta(x = 0, y) = 1/2$.
- $\theta(x = 1, y, \omega) = -1/2 + \theta'(y, \omega)$.

$$\langle\theta'(y)\theta'(y')\rangle = \sigma_\theta^2 \exp[-|y - y'|/L], \quad \theta' \sim N(0, \sigma_\theta^2).$$

BC and solution representations

$$\theta'(y,\xi) = \sum_{i=1}^{N} \sqrt{\lambda_i}\widetilde{\theta}_i(y)\xi_i = \sum_{k=0}^{P} \theta_k(y)\Psi_k(\xi).$$

$$(\boldsymbol{u}, p, \theta)(\xi) = \sum_{k=0}^{P} (\boldsymbol{u}, p, \theta)_k \Psi_k(\xi).$$

- $\xi_i \sim N(0,1) \longrightarrow$ **Hermite polynomials**.
- Stochastic dimension N.
- Expansion order $\mathrm{No} \longrightarrow \mathrm{P}+1 = (\mathrm{N}+\mathrm{No})!/(\mathrm{N}!\mathrm{No}!)$.

Galerkin projection

Implementation and solver

BC and solution representations

Galerkin projection

$$\frac{\partial \boldsymbol{u}_k}{\partial t} + \sum_{i,j=0}^{\mathrm{P}} \boldsymbol{u}_i \cdot \nabla \boldsymbol{u}_j \frac{\langle \Psi_i \Psi_j, \Psi_k \rangle}{\langle \Psi_k, \Psi_k \rangle} = -\nabla p_i + \frac{\mathrm{Pr}}{\sqrt{\mathrm{Ra}}} \nabla^2 \boldsymbol{u}_k + \mathrm{Pr}\,\theta_k \boldsymbol{y}$$

$$\frac{\partial \theta_k}{\partial t} + \sum_{i,j=0}^{\mathrm{P}} \boldsymbol{u}_i \cdot \nabla \theta_j \frac{\langle \Psi_i \Psi_j, \Psi_k \rangle}{\langle \Psi_k, \Psi_k \rangle} = \frac{1}{\sqrt{\mathrm{Ra}}} \nabla^2 \theta_k$$

$$\nabla \cdot \boldsymbol{u}_k = 0$$

- $\mathrm{P}+1$ **coupled** momentum and energy equations.
- $\mathrm{P}+1$ **uncoupled** divergence constraints and BCs.

Implementation and solver

BC and solution representations

Galerkin projection

Implementation and solver

Discretization

- Uniform grid, staggered arrangement and 2nd order FD
- Semi-**explicit** second order Adams-Bashford time-scheme

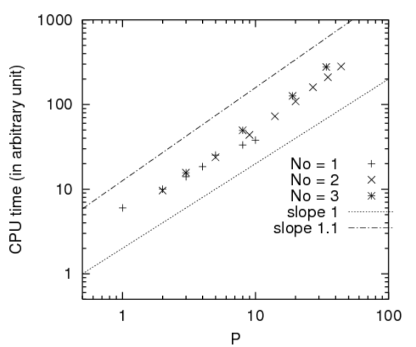
Incompressibility Treatment

- Prediction / Projection method [Chorin, 1971]
- FFT based solver for the elliptic pressure equations

CPU: essentially projection of **uncoupled** modes:

Stochastic $\simeq$ $(\mathrm{P}+1) \times$ deterministic.

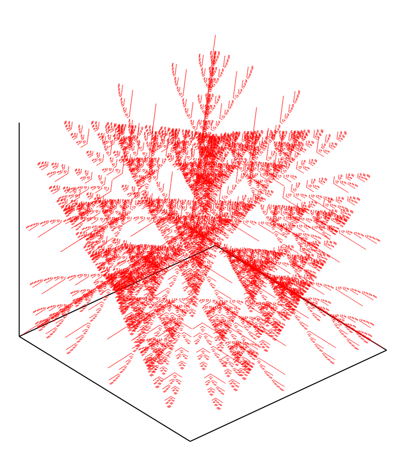
Convergence and performance (unsteady solver)



- $\mathrm{N} = 4 \sim 6$ is enough for $L \geq 1/3$
- $\mathrm{No} = 3 \rightarrow$ relative error on variance $< 10^{-4}$
- $\sim$ 1000 times more efficient than MC (LHS)
- $\sim$ 10 times more efficient than NISP + GH quadrature (sparse grid?)
- **Parallelization**

[olm *et al*, 2001]

Parallelization

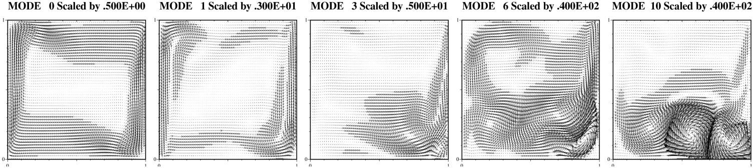


Structure of $\langle \Psi_l \Psi_m, \Psi_k \rangle$

- Distribution of modes resolution
- **Not scalable** with increasing P
- assembly of rhs needs too many communications
- load balancing
- Domain decomposition?

Example of velocity modes

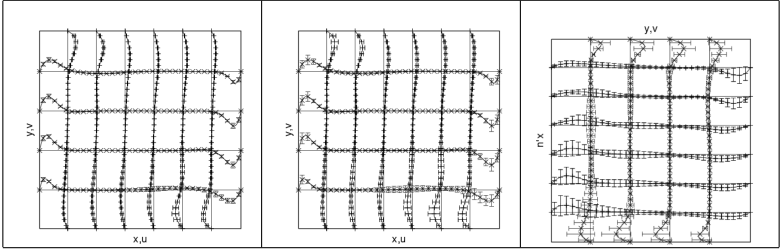
$\mathrm{Ra} = 10^6, L = 1 \; - \; \sigma_\theta = 0.25.$



Uncertainty bars

$L = 1.$

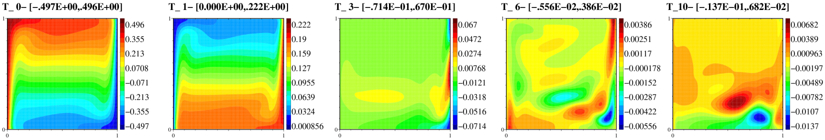
$\sigma_\theta = 0.125$	$\sigma_\theta = 0.25$	$\sigma_\theta = 0.5$



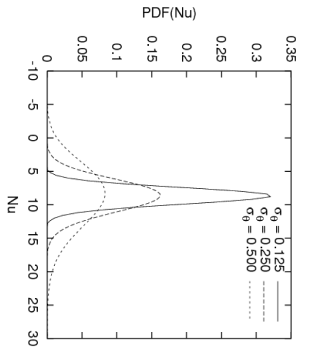
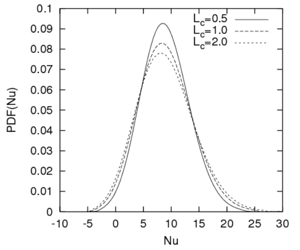
[olm *et al*, 2002]

Example of temperature modes

$\mathrm{Ra} = 10^6, L = 1 \; - \; \sigma_\theta = 0.25.$



Heat-transfer density

$L = 1 \; - \; \neq \sigma_\theta$	$\neq L \; - \; \sigma_\theta = 0.25$
	

olm et al, 2002]

Some issues stochastic CFD models

1. **Bifurcation(s)** in the uncertain parameter range:
   - compromise the convergence of spectral expansions
   - require piecewise polynomial expansions with eventually an adaptive strategy
2. **Existence of multiple solutions**
   - what to we want to measure?
   - how to force the selection of a given solution branch?
   - common to any approach of UQ.

Return

Stochactic spectral solvers
for incompressible Navier-Stokes equations

Galerkin projection of the Navier-Stokes Equation:
General form of the problem for mode k

$$\frac{\partial \boldsymbol{u}_k}{\partial t} + \sum_{l,m} \mathcal{M}_{klm} \boldsymbol{u}_l \boldsymbol{\nabla} \boldsymbol{u}_m = -\boldsymbol{\nabla} p_k + \sum_{l,m} \mathcal{M}_{klm} \nu_l \nabla^2 \boldsymbol{u}_m + \boldsymbol{f}_k, \quad \boldsymbol{\nabla} \cdot \boldsymbol{u}_k = 0$$

where $\mathcal{M}_{klm} := \frac{\langle \Psi_l \Psi_m, \Psi_m \rangle}{\langle \Psi_m, \Psi_m \rangle}$

Treatment of the nonlinear part:

- explicit treatment, *e.g.* using $\boldsymbol{u}_l^n \boldsymbol{\nabla} \boldsymbol{u}_m^n$
- semi-implicit, $\boldsymbol{u}_l^n \boldsymbol{\nabla} \boldsymbol{u}_m^{n+1}$, $\longrightarrow$ set of linear unsymmetric coupled problems: **stabilization, ?**
- other semi-implicit form:

$$\left(\sum_{l,m} \mathcal{M}_{klm} \boldsymbol{u}_l \boldsymbol{\nabla} \boldsymbol{u}_m \right)^{n+1} \approx \boldsymbol{u}_0^n \boldsymbol{\nabla} \boldsymbol{u}_k^{n+1} + \sum_{l>0,m} \mathcal{M}_{klm} \boldsymbol{u}_l^n \boldsymbol{\nabla} \boldsymbol{u}_m^n$$

$\longrightarrow$ **mean-flow based stabilization (*e.g. upwinding*).**

Stochastic unsteady Stoked problem for mode k

$$\frac{\partial \boldsymbol{u}_k}{\partial t} + \boldsymbol{\nabla} p_k - \sum_{l,m} \mathcal{M}_{klm} \nu_l \nabla^2 \boldsymbol{u}_m = \boldsymbol{\mathcal{R}}_k, \quad \boldsymbol{\nabla} \cdot \boldsymbol{u}_k = 0$$

Set of $\mathrm{P}+1$ coupled Stokes-like problems.
Spatial / time discretization results in a discrete system of the form

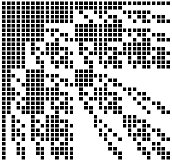
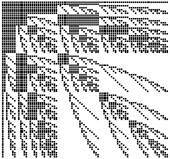
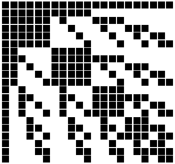
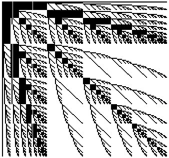
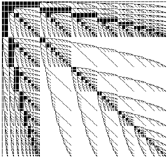
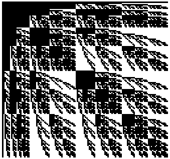
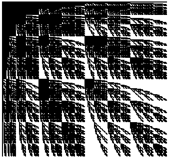
$$\mathbb{A}\boldsymbol{X} = \boldsymbol{B}, \quad \boldsymbol{X} = (\boldsymbol{X}_0 \dots \boldsymbol{X}_{\mathrm{P}})^T, \quad \boldsymbol{X}_k := (\boldsymbol{u}_k p_k)^T$$

$\mathbb{A}$ has a block structure and $[\mathbb{A}]_{0<k,l<\mathrm{P}}$ has a similar or sparser non-zero pattern than the deterministic Stokes problem.

Structure of the Galerkin system:

- The Galerkin product tensor $\mathcal{M}$ is sparse

(examples for $\mathrm{No} = 3$ -left- and $\mathrm{N} = 5$ -right-)

$\mathrm{N} = 4$-$\mathrm{P} = 35$	$\mathrm{N} = 6$-$\mathrm{P} = 84$	$\mathrm{No} = 2$-$\mathrm{P} = 20$	$\mathrm{No} = 3$-$\mathrm{P} = 55$
			
$\mathrm{N} = 8$-$\mathrm{P} = 164$	$\mathrm{N} = 10$-$\mathrm{P} = 285$	$\mathrm{No} = 4$-$\mathrm{P} = 126$	$\mathrm{No} = 5$-$\mathrm{P} = 251$
			

Resolution of the Galerkin system

Rewrite stochastic Stokes problem as

$$\sum_{l=0}^{\mathrm{P}} \sum_{m=0}^{\mathrm{P}} \mathcal{M}_{klm}[S]_l \boldsymbol{X}_m = \boldsymbol{B}_k, \quad \text{for } k = 0, \ldots, \mathrm{P}$$

where $[S](\xi)$ is the operator resulting from the determinsitic discretization of continuous stokes problem with a viscosity $\nu(\xi)$, so

$$[S](\xi) = \sum_{l=0}^{\mathrm{P}} [S]_l \Psi_l(\xi).$$

Note that $[\mathbb{A}]_{km} = \sum_l \mathcal{M}_{klm}[S]_l$.

Resolution of the Galerkin system

$$\sum_{l=0}^{\mathrm{P}} \mathcal{M}_{k0m}[S]_0 \boldsymbol{X}_m + \sum_{l=1}^{\mathrm{P}} \sum_{m=0}^{\mathrm{P}} \mathcal{M}_{klm}[S]_l \boldsymbol{X}_m = \boldsymbol{B}_k, \quad \text{for } k = 0, \ldots, \mathrm{P}$$

Resolution of the Galerkin system

$$[S]_0 \boldsymbol{X}_k = \boldsymbol{B}_k - \sum_{l=1}^{\mathrm{P}} \sum_{m=0}^{\mathrm{P}} \mathcal{M}_{klm} [S]_l \boldsymbol{X}_m, \quad \text{for } k = 0, \dots, \mathrm{P}$$

- Suggest Jacobi type iterations
- Factorization of $[S]_0 = \mathbb{E}\left[[S](\xi)\right]$ only
- Other iterative (Krylov-type) methods with preconditioner $\mathbb{P} = diag(\mathbb{E}\left[[S]\right])$
- Efficiency depends on the variability of $[S](\xi)$

[Powell *et al*, 2009]

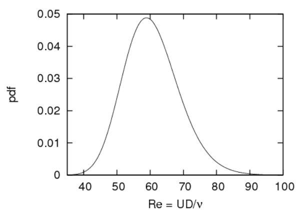
Steady problem

Solve the **nonlinear set of equations**

$$\sum_{l,m} \mathcal{M}_{klm} \left(\boldsymbol{u}_l \boldsymbol{\nabla} \boldsymbol{u}_m - \nu_l \nabla^2 \boldsymbol{u}_m \right) + \boldsymbol{\nabla} p_k = \boldsymbol{f}_k, \quad \boldsymbol{\nabla} \cdot \boldsymbol{u}_k = 0.$$

- **Very large** problem
- Iterative approach mandatory (Newton-like)
- Construction of approximate tangent operator (matrix-free)
- Derive appropriate preconditioners, *e.g.* based on time-stepper [olm, 2009]

Steady Flow around a circular cylinder - Vorticity formulation



Uncertain Reynolds: $\mathrm{Re} = \mathrm{Re}(\xi) \sim LN$
(Median above critical value)
stochastic basis:
Wiener-Hermite

Numerical Method:
Newton Iterations (with Unstd. stoch. Stokes prec.)
$\psi - \omega$ formulation + influence matrix for BCs

$$\boldsymbol{u}(\xi)\boldsymbol{\nabla}\omega(\xi) - \frac{1}{\mathrm{Re}(\xi)}\nabla^2\omega(\xi) = 0.$$

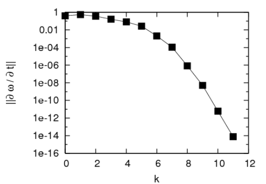
Centered Finite differences $\mathcal{O}(\Delta x^2)$
Uniform mesh (512×360) and direct FFT-based solvers

Convergence of Newton iterates

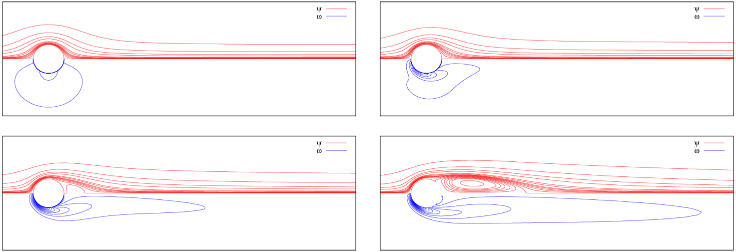
Wiener-Hermite $\mathrm{No} = 4$

L_2 Residual of stochastic equation:

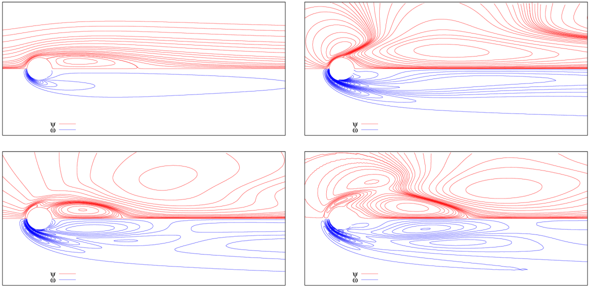
$$\boldsymbol{u}(\xi)\boldsymbol{\nabla}\omega(\xi) - \frac{1}{\mathrm{Re}(\xi)}\nabla^2\omega(\xi) = 0.$$



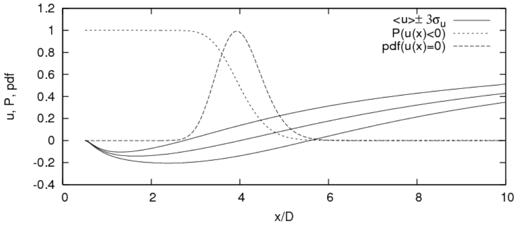
Convergence of the mean mode: (first 4 iterations)



First 4 stoch. modes: $u(\boldsymbol{x},\xi) = \sum u_k(\boldsymbol{x})\Psi_k(\xi)$



Near wake statistics:



Stochastic Galerkin Method
for low-Mach approxmation

With: O. Knio (JHU, Baltimore), H. Najm & B. Debusschere (SANDIA, Livermore) and R. Ghanem (USC, Los Angeles).

So far we have seen problems with **quadratic nonlinearities**, but model may involve more general ones `[Debusschere et al, 2003]`

- Galerkin methods need specific treatment for the projection of nonlinearities
- Projection of nonlinearities can be achieved through:
  1. Non-intrusive projections (but why mixing Galerkin and non-intrusive approaches?)
  2. By means of pseudo-spectral (P-S) calculations

     `[Debusschere et al, 2004]`
- Different (P-S) alternative possible: need be carefully verified to check in particular **convergence and consistency**.
- **Example: Low-Mach number model**.

Low-Mach approximation [Majda and Stehian, 1985]

- **Formulation**

$$
\begin{aligned}
\frac{\partial \rho}{\partial t} &= \frac{1}{\gamma T}\frac{dP}{dt} + \frac{1}{T}\left(\rho \boldsymbol{u}\cdot\boldsymbol{\nabla} T - \frac{1}{\mathrm{Pr}\sqrt{\mathrm{Ra}}}\boldsymbol{\nabla}\cdot(\kappa\boldsymbol{\nabla} T)\right)\\
\frac{dP}{dt} &= -\gamma\int_\Omega \frac{1}{T}\left(\rho \boldsymbol{u}\cdot\boldsymbol{\nabla} T - \frac{1}{\mathrm{Pr}\sqrt{\mathrm{Ra}}}\boldsymbol{\nabla}\cdot(\kappa\boldsymbol{\nabla} T)\right) d\Omega \Big/ \int_\Omega \frac{1}{T} d\Omega\\
\frac{\partial \rho u}{\partial t} &= -\frac{\partial \rho u^2}{\partial x} - \frac{\partial \rho uv}{\partial y} - \frac{\partial \Pi}{\partial x} + \frac{1}{\sqrt{\mathrm{Ra}}}\Phi_x\\
\frac{\partial \rho v}{\partial t} &= -\frac{\partial \rho uv}{\partial x} - \frac{\partial \rho v^2}{\partial y} - \frac{\partial \Pi}{\partial y} + \frac{1}{\sqrt{\mathrm{Ra}}}\Phi_y - \frac{1}{\mathrm{Pr}}\frac{\rho-1}{2\epsilon}\\
T &= \frac{P}{\rho}
\end{aligned}
$$

- **Main difficulties of stochastic extension:** [olm *et al.*, 2004]

- **Stochastic inverses**
- **Mass-conservation** (mean sense is not enough).

Differentiation of the equation of state, combined with energy equation gives :

[Najm, Knio *et al*, 1998 & 1999]

$$
\begin{aligned}
\frac{\partial \rho}{\partial t} &= \frac{1}{\gamma T}\frac{dP}{dt} + \frac{1}{T}\left(\rho \boldsymbol{u}\cdot\boldsymbol{\nabla} T - \frac{1}{\mathrm{Pr}\sqrt{\mathrm{Ra}}}\boldsymbol{\nabla}\cdot(\kappa \boldsymbol{\nabla} T)\right) \\
\frac{dP}{dt} &= -\gamma \frac{\int_\Omega \frac{1}{T}\left(\rho \boldsymbol{u}\cdot\boldsymbol{\nabla} T - \frac{1}{\mathrm{Pr}\sqrt{\mathrm{Ra}}}\boldsymbol{\nabla}\cdot(\kappa \boldsymbol{\nabla} T)\right) d\Omega}{\int_\Omega \frac{1}{T} d\Omega} \\
\frac{\partial \rho u}{\partial t} &= -\frac{\partial \rho u^2}{\partial x} - \frac{\partial \rho u v}{\partial y} - \frac{\partial \Pi}{\partial x} + \frac{1}{\sqrt{\mathrm{Ra}}}\Phi_x \\
\frac{\partial \rho v}{\partial t} &= -\frac{\partial \rho u v}{\partial x} - \frac{\partial \rho v^2}{\partial y} - \frac{\partial \Pi}{\partial y} + \frac{1}{\sqrt{\mathrm{Ra}}}\Phi_y - \frac{1}{\mathrm{Pr}}\frac{\rho - 1}{2\epsilon} \\
T &= \frac{P}{\rho} \\
&+ \text{Boundary and Initial Conditions.}
\end{aligned}
$$

- **Galerkin Projection**
  1) insertion of the spectral expansions
  2) projection of resulting equations onto the spectral basis:

$$\begin{cases} \dfrac{\partial \rho_k}{\partial t} = \mathcal{H}_k & , \quad \dfrac{dP_k}{dt} = \mathcal{G}_k \\ \dfrac{\partial \rho u_k}{\partial t} = \mathcal{X}_k - \dfrac{\partial \Pi_k}{\partial x} & , \quad \dfrac{\partial \rho v_k}{\partial t} = \mathcal{Y}_k - \dfrac{\partial \Pi_k}{\partial y} \\ T_k = \left(\dfrac{P}{\rho}\right)_k & , \quad k = 0, \ldots, \mathrm{P} \end{cases}$$

- **Strategy : explicit time scheme**
  - Evaluation of non-linearities
  - Exact enforcement of mass conservation

- **Update density and thermodynamic pressure :**

$$\rho_k^{n+1} = \rho_k^n + \Delta t \left(\frac{3}{2}\mathcal{H}_k^n - \frac{1}{2}\mathcal{H}_k^{n-1} \right) , \quad P_k^{n+1} = P_k^n + \Delta t \left(\frac{3}{2}\mathcal{G}_k^n - \frac{1}{2}\mathcal{G}_k^{n-1} \right)$$

- **Deduce temperature :** $T_k^{n+1} = \left(\frac{P}{\rho}\right)_k^{n+1}$
- **Predictions on momentum :**

$$(\rho u)_k^* = (\rho u)_k^n + \Delta t \left(\frac{3}{2}\mathcal{X}_k^n - \frac{1}{2}\mathcal{X}_k^{n-1} \right) , (\rho v)_k^* = (\rho v)_k^n + \Delta t \left(\frac{3}{2}\mathcal{Y}_k^n - \frac{1}{2}\mathcal{Y}_k^{n-1} \right)$$

- **Correction step · (decoupled elliptic systems)**

$$\nabla^2 \Pi_k = \frac{1}{\Delta t} \left[\boldsymbol{\nabla} \cdot (\rho \boldsymbol{u})_k^* + \left.\frac{\partial \rho_k}{\partial t}\right|^{n+1} \right], \quad \text{where } \left.\frac{\partial \rho_k}{\partial t}\right|^{n+1} = \frac{3\rho_k^{n+1} - 4\rho_k^n + \rho_k^{n-1}}{\Delta t},$$

$$(\rho u)_k^{n+1} = (\rho u)_k^* - \Delta t \frac{\partial \Pi_k}{\partial x}, \qquad (\rho v)_k^{n+1} = (\rho v)_k^* - \Delta t \frac{\partial \Pi_k}{\partial y}$$

$$u_k^{n+1} = \left(\frac{(\rho u)^{n+1}}{\rho^{n+1}} \right)_k , \qquad v_k^{n+1} = \left(\frac{(\rho v)^{n+1}}{\rho^{n+1}} \right)_k .$$

Pressure solvability and mass conservation :

- Closed Cavity : the pressure solvability constraint is

$$\int_{\Omega} \frac{\partial \rho_k}{\partial t}\, d\Omega = 0, \quad k = 0, \dots, \mathrm{P},$$

i.e. Global Mass Conservation of each modes

- Mass conservation enforcement: $\frac{\partial \rho_k}{\partial t} = \mathcal{H}_k$, with
$\mathcal{H}_k = \frac{1}{\gamma T}\frac{dP_k}{dt} + \left[\frac{1}{T}\left(\rho \boldsymbol{u}\cdot\boldsymbol{\nabla} T - \frac{1}{\mathrm{Pr}\sqrt{\mathrm{Ra}}}\boldsymbol{\nabla}\cdot(\kappa\boldsymbol{\nabla} T)\right)\right]_k$

Well-posedness requires that dP/dt s.t.

$$\frac{dP}{dt}\int_{\Omega}\frac{1}{\gamma T} d\Omega = (\delta\mathcal{P})\mathcal{T} = -\int_{\Omega}\frac{1}{T}\left(\rho \boldsymbol{u}\cdot\boldsymbol{\nabla} T - \frac{1}{\mathrm{Pr}\sqrt{\mathrm{Ra}}}\boldsymbol{\nabla}\cdot(\kappa\boldsymbol{\nabla} T)\right) d\Omega = \mathcal{S}.$$

Using $\delta\mathcal{P} = \mathcal{S}\mathcal{T}^{-1}$ **leads to blow-up**. Instead **inversion of the true Galerkin product** :

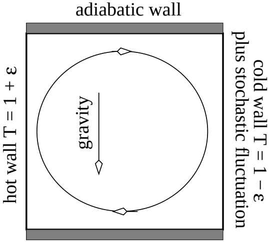
$$\sum_{l}\sum_{m}(\delta\mathcal{P})_l\,\mathcal{T}_m C_{ijk} = \sum_{l}\mathcal{A}_{kl}(\delta\mathcal{P})_l = \mathcal{S}_k \Rightarrow \delta\mathcal{P} = \mathcal{A}^{-1}\mathcal{S}.$$

Limsi cnrs

Boundary conditions : Stochastic temperature distribution on cold wall

- Gaussian, $COV = 0.25\epsilon$
- Correlation length $L_c = 1$ (exponential kernel);
- **KL decomposition**.

$$T_c(y, \boldsymbol{\xi}) \approx 1 + \epsilon + \sum_{i=1}^{N_{KL}=4} \epsilon \sqrt{\lambda_i} f_i(y) \xi_i .$$



- **Galerkin projection of the BC**

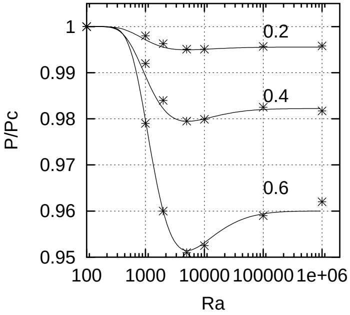
$$\frac{\partial T_k}{\partial y} = 0, \quad k = 0, \ldots, P \quad \text{for } y = 0, \text{ and } y = 1$$
$$T_0(0, y) = 1 + \epsilon, \qquad T_0(1, y) = 1 - \epsilon$$
$$T_k(0, y) = 0, \quad T_k(1, y) = \epsilon \sqrt{\lambda_k} f_k(y) \qquad \text{for } k = 1, \ldots, N_{KL}$$
$$T_k(0, y) = T_k(1, y) = 0 \qquad \text{for } k > N_{KL}$$

Validation 1 : Deterministic problem ($No = 0$)

- Convergence with grid resolution$\epsilon = 0.6$, $\mathrm{Ra} = 10^6$

$N_x \times N_y$	80×80	120×120	160×160
Nu_{av}	8.744	8.688	8.651
Nu_{min}-(hot/cold)	(1.057-0.663)	(1.064-0.677)	(1.064-0.691)
Nu_{max}-(hot/cold)	(21.81-14.77)	(21.00-15.38)	(20.70-15.48)

- Thermodynamic pressure



Solid lines : [Chenoweth & Paolucci, 1986]

Validation 2 : stochastic problem

- **Comparison with Boussinesq approximation** $\epsilon = 0.001$, $\mathrm{No} = 2$, $\mathrm{N}_{KL} = 6$, $\mathrm{Ra} = 10^6$

	N.B. 80×80	N.B. 140×100	Boussinesq 140×100
$\langle \mathrm{Nu}_{av} \rangle$	9.0794	8.9716	8.9729
$\sigma(\mathrm{Nu}_{av})$	2.4993	2.4602	2.4632

Use 120×100 spatial discretization.

Influence of ϵ for $\mathrm{Ra} = 10^6$, $COV = 0.25\epsilon$ and $\mathrm{N}_{KL} = 6$.

- Global heat flux and thermodynamic pressure

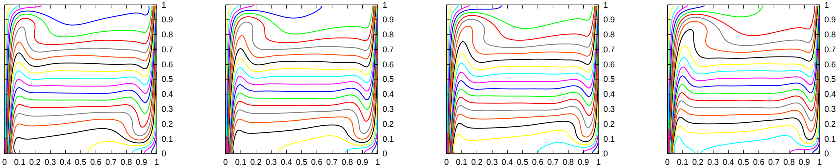
	$\langle \mathrm{Nu}_{av} \rangle$	$\sigma(\mathrm{Nu}_{av})$	$\langle P \rangle$	$\sigma(P)$
$\mathrm{No} = 1$				
$\epsilon = 0.01$	8.990	2.479	0.9999	0.0022
$\epsilon = 0.10$	9.018	2.531	0.9959	0.0232
$\epsilon = 0.20$	9.055	2.591	0.9833	0.0501
$\epsilon = 0.30$	9.103	2.653	0.9612	0.0819
$\mathrm{No} = 2$				
	$\langle \mathrm{Nu}_{av} \rangle$	$\sigma(\mathrm{Nu}_{av})$	$\langle P \rangle$	$\sigma(P)$
$\epsilon = 0.01$	8.992	2.472	0.9999	0.0022
$\epsilon = 0.10$	9.019	2.529	0.9959	0.0232
$\epsilon = 0.20$	9.058	2.598	0.9832	0.0538
$\epsilon = 0.30$	9.108	2.676	0.9609	0.0829

[olm *et al*, 2004]

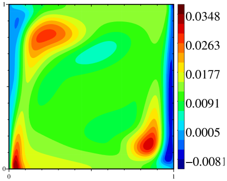
Influence of ϵ ($\mathrm{Ra} = 10^6$, $COV = 0.25\epsilon$, $\mathrm{N}_{KL} = 6$)

- Standard deviation of T

$\epsilon = 0.01$	$\epsilon = 0.1$	$\epsilon = 0.2$	$\epsilon = 0.3$



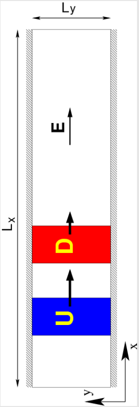
- Differences between Std-fields of T at $\epsilon = 0.01$ and $\epsilon = 0.3$.



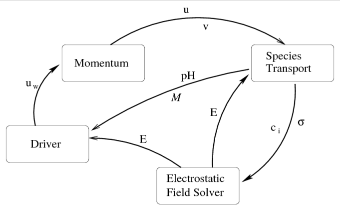
[olm *et al*, 2004]

Electrophoresis Debusschere *et al*, Phys. Fluids (2003)

Problem



Code structure



Multi-physics: NS, diffusion convection, electro-osmotic flow, chemistry (finite & infinite rates).

Uncertainties

- ζ potential (BCs).
- Tension at channel ends.
- Reaction rates.
- Initial conditions.

Spectral UQ (Galerkin)

Respective influences of $\neq$ uncertainty sources.

Return

Stochastic Particle method
for stochastic Navier-Stokes equations

With: Omar Knio (Johns Hopkins University, Baltimore).

Lagrangian techniques for Navier-Stokes

Particle methods

- Solve (incompressible) N-S equations in rotational form.
- Theoretically well grounded.
- Deal with complex/moving boundary problems, infinite domains, . . .
- Immediate extension to low diffusivity/inviscid flows without requiring stabilisation or flux limiters.
- Handle transport and reactions.

Can we extend particle methods to propagate uncertainty?

▸ Zap determ

2D incompressible Navier-Stokes equations

Rotational Form

$$\begin{cases} \dfrac{\partial \omega}{\partial t} + \boldsymbol{\nabla} \cdot (\boldsymbol{u}\omega) = \nu \Delta \omega, \\ \Delta \psi = -\omega, \\ \boldsymbol{u} = \boldsymbol{\nabla} \wedge (\psi \boldsymbol{e}_z), \\ \omega(\boldsymbol{x}, 0) = (\boldsymbol{\nabla} \wedge \boldsymbol{u}(\boldsymbol{x}, 0)) \cdot \boldsymbol{e}_z \\ \boldsymbol{u}, \omega \to 0 \quad \text{as } |\boldsymbol{x}| \to \infty. \end{cases}$$

Velocity kernel (Biot-Savart)

$$\boldsymbol{u} = \frac{-1}{2\pi} \mathcal{K} \star \omega = \frac{-1}{2\pi} \int_{\mathbb{R}^2} \mathcal{K}(\boldsymbol{x}, \boldsymbol{y}) \wedge (\omega \boldsymbol{e}_z) d\boldsymbol{y}, \quad \mathcal{K}(\boldsymbol{x}, \boldsymbol{y}) = (\boldsymbol{x} - \boldsymbol{y})/|\boldsymbol{x} - \boldsymbol{y}|^2.$$

Particle approximation

Smooth approximation

Particles : position $\boldsymbol{X}_i(t)$, circulation $\Gamma_i(t)$, core size ϵ :

$$\omega(\boldsymbol{x}, t) = \sum_{i=1}^{\text{Np}} \Gamma_i(t)\zeta_\epsilon(\boldsymbol{x} - \boldsymbol{X}_i(t)), \quad \lim_{\epsilon \to 0} \zeta_\epsilon(\boldsymbol{x}) = \delta(\boldsymbol{x}).$$

Solution technique

Split convection and diffusion processes:

- Convection : transport particles with flow velocity.
- Diffusion : update particle circulations to account for diffusion (Particle Strength Exchange method).

▸ Zap details

Solution method

Convection step

$$\frac{d\boldsymbol{X}_i}{dt} = \frac{-1}{2\pi}\sum_{j=1}^{\mathrm{Np}} \Gamma_j \mathcal{K}_\epsilon(\boldsymbol{X}_i, \boldsymbol{X}_j), \qquad \frac{d\Gamma_i}{dt} = 0.$$

- $\mathcal{K}_\epsilon$: regularised Biot-Savart kernel.
- Reduce to ODE, but **complexity in $\mathcal{O}(\mathrm{Np}^2)$**.

Acceleration of velocity computation

- Multipoles expansion $\to \mathcal{O}(\mathrm{Np})$.
- **Particle-mesh techniques**:
  1. Project circulations Γ_i on an Eulerian mesh.
  2. Solve $\nabla^2\Psi = -\omega$ (using FFT based solver for instance).
  3. Interpolate at $\boldsymbol{X}_i$ to obtain particle velocities.

Solution method

Integral representation of differential operators

Let $\eta(\boldsymbol{x})$ a radial function such that

$$\int_{\mathbb{R}^2} x^2 \eta(\boldsymbol{x}) d\boldsymbol{x} = \int_{\mathbb{R}^2} y^2 \eta(\boldsymbol{x}) = 2,$$

$$\int_{\mathbb{R}^2} x^{\alpha_1} y^{\alpha_2} \eta(\boldsymbol{x}) d\boldsymbol{x} = 0, \quad 1 \leq \alpha_1 + \alpha_2 \leq m+1,\ \alpha_1, \alpha_2 \neq 2,$$

then for positive integer multi-index β and $\eta_\epsilon(\boldsymbol{x}) \equiv \eta(\boldsymbol{x}/\epsilon)/\epsilon^2$ we have

$$\frac{\partial^{|\beta|}}{\partial x_1^{\beta_1} \dots \partial x_d^{\beta_d}} f(\boldsymbol{x}) = \frac{1}{\epsilon^{|\beta|}} \int [f(\boldsymbol{y}) + (-1)^{|\beta|+1} f(\boldsymbol{x})] \eta_\epsilon^{(\beta)}(\boldsymbol{x} - \boldsymbol{y}) d\boldsymbol{y} + \mathcal{O}(\epsilon^m).$$

Degond & Mas-Gallic (1989), Eldredge *et al* (2002).

Solution method

Diffusion term

$$\frac{d\Gamma_i}{dt} = \nu \sum_{j=1}^{\mathrm{Np}} \mathcal{L}(\boldsymbol{X}_i - \boldsymbol{X}_j) S \left[\Gamma_j - \Gamma_i\right] .$$

- Use compact functions η so only particles within a few core-size distances contribute.

Summary

$$\frac{d\boldsymbol{X}_i}{dt} = \frac{-1}{2\pi} \sum_{j=1}^{\mathrm{Np}} \Gamma_j \mathcal{K}_\epsilon(\boldsymbol{X}_i, \boldsymbol{X}_j),$$

$$\frac{d\Gamma_i}{dt} = \nu \sum_{j=1}^{\mathrm{Np}} \mathcal{L}(\boldsymbol{X}_i - \boldsymbol{X}_j) S \left[\Gamma_j - \Gamma_i\right] .$$

Direct spectral expansion : the bad way!

Set **both particle positions and circulations as uncertain**:

$$\boldsymbol{X}_i(t,\xi) = \sum_k [\boldsymbol{X}_i]_k(t)\Psi_k(\xi), \quad \Gamma_i(t,\xi) = \sum_k [\Gamma_i]_k(t)\Psi_k(\xi).$$

Apply Galerkin projection to particle problem:

$$\left\langle \Psi_k^2 \right\rangle \frac{d[\boldsymbol{X}_i]_k}{dt} = \frac{-1}{2\pi} \sum_{j=1}^{\mathrm{Np}} \left\langle \Psi_k(\xi)\Gamma_j(\xi)\mathcal{K}_\epsilon(\boldsymbol{X}_i(\xi), \boldsymbol{X}_j(\xi)) \right\rangle,$$

$$\left\langle \Psi_k^2 \right\rangle \frac{d[\Gamma_i]_k}{dt} = \left\langle \Psi_k(\xi)\nu(\xi) \sum_{j=1}^{\mathrm{Np}} \mathcal{L}(\boldsymbol{X}_i(\xi) - \boldsymbol{X}_j(\xi)) S\left[\Gamma_j(\xi) - \Gamma_i(\xi)\right] \right\rangle.$$

- Requires **stochastic projection of the kernels**.
- Fast algorithms for velocity estimation are impossible.

Untractable problem

Continuous stochastic problem: a better approach Let's go back to the **continuous vorticity equation**:

$$\frac{\partial \omega(\xi)}{\partial t} + \boldsymbol{u}(\xi)\boldsymbol{\nabla}\omega(\xi) = \nu(\xi)\nabla^2\omega(\xi), \quad \omega(\boldsymbol{x}, t, \xi) = \sum_k [\omega]_k(\boldsymbol{x}, t)\Psi_k(\xi).$$

The Galerkin projection gives:

$$\frac{\partial [\omega]_k}{\partial t} + \sum_{i,j} C_{ijk}[\boldsymbol{u}]_i \boldsymbol{\nabla}[\omega]_j = \sum_{i,j} C_{ijk}[\nu]_i \nabla^2[\omega]_j, \quad C_{ijk} = \frac{\langle \Psi_i \Psi_j \Psi_k \rangle}{\langle \Psi_k^2 \rangle},$$

or, since by convention $\Psi_0 = 1 \Rightarrow C_{0jk} = \delta_{jk}$ and

$$\frac{\partial [\omega]_k}{\partial t} + [\boldsymbol{u}]_0 \boldsymbol{\nabla}[\omega]_k = -\sum_{i \neq 0,j} C_{ijk}[\boldsymbol{u}]_i \boldsymbol{\nabla}[\omega]_j + \sum_{i,j} C_{ijk}[\nu]_i \nabla^2[\omega]_j.$$

- Stochastic modes are **convected with the mean flow** $[\boldsymbol{u}]_0$.
- Interactions with other modes are treated as **source terms using integral approximations** (PSE).

Particles with **stochastic strengths** $\Gamma_i(t,\xi) = \sum_k [\Gamma_i]_k(t)\Psi_k(\xi)$.

$$\frac{d\boldsymbol{X}_i}{dt} = [\boldsymbol{U}_i]_0,$$

$$\frac{d[\Gamma_i]_k}{dt} = - \sum_{j=1}^{\mathrm{Np}} \sum_{l=1}^{\mathrm{P}} \sum_{m=0}^{\mathrm{P}} C_{klm} S \left\{ \mathcal{G}^x(\boldsymbol{X}_i - \boldsymbol{X}_j) \left([U_i]_l [\Gamma_i]_m + [U_j]_l [\Gamma_j]_m \right) + \mathcal{G}^y(\boldsymbol{X}_i - \boldsymbol{X}_j) \left([V_i]_l [\Gamma_i]_m + [V_j]_l [\Gamma_j]_m \right) \right\} + \sum_{j=1}^{\mathrm{Np}} \sum_{l=0}^{\mathrm{P}} \sum_{m=0}^{\mathrm{P}} C_{klm} S [\nu]_l \mathcal{L}(\boldsymbol{X}_i - \boldsymbol{X}_j) \left([\Gamma_j]_m - [\Gamma_i]_m \right),$$

$$[\boldsymbol{U}_i]_k = \frac{-1}{2\pi} \sum_{j=1}^{\mathrm{Np}} [\Gamma_j]_k \mathcal{K}_\epsilon(\boldsymbol{X}_i, \boldsymbol{X}_j).$$

- Kernels are evaluated only once for all modes.
- Fast algorithms for velocity computation are still possible.
- Formulation is conservative.

Lagrangian formulation

Particle method

Particles with

- deterministic positions,
- **stochastic strengths** (circulation & heat).

Time-integration: RK-3

- Particles convected by the mean flow.
- Integral representation of stochastic modes interactions.

Code efficiency

- Stable and diffusion free convection step.
- Fast algorithms for stochastic velocity calculation (*e.g.* FFT based, multipole expansion): $\mathcal{O}(n \log n)$.
- Conservative method (regridding).

Results (I) Convection of a passive scalar

Stochastic equations

$$\frac{\partial c}{\partial t} + \boldsymbol{U} \cdot \boldsymbol{\nabla} c = 0,$$

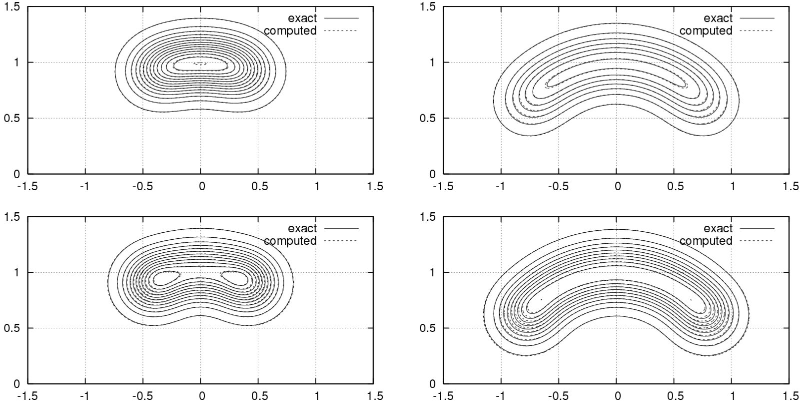
$$c(\boldsymbol{x}, t, \xi) = \exp\left[-\|\boldsymbol{x} - \boldsymbol{x}_0\|^2/\pi d^2 \|\boldsymbol{x}_0\|\right], \quad \boldsymbol{x}_0 = \boldsymbol{e}_y,$$

$$\boldsymbol{U}(\boldsymbol{x}, \xi) = -(1 + 0.075\xi)\boldsymbol{x} \wedge \boldsymbol{e}_z, \quad \xi \sim U[-1, 1].$$

Discretization

- Particle positions $\boldsymbol{X}_i(t)$, $\epsilon = 0.025$.
- Particle strengths $C_i(t, \xi) = \sum_k [C_i]_k(t)\Psi_k(\xi)$.
- Stochastic basis: Legendre polynomial.
- Stochastic order up to $\mathrm{No} = 20$.
- RK-3 with $\Delta t = 2\pi/400$.

Mean and Standard deviation of $c(\boldsymbol{x}, t, \xi)$.



Mean (top row) and standard deviation (bottom row) of the scalar field after 1 revolution (left) and 2 revolutions (right). $\mathrm{No} = 20$.

Results (II) Evolution of a radial vortex

Equations

$$\frac{\partial \omega}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} \omega = \nu \nabla^2 \omega,$$

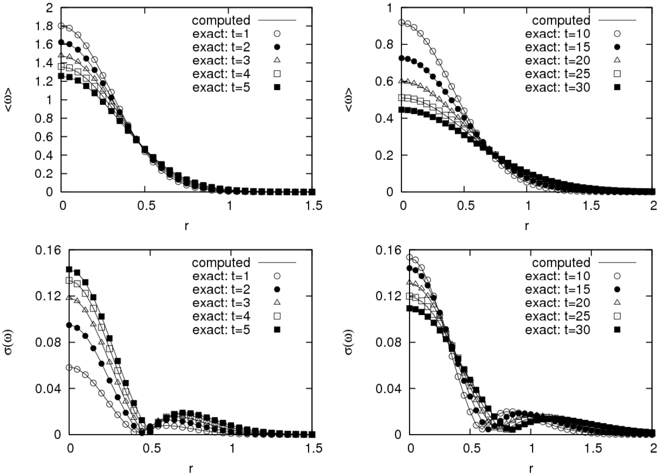
$$\omega(\boldsymbol{x}, t = 0) = \frac{\exp[-\|\boldsymbol{x}\|^2/d]}{\pi d},$$

$$\nu = 0.005 + 0.0025\xi, \quad \xi \sim U(-1, 1).$$

Discretization

- $\epsilon = 0.05$, remeshing every 10 iterations.
- Simulation for $t \in [0, 30]$, $\Delta t = 0.02$ with RK-3.
- Velocities computed with particle-mesh scheme $h_g = \epsilon$.
- Wiener Legendre expansion with $\mathrm{No} = 5$.
- Check the invariants of the flow.

Mean and Standard deviation of $\omega(\boldsymbol{x}, t, \xi)$.



Mean (top row) and standard deviation (bottom row) at different times.

Results (III) Natural convection problem

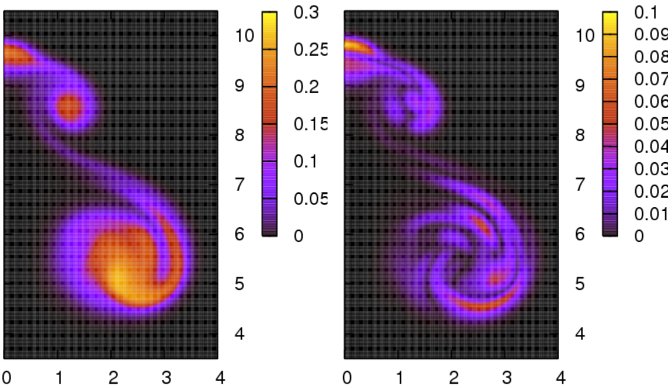
Equations

- Evolution of a compact hot patch of air in infinite medium.
- Boussinesq approximation: incompressible Navier-Stokes + buoyancy terms and heat transport equation.
- Uncertainty and the Rayleigh number in the $\mathrm{Ra} \sim U[2.10^5, 3.10^5]$.

Discretization

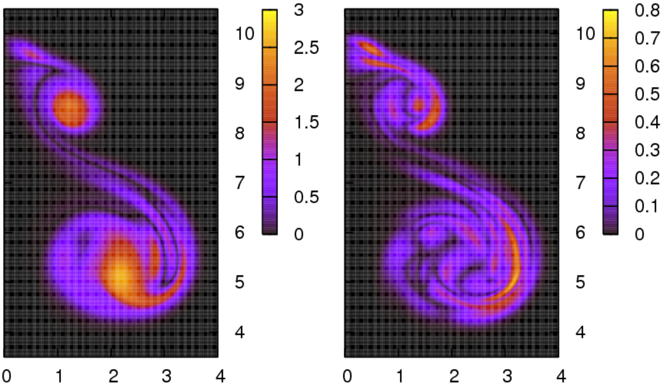
- $\epsilon = 1/30$.
- Simulation for $t \in [0, 28]$, $\Delta t = 0.2$ with RK-2.
- Remeshing every 4 iterations: $\mathrm{Np} > 200,000$ at the end of the simulation.
- Velocities computed with particle-mesh scheme $h_g = \epsilon$.
- Wiener Legendre expansion with up to $\mathrm{No} = 12$.

Mean and Standard deviation of the temperature field.



Temperature mean (left) and standard deviation (right)at $t = 20$.

Mean and Standard deviation of the vorticity field.



Vorticity mean (left) and standard deviation (right)at $t = 20$.

Return