Introduction

Spectral UQ

Examples : Fluid flows

Advanced Topics Conclusive remarks

Méthodes Spectrales pour la Propagation et la Quantification d'Incertitudes Applications aux Écoulements

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Journées Incertitudes, 10/2007

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- Simulation and errors
- Data uncertainty
- Alternative UQ methods

2 Spectral UQ

- Generalized PC expansion
- Application to spectral UQ
- Solution Techniques
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 - Multi-resolution-analysis
 - Adaptive Techniques
 - A posterior error estimation
 - Conclusive remarks

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Simulation and errors				

Simulation framework.

Basic ingredients

- Understanding of the physics involved (optional ?) : selection of the mathematical model.
- Numerical method(s) to solve the model.
- Specify a set of data :

select a system among the class spanned by the model.

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Simulation and errors				

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Simulation errors

- Model errors : physical approximations and simplifications.
- Numerical errors : discretization, approximate solvers, finite arithmetics.
- **Data error** : boundary/initial conditions, model constants and parameters, external forcings, ...

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Data uncertainty				

Sources of data uncertainty

- Inherent variability (e.g. industrial processes).
- Epistemologic uncertainty (e.g. model constants).
- May not be fully reductible, even theoretically.

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Data uncertainty				

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Probabilistic framework

- Define an abstract probability space $(\Omega, \mathcal{A}, d\mu)$.
- Consider data *D* as random quantity : $D(\omega), \ \omega \in \Omega$.
- Simulation output *S* is random and on $(\Omega, \mathcal{A}, d\mu)$.

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- Consider data *D* as random quantity : $D(\omega)$, $\omega \in \Omega$.
- Simulation output *S* is random and on $(\Omega, \mathcal{A}, d\mu)$.
- Data *D* and simulation output *S* are dependent random quantities (through the mathematical model *M*):

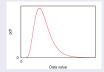
$$\mathcal{M}(\mathcal{S}(\omega), \mathcal{D}(\omega)) = \mathbf{0}, \quad \forall \omega \in \Omega.$$

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Data uncertainty

Propagation and Quantification of data uncertainty

Data density

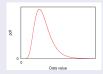


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Data uncertainty

Propagation and Quantification of data uncertainty

Data density



$$\mathcal{M}(S,D) = 0$$

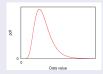
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Data uncertainty

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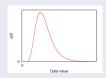
Solution density



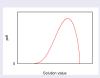




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Propa	agation and	Quantification of d	lata uncertainty	
Dat	ta density		Solution of	density



 $\mathcal{M}(S,D)=0$



- Variability in model output : numerical error bars.
- Assessment of predictability.
- Support decision making process.
- What type of information (abstract quantities, confidence intervals, density estimations, structure of dependencies, ...) one needs?

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Alternative LIO metho	de			

Deterministic methods

- Sensitivity analysis (adjoint based, AD, ...) : local.
- Perturbation techniques : limited to low order and simple data uncertainty.
- Neuman expansions : limited to low expansion order.
- Moments method : closure problem (non-Gaussian / non-linear problems).

Simulation techniques

Monte-Carlo

Spectral Methods

Spectral UQ

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Alternative UQ methods

Deterministic methods

Simulation techniques

Monte-Carlo

- Generate a sample set of data realizations and compute the corresponding sample set of model ouput.
- Use sample set based random estimates of abstract characterizations (moments, correlations, ...).
- Plus : Very robust and re-use deterministic codes : (parallelization, complex data uncertainty).
- Minus : **slow convergence of the random estimates** with the sample set dimension.

Spectral Methods

Alternative UQ methods

Deterministic methods

Simulation techniques

Monte-Carlo

Spectral Methods

- Parametrization of the data with random variables (RVs).
- \perp projection of solution on the space spanned by the RVs.
- Plus : arbitrary level of uncertainty, deterministic approach, convergence rate, information contained.
- Minus : parametrizations (limited # of RVs), adaptation of simulation tools (legacy codes), robustness (non-linear problems, non-smooth output, ...).
- Constant developments and improvements (be faithfull !).

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Polynomial Chaos expansion



Any well behaved RV $\theta(\omega)$ (*e.g.* 2nd order one) defined on $(\Omega, \mathcal{A}, d\mu)$ has a **convergent expansion** of the form :

$$\theta(\omega) = u_0 \Gamma_0 + \sum_{i_1=1}^{\infty} \theta_{i_1} \Gamma_1(\xi_{i_1}(\omega)) + \sum_{i_1=1}^{\infty} \sum_{i_2=1}^{i_1} \theta_{i_1,i_2} \Gamma_2(\xi_{i_1}(\omega),\xi_{i_2}(\omega))$$

+
$$\sum_{i_1=1}^{\infty} \sum_{i_2=1}^{i_1} \sum_{i_3=1}^{i_2} \theta_{i_1,i_2,i_3} \Gamma_3(\xi_{i_1}(\omega),\xi_{i_2}(\omega),\xi_{i_3}(\omega)) + \dots$$

- $\{\xi_1, \xi_2, \ldots\}$: independent normalized Gaussian RVs.
- Γ_p polynomials with degree p, orthogonal to Γ_q, ∀q < p.
- Convergence in the **mean square sense** (Cameron and Martin, 1947).

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Generalized PC expansion

Polynomial Chaos expansion

Wiener-1938

Truncated PC expansion at order *p* and *n* RVs :

$$\theta(\omega) \approx \sum_{k=0}^{P} \theta_k \Psi_k(\boldsymbol{\xi}(\omega)), \quad \boldsymbol{\xi} = \{\xi_1, \dots, \xi_n\}, \quad \mathbf{P} = \frac{(n+p)!}{n!p!}.$$

- $\{\theta_k\}_{k=0,\dots,P}$: **deterministic** expansion coefficients,
- {Ψ_k}_{k=0,...,P} : ⊥ random polynomials for the inner product defined with the density of ξ as weight :

$$\begin{array}{ll} \langle \Psi_{k}\Psi_{l}\rangle &\equiv& \int_{\Omega}\Psi_{k}(\boldsymbol{\xi}(\omega))\Psi_{l}(\boldsymbol{\xi}(\omega))d\mu(\omega)\\ &=& \int\Psi_{k}(\boldsymbol{\xi})\Psi_{l}(\boldsymbol{\xi})p(\boldsymbol{\xi})d\boldsymbol{\xi}=\delta_{kl}\left\langle \Psi_{k}^{2}\right\rangle. \end{array}$$

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Polynomial Chaos expansion

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angle &\equiv& \int_\Omega \Psi_k(m{\xi}(\omega)) \Psi_l(m{\xi}(\omega)) d\mu(\omega) \ &=& \int \Psi_k(m{\xi}) \Psi_l(m{\xi}) p(m{\xi}) dm{\xi} = \delta_{kl} \left< \Psi_k^2 \right>. \end{array}$$

• $p(\xi) = \prod_{i=1}^{n} \frac{\exp(-\xi_i^2/2)}{\sqrt{2\pi}} \Longrightarrow \Psi_k(\xi)$: Hermite polynomials

Wiener-1938

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Polynomial Chaos expansion

Wiener-1938

Truncated PC expansion :

$$\theta(\omega) \approx \sum_{k=0}^{P} \theta_k \Psi_k(\boldsymbol{\xi}(\omega)).$$

- Convention $\Psi_0 \equiv 1$: mean mode.
- **Expectation** of θ :

$$\boldsymbol{E}[\theta] \equiv \int_{\Omega} \theta(\omega) d\mu(\omega) \approx \sum_{k=0}^{\mathrm{P}} \theta_k \int_{\Omega_{\boldsymbol{\xi}}} \Psi_k(\boldsymbol{\xi}) \boldsymbol{p}(\boldsymbol{\xi}) d\boldsymbol{\xi} = \theta_0.$$

• Variance of θ :

$$V[\theta] = E[\theta^2] - E[\theta]^2 \approx \sum_{k=1}^{\mathrm{P}} \theta_k^2 \langle \Psi_k \Psi_k \rangle.$$

Extension to random vectors & stochastic processes :

$$\begin{pmatrix} \theta_1 \\ \vdots \\ \theta_m \end{pmatrix} (\omega, \boldsymbol{x}, t) \approx \sum_{k=0}^{P} \begin{pmatrix} \theta_1 \\ \vdots \\ \theta_m \end{pmatrix}_k (\boldsymbol{x}, t) \, \Psi_k(\boldsymbol{\xi}(\omega))$$

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Generalized PC expansion

Generalized PC expansion

Xiu and Karniadakis-2002

Askey	scheme
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Distribution of ξ_i	Polynomial familly
Gaussian	Hermite
Uniform	Legendre
Exponential	Laguerre
β -distribution	Jacobi

Also : discrete RVs (Poisson process).

$$heta(\omega) pprox \sum_{k=0}^{\mathrm{P}} heta_k \Psi_k(m{\xi}(\omega))$$

where Ψ_k : classical (or mixture of) polynomials.

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Application to spectral UQ

Data parametrization

Parametrization of *D* using $N < \infty$ independent RVs with prescribed distribution $p(\xi)$:

$$D(\omega) = D(\boldsymbol{\xi}(\omega)), \quad \boldsymbol{\xi} = (\xi_1, \dots, \xi_N) \in \Omega_{\boldsymbol{\xi}}.$$

- Transformation of random variables : $D(\omega)$ RV.
- Karhunen-Loève expansion : $D(\mathbf{x}, \omega)$ stochastic process.
- Independent components analysis.

Model

Solution expansion

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Data parametrization

Model

We assume that $\forall \boldsymbol{\xi}(\omega) \in \Omega_{\boldsymbol{\xi}}$, the problem $\mathcal{M}(\boldsymbol{S}, \boldsymbol{D}(\boldsymbol{\xi}(\omega)) = \boldsymbol{0}$

- is well-posed,
- 2 has a unique solution, denoted $S(\xi(\omega))$,

and that the random solution $S \in L_2(\Omega_{\xi}, p_{\xi})$:

$$\left\langle \mathcal{S}^2 \right
angle = \int_\Omega \mathcal{S}^2(oldsymbol{\xi}(\omega)) d\mu(\omega) = \int_{\Omega_\xi} \mathcal{S}^2(oldsymbol{\xi}) p(oldsymbol{\xi}) doldsymbol{\xi} < +\infty.$$

Solution expansion

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Data parametrization

Model

Solution expansion

Let $\{\Psi_0, \Psi_1, \ldots\}$ be a Hilbert basis of $L_2(\Omega_{\xi}, p_{\xi})$ then

$$S(\boldsymbol{\xi}(\omega)) = \sum_{k} S_{k} \Psi_{k}(\boldsymbol{\xi}(\omega)).$$

- Knowledge of the spectral coefficients S_k fully determine the random solution.
- Makes explicit the dependence between $D(\xi)$ and $S(\xi)$.

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- Knowledge of the spectral coefficients S_k fully determine the random solution.
- Makes explicit the dependence between $D(\xi)$ and $S(\xi)$.
- Need efficient procedure to compute the S_k.

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Solution Technic	lues			
Non	intrusive tecl	hniques		
		nate spectral coeffi nodel solutions.	cients <i>via</i> a set o	of
•	Requires a <mark>de</mark>	terministic solver o	nlv	

- Overcome issues related to non-linearities.
- Suffers from the curse of dimensionnality.

Galerkin projection

- Weak solution of the stochastic problem $\mathcal{M}(S, D) = 0$.
- Needs adaptation of deterministic codes.
- Usually more efficient than NI techniques.
- Better suited to improvement (error estimate, optimal and basis reduction, ...), thanks to spectral theory and functional analysis.



- ① Introduce truncated expansions in model equations.
- ^② Require residual to be \perp to the subspace.

$$\left\langle \mathcal{M}\left(\sum_{k=0}^{\mathsf{P}} S_k \Psi_k(\boldsymbol{\xi}), D(\boldsymbol{\xi})\right) \Psi_m(\boldsymbol{\xi}) \right\rangle = 0 \quad \text{for } m = 0, \dots, \mathsf{P}.$$

Set of P + 1 **coupled** problems.

Plus

- Implicitly account for modes' coupling.
- Often inherit properties of the deterministic model.

Minus

- Requires adaptation of deterministic solvers.
- Treatment of non-linearities.

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Examples of Application to Fluid Flows

- Natural convection : Boussinesq approximation Goto example
- Natural convection : Low-Mach approximation Goto example
- Electrophoresis : coupled physical problems
 Goto example
- Lagrangian formulation :

particle method • Goto example

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Multi-resolution-ar	nalysis			
Motivatio	ns			

GPC expansions fail for some problems because of :



- Non-linearities requiring large polynomial orders for global approximation over uncertainty range.
- Non-smooth or steep dependences of the solution w.r.t. the uncertain data (*e.g.* parametric bifurcations, absolute value, threshold effect, ...).
- ③ Oscillating character of the polynomials.

Response :

Le Maître et al, JCPs (2004).

Wiener-type orthogonal expansion (multiwavelets) using Multi-Resolution-Analysis

- ✓ Piecewise polynomial.
- ✓ Convergence in polynomial order and resolution level.
- ✓ Discontinuous dependences.
- ✓ Local control of the resolution.
- ✓ Adaptive strategy.

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Multi-resolution-anal	veie			

Multi-resolution space

For No = 0, 1, ... and $k = 0, 1, ..., \mathbf{V}_k^{\text{No}}$ is the space of **piecewise polynomial functions** $f : x \in [-1, 1] \mapsto \mathbb{R}$:

$$\mathbf{V}_k^{ ext{No}} \equiv \left\{ f: ext{ the restriction of } f ext{ on } (2^{-k}l, 2^{-k}(l+1)) \in \mathbb{P}_{ ext{No}}
ight.$$
for $l = 0, \dots, 2^k - 1
ight\}$,

where \mathbb{P}_{No} is the space of polynomials with degree $\leq \mathrm{No}.$ We have :

•
$$Dim(\mathbf{V}_k^{No}) = (No + 1)(2^k),$$

• $\mathbf{V}_0^{No} \subset \mathbf{V}_1^{No} \subset \cdots \subset \mathbf{V}_k^{No} \subset \cdots$

• $\mathbf{V}^{\text{No}} \equiv \overline{\bigcup}_{k \ge 0} \mathbf{V}_k^{\text{No}}$ is dense in $L_2([0, 1])$ with the scalar product

$$\langle f,g\rangle=\int_0^1f(x)g(x)dx.$$

Multi-way	velet space			
Multi-resolution-ar	nalysis			
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Let us denote \mathbf{W}_{k}^{No} , k = 0, 1, 2, ..., the orthogonal complement of \mathbf{V}_{k}^{No} in \mathbf{V}_{k+1}^{No} :

$$\mathbf{V}_{k}^{\mathrm{No}} \oplus \mathbf{W}_{k}^{\mathrm{No}} = \mathbf{V}_{k+1}^{\mathrm{No}}, \quad \mathbf{W}_{k}^{\mathrm{No}} \perp \mathbf{V}_{k}^{\mathrm{No}},$$

SO

$$\mathbf{V}_0^{\mathrm{No}} \bigoplus_{k \ge 0} \mathbf{W}_k^{\mathrm{No}} = L^2([0,1]).$$

Let $\{\psi_0,\psi_1,\ldots,\psi_{No}\}$ be an orthonormal basis of \bm{W}_0^{No} :

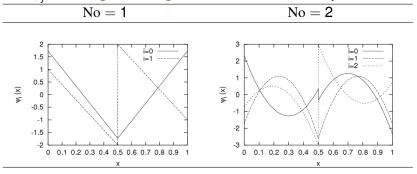
$$\langle \psi_i(\mathbf{x}), \psi_j(\mathbf{x}) \rangle = \delta_{ij},$$

and since $\mathbf{W}_0^{\mathrm{No}} \perp \mathbf{V}_0^{\mathrm{No}}$ we have

$$\left\langle \psi_j, \boldsymbol{x}^i \right\rangle = \mathbf{0}, \quad \mathbf{0} \leq i, j \leq \mathrm{No}.$$



The ψ_i are the **generating functions** of the MRA system.



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The ψ_i are the **generating functions** of the MRA system.

Multi-wavelets

 ψ_i

$$\psi_{jl}^{k}(x) = 2^{k/2}\psi_{j}(2^{k}x - l), \quad j = 0, \dots, \text{No}, \text{ and } l = 0, \dots, 2^{k} - 1.$$

• Supp
$$(\psi_{jl}^k) = [2^{-k}l, 2^{-k}(l+1)].$$

•
$$\left\langle \psi_{il}^{k}, \psi_{jm}^{k'} \right\rangle = \delta_{ij} \delta_{lm} \delta_{kk'}.$$

Basis of V_0^{No}

Legendre polynomials

$$\phi_i(x) = rac{\mathcal{L}e_i(2x-1)}{L_i}, \quad i = 0, 1, \dots, \mathrm{No}, \ \langle \phi_i(x), \phi_j(x)
angle = \delta_{ij} ext{ for } i, j = 0, \dots, \mathrm{No}.$$



Let us denote $f^{No,Nr}$ the projection of f on \mathbf{V}_{Nr}^{No} :

$$f^{\mathrm{No,Nr}}(x) \equiv \mathcal{P}_{\mathrm{Nr}}^{\mathrm{No}}[f] = \sum_{i=0}^{\mathrm{No}} f_i \psi_i(x) + \sum_{k=0}^{\mathrm{Nr}-1} \sum_{l=0}^{2^k-1} \left(\sum_{i=0}^{\mathrm{No}} \delta f_{il}^k \psi_{il}^k(x) \right),$$

where

$$f_{i} = \langle f, \phi_{i} \rangle$$
, and $\delta f_{il}^{k} = \left\langle \left\{ \mathcal{P}_{k+1}^{\mathrm{No}}\left[f\right] - \mathcal{P}_{k}^{\mathrm{No}}\left[f\right] \right\}, \psi_{il}^{k} \right\rangle$.

For $f \in L_2([0, 1])$, the projection error can be made arbitrarily small by increasing the expansion order No and/or resolution level Nr.

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Multi-resolution-analysis

Application of MRA to UQ

One-dimensional case

- $\xi(\omega)$: RV with density $pdf(\xi)$, CDF $q(\xi) = \int_{-\infty}^{\xi} pdf(\xi') d\xi'$.
- $\theta(\xi) \in L_2(\Omega_{\xi}).$
- $\theta(\xi) = \theta(q^{-1}(x)) = \widetilde{\theta}(x)$ for $x \sim U(0, 1)$.
- $\widetilde{\theta}(x) \in L_2([0,1]).$

$$\widetilde{ heta}(x(\omega)) \approx \sum_{k} \widetilde{ heta}_{k} W_{k}(x(\omega)), \quad x \sim U(0,1),$$

 W_k elements of the MRA system.

Multi recolution of				
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Application of MRA to UQ

N-dimensionnal case

• Proceed by tensorization of 1-D MRA system.

•
$$\tilde{\theta}(\boldsymbol{x}) \equiv \tilde{\theta}(\boldsymbol{x}_1, \dots, \boldsymbol{x}_N) \approx \sum_{\boldsymbol{k}} \tilde{\theta}_{\boldsymbol{k}} \mathcal{M}^{\boldsymbol{w}}_{\boldsymbol{k}}(\boldsymbol{x}_1, \dots, \boldsymbol{x}_N).$$

•
$$\mathcal{M}^{w}_{\mathbf{k}}(\mathbf{x}) = W_{k_{1}}(x_{1}) \times \cdots \times W_{k_{N}}(x_{N}).$$

Summary

- Expansion in terms of CDF of random parameters.
- Piecewise polynomial approximation.
- Error reduction through *p* (No) or *h* (Nr) refinement.
- Fast increase with No, Nr and N of approximation space's dimension (calls for adaptive techniques).



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Rayleigh-Bénard Instability

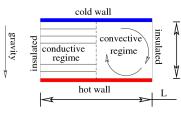
- * Aspect ratio : A = L/H = 2;
- * Prandtl number : $\Pr = \frac{\mu C_{P}}{\kappa} = 0.7$;
- * Rayleigh number : Ra = $\frac{\rho g \beta \Delta T H^3}{\mu \kappa}$

Model : **Boussinesq equations.** Parameter and uncertainty :

- Ra = 2150 (slightly above critical)
- $\Theta_{\text{hot}}(\xi) = \frac{1}{2} + 0.2\xi$, ξ U.D. in [-1, 1]

Both conductive **and** convective regimes are explored.

The process has a **discontinuity** in the uncertainty range.



Spectral UQ

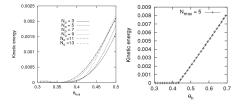
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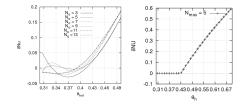
Multi-resolution-analysis

Comparison Legendre / Wiener-Haar (Nr = 5) solutions.

Kinetic energy as function of $\theta_{hot}(\xi)$.

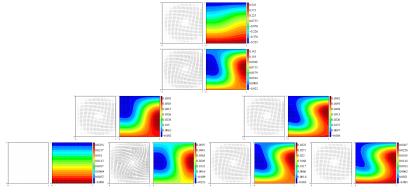


Heat transfer enhancement as a function of $\theta_{hot}(\xi)$.



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Hierarchy of velocity and temperature modes (Wiener-Haar)



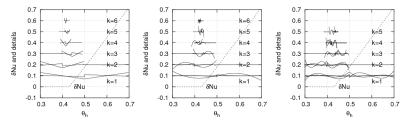
Cold

Hot

00000 Multi-resolution-a	000000		000000000000000000000000000000000000000	00000
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Heat-transfer enhancement (from conduct. solution).

Adaptive MRA scheme for No = 1, 2 and 3



Only details around critical points are computed.

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Limitations of MRA

- ✓ Fast increase of the basis dimension with No and resolution level Nr.
- Adaptivity possible but quickly cumbersome with increasing N(number of stochastic dimensions).

A More efficient approach

Remark : Spectral problems present **no differential operator along stochastic dimensions**. (Model solutions for different data are independent)

⇒ Strongly suggests a **domain decomposition** technique in the parameter space $\Omega_{\xi} = [0, 1]^{N}$.

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Adaptive Techniques

Partition of the random parameter space

Domain decomposition.

- Basic principle : zooming.
 - $\checkmark\,$ Define a generic expansion basis for $[0,1]^{\rm N}$:

N-Dimensional Legendre basis

1-D first resolution level Multi-Wavelets.

- ✓ Rescale and translate this basis to expand locally the solution on non-overlapping sub-domains Ω_i ⊂ [0, 1]^N.
- ✓ Decide if the expansion is sufficient over Ω_i ; If not :

break it into smaller sub-domains along under-resolved dimensions only

✓ Refinement strategy based on 1-D details.

Introduc 00000	tion	Spectral UQ 000000	Examples : Fluid flows	Advanced Topics	Conclusive remarks
Adaptive	e Techniques				

Reaction surface problem

No = 3

Convergence with ϵ_r :

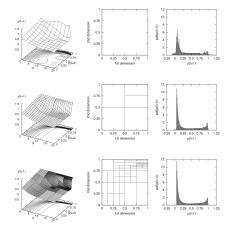
Governing equations :

$$\begin{cases} \frac{d\rho}{dt} = \alpha(1-\rho) - \gamma\rho \\ -\beta(\rho-1)\rho^2 \\ \rho(t=0) = \rho_0 \end{cases}$$

Uncertainty

✓ $\rho_0 \sim U(0, 1)$. ✓ $\beta \sim U(0, 20)$. ✓ ρ_0, β ind. RVs.

 \Rightarrow 2 Stochastic dim.



Applied for up to 8 stochastic dimensions and a complex chemical mechanism (Le Maître *et al*, J. Sci. Comp. 2007.)

Introduction	Spectral UQ 000000	Examples : Fluid flows	Advanced Topics	Conclusive remarks	
A posterior error estimation					

(Lionel Mathelin, LIMSI-CNRS)

Objective : design less heuristic criteria / error indicator.

Variational framework

Solve for $U(\mathbf{x} \in \Omega_x, \mathbf{\xi} \in \Omega_{\mathbf{\xi}}) \in \mathcal{V}_{\mathbf{x}} \otimes \mathcal{V}_{\mathbf{\xi}}$

$$oldsymbol{A}(U;\Phi|D)=oldsymbol{B}(\Phi|D)\quad orall\Phi\in\mathcal{V}_{oldsymbol{x}}\otimes\mathcal{V}_{oldsymbol{\xi}},$$

where :

- \mathcal{V}_x suitable deterministic Hilbert space,
- $\mathcal{V}_{\xi} \equiv L_2(\Omega_{\xi}, p_{\xi})$ space of 2nd order RV,
- $A(U;\Phi|D) = \int_{\Omega_{\xi}} a(U(\xi);\Phi(\xi)|D(\xi))p_{\xi}(\xi)d\xi,$
- $B(\Phi|D) = \int_{\Omega_{\xi}} b(\Phi(\xi)|D(\xi)) p_{\xi}(\xi) d\xi$,
- *a*(.;.|.) a deterministic semi-linear form,
- b(.|.) a linear form.

Introduction	Spectral UQ	Examples : Fluid flows	Advance

Advanced Topics Conclusive remarks

A posterior error estimation

Deterministic finite element space

•
$$\Omega_x = \bigcup_{l=1}^{N_x} \Omega_x^{(l)}$$
.
• $U^h(x \in \Omega_x^{(l)}) = \sum_{i=1}^{\mathrm{Nd}(l)} U_i^{(l)} \mathcal{N}_i^{(l)}(x)$.
 $\mathcal{V}_x^h = \mathrm{span}\left(\{\mathcal{N}_i^{(l)}\}, \ 1 \le l \le N_x, \ 1 \le i \le \mathrm{Nd}(l)\right)$.

Stochastic space

•
$$\Omega_{\xi} = \bigcup_{m=1}^{Nb} \Omega_{\xi}^{(m)},$$

• $\Omega_{\xi}^{(m)} = [\xi_{1}^{(m),-},\xi_{1}^{(m),+}] \times \cdots \times [\xi_{N}^{(m),-},\xi_{N}^{(m),+}],$
• $U^{h}(\xi \in \Omega_{\xi}^{(m)}) = \sum_{k=0}^{P(m)} u_{k}^{(m)} \Psi_{k}^{(m)}(\xi),$
 $\overline{\mathcal{V}_{\xi}^{h}} = \operatorname{span}\left(\left\{\Psi_{k}^{(m)}\right\}, \ 1 \le m \le Nb, \ 0 \le k \le P(m)\right)$

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Approximation space

$$\mathcal{V}^h = \mathcal{V}^h_x \otimes \mathcal{V}^h_\xi.$$

The approximate solution at point (x, ξ) of $\Omega \equiv \Omega_x \times \Omega_{\xi}$, is $U^h\left(x \in \Omega_x^{(l)}, \xi \in \Omega_{\xi}^{(m)}\right) = \sum_{i=1}^{\operatorname{Nd}(l)} \sum_{k=0}^{\operatorname{P}(m)} u_{i,k}^{(l,m)} \mathcal{N}_i^{(l)}(x) \Psi_k^{(m)}(\xi)$ and solves

$$\mathcal{A}(U^h;\Phi^h|D^h)=\mathcal{B}(\Phi^h|D^h)\quad orall \Phi^h\in\mathcal{V}^h.$$

Error estimation

For $\mathcal{J} : \Omega_x \times \Omega_{\xi} \mapsto \mathbb{R}$, the approximation error is measured as $\eta = \left| \mathcal{J}(U) - \mathcal{J}(U^h) \right|$.

The exact solution being unknown η has to be estimated.

Introduction	Spectral UQ	Examples : Fluid flows	Advanced Topics	Conclusive remarks
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Dual-based error estimate

$$\mathcal{J}(\boldsymbol{U}) - \mathcal{J}(\boldsymbol{U}^h) \approx \boldsymbol{B}(\widetilde{\boldsymbol{Z}} - \boldsymbol{Z}^h | \boldsymbol{D}^h) - \boldsymbol{A}(\boldsymbol{U}^h; \widetilde{\boldsymbol{Z}} - \boldsymbol{Z}^h | \boldsymbol{D}^h),$$

where

• Z^h is the approximate dual solution satisfying $\mathcal{J}'(U^h; \Phi) - \mathcal{A}'(U^h; \Phi, Z^h | D^h) = 0 \quad \forall \Phi \in \mathcal{V}^h,$

• $\widetilde{Z} \in \mathcal{V}^{\widetilde{h}} \supset \mathcal{V}^{h}$ an estimate of the exact dual solution : $\mathcal{J}'(U^{h}; \widetilde{\Phi}) - A'(U^{h}; \widetilde{\Phi}, \widetilde{Z} | D^{\widetilde{h}}) = 0 \quad \forall \widetilde{\Phi} \in \mathcal{V}^{\widetilde{h}}.$

In practice : \mathcal{V}^h is constructed by increasing the stochastic and finite element orders of \mathcal{V}^h .

Remark : Dual problems are linear, primes denote Gateau derivatives :

$$\mathcal{J}'(\boldsymbol{U}, \Phi) = \lim_{\epsilon o 0} rac{\mathcal{J}(\boldsymbol{U}) - \boldsymbol{J}(\boldsymbol{U} + \epsilon \Phi)}{\epsilon}$$

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Local error estimate

$$\eta = \left| \mathcal{J}(U) - \mathcal{J}(U^h) \right| \leq \sum_{l=1}^{N_x} \sum_{m=1}^{Nb} \eta_{l,m},$$

where $\eta_{l,m}$ is the local contribution of $\left(\Omega_x^{(l)} \times \Omega_{\xi}^{(m)}\right)$ to the aposteriori error estimation.

To ensure $\eta < \epsilon$, the approximation space \mathcal{V}^h is refined such that

$$\eta_{l,m} < \frac{\epsilon_{\eta}}{N_x N b} = \epsilon, \quad \forall l, m \in [1, N_x] \times [1, N b].$$

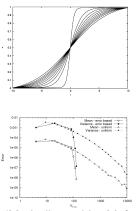
Refinement scheme

- Refine \mathcal{V}_x or \mathcal{V}_{ξ} ?
- What type of refinement : h or p?
- If h_ξ, then along which stochastic dimension(s)?

Introduction	Spectral UQ	Examples : Fluid flows	Advanced Topics	Conclusive remarks
A posterior error estimation				

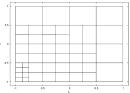
Example : Burger's equation with uncertain viscosity (N = 2).

- \mathcal{V}_{x}^{h} : 10 spectral finite elements (order 15).
- Stochastic order No = 2 with isotropic h_{ξ} -refinement.



$$u(\theta)\frac{\partial u(\theta)}{\partial x} = \nu(\theta)\frac{\partial^2 x(\theta)}{\partial x^2}$$

Errors on computed mean and variance as a function of the number of primal and dual problems solved. Comparison of adaptive and uniform refinements.



(Mathelin and Le Maître, Com. Appl. Math and Comp., 2007)

Introduction	Spectral UQ 000000	Examples : Fluid flows	Advanced Topics	Conclusive remarks
A posterior error estimation				
Outline				



Introduction

- Simulation and errors
- Data uncertainty
- Alternative UQ methods
- 2 Spectral UQ
 - Generalized PC expansion
 - Application to spectral UQ
 - Solution Techniques
 - Examples : Fluid flows
- Advanced Topics
 - Multi-resolution-analysis
 - Adaptive Techniques
 - A posterior error estimation
 - Conclusive remarks

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Improvement of Spectral UQ

- Computational efficiency (steady-solvers, pre-conditioning, multigrid techniques,...).
- Development of directional error estimates to improve adaptive techniques.
- Construction of reduced basis.
- Adaptive non-intrusive technique.

Open problems

- Existence/treatment of multiple solutions !
- Stochastic eigen-value problems (many issues remaining to be addressed).
- ...

Introduction 00000	Spectral UQ	Examples : Fluid flows	Advanced Topics	Conclusive remarks
Acknowl	ormonto			

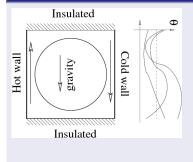
- Omar Knio, The Johns Hopkins University (Baltimore).
- Roger Ghanem, University of Southern California (Los Angeles).
- Habib Najm and Bert Debusschere, Sandia National Labs (Livermore).
- Lionel Mathelin, LIMSI (Orsay).
- Jean-Marc Martinez, CEA (saclay).

Boussinesq approximation

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

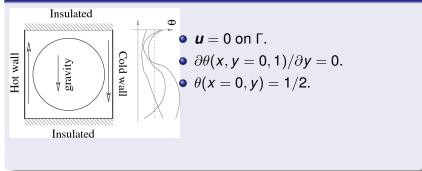
Boussinesq approximation

Governing equations



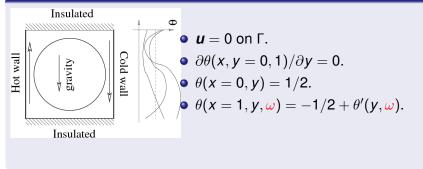
Boussinesq approximation

Governing equations



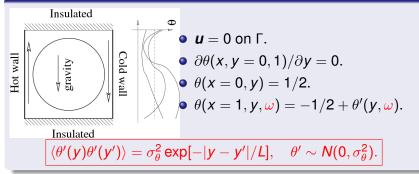
Boussinesq approximation

Governing equations



Boussinesq approximation

Governing equations



BC and solution representations

$$egin{aligned} η'(m{y},m{\xi}) = \sum_{i=1}^{\mathrm{N}} \sqrt{\lambda_i} \widetilde{ heta}_i(m{y}) \xi_i = \sum_{k=0}^{\mathrm{P}} heta_k(m{y}) \Psi_k(m{\xi}). \ & (m{u},m{p}, heta)(m{\xi}) = \sum_{k=0}^{\mathrm{P}} (m{u},m{p}, heta)_k \Psi_k(m{\xi}). \end{aligned}$$

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

Galerkin projection

Implementation and solver

BC and solution representations

Galerkin projection

$$\frac{\partial \boldsymbol{u}_{i}}{\partial t} + \sum_{j=0}^{P} \sum_{k=0}^{P} \boldsymbol{u}_{j} \cdot \boldsymbol{\nabla} \boldsymbol{u}_{k} \frac{\langle \boldsymbol{\Psi}_{i} \boldsymbol{\Psi}_{j} \boldsymbol{\Psi}_{k} \rangle}{\langle \boldsymbol{\Psi}_{i} \boldsymbol{\Psi}_{i} \rangle} = -\boldsymbol{\nabla} \boldsymbol{p}_{i} + \frac{\Pr}{\sqrt{\operatorname{Ra}}} \boldsymbol{\nabla}^{2} \boldsymbol{u}_{i} + \Pr \theta_{i} \boldsymbol{y}$$
$$\frac{\partial \theta_{i}}{\partial t} + \sum_{j=0}^{P} \sum_{k=0}^{P} \boldsymbol{u}_{j} \cdot \boldsymbol{\nabla} \theta_{k} \frac{\langle \boldsymbol{\Psi}_{i} \boldsymbol{\Psi}_{j} \boldsymbol{\Psi}_{k} \rangle}{\langle \boldsymbol{\Psi}_{i} \boldsymbol{\Psi}_{i} \rangle} = \frac{1}{\sqrt{\operatorname{Ra}}} \boldsymbol{\nabla}^{2} \theta_{i}$$
$$\boldsymbol{\nabla} \cdot \boldsymbol{u}_{i} = 0$$

- P + 1 coupled momentum and energy equations.
- 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.

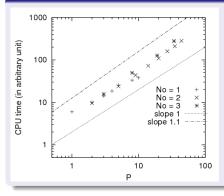
Incompressibility Treatment

- Prediction / Projection method (Chorin).
- FFT based solver for the elliptic pressure equations.

CPU : essentially projection of uncoupled modes :

Stochastic \simeq (P + 1) \times deterministic.

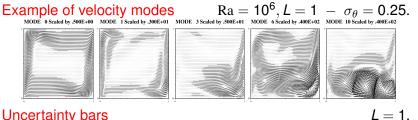
Convergence and performance



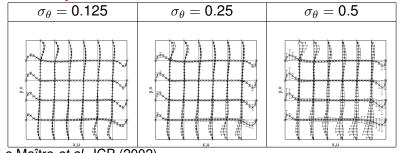
Le Maître et al, JCP (2001).

(unsteady solver)

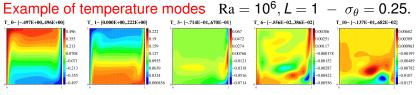
- N = 4 \sim 6 is enough for $L \ge 1/3$.
- No = 3 \rightarrow relative error on variance $< 10^{-4}$.
- ~ 1000 times more efficient than MC (LHS).
- \sim 10 times more efficient than NISP + GH quadrature.



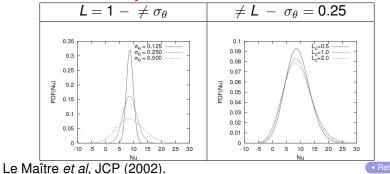
Uncertainty bars



Le Maître et al, JCP (2002).



Heat-transfert density



Appendix

Natural convection

Low-Mach approximation

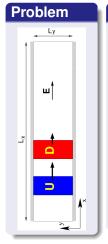
- Formulation (Najm et al, J. Comp. Phys., 1998 & 1999). $\frac{\partial \rho}{\partial t} = \frac{1}{\gamma T} \frac{dP}{dt} + \frac{1}{T} \left(\rho \boldsymbol{u} \cdot \boldsymbol{\nabla} T - \frac{1}{\Pr \sqrt{Ra}} \boldsymbol{\nabla} \cdot (\kappa \boldsymbol{\nabla} T) \right)$ $\frac{dP}{dt} = -\gamma \int_{\Omega} \frac{1}{T} \left(\rho \boldsymbol{u} \cdot \boldsymbol{\nabla} T - \frac{1}{\Pr \sqrt{Ra}} \boldsymbol{\nabla} \cdot (\kappa \boldsymbol{\nabla} T) \right) d\Omega / \int_{\Omega} \frac{1}{T} d\Omega$ $\frac{\partial \rho u}{\partial t} = -\frac{\partial \rho u^2}{\partial x} - \frac{\partial \rho u v}{\partial y} - \frac{\partial \Pi}{\partial x} + \frac{1}{\sqrt{Ra}} \Phi_x$ $\frac{\partial \rho \mathbf{v}}{\partial t} = -\frac{\partial \rho u \mathbf{v}}{\partial \mathbf{x}} - \frac{\partial \rho \mathbf{v}^2}{\partial \mathbf{y}} - \frac{\partial \Pi}{\partial \mathbf{y}} + \frac{1}{\sqrt{Ra}} \Phi_{\mathbf{y}} - \frac{1}{Pr} \frac{\rho - 1}{2\epsilon}$ $T = \frac{P}{-}$
- Difficulty : non-linearities
- **D** Exact inversion of the Galerkin product.
- **Exact mass-conservation** (mean sense is not enough).

Le Maître et al., J. Sci. Comp., 2004.



Electrophoresis

Debusschere et al, Phys. Fluids (2003)



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.



Stochastic spectral methods for uncertainty quantification

Methodological developments

- 90s : Wiener-Hermite expansion of model solutions (Ghanem & Spanos).
- Applications to linear models (elasticity, thermal sciences, porous media, ...)
- 2000 : application to non-linear models : Navier-Stokes equations, porous media, reacting flows.
- 2004 : development of alternative expansion basis (generalised polynomial chaos, piecewise polynomial expansions, wavelets).
- Essentially rely on Eulerian formulations/models.

Are spectral expansions amenable to Lagrangian models?

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?

2D incompressible Navier-Stokes equations

Rotational Form

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

Velocity kernel (Biot-Savart)

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

Particle approximation

Smooth approximation

Particles : position $X_i(t)$, circulation $\Gamma_i(t)$, core size ϵ :

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

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).



Solution method

Convection step

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

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

Acceleration of velocity computation

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

Solution method

Integral representation of differential operators

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

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

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

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

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

Summary

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

$$\frac{d\Gamma_{i}}{dt} = \nu \sum_{j=1}^{Np} \mathcal{L}(\boldsymbol{X}_{i} - \boldsymbol{X}_{j}) S[\Gamma_{j} - \Gamma_{i}].$$

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 :

$$\begin{split} \langle \Psi_k^2 \rangle \, \frac{d[\boldsymbol{X}_i]_k}{dt} &= \frac{-1}{2\pi} \sum_{j=1}^{N_p} \left\langle \Psi_k(\xi) \Gamma_j(\xi) \mathcal{K}_\epsilon(\boldsymbol{X}_i(\xi), \boldsymbol{X}_j(\xi)) \right\rangle, \\ \langle \Psi_k^2 \rangle \, \frac{d[\Gamma_i]_k}{dt} &= \left\langle \Psi_k(\xi) \nu(\xi) \sum_{j=1}^{N_p} \mathcal{L}(\boldsymbol{X}_i(\xi) - \boldsymbol{X}_j(\xi)) \mathcal{S}[\Gamma_j(\xi) - \Gamma_i(\xi)] \right\rangle. \end{split}$$

- 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 [u]₀.
- Interactions with other modes are treated as source terms using integral approximations (PSE).

Particle approximation of the stochastic problem

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

$$\begin{aligned} \frac{d\boldsymbol{X}_{i}}{dt} &= [\boldsymbol{U}_{i}]_{0}, \\ \frac{d[\Gamma_{i}]_{k}}{dt} &= -\sum_{j=1}^{N_{p}} \sum_{l=1}^{P} \sum_{m=0}^{P} C_{klm} S\left\{\mathcal{G}^{x}(\boldsymbol{X}_{i} - \boldsymbol{X}_{j})\left([U_{i}]_{l}[\Gamma_{i}]_{m} + [U_{j}]_{l}[\Gamma_{j}]_{m}\right)\right. \\ &+ \mathcal{G}^{y}(\boldsymbol{X}_{i} - \boldsymbol{X}_{j})\left([V_{i}]_{l}[\Gamma_{i}]_{m} + [V_{j}]_{l}[\Gamma_{j}]_{m}\right)\right\} \\ &+ \sum_{j=1}^{N_{p}} \sum_{l=0}^{P} \sum_{m=0}^{P} C_{klm} S[\nu]_{l} \mathcal{L}(\boldsymbol{X}_{i} - \boldsymbol{X}_{j})\left([\Gamma_{j}]_{m} - [\Gamma_{i}]_{m}\right), \\ [\boldsymbol{U}_{i}]_{k} &= -\frac{1}{2\pi} \sum_{j=1}^{N_{p}} [\Gamma_{j}]_{k} \mathcal{K}_{\epsilon}(\boldsymbol{X}_{i}, \boldsymbol{X}_{j}). \end{aligned}$$

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

Lagrangian formulation Le Maître and Knio, J. Comp. Phys. (2007)

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) : O(n log n).
- Conservative method (regridding).

Results (I)

Convection of a passive scalar

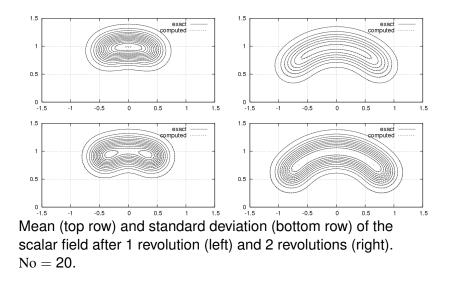
Stochastic equations

$$\begin{aligned} \frac{\partial \boldsymbol{c}}{\partial t} + \boldsymbol{U} \cdot \boldsymbol{\nabla} \boldsymbol{c} &= \boldsymbol{0}, \\ \boldsymbol{c}(\boldsymbol{x}, t, \xi) &= \exp\left[-\|\boldsymbol{x} - \boldsymbol{x}_0\|^2 / \pi d^2 \|\boldsymbol{x}_0\|\right], \quad \boldsymbol{x}_0 = \boldsymbol{e}_y, \\ \boldsymbol{U}(\boldsymbol{x}, \xi) &= -(1 + 0.075\xi)\boldsymbol{x} \wedge \boldsymbol{e}_z, \quad \xi \sim \boldsymbol{U}[-1, 1]. \end{aligned}$$

Discretization

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

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



Results (II)

Evolution of a radial vortex

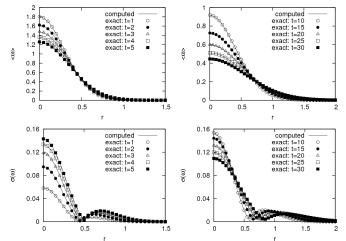
Equations

$$\begin{aligned} \frac{\partial \omega}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} \omega &= \nu \nabla^2 \omega, \\ \omega(\boldsymbol{x}, t = 0) &= \frac{\exp[-\|\boldsymbol{x}\|^2/d]}{\pi d}, \\ \nu &= 0.005 + 0.0025\xi, \quad \xi \sim U(-1, 1). \end{aligned}$$

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 No = 5.
- Check the invariants of the flow.

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



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

Results (III)

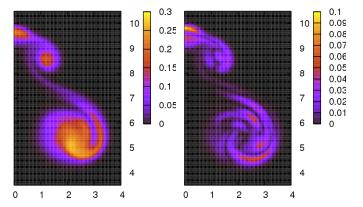
Equations

- 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 Ra ~ U[2.10⁵, 3.10⁵].

Discretization

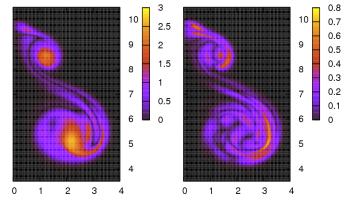
- *ϵ* = 1/30.
- Simulation for $t \in [0, 28]$, $\Delta t = 0.2$ with RK-2.
- Remeshing every 4 iterations : Np > 200,000 at the end of the simulation.
- Velocities computed with particle-mesh scheme $h_g = \epsilon$.
- Wiener Legendre expansion with up to No = 12.

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.

(Non-intrusive techniques)

Regression

- Let {ξ⁽¹⁾,...,ξ^(m)} be the set of regression points, such that ξ⁽ⁱ⁾ ∈ Ω_ξ, i = 1,...,m.
- Let $S^{(i)}$ be the solution of deterministic problem $\mathcal{M}\left(s^{(i)}, D(\xi^{(i)})\right) = 0$, for i = 1, ..., m.
- Determine S_k , k = 0, ..., P, that minimizes the distance

$$d^{2} = \sum_{i=1}^{m} w_{i} \left(S^{(i)} - \sum_{k=0}^{P} S_{k} \Psi_{k} \left(\boldsymbol{\xi}^{(i)} \right) \right)^{2}$$

Advantages/issues

- Works with a subset of the solution or by-products.
- Convergence with number of regression points m.
- Selection of the regression points.
- Error estimate.

Return

Non intrusive projection

Make use of the orthogonality of the basis : $\langle S\Psi_k \rangle = \langle \Psi_k^2 \rangle S_k = \int_{\Omega_{\xi}} S(\xi) \Psi_k(\xi) p(\xi) d\xi.$

Computation of P + 1 N-dimensional integrals

Non intrusive projection

Make use of the orthogonality of the basis :

$$\left\langle S\Psi_{k}
ight
angle =\left\langle \Psi_{k}^{2}
ight
angle S_{k}=\int_{\Omega_{\xi}}S(\xi)\Psi_{k}(\xi)p(\xi)d\xi.$$

Computation of P + 1 N-dimensional integrals

(Quasi) Monte-Carlo sampling

$$\langle S\Psi_k \rangle \approx \frac{1}{m} \sum_{i=1}^m w^{(i)} S\left(\xi^{(i)}\right) \Psi_k\left(\xi^{(i)}\right).$$

- Convergence rate.
- Error estimate
- Optimal sampling strategy.

Non intrusive projection

Make use of the orthogonality of the basis :

$$\langle S\Psi_k \rangle = \left\langle \Psi_k^2 \right\rangle S_k \approx \sum_{i=1}^{N_O} w^{(i)} S\left(\boldsymbol{\xi}^{(i)}\right) \Psi_k\left(\boldsymbol{\xi}^{(i)}\right).$$

Computation of P + 1 N-dimensional integrals

Numerical quadrature

Quadrature points $\boldsymbol{\xi}^{(i)}$ and weights $\boldsymbol{w}^{(i)}$ obtained by

- full tensorisation of *n* points 1-D quadrature formula (*e.g.* Gauss formula) : $N_Q = n^N$.
- partial tensorization of nested 1-D quadrature formula (Féjer, Clenshaw-Curtis) :
- Cost for large stochastic dimension N.
- Projection of non-polynomial solutions.

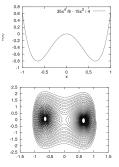
Example of GPC failure

Rolling-ball problem

$$\frac{d^2X}{dt^2} + f\frac{dX}{dt} = -\frac{dh}{dX} \equiv -\frac{35}{2}X^3 + \frac{15}{2}X,$$

with friction $f \ge 0$. Uncertain initial conditions :

$$X(t=0,\xi)=X_0+\Delta X\xi,\quad \left.\frac{dX}{dt}\right|_{t=0}=0,$$



with ξ U.D. on [-1, 1] (Legendre basis).

Solution : The system has two stable fixed points

 $(X^2 = 15/35)$. Uncertainty in IC can lead to one fixed point **or** the other !

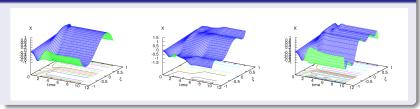
Stochastic solution may exhibit discontinuities.

Legendre solution

Parameters and solution method

 $f = 2., X_0 = 0.05, \Delta X = 0.2$; equation is time integrated using RK(3) and Galerkin projection.

Results for No = 3,5 and 9



Conclusion

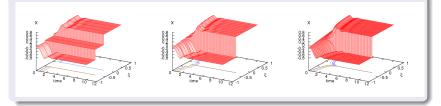
Global polynomials (C^{∞}) can hardly represent discontinuous solution (Gibbs' oscillations).

Wiener-Haar solution

Parameters and solution method

 $f = 2., X_0 = 0.05, \Delta X = 0.2$; equation is time integrated using RK(3) and Galerkin projection.

Results for Nr = 2, 3 and 5



Remark

Details are not necessary evrywhere : adaptive method. <a>Return