Incertitudes et Simulation
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Introduction to Stochastic Spectral Methods

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- Introduction
- Strong and weak form of stochastic PDEs
- Stochastic spectral representations (Karhunen-Loève & Polynomial Chaos)
- Resolution methods (Galerkin & collocation approaches)
- Application to CFD: spatially developing mixing layer with random BCs
- Conclusion

Need for Uncertainty Quantification (UQ)

- Modeling errors/uncertainties, numerical errors and data errors/uncertainties can interact (non-linearly).
- Aleatoric (not reducible) or epistemic (incomplete knowledge) uncertainty.
- Need to quantitatively access the impact of uncertain data on simulation outputs ⇒ use of stochastic / probabilistic methods.
- In case of the lack of a reference solution, the validity of the model can be established only if uncertainty in numerical predictions due to uncertain input parameters can be quantified.
- Difficulty: not looking for the unique solution. Now interested in finding the space of all possible solutions spanned by the uncertain parameters.
- Possible sources: simulation constants/parameters, transport coefficients, physical properties, boundary/initial conditions, geometry, models, numerical schemes, ...

Stochastic process representations

Outline
Introduction
Stochastic PDEs
Computational Approach
Stochastic spectral representation
Resolution methods
Post-processing
Application
Conclusion

Statistical methods:

<u>*(Brute-force)* Monte Carlo method:</u>

• Converges as $1/\sqrt{N}$; Convergence rate is independent of number of RVs. Robust. Parallelizable.

<u>Monte Carlo based methods:</u>

• QMC (*Quasi-MC*), MCMC (*Markov chain MC*).

• importance sampling, correlated sampling, conditional sampling.

Latin hypercube sampling, etc. (Fishman 1996)

Variance reduction technique: (limitation with large number of RVs)

<u>RSM (*Response Surface Method*):</u>

• realizations reduced by interpolation in state space; same limitation with large number of RVs.

Non-statistical methods:

"Indirect" methods:

<u>Fokker-Planck equation:</u> Solves for distribution function; Challenging in high dimensions (computational cost), BCs.

<u>Moments equations:</u> Closure of equations is key. Good for linear problems with Gaussian RVs.

"Direct" methods (e.g. SFEM, stochastic finite element method):

<u>Interval analysis:</u> "maximum" output bounds

<u>Perturbation-based methods:</u>

Taylor expansion around means. Differ at the local representation of randomness: mid-point, local average, piecewise polynomial, etc.

<u>Operator-based methods:</u>

Weighted integral method; Neumann expansion.

<u>Stochastic spectral methods: Polynomial chaos, Wiener-Askey chaos & Karhunen-Loève decomposition</u> (Wiener, *The homogeneous chaos* 1938, Ghanem & Spanos, *Stochastic Finite Elements: a Spectral Approach* 1991, Loève, *Probability Theory* 1977).

Complete probability space: $(\Omega, \mathcal{A}, P)$, where Ω is the event space, $\mathcal{A} \subset 2^{\Omega}$ the σ-algebra and P the probability measure.
Random variable $X(\omega)$:

$$X : (\Omega, \mathcal{A}, P) \to \mathbb{R},$$

with probability density function (pdf) f_X and cumulative density function (cdf) F_X.

$$F_X(x) = \int_{-\infty}^{x} f_X(x)dx.$$

Random vector:

$$\boldsymbol{X} = \{X_i(\omega)\}_{i=1}^{N}, N \in \mathbb{N}.$$

Two RVs X_1 and X_2:

- uncorrelated if: $\mathbb{E}(\tilde{X}_1 \otimes \tilde{X}_2) = 0$
- independent if: $\mathbb{E}[\phi_1(X_1)\,\phi_2(X_2)] \equiv \mathbb{E}[\phi_1(X_1)]\,\mathbb{E}[\phi_2(X_2)]$

We consider a functional $X = u(X) = u(\omega)$.
Expectation operator:

$$\mathbb{E}[u] =< u >= \int_{\Omega} u(\omega)dP(\omega) = \int_{\mathbb{R}} u(x)f_X(x)dx$$

1. $\bar{u} = \mathbb{E}[u]$
2. $\text{var}_u = \mathbb{E}[\tilde{u}^2]$ where $\tilde{u} = u - \bar{u}$
3. $P(u \leq u_0) = P(\{\omega \in \Omega : u(\omega) \leq u_0\}) = \mathbb{E}[\mathbf{1}_{\{u \leq u_0\}}]$

Random process (RP)

We consider a continuous random process $u(\boldsymbol{x}, \omega)$ indexed by a bounded domain $\mathcal{D} \subset \mathbb{R}^d$ on the probability space $(\Omega, \mathcal{A}, P)$.

1. For each $\boldsymbol{x} = \boldsymbol{x_0}$, $u(\boldsymbol{x} = \boldsymbol{x_0}, \omega)$ is a random variable on Ω.
2. u is a function of $\mathcal{D} \times \Omega$ with value $u(\boldsymbol{x}, \omega)$ for given $\boldsymbol{x} \in \mathcal{D}$ and $\omega \in \Omega$.
3. For each fixed $\omega \in \Omega$, $u(\boldsymbol{x}, \omega)$ is a function - a *realization* - of $\boldsymbol{x}$ in $\mathcal{D}$.

Expectation operator:

$$\mathbb{E}[u] =< u(\boldsymbol{x}) >= \int_\Omega u(\boldsymbol{x}, \omega) dP(\omega) = \int_\mathbb{R} u(\boldsymbol{x}, x) f_X(x) dx$$

1. $\bar{u}(\boldsymbol{x}) = \mathbb{E}[u(\boldsymbol{x})]$
2. $\text{var}_u(\boldsymbol{x}) = \mathbb{E}[\tilde{u}(\boldsymbol{x})^2]$ where $\tilde{u}(\boldsymbol{x}) = u(\boldsymbol{x}) - \bar{u}(\boldsymbol{x})$
3. $P(u(\boldsymbol{x}) \leq u_0) = P(\{\omega \in \Omega : u(\boldsymbol{x}, \omega) \leq u_0\}) = \mathbb{E}[\mathbf{1}_{\{u(\boldsymbol{x}) \leq u_0\}}]$

Stochastic PDE and variational form

- Find $u(\boldsymbol{x},t,\omega)$ with $t \in [0,T]$, $\omega \in \Omega$, such that:

$$\begin{aligned} \mathcal{L}(\boldsymbol{x},t,\omega;u) &= f(\boldsymbol{x},t,\omega) \quad \text{with} \quad \boldsymbol{x} \in \mathcal{D}, \\ \mathcal{B}(\boldsymbol{x},t,\omega;u) &= g(\boldsymbol{x},t,\omega) \quad \text{with} \quad \boldsymbol{x} \in \partial\mathcal{D}. \end{aligned}$$

- Random inputs $\leftarrow$ $\mathcal{L}$, $\mathcal{B}$, f, g, $\mathcal{D}$, random parameter R, ...

- *Finite dimensional noise assumption*: $R(\omega) = R(X_1(\omega), X_2(\omega), \ldots, X_N(\omega))$
  Each random variable is a function $X_i : \omega \in \Omega \to \mathbb{R}$

  One possible choice: KL decomposition - RVs are pairwise uncorrelated but not necessarily mutually independent.

  $u(\boldsymbol{x},t,\omega) \approx u(\boldsymbol{x},t,X_1(\omega),X_2(\omega),\ldots,X_N(\omega))$

- $\boldsymbol{X}(\omega) = (X_1(\omega), X_2(\omega), \ldots, X_N(\omega))$: set of $i.i.d$ continuous random variables with PDF:

  $\rho(\boldsymbol{X}) = \rho_1(X_1)\rho_2(X_2)\cdots\rho_N(X_N) = \prod_{i=1}^N \rho_i(X_i)$ and support:

  $\Gamma \equiv \prod_{i=1}^N X_i(\Omega) \subset \mathbb{R}^N$

Stochastic PDE and variational form

- Strong form: find $u(\boldsymbol{x}, t, \boldsymbol{X})$, such that:

$$\begin{aligned} \mathcal{L}(\boldsymbol{x}, t, \boldsymbol{X}; u) &= f(\boldsymbol{x}, t, \boldsymbol{X}) \quad \text{with} \quad \boldsymbol{x} \in \mathcal{D},\ t \in [0, T],\ \boldsymbol{X} \in \Gamma \\ \mathcal{B}(\boldsymbol{x}, t, \boldsymbol{X}; u) &= g(\boldsymbol{x}, t, \boldsymbol{X}) \quad \text{with} \quad \boldsymbol{x} \in \partial\mathcal{D}. \end{aligned}$$

- Finite dimensional subspace $V_\Gamma \subset L^2_\rho(\Gamma)$ of all square integrable function in Γ with respect to the measure $\rho(\boldsymbol{X})d\boldsymbol{X}$

- Weak form: find $u_V(\boldsymbol{x}, t, \boldsymbol{X}) \in V_\Gamma(\boldsymbol{X})$, such that:

$$\begin{aligned} \int_\Gamma \mathcal{L}(\boldsymbol{x}, t, \boldsymbol{X}; u_V)\phi(\boldsymbol{X})\rho(\boldsymbol{X})d\boldsymbol{X} &= \int_\Gamma f(\boldsymbol{x}, t, \boldsymbol{X})\phi(\boldsymbol{X})\rho(\boldsymbol{X})d\boldsymbol{X},\ \forall\, \phi(\boldsymbol{X}) \in V_\Gamma,\ \boldsymbol{x} \in \mathcal{D},\ t \in [0, T] \\ \int_\Gamma \mathcal{B}(\boldsymbol{x}, t, \boldsymbol{X}; u_V)\phi(\boldsymbol{X})\rho(\boldsymbol{X})d\boldsymbol{X} &= \int_\Gamma g(\boldsymbol{x}, t, \boldsymbol{X})\phi(\boldsymbol{X})\rho(\boldsymbol{X})d\boldsymbol{X},\ \forall\, \phi(\boldsymbol{X}) \in V_\Gamma,\ \boldsymbol{x} \in \mathcal{D},\ t \in [0, T] \end{aligned}$$

Karhunen-Loève representation

The Karhunen-Loève (KL) expansion [Loeve 1977] is based on the spectral expansion of the covariance function of a random process.

We consider a second-order RP $u(\boldsymbol{x}, \omega) \Rightarrow \mathbb{E}[u(\boldsymbol{x})^2] < +\infty, \forall \boldsymbol{x} \in \mathcal{D}$ and its covariance function $R_u(\boldsymbol{x}_1, \boldsymbol{x}_2)$.

$$R_u(\boldsymbol{x}_1, \boldsymbol{x}_2) = \mathbb{E}(u(\boldsymbol{x}_1, \omega) \otimes u(\boldsymbol{x}_2, \omega))$$

The covariance kernel is *real*, *symmetric* and *positive-definite*. Spectrum of $\{\lambda_i\} \subset \mathbb{R}_+$ and *orthogonal* eigenfunctions $\phi_i(x)$ (complete basis).

Spectral representation of the kernel:

$$R_u(\boldsymbol{x}_1, \boldsymbol{x}_2) = \sum_{i=1}^{\infty} \lambda_i \phi_i(\boldsymbol{x}_1) \phi_i(\boldsymbol{x}_2)$$

Second-order Fredholm equation:

$$\int_{\mathcal{D}} R_u(\boldsymbol{x}_1, \boldsymbol{x}_2) \phi_i(\boldsymbol{x}_2) d\boldsymbol{x}_2 = \lambda_i \phi_i(\boldsymbol{x}_1) \quad \text{with} \quad \int_{\mathcal{D}} \phi_i(\boldsymbol{x}) \phi_j(\boldsymbol{x}) d\boldsymbol{x} = \delta_{ij}.$$

Karhunen-Loève representation

$$u(\boldsymbol{x},\omega) = \bar{u}(\boldsymbol{x}) + \sigma_u \sum_{i=1}^{\infty} \sqrt{\lambda_i}\phi_i(\boldsymbol{x})X_i(\omega),$$

with X_i: centred, normalized, uncorrelated RVs (but not necessarily *independent*!); $\mathbb{E}X_i = 0$, $\mathbb{E}(X_i\,X_j) = \delta_{ij}$.

$$X_i(\omega) = \frac{1}{\lambda_i}\int_{\mathcal{D}} \big(u(\boldsymbol{x},\omega) - \bar{u}(\boldsymbol{x})\big)\phi_i(\boldsymbol{x})d\boldsymbol{x}$$

Remark: If $u(\boldsymbol{x},\omega)$ is a Gaussian RP. It has a KL representation with RVs $X_i(\omega)$: Gaussian vector. These *Gaussian* RVs are *uncorrelated* $\Rightarrow$ *independent*.

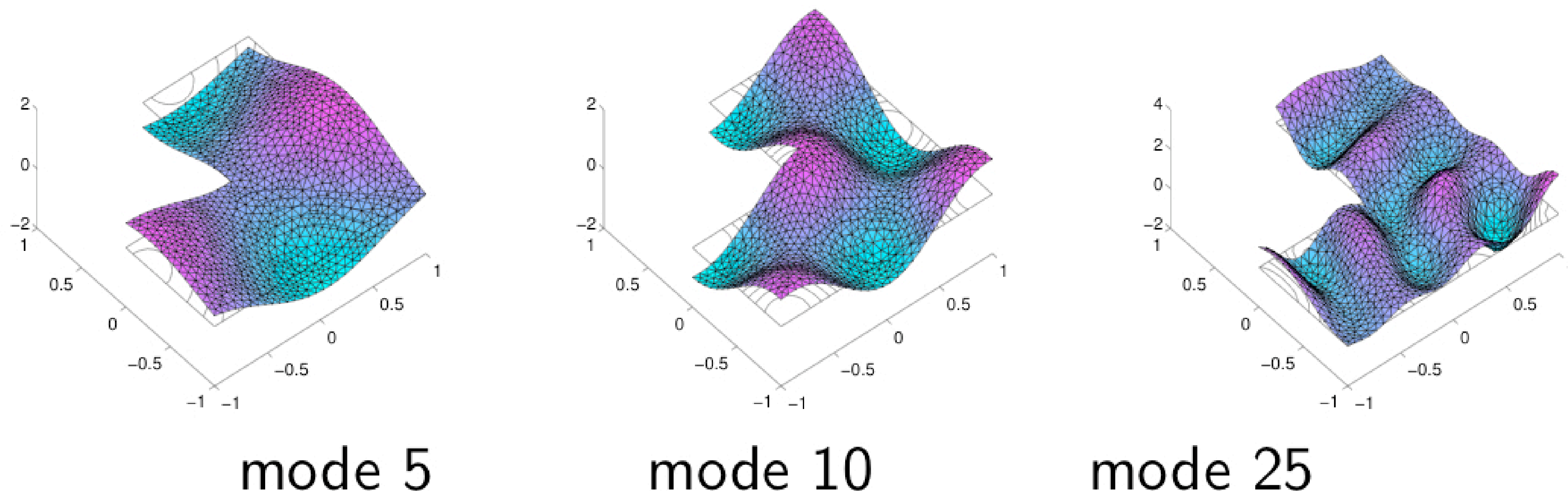
$$u(\boldsymbol{x},\omega) = \bar{u}(\boldsymbol{x}) + \sigma_u \sum_{i=1}^{N} \sqrt{\lambda_i}\phi_i(\boldsymbol{x})X_i(\omega),$$

Error minimizing property: truncate after N largest eigenvalues $\Rightarrow$ *optimal* - in variance - expansion in N RVs.

$$\epsilon_N^2 = \sum_{i>N} \lambda_i$$

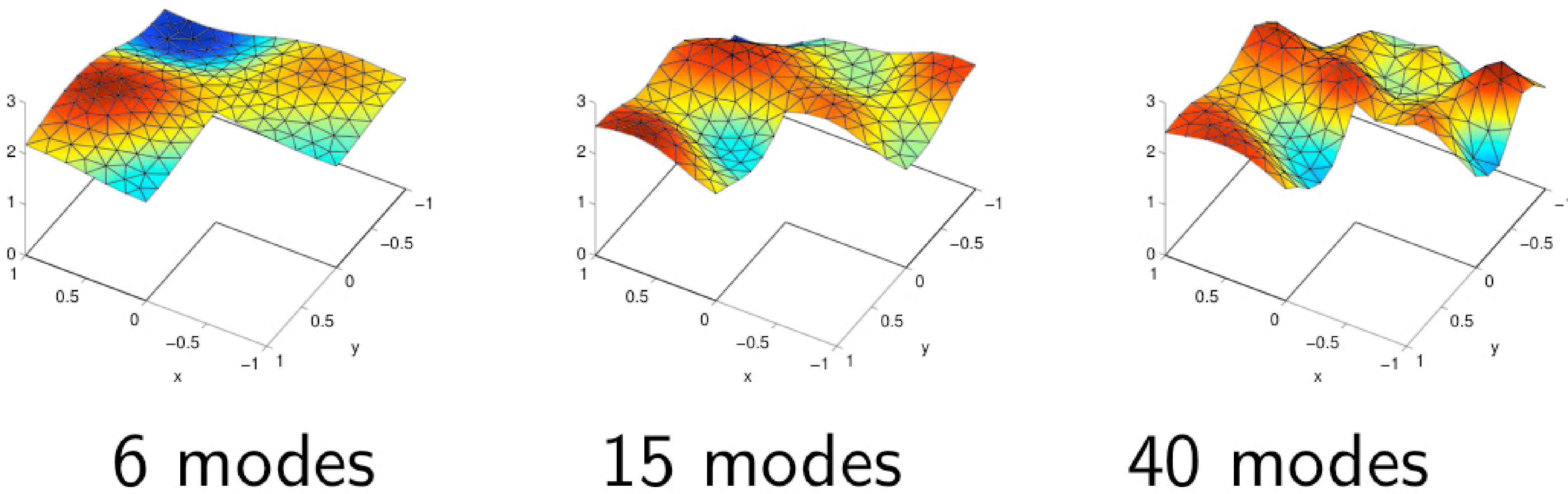
Convergence rate of the spectrum: inversely proportional to *correlation length* and depends on the regularity of the covariance kernel.

Example: groundwater flow stochastic conductivity - Modal decomposition



H. Matthies (Institute of Scientific Computing, TU Braunschweig)

Example: groundwater flow stochastic conductivity - Realizations



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Homogeneous Chaos

Theorem [N. Wiener]: any RV $u(\omega) \in L_2(\Omega, \mathcal{A}, P)$ (with finite variance) can be represented in orthogonal polynomials of *Gaussian* RVs $\boldsymbol{X} = \{X_i(\omega)\}_{i=1}^{\infty}$.

$$u(\omega) = \sum_{k=0}^{\infty} \hat{u}_k H_k(\boldsymbol{X}(\omega))$$

- The type of $H_k(\boldsymbol{X})$ are *Hermite* polynomials
- Convergence in $L_2(\Omega, \mathcal{A}, P)$ (Cameron & Martin, 1947)
- Orthogonality condition: $< H_i, H_j >= \mathbb{E}[H_i, H_j] = \mathbb{E}[H_i^2]\, \delta_{ij}$
- Expectation operator: $\mathbb{E}\,[\cdot, f] = \int_\Omega f(\boldsymbol{X})\rho(\boldsymbol{X})\, d\boldsymbol{X}$

generalized Polynomial Chaos (gPC)

$$u(\boldsymbol{x}, t, \omega) = \sum_{k=0}^{\infty} \hat{u}_k(\boldsymbol{x}, t) \Phi_k(\boldsymbol{X})$$

- Generalization to the Askey scheme family of polynomials [Xiu & Karniadakis, 2002].
- Orthogonality condition: $\mathbb{E}[\Phi_i, \Phi_j] = \mathbb{E}[\Phi_i^2]\,\delta_{ij}$
- Expectation operator: $\mathbb{E}\,[\cdot, f] = \int_\Omega f(\boldsymbol{X}) \rho(\boldsymbol{X})\, d\boldsymbol{X}$
- The type of polynomial $\Phi_k(\boldsymbol{X})$ is determined by $\rho_k(X_i)$

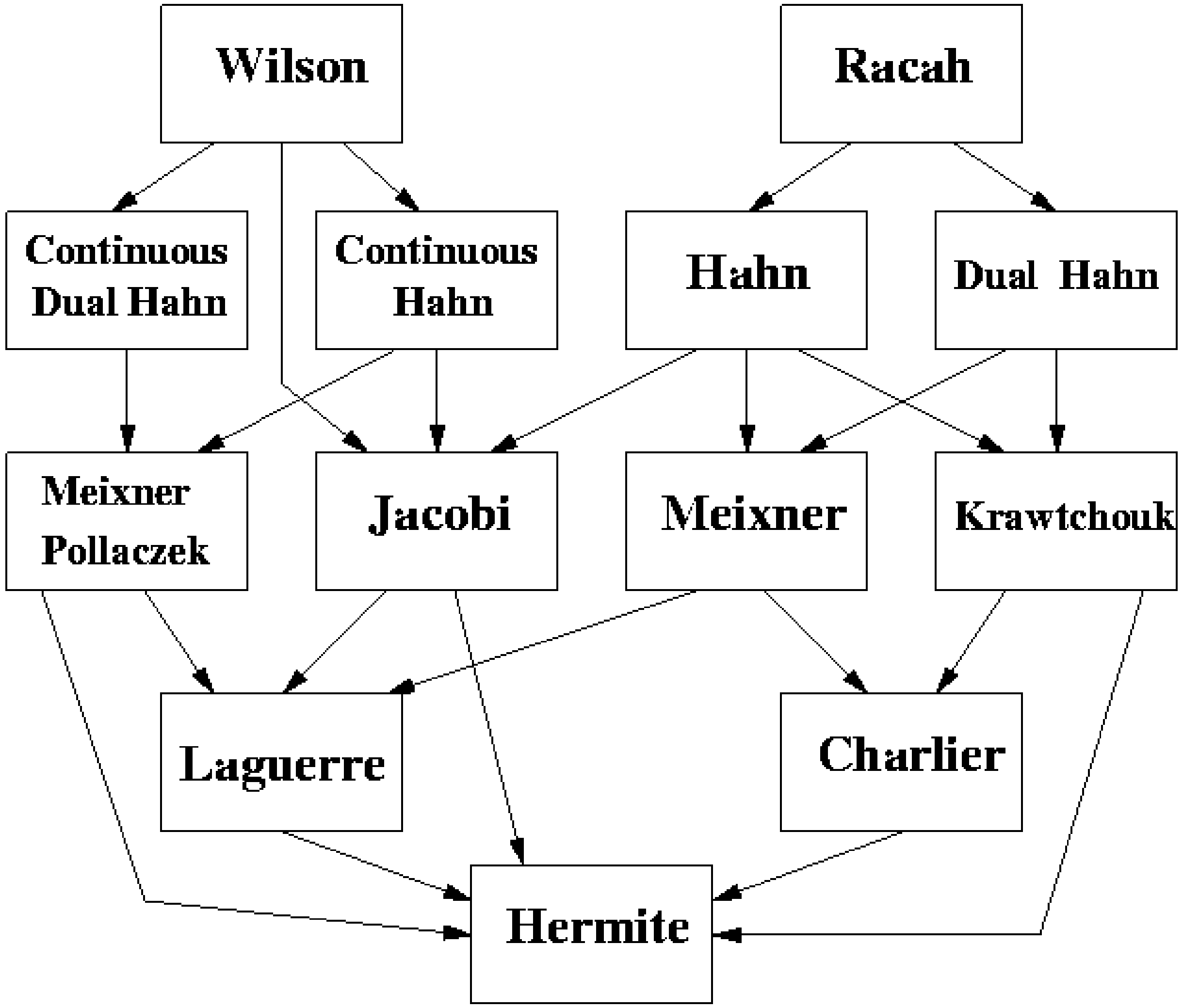
Numerically, we have to truncate the representation:

$$u(\boldsymbol{x}, t, \omega) \approx \sum_{k=0}^{M} \hat{u}_k(\boldsymbol{x}, t), \Phi_k(\boldsymbol{X})$$

where M depends on the number of random dimensions N and the highest polynomial order P of the polynomial basis:

$$M(N, P) = \frac{(N+P)!}{N!\,P!} - 1$$

Choice of orthogonal (hypergeometric) polynomials: the Askey Scheme [Askey 1985, Schoutens 1999]

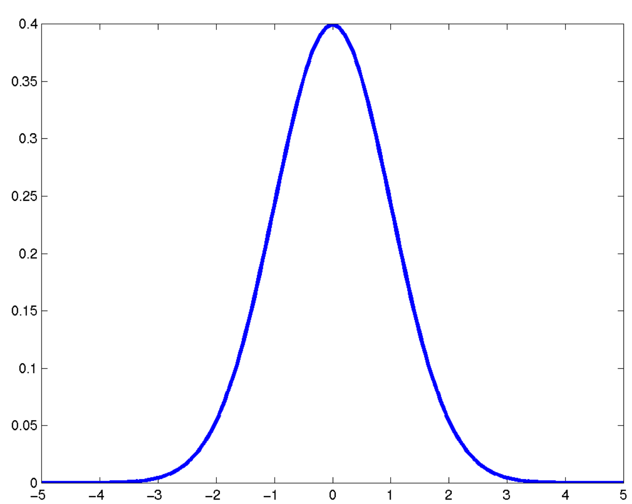


Correspondence between Orthogonal Polynomials and Probability Distributions

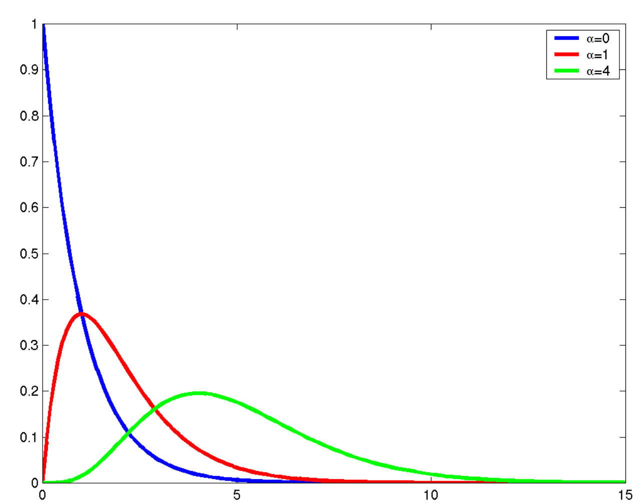
Continuous Cases:

- Hermite Polynomials ➡ Gaussian Distribution
- Laguerre Polynomials ➡ Gamma Distribution

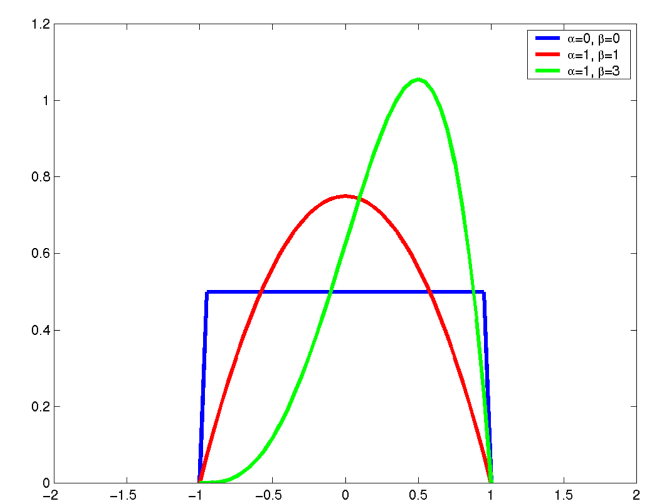
  (special case: exponential distribution)
- Jacobi Polynomials ➡ Beta Distribution
- Legendre Polynomials ➡ Uniform Distribution



Gaussian distribution



Gamma distribution

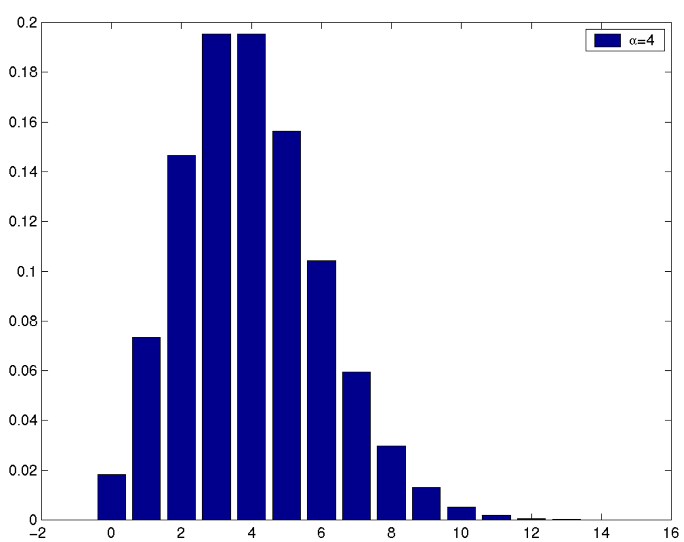


Beta distribution

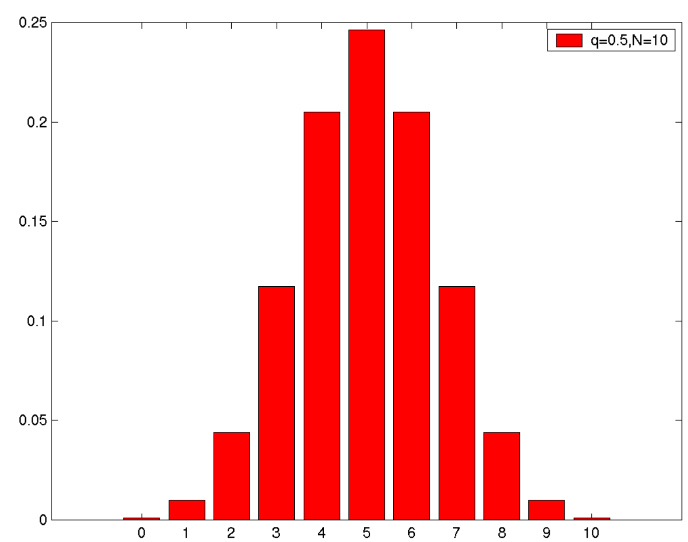
Correspondence between Orthogonal Polynomials and Probability Distributions

Discrete Cases:

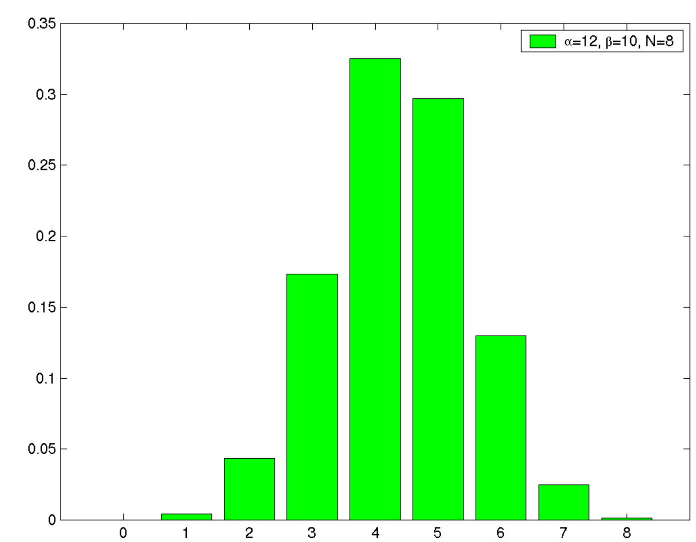
- Charlier Polynomials ➠ Poisson Distribution
- Krawtchouk Polynomials ➠ Binomial Distribution
- Hahn Polynomials ➠ Hypergeometric Distribution
- Meixner Polynomials ➠ Pascal Distribution



Poisson distribution



Binomial distribution



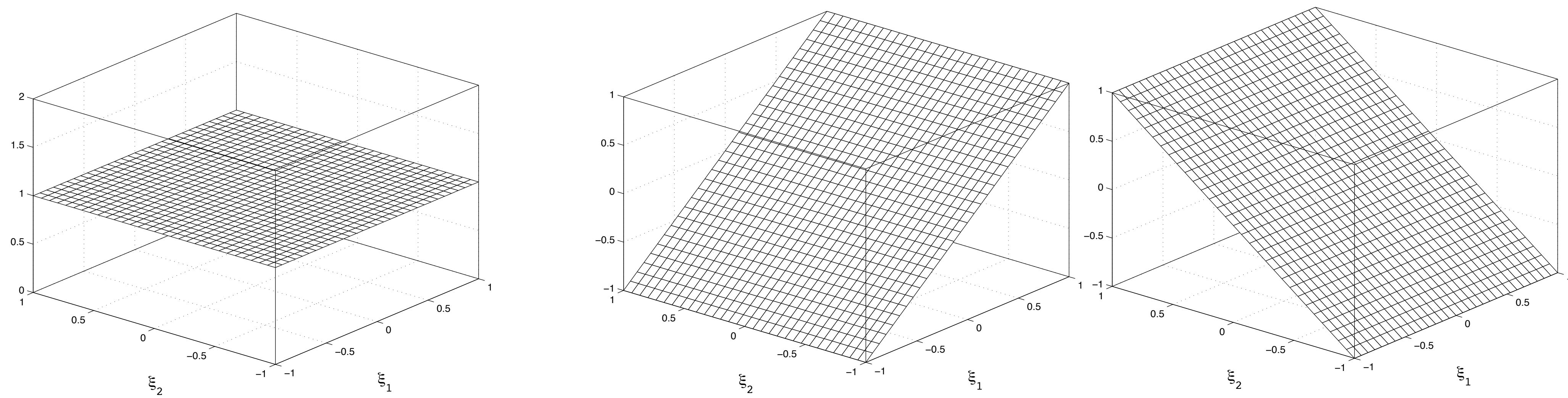
Hypergeometric distribution

Example: 2-dimensional Legendre polynomials

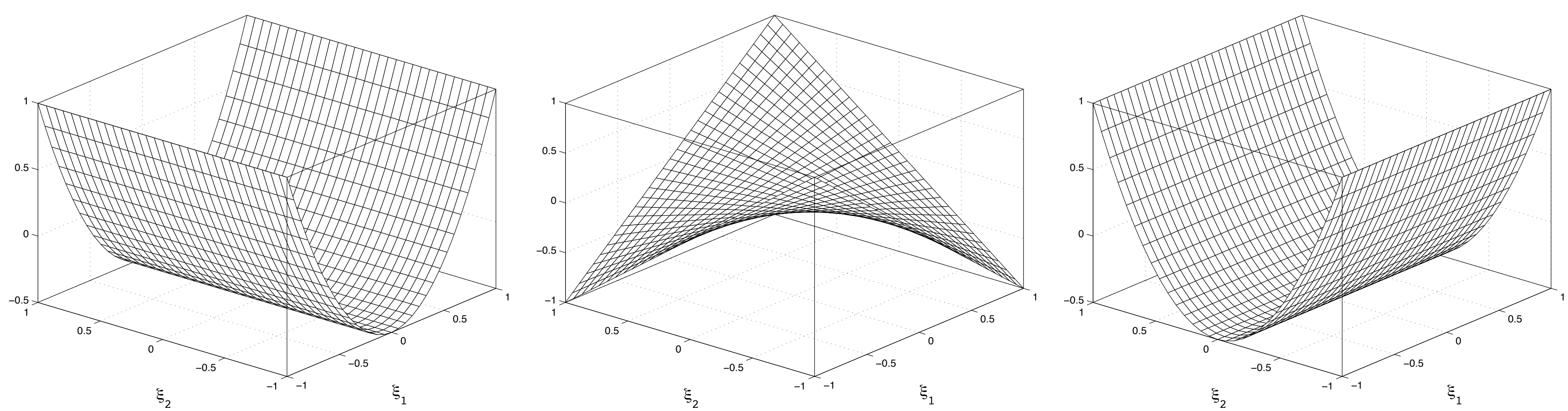
$$
\begin{aligned}
\Phi_0(X_1,X_2) &= 1\\
\Phi_1(X_1,X_2) &= X_1\\
\Phi_2(X_1,X_2) &= X_2\\
\Phi_3(X_1,X_2) &= \frac{3}{2}X_1^2-\frac{1}{2}\\
\Phi_4(X_1,X_2) &= X_1X_2\\
\Phi_5(X_1,X_2) &= \frac{3}{2}X_2^2-\frac{1}{2}\\
\Phi_6(X_1,X_2) &= \frac{5}{2}X_1^3-\frac{3}{2}X_1\\
\Phi_7(X_1,X_2) &= \frac{3}{2}X_1^2X_2-\frac{1}{2}X_2\\
\Phi_8(X_1,X_2) &= \frac{3}{2}X_1X_2^2-\frac{1}{2}X_1\\
\Phi_9(X_1,X_2) &= \frac{5}{2}X_2^3-\frac{3}{2}X_2\\
\Phi_{10}(X_1,X_2) &= \frac{35}{8}X_1^4-\frac{15}{4}X_1^2+\frac{3}{8}\\
\Phi_{11}(X_1,X_2) &= \frac{5}{2}X_1^3X_2-\frac{3}{2}X_1X_2\\
\Phi_{12}(X_1,X_2) &= \frac{9}{4}X_1^2X_2^2-\frac{3}{4}X_1^2-\frac{3}{4}X_2^2+\frac{2}{8}\\
\Phi_{13}(X_1,X_2) &= \frac{5}{2}X_1X_2^3-\frac{3}{2}X_1X_2\\
\Phi_{14}(X_1,X_2) &= \frac{35}{8}X_2^4-\frac{15}{4}X_2^2+\frac{3}{8}
\end{aligned}
$$

2-dimensional Legendre polynomials

P=Zero & P=1st order

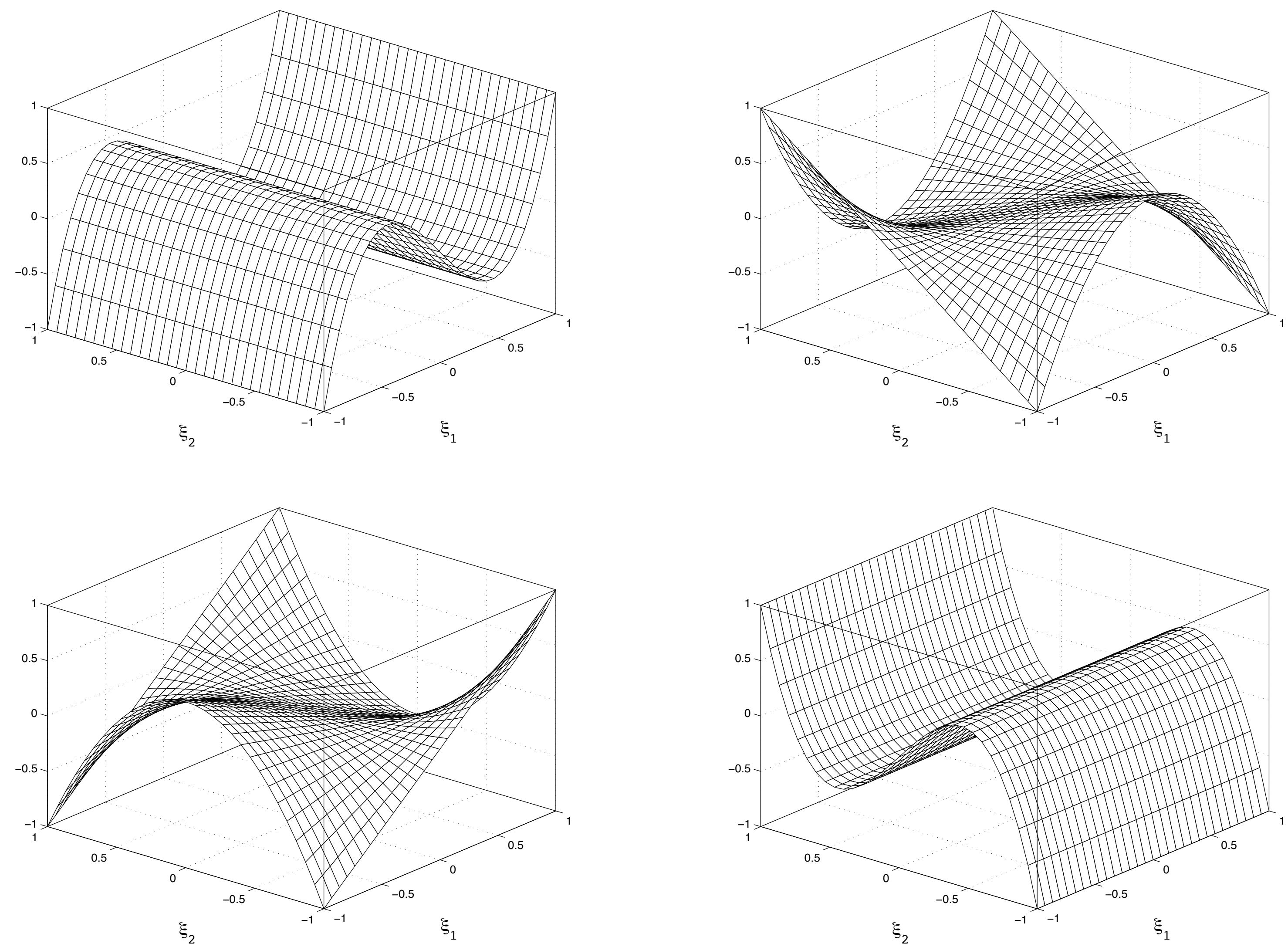


P=2nd order



2-dimensional Legendre polynomials

<u>P=3rd order</u>



Multi-dimensional polynomials construction

- Based on the finite number of random dimensions $\boldsymbol{X} = \{X_i(\omega)\}_{i=1}^{d=N}, N \in \mathbb{N}$,
- there exists an ensemble $\Gamma_P^{(N)}$ of $(M+1) = (N+P)!/(N!P!)$ polynomials $\Phi(\boldsymbol{X})$ at most of degree P.
- A simple way to construct the k^{th} polynomial $\Phi_k(\boldsymbol{X})$ is to tensorize one-dimensional polynomials $\Phi^{\text{d=1}}_{\alpha_k(i)}(X_i)$, where we define the multi-index: $\boldsymbol{\alpha}_k = \{\alpha_{k_1}, \ldots \alpha_{k_i}, \ldots \alpha_{k_N}\}$, such that:

$$\Phi_k(\boldsymbol{X}) = \prod_{i=1}^{N} \Phi^{\text{d=1}}_{\alpha_{k_i}}(X_i),$$

- $\boldsymbol{\alpha}_k := \{\alpha_{k_i}\}_{i=1}^{N}$ is an array whose each component refers to the degree of the i^{th} one-dimensional polynomial $\Phi^{\text{d=1}}(X_i)$ contributing to $\Phi_k(\boldsymbol{X})$.
- Each $\boldsymbol{\alpha}_k$ satisfy: $\forall k \sum_{i=1}^{N} \alpha_{k_i} \leq P$. We have:

$$\Gamma_P^{(N)} = \left\{ \bigcup_{k=0}^{M} \prod_{i=1}^{N} \Phi^{\text{1d}}_{\alpha_{k_i}}(X_i) \right\}$$

Stochastic PDE and variational form

- Strong form: find $u(\boldsymbol{x}, t, \boldsymbol{X})$, such that:

$$\begin{aligned} \mathcal{L}(\boldsymbol{x}, t, \boldsymbol{X}; u) &= f(\boldsymbol{x}, t, \boldsymbol{X}) \quad \text{with} \quad \boldsymbol{x} \in \mathcal{D},\ t \in [0, T],\ \boldsymbol{X} \in \Gamma \\ \mathcal{B}(\boldsymbol{x}, t, \boldsymbol{X}; u) &= g(\boldsymbol{x}, t, \boldsymbol{X}) \quad \text{with} \quad \boldsymbol{x} \in \partial\mathcal{D}. \end{aligned}$$

- Finite dimensional subspace $V_\Gamma \subset L^2_\rho(\Gamma)$ of all square integrable function in Γ with respect to the measure $\rho(\boldsymbol{X})d\boldsymbol{X}$
- Weak form: find $u_V(\boldsymbol{x}, t, \boldsymbol{X}) \in V_\Gamma(\boldsymbol{X})$, such that:

$$\begin{aligned} \int_\Gamma \mathcal{L}(\boldsymbol{x}, t, \boldsymbol{X}; u_V)\phi(\boldsymbol{X})\rho(\boldsymbol{X})d\boldsymbol{X} &= \int_\Gamma f(\boldsymbol{x}, t, \boldsymbol{X})\phi(\boldsymbol{X})\rho(\boldsymbol{X})d\boldsymbol{X},\ \forall\, \phi(\boldsymbol{X}) \in V_\Gamma,\ \boldsymbol{x} \in \mathcal{D},\ t \in [0, T] \\ \int_\Gamma \mathcal{B}(\boldsymbol{x}, t, \boldsymbol{X}; u_V)\phi(\boldsymbol{X})\rho(\boldsymbol{X})d\boldsymbol{X} &= \int_\Gamma g(\boldsymbol{x}, t, \boldsymbol{X})\phi(\boldsymbol{X})\rho(\boldsymbol{X})d\boldsymbol{X},\ \forall\, \phi(\boldsymbol{X}) \in V_\Gamma,\ \boldsymbol{x} \in \mathcal{D},\ t \in [0, T] \end{aligned}$$

Stochastic Galerkin method
Intrusive approach

$$u(\boldsymbol{x},t,\omega) = \sum_{k=0}^{M} \hat{u}_k(\boldsymbol{x},t)\Phi_k(\boldsymbol{X})$$

$$M(N,P) = \frac{(N+P)!}{N!\,P!} - 1$$

- Substitute in the weak form of the model problem. We have for $i = 1,2,\dots M$:

$$\int_\Gamma \mathcal{L}\big(\boldsymbol{x},t,\boldsymbol{X};\sum_{k=0}^{M}\hat{u}_k(\boldsymbol{x},t)\Phi_k(\boldsymbol{X})\big)\Phi_i(\boldsymbol{X})\rho(\boldsymbol{X})d\boldsymbol{X} = \int_\Gamma f(\boldsymbol{x},t,\boldsymbol{X})\Phi_i(\boldsymbol{X})\rho(\boldsymbol{X})d\boldsymbol{X}.$$

- Orthogonality condition $\Rightarrow$ system of $(M+1)$ *deterministic* equations for $\hat{u}_i(\boldsymbol{x},t)$.

  1. System is coupled unless the problem is linear (in random space)
  2. any standard numerical method can be used to solve this deterministic system

- Variations of the stochastic Galerkin method when poor convergence (discontinuity, stochastic bifurcation): multi-element formulation [Karniadakis], multi-resolution (wavelets) formulation [Le Maitre].

Multi-elements gPC [Wan & Karniadakis 2005]

- $\boldsymbol{X}(\omega) = (X_1(\omega), X_2(\omega), \ldots, X_N(\omega))$: set of i.i.d *uniform* continuous RVs with support $\Gamma \equiv \prod_{i=1}^{N} X_i(\Omega) \subset [-1,1]^N$
- **D**: a decomposition of Γ with N_e *non-overlapping* elements

$$\mathbf{D} = \begin{cases} B_l = [a_1^l, b_1^l] \times [a_2^l, b_2^l] \times \cdots \times [a_N^l, b_N^l], \\ B = \bigcup_{l=1}^{N} B_l, \\ B_{l_1} \bigcap B_{l_2} = \emptyset, \text{ if } l_1 \neq l_2, \end{cases}$$

where $l, l_1, l_2 = 1, 2, \cdots, N_e$.

- Indicator random variables

$$I_{B_l} = \begin{cases} 1 \text{ if } \boldsymbol{X} \in B_l, \\ 0 \text{ otherwise.} \end{cases}$$

such that $\Omega = \bigcup_{l=1}^{N_e} I_{B_l}^{-1}(1)$ is a decomposition of the sample space Ω into the N_e elements.

Multi-elements gPC [Wan & Karniadakis 2005]

- We now define a new $\mathbb{R}^N$-valued *local* random vector $\boldsymbol{Z^l} = (Z_1^l, Z_2^l, \ldots, Z_N^l)$ such that $Z_i^l : I_{B_l}^{-1}(1) \rightarrow B_l$ on the probability space $(I_{B_l}^{-1}(1), \mathcal{F} \cap I_{B_l}^{-1}, P(\cdot|I_{B_l}=1))$ subject to a *conditional* PDF

$$\hat{\rho}_l(y|I_{B_l=1}) = \frac{\rho(y)}{P(I_{B_l}=1)}.$$

- Spectral representation:

$$u(\boldsymbol{x}, t, \omega) = \sum_{l=1}^{N_e} P(I_{B_l}=1) \sum_{k=0}^{\infty} \hat{u}_{l,k}(\boldsymbol{x}, t) \Phi_{l,k}(\boldsymbol{Z^l}),$$

with: $\mathbb{E}[\Phi_{l,i}, \Phi_{l,j}] = \mathbb{E}[\Phi_{l,i}^2]\, \delta_{ij}$.

- Moments of the global solution, e.g.:

$$\mathbb{E}[u(\boldsymbol{x}, t)] = \sum_{l=1}^{N_e} P(\boldsymbol{X} \in B_l)\; \mathbb{E}[u_l(\boldsymbol{x}, t)].$$

Stochastic PDE and variational form

- Strong form: find $u(\boldsymbol{x}, t, \boldsymbol{X})$, such that:

$$\begin{aligned} \mathcal{L}(\boldsymbol{x}, t, \boldsymbol{X}; u) &= f(\boldsymbol{x}, t, \boldsymbol{X}) \quad \text{with} \quad \boldsymbol{x} \in \mathcal{D},\ t \in [0, T],\ \boldsymbol{X} \in \Gamma \\ \mathcal{B}(\boldsymbol{x}, t, \boldsymbol{X}; u) &= g(\boldsymbol{x}, t, \boldsymbol{X}) \quad \text{with} \quad \boldsymbol{x} \in \partial\mathcal{D}. \end{aligned}$$

- Finite dimensional subspace $V_\Gamma \subset L^2_\rho(\Gamma)$ of all square integrable function in Γ with respect to the measure $\rho(\boldsymbol{X})d\boldsymbol{X}$

- Weak form: find $u_V(\boldsymbol{x}, t, \boldsymbol{X}) \in V_\Gamma(\boldsymbol{X})$, such that:

$$\begin{aligned} \int_\Gamma \mathcal{L}(\boldsymbol{x}, t, \boldsymbol{X}; u_V)\phi(\boldsymbol{X})\rho(\boldsymbol{X})d\boldsymbol{X} &= \int_\Gamma f(\boldsymbol{x}, t, \boldsymbol{X})\phi(\boldsymbol{X})\rho(\boldsymbol{X})d\boldsymbol{X},\ \forall\, \phi(\boldsymbol{X}) \in V_\Gamma,\ \boldsymbol{x} \in \mathcal{D},\ t \in [0, T] \\ \int_\Gamma \mathcal{B}(\boldsymbol{x}, t, \boldsymbol{X}; u_V)\phi(\boldsymbol{X})\rho(\boldsymbol{X})d\boldsymbol{X} &= \int_\Gamma g(\boldsymbol{x}, t, \boldsymbol{X})\phi(\boldsymbol{X})\rho(\boldsymbol{X})d\boldsymbol{X},\ \forall\, \phi(\boldsymbol{X}) \in V_\Gamma,\ \boldsymbol{x} \in \mathcal{D},\ t \in [0, T] \end{aligned}$$

Stochastic Collocation method
Non-intrusive approach

$$u(\boldsymbol{x}, t, \omega) = \sum_{k=0}^{M} \hat{u}_k(\boldsymbol{x}, t)\Phi_k(\boldsymbol{X})$$

$$M(N, P) = \frac{(N+P)!}{N!\,P!} - 1$$

- A set of collocation points $\{\boldsymbol{X_j}\}_{j=1}^{N_q}$ is defined on the space Γ and collocation projections are performed on the model problem.

$$\mathcal{L}(\boldsymbol{x}, t, \boldsymbol{X_j}; u) = f(\boldsymbol{x}, t, \boldsymbol{X_j}) \quad \text{for } j = 1, 2, \ldots, N_q$$

- A system of N_q *deterministic* equations is obtained.
  1. this system is always uncoupled
  2. each solution $u(\boldsymbol{x}, t, \boldsymbol{X_j})$ may be found using a suitable deterministic solver

Stochastic Collocation method
Non-intrusive approach

- The solution $u(\boldsymbol{x}, t, \boldsymbol{X})$ can be approximated by interpolation on the $\{\boldsymbol{y_j}\}$:

$$\hat{u}_k(\boldsymbol{x}, t) = \frac{\mathbb{E}[u(\boldsymbol{x}, t, \boldsymbol{X})\, \Phi_k(\boldsymbol{X})]}{\mathbb{E}[\Phi_k^2]} = \frac{< u(\boldsymbol{x}, t, \boldsymbol{X}), \Phi_k(\boldsymbol{X}) >}{< \Phi_k^2(\boldsymbol{X}) >}$$

$$= \frac{\int_\Gamma u(\boldsymbol{x}, t, \boldsymbol{X}) \Phi_k(\boldsymbol{X}) \rho(\boldsymbol{X}) d\boldsymbol{X}}{\int_\Gamma \Phi_k^2(\boldsymbol{X}) \rho(\boldsymbol{X}) d\boldsymbol{X}} = \frac{\int_\Gamma u(\boldsymbol{x}, t, \boldsymbol{X}) \big(\prod_{i=1}^N \Phi_{\alpha_{k_i}}^{\mathrm{d}=1}(X_i) \big) \big(\prod_{i=1}^N \rho(X_i) \big) d\boldsymbol{X}}{\int_\Gamma \Phi_k^2(\boldsymbol{X}) \rho(\boldsymbol{X}) d\boldsymbol{X}}$$

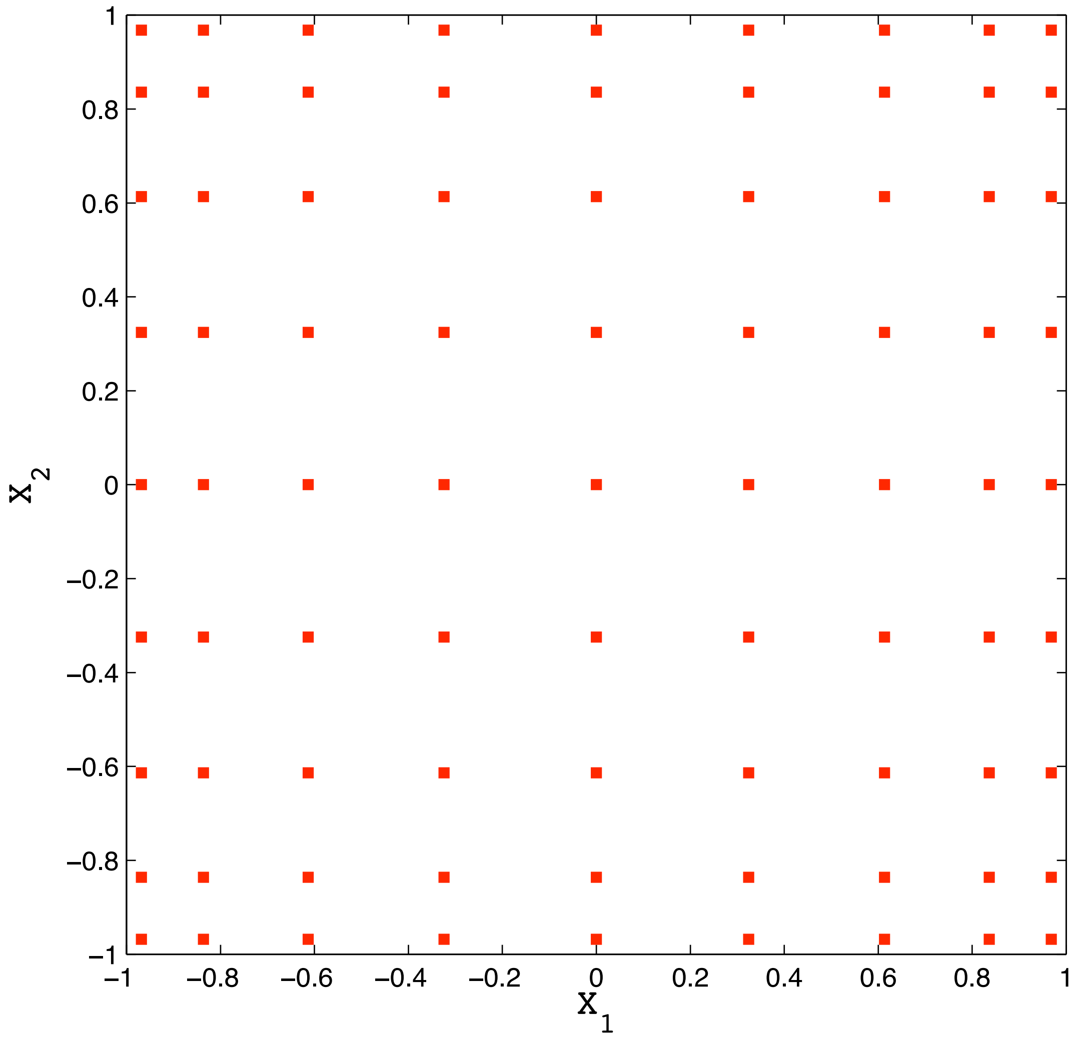
- Different multi-dimensional integration methods can be used (e.g. Gauss-type numerical quadrature). For the numerator we have:

$$\int_\Gamma u(\boldsymbol{x}, t, \boldsymbol{X}) \big(\prod_{i=1}^N \Phi_{\alpha_{k_i}}^{\mathrm{d}=1}(X_i) \big) \big(\prod_{i=1}^N \rho(X_i) \big) d\boldsymbol{X} = \sum_j^{N_q} \omega_j \Big(u(\boldsymbol{x}, t, \boldsymbol{Z}^{(j)}) \big(\prod_{i=1}^N \Phi_{\alpha_{k_i}}^{\mathrm{d}=1}(\boldsymbol{Z}^{(j)}) \big) \Big)$$

Goal: evaluate $I^N f := \int_\Omega f(\boldsymbol{x})d\boldsymbol{x}$

1D: a polynomial function of order **p ≤ 2$\mathbf{n_q}$-1** is exactly integrated with a Gauss quadrature with **$\mathbf{n_q}$** quadrature points.

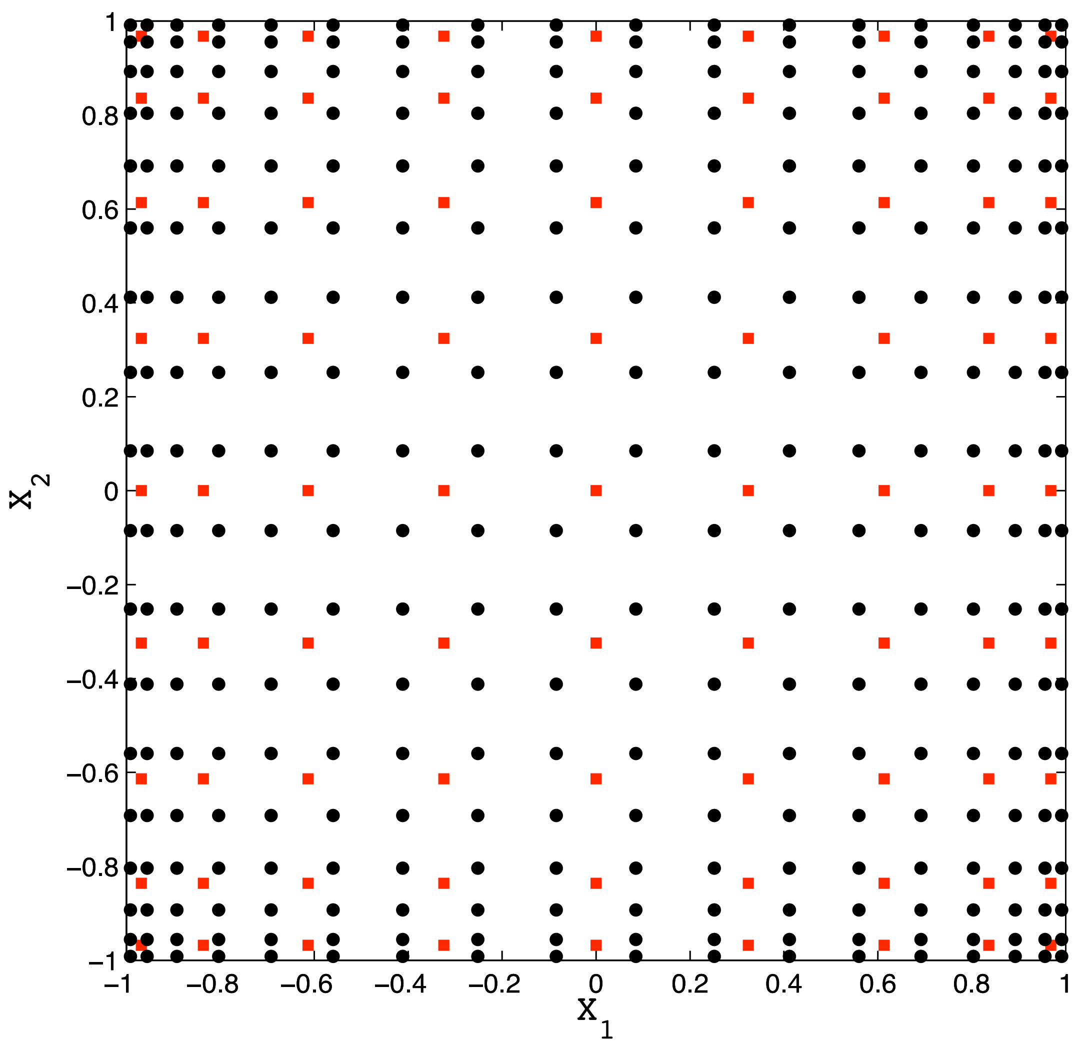
2D: uniform distribution over a square domain.



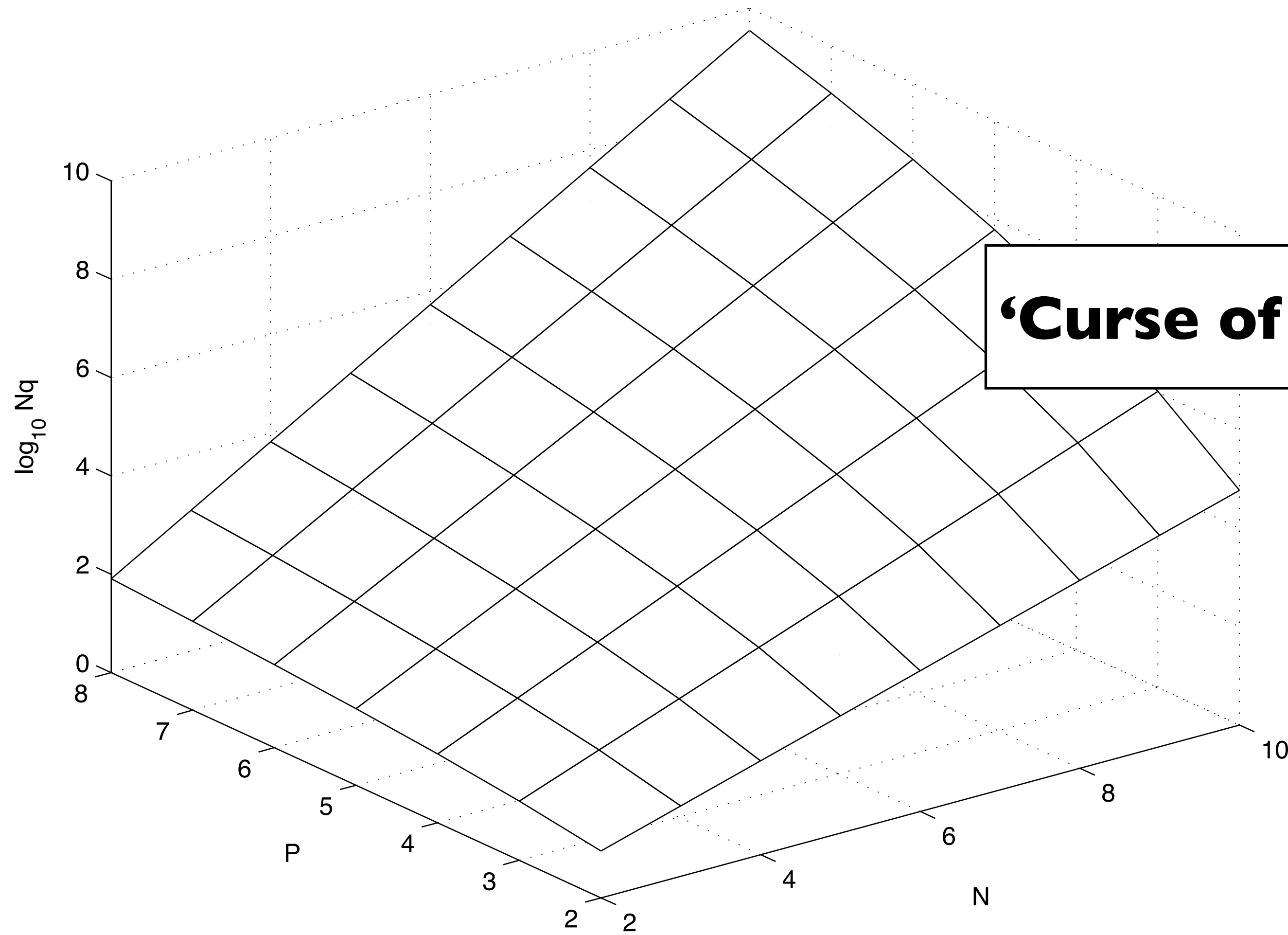
Goal: evaluate $I^N f := \int_\Omega f(\boldsymbol{x}) d\boldsymbol{x}$

1D: a polynomial function of order $\mathbf{p \leq 2n_q - 1}$ is exactly integrated with a Gauss quadrature with $\mathbf{n_q}$ quadrature points.

2D: uniform distribution over a square domain.



Stochastic Collocation method - Gauss quadrature



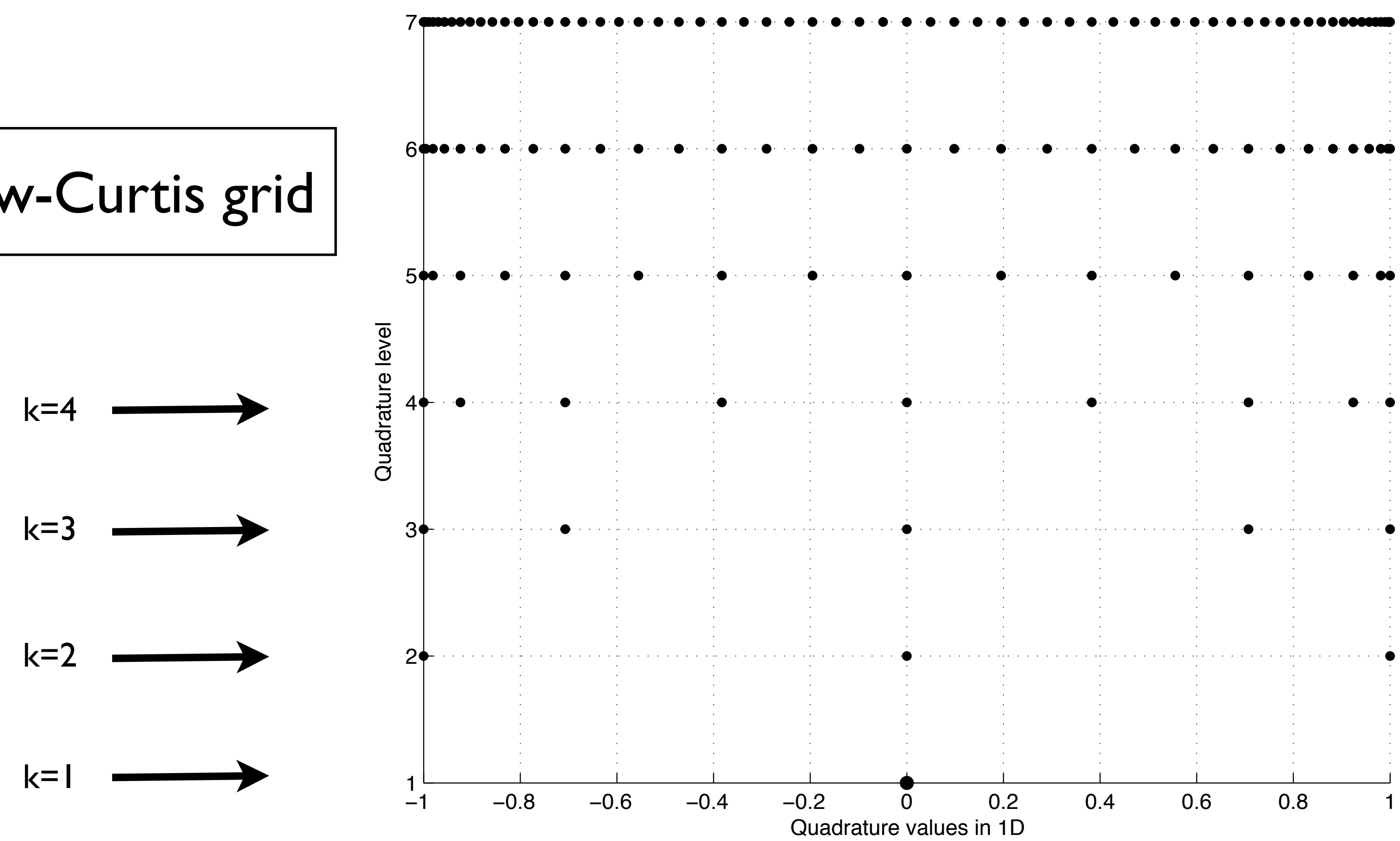
'Curse of dimensionality'!

Multi-D: minimum number of Gauss quadrature points $\mathbf{N_q}$ required to compute exactly the M modal coefficients of the representation of a **N**-dimensional polynomial fonction of degree $\mathbf{p} \leq \mathbf{P}$.

Sparse quadrature - How to reduce the cost?

Approximate the integral with a linear combination of tensor product formulas with key properties: only products with a small number of points are used and the combination is chosen | that the interpolation property for N=1 is preserved for N>1.

Clenshaw-Curtis grid



Sparse quadrature - Smolyak algorithm

In 1D:

$$Q_k(f) := \sum_{i=1}^{m_k} w_i^k\, f(x_i^k), \qquad \Gamma_k := \{x_i^k : 1 \le i \le m_k\} \subset [-1,1].$$

In Multi-D:

$$Q_k^n(f) := \sum_{i=1}^{m_k^n} w_i^k\, f(x_i^k), \qquad \Gamma_k^n := \{x_i^k : 1 \le i \le m_k^n\} \subset [-1,1]^N$$

$$(Q_k^1 \otimes \ldots \otimes Q_k^N)(f) = \sum_{j^1=1}^{m_k^1} \ldots \sum_{j^N=1}^{m_k^N} (w_{j^1}^{k^1} \ldots w_{j^N}^{k^N}) \cdot f(x_{j^1}^{k^1} \ldots x_{j^N}^{k^N})$$

$$\Delta_k^n(f) := (Q_k^n - Q_{k-1}^n)(f),$$

$$I^N f \equiv A(q,N) = \sum_{|\boldsymbol{k}| \le q} (\Delta_k^1 \otimes \ldots \otimes \Delta_k^N)(f),$$

pour $q \in \mathbb{N}$ et $\underline{q \ge N}$, $\boldsymbol{k} \in \mathbb{N}^N$ et $|\boldsymbol{k}| = k^1 + \ldots + k^N$.

Sparse quadrature - Smolyak algorithm

$$A(q,N) = \sum_{q-N+1 \leq |\boldsymbol{k}| \leq q} (-1)^{q-|\boldsymbol{k}|}\, C(N-1, q-|\boldsymbol{k}|)\, (Q_k^1 \otimes \ldots \otimes Q_k^N)(f).$$

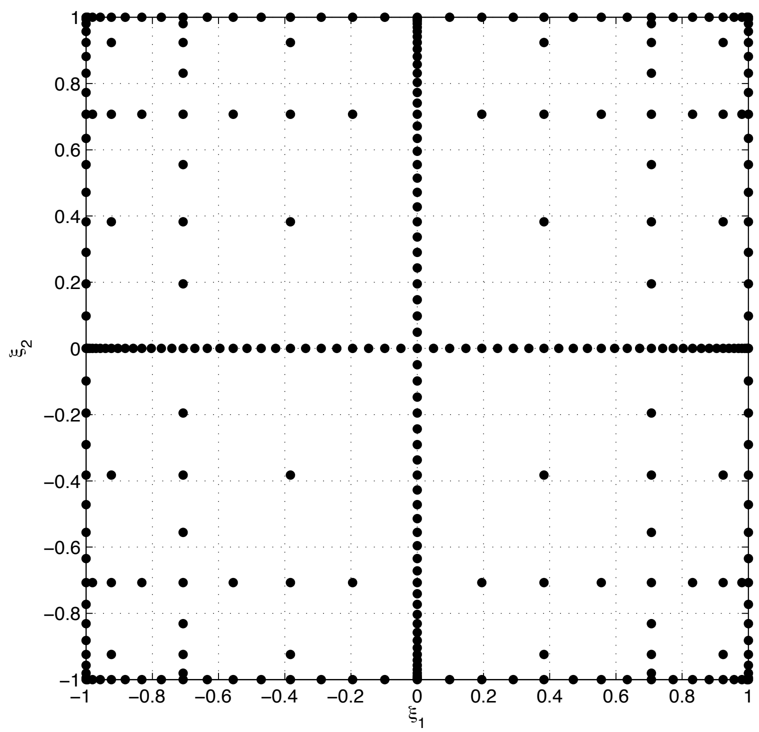
Le produit des tenseurs $(Q_k^1 \otimes \ldots \otimes Q_k^N)$ doit être calculé sur la grille $(\Gamma_k^1 \times \ldots \times \Gamma$
c'est-à-dire que $A(q,d)$ dépend des valeurs de la fonction sur l'union :

$$U(q,d) = \bigcup_{q-d+1 \leq |\boldsymbol{k}| \leq q} (\Gamma_k^1 \times \ldots \times \Gamma_k^N) \subset [-1,1]^N.$$

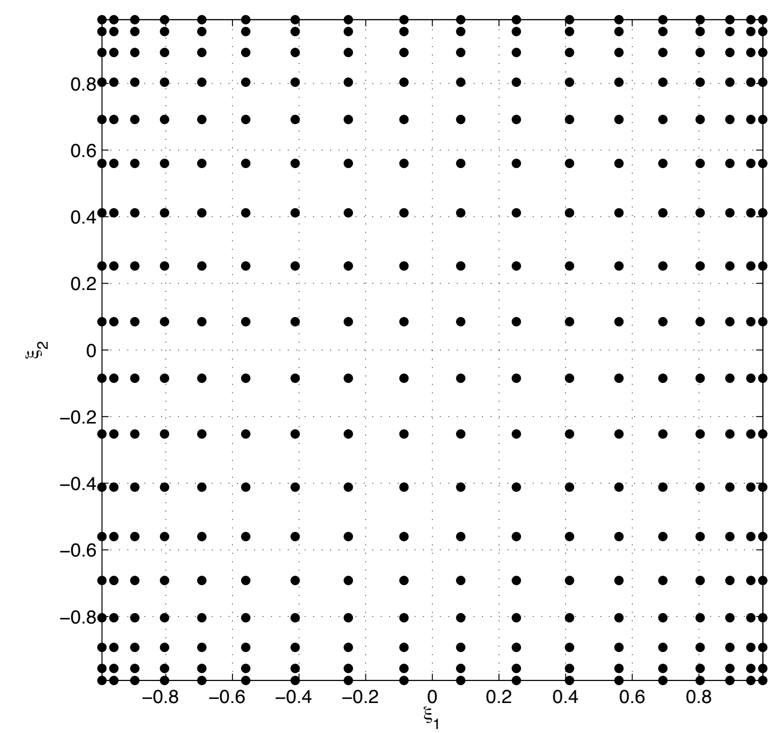
Si les grilles sont emboîtées alors $\Gamma_k^n \subset \Gamma_{k+1}^n$ et $U(q,d) \subset U(q+1,d)$ et donc :

$$U(q,d) = \bigcup_{|\boldsymbol{k}|=q} (\Gamma_k^1 \times \ldots \times \Gamma_k^N) \subset [-1,1]^N,$$

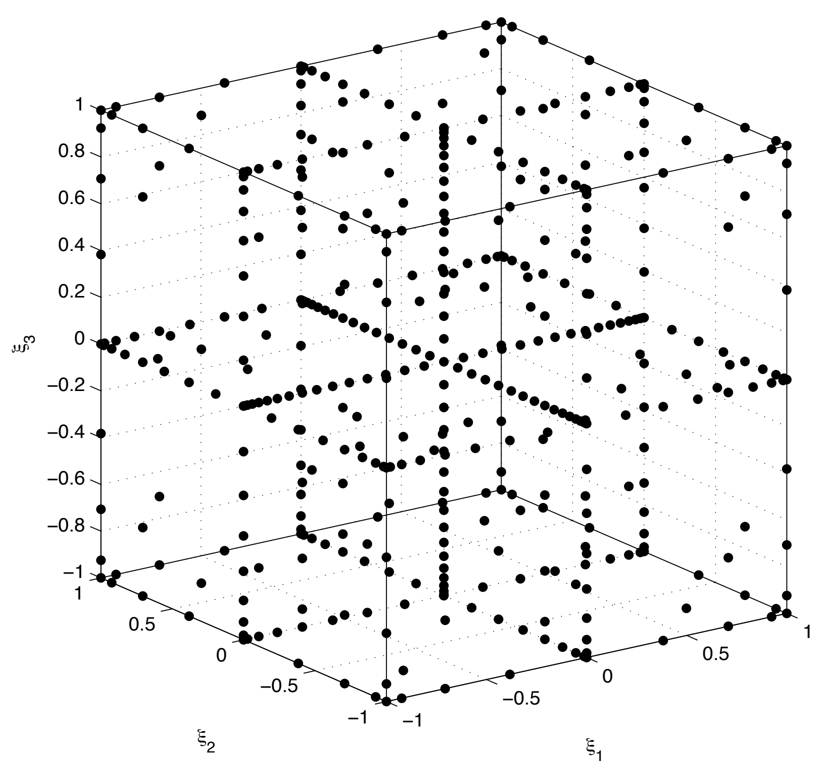
A(N+l,N): N=2, l=8; Nq=321 points



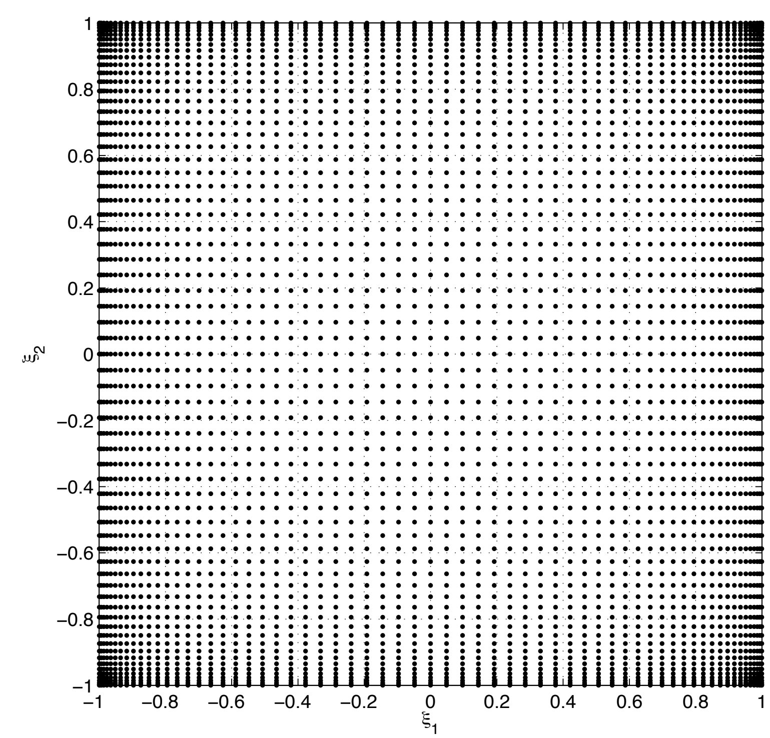
QG N=2, nq=18; Nq=324 points



A(N+l,N): N=3, l=8; Nq=441 points



QG N=2, nq=65; Nq=4425 points



Sparse quadrature - accuracy and cost comparison

We introduce the notation: $q=N+l$ and we have $A(N+l,N)$ where the level l is called the stage.

Smolyak/Clenshaw-Curtis $A(N+l,N)$ is exact for all polynomials π_N^{2l+1}, i.e. N-dimensional polynomials of degree at most $p=2l+1$ (Novak & Ritter, Constructive Approximation 1999)

$$Nq_{\mathrm{SCC}} \sim \frac{2^l}{l!} N^l \quad \text{si } l \text{ fixé et } N \gg 1$$

$dim(\pi_N^l) = C(N+l,N) \sim N^l / l!$ for large N.

$A(N+l,N)$ uses about 2^l times more points than degrees of freedom of π_N^l.

This factor is independent of N. Therefore the algorithm is considered optimal.

N	l	M	Nq_{SCC}	Nq_{QG}	$Nq_{\mathrm{QG}}/Nq_{\mathrm{SCC}}$
2	1	3	5	4	< 1
	2	6	13	9	< 1
	3	10	29	16	< 1
	4	15	65	25	< 1
	5	21	145	36	< 1
5	1	6	11	32	≈ 3
	2	21	61	243	≈ 4
	3	56	241	1 024	≈ 4
	4	126	801	3 125	≈ 4
	5	252	2 433	7 776	≈ 3
10	1	11	21	1 024	≈ 49
	2	66	221	59 049	≈ 267
	3	286	1 581	1 048 576	≈ 663
	4	1 001	8 801	9 765 625	$\approx 1\,110$
	5	3 003	41 265	60 466 176	$\approx 1\,465$

Once we hold the spectral PC representation... Post-processing I

- Auto-correlation R_u:

$$\begin{aligned} R_u(\boldsymbol{x_1}, \boldsymbol{x_2}, t) &= \; < u(\boldsymbol{x_1}, t, \omega), u(\boldsymbol{x_2}, t, \omega) > \\ &= \sum_{k=0}^{M} \hat{u}_k(\boldsymbol{x_1}, t)\hat{u}_k(\boldsymbol{x_2}, t) < \Phi_i^2 > \end{aligned}$$

- Expected values:

1. $\mu_u = \mathbb{E}[u(\boldsymbol{x}, t, \boldsymbol{X})] = \hat{u}_0$
2. $\sigma_u^2 = \mathbb{E}[u(\boldsymbol{x}, t, \boldsymbol{X})^2] = \sum_{k=1}^{M} \hat{u}_k^2 \, \mathbb{E}[\Phi_k^2]$
3. $\delta_u = \frac{1}{\sigma_u^3}\mathbb{E}[u(\boldsymbol{x}, t, \boldsymbol{X})^3] = \frac{1}{\sigma_u^3} \sum_{i=1}^{M} \sum_{j=1}^{M} \sum_{k=1}^{M} \hat{u}_i \hat{u}_j \hat{u}_k \, \mathbb{E}[\Phi_i \Phi_j \Phi_k]$
4. $\kappa_u = \frac{1}{\sigma_u^4}\mathbb{E}[u(\boldsymbol{x}, t, \boldsymbol{X})^4] = \frac{1}{\sigma_u^4} \sum_{i=1}^{M} \sum_{j=1}^{M} \sum_{k=1}^{M} \sum_{l=1}^{M} \hat{u}_i \hat{u}_j \hat{u}_k \hat{u}_l \, \mathbb{E}[\Phi_i \Phi_j \Phi_k \Phi_l]$

Post-processing II

- Sensitivity analysis:

  Variance-based: Sobol' sensitivity indices $S_i = \text{var}(\mathbb{E}[u|X_i])/\sigma_u^2$ (analytically computed from gPC coefficients)

- Distributions and conditional densities:

  1. Histogram
  2. Kernel-smoothing density estimate
  3. $f_u(\boldsymbol{x}, t, x) = \sum_n \frac{f_X(X_n)}{\left|\frac{\partial u(\boldsymbol{x},t,X)}{\partial X}|_{X=X_n}\right|}$ with X_n roots of $u(\boldsymbol{x}, t, X) = \sum_{i=0}^{M} \hat{u}_k \Phi_k = x$.

- Reliability analysis:

  1. Probability failure P_f of u:

  $$P_f = \int_D f_X(\boldsymbol{X}) d\boldsymbol{X} = \mathbb{E}[\mathbf{1}_D(u)] \text{ with } D = \{G(\boldsymbol{X}) = R - u(\boldsymbol{x}, t, \boldsymbol{X}) < 0\}$$

  2. α-Quantile u_α:

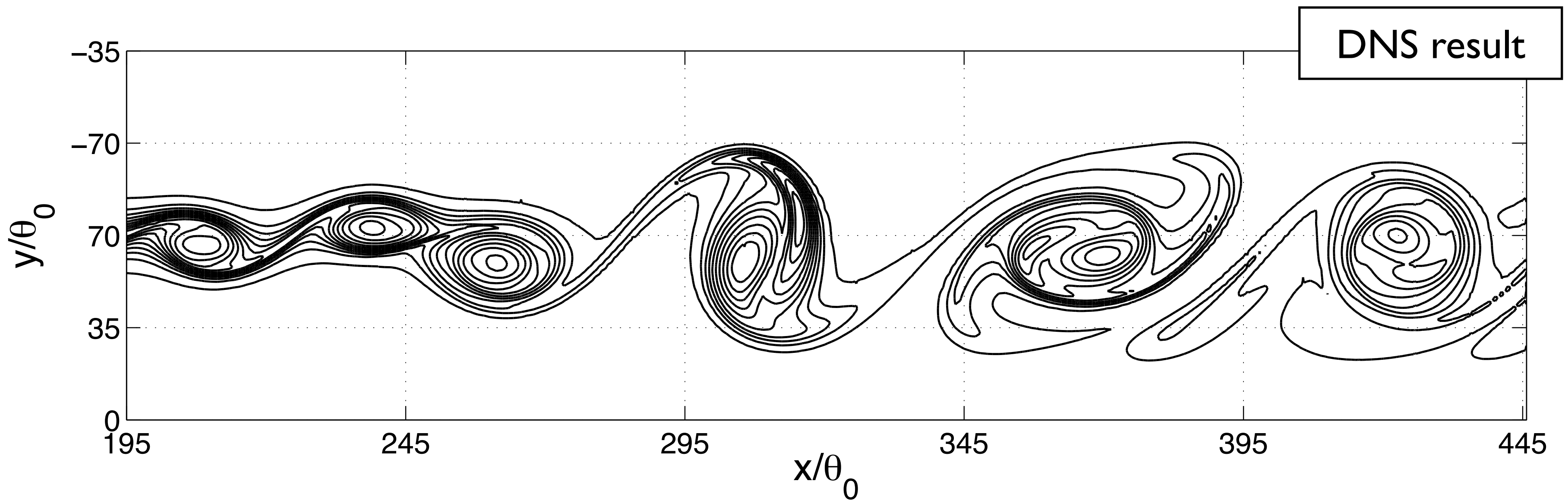
  $$P(u(\boldsymbol{x}, t, \boldsymbol{X}) \leq u_\alpha(\boldsymbol{x}, t) = \alpha \text{ i.e. } u_\alpha = \mathbf{inf}\{u(\boldsymbol{x}, t), F\big(u(\boldsymbol{x}, t)\big) > \alpha\}$$

Possible applications (in mechanical engineering!) so far...

- Solid mechanics (Ghanem & Spanos 1989-91).
- Flow through porous media (Ghanem & Dham 1998, Zhang & Lu 2004).
- Heat diffusion in stochastic media (Hien & Kleiber 1997-98, Xiu & Karniadakis 2003).
- Incompressible flows (Le Maître et al, Karniadakis et al, Hou et al).
- Fluid-Structure interaction (Karniadakis et al, Lucor et al).
- Micro-fluid systems (Debusschere et al 2001).
- Reacting flows & combustion (Reagan et al 2001).
- 0-Mach flows & thermo-fluid problems (Le Maître et al 2003).

Sensitivity of spatially developing plane mixing layer with respect to uncertain inflow conditions (Collaboration with Jordan Ko & Pierre Sagaut)

$$\overline{u}_{\rm in}(y) = 1 + \lambda \tanh(y/2) \qquad \lambda = \triangle U / 2\overline{U}$$
$$\overline{v}_{\rm in}(y) = 0,$$



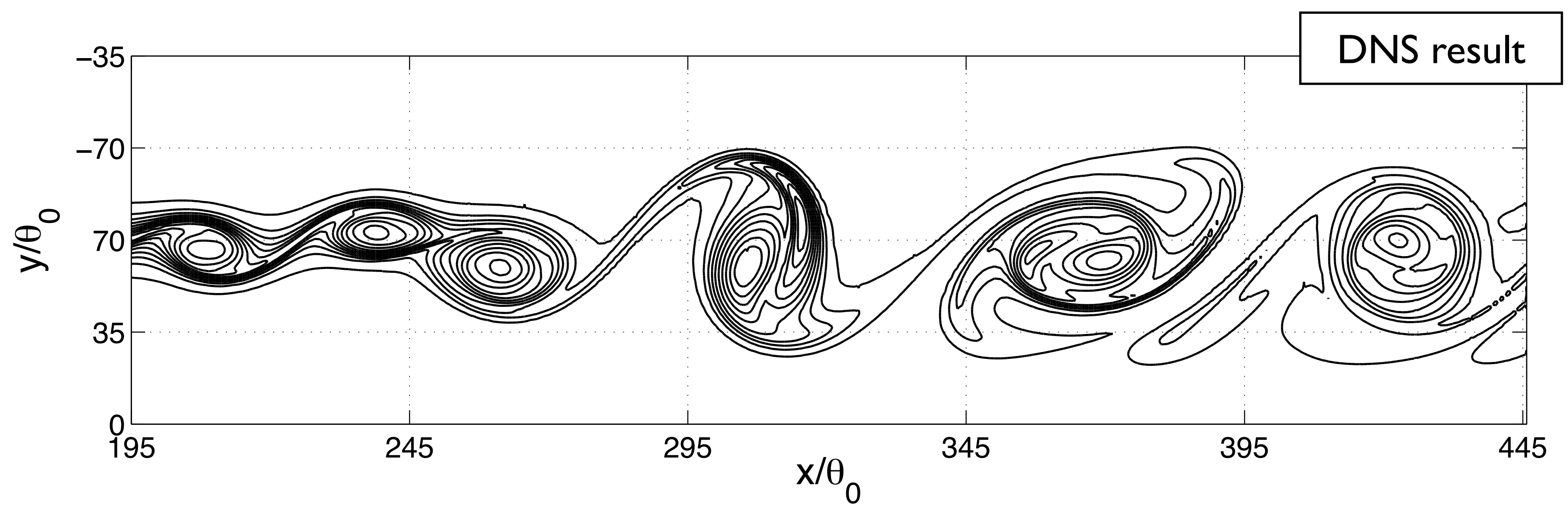
Sensitivity of spatially developing plane mixing layer with respect to uncertain inflow conditions

$$u_{\text{in}}(y,t) = \overline{u}_{\text{in}}(y) + \sum_{i=1}^{N_p} \epsilon_i [\cos(n_i y) f(y) \sin(\omega_i t) + \gamma_i]$$
$$v_{\text{in}}(y,t) = \overline{v}_{\text{in}}(y)$$

LST

Forcing

$$\overline{u}_{\text{in}}(y) = 1 + \lambda \tanh(y/2) \qquad \lambda = \Delta U / 2\overline{U}$$
$$\overline{v}_{\text{in}}(y) = 0,$$



Sensitivity of spatially developing plane mixing layer with respect to uncertain inflow conditions

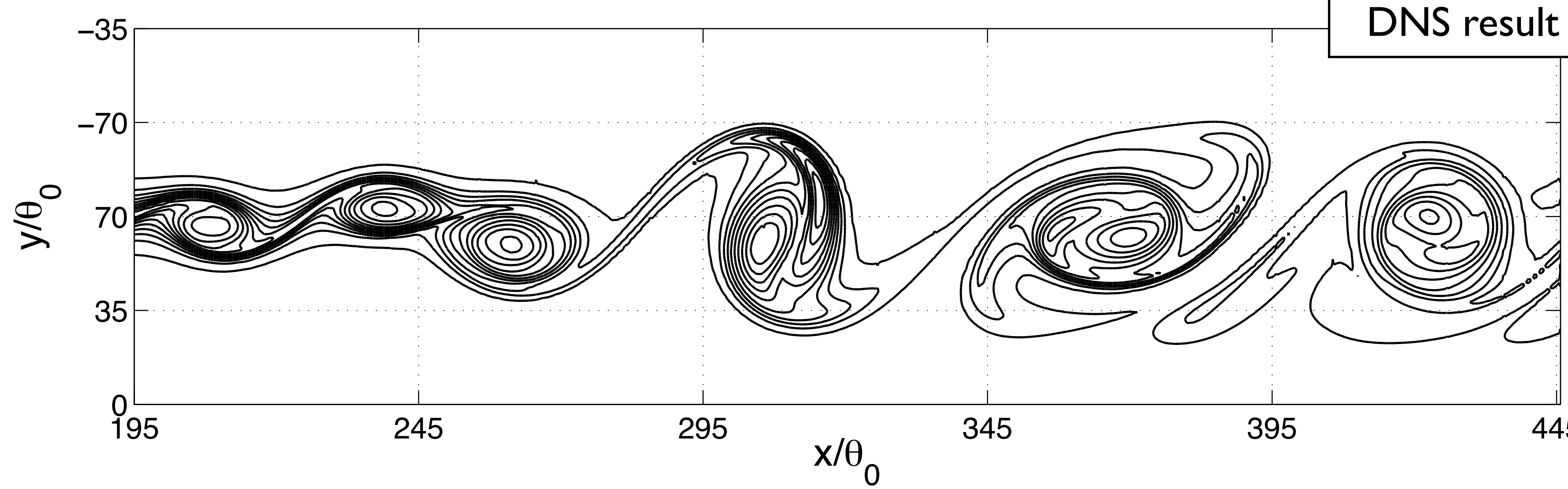
$$u_{\text{in}}(y,t) = \overline{u}_{\text{in}}(y) + \sum_{i=1}^{N_p} \epsilon_i \left[\cos(n_i y) f(y) \sin(\omega_i t) + \gamma_i\right]$$
$$v_{\text{in}}(y,t) = \overline{v}_{\text{in}}(y)$$

LST

Forcing

$$\overline{u}_{\text{in}}(y) = 1 + \lambda \tanh(y/2) \qquad \lambda = \Delta U / 2\overline{U}$$
$$\overline{v}_{\text{in}}(y) = 0,$$

DNS result

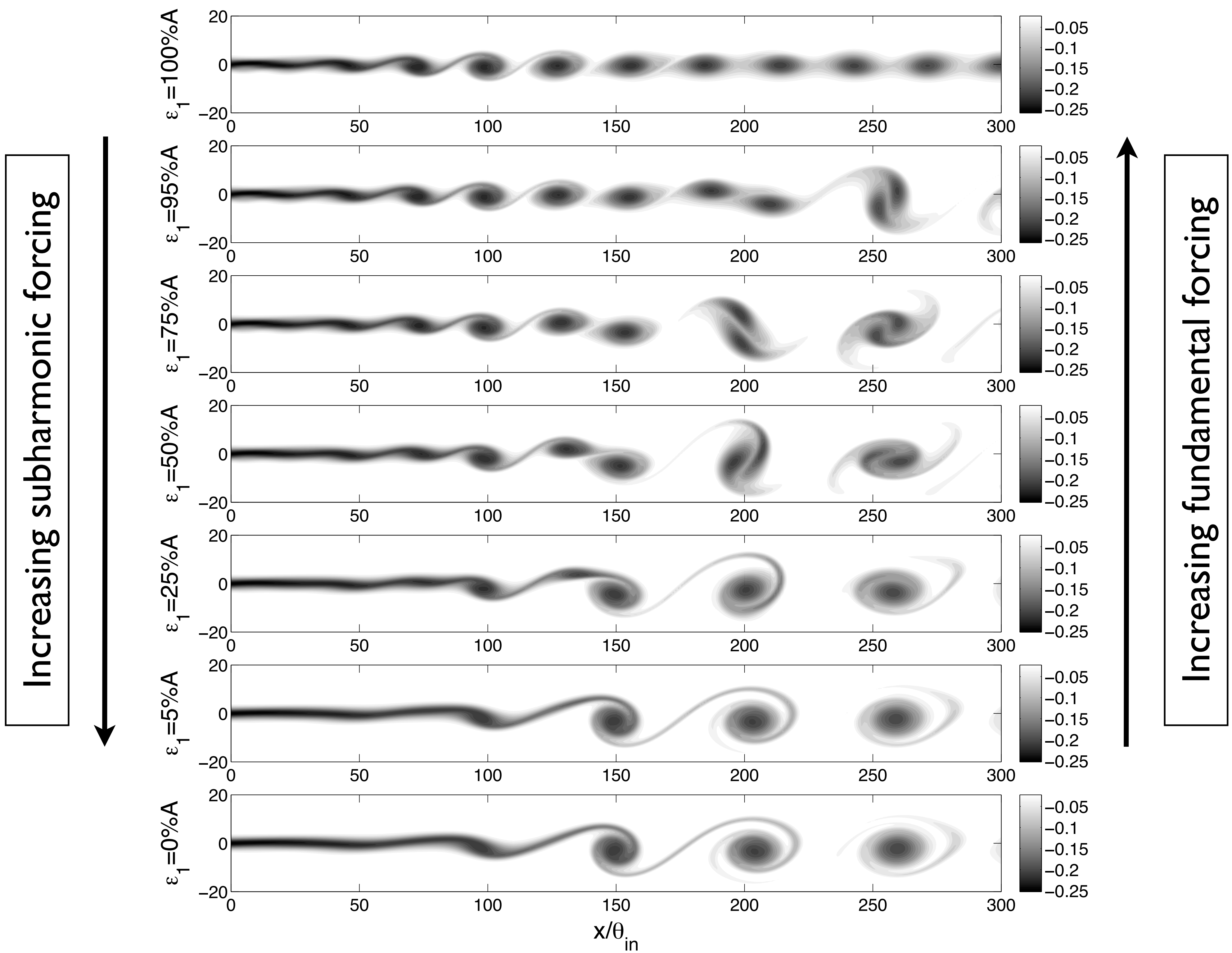


Quantities of interest:
momentum and vorticity thicknesses

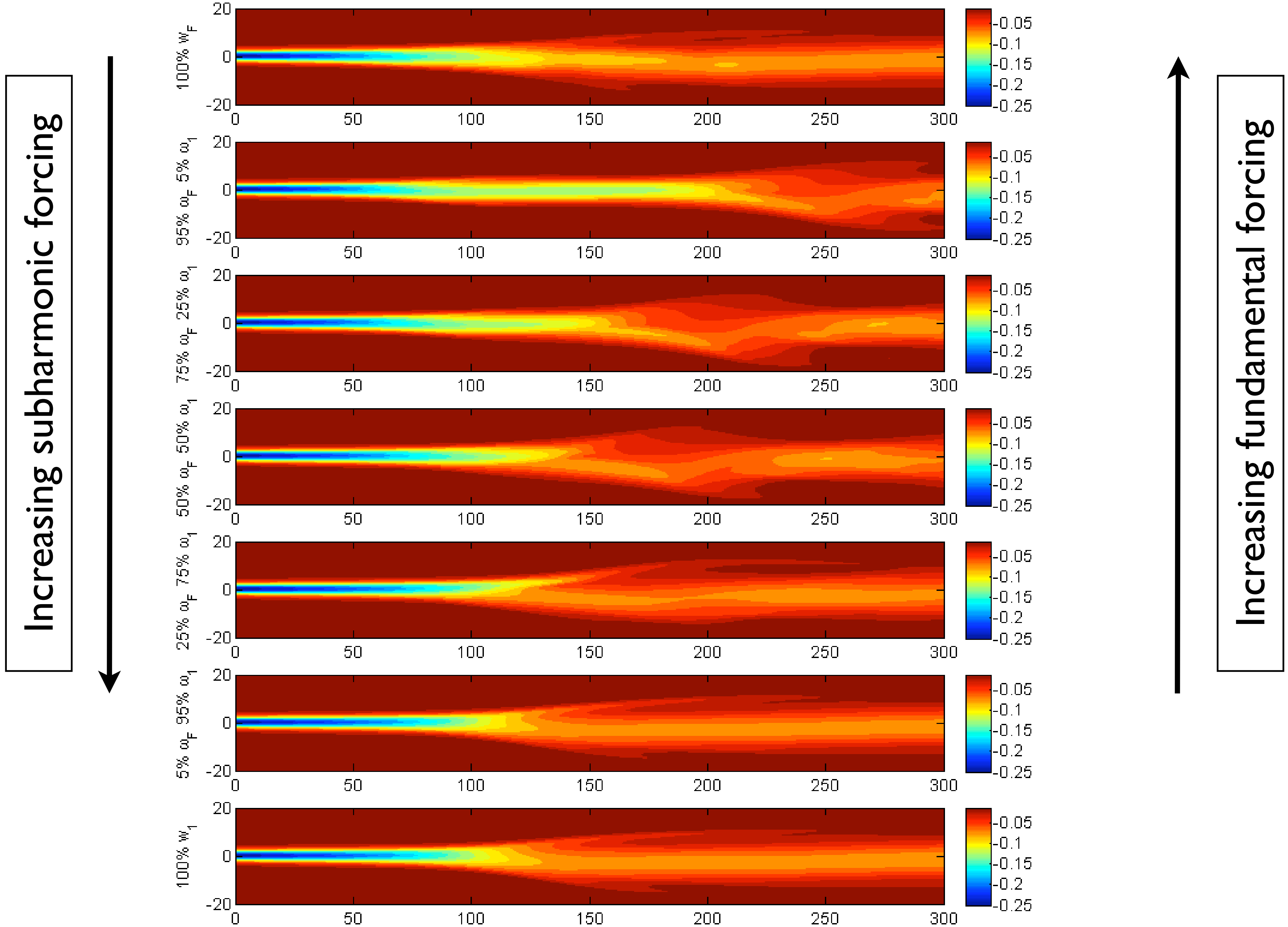
$$\theta = \frac{-1}{\Delta U^2} \int_{-\infty}^{\infty} (u(y) - U_H)(u(y) - U_L)\, dy$$

$$\delta_\omega = \frac{\Delta U}{[\partial u(y)/\partial y]_{\max}}$$

Stochastic mixing layer
Bi-modal perturbation forcing



Stochastic mixing layer
Bi-modal perturbation forcing



Stochastic mixing layer
Numerical parameters

Random forcing magnitudes ϵᵢ: *uniform* ind. random variables

Re	λ	$\overline{\epsilon_i}$	σ_i	ω_f	n_1	n_2	n_3
100	0.5	5.0%	5.0%	0.22	0.4π	0.3π	$[0.2\pi]$

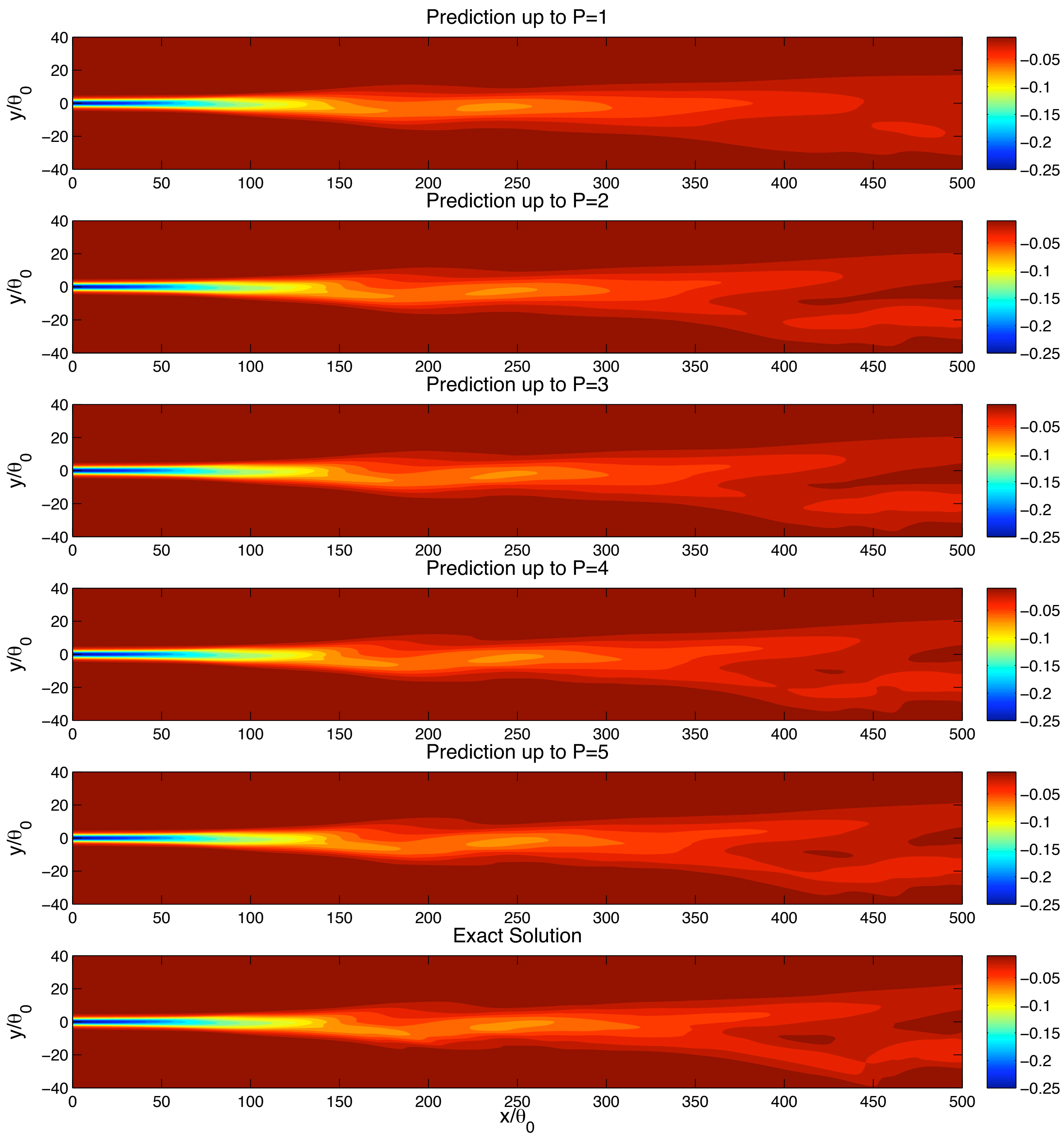
Deterministic parameters per realization

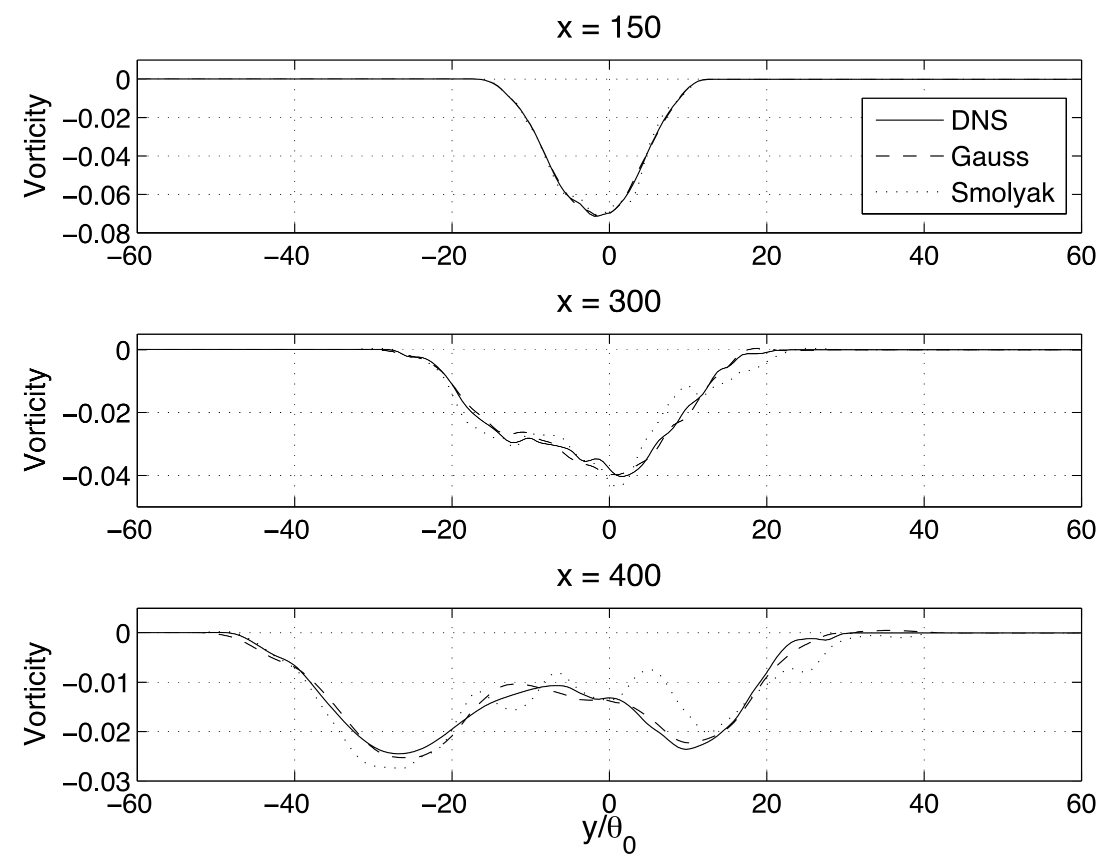
	Bi-modal	Tri-modal
Domain Size (in θ_0 units)	360×240	600×480
Mesh Resolution (in θ_0 units)	0.83×0.83	0.91×0.91
DOF	438 048	1 244 160
Integration Time	24 (8) T_f	40 (12) T_f
Run Time	18 hours	64 hours

Stochastic Parameters

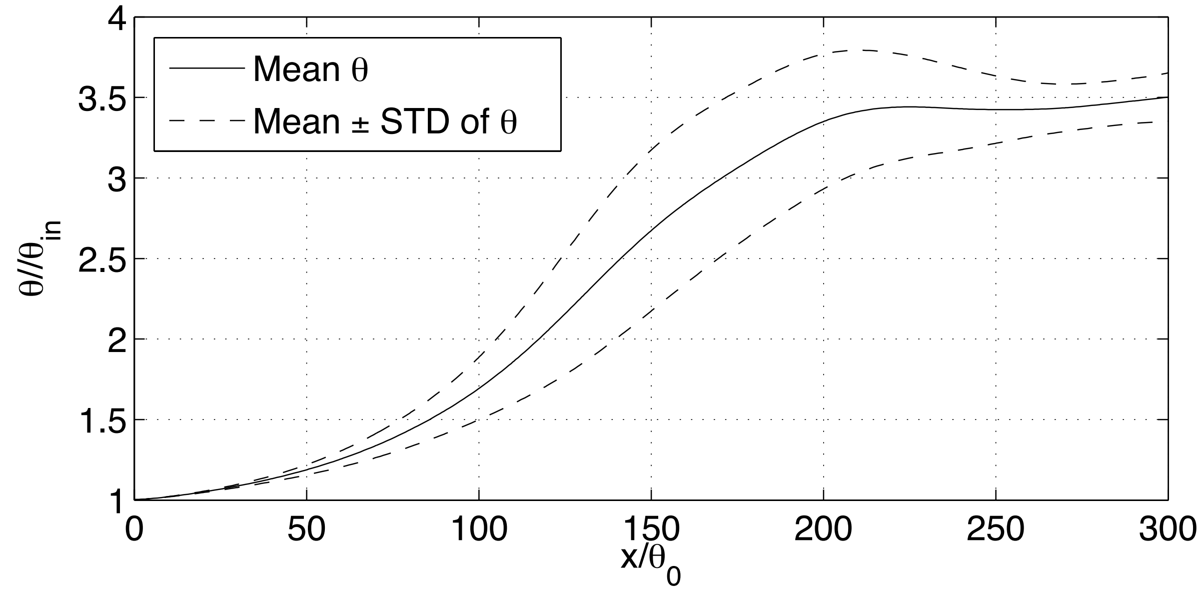
	Bi-modal Full	Bi-modal Sparse	Tri-modal Full	Tri-modal Sparse
Quadrature Level	9	6	10	5
Samples	81(100)	145(321)	[216]1000(1331)	177(441)
Legendre Poly. Order	7	4	8	3
Total gPC Terms	36	15	165	20

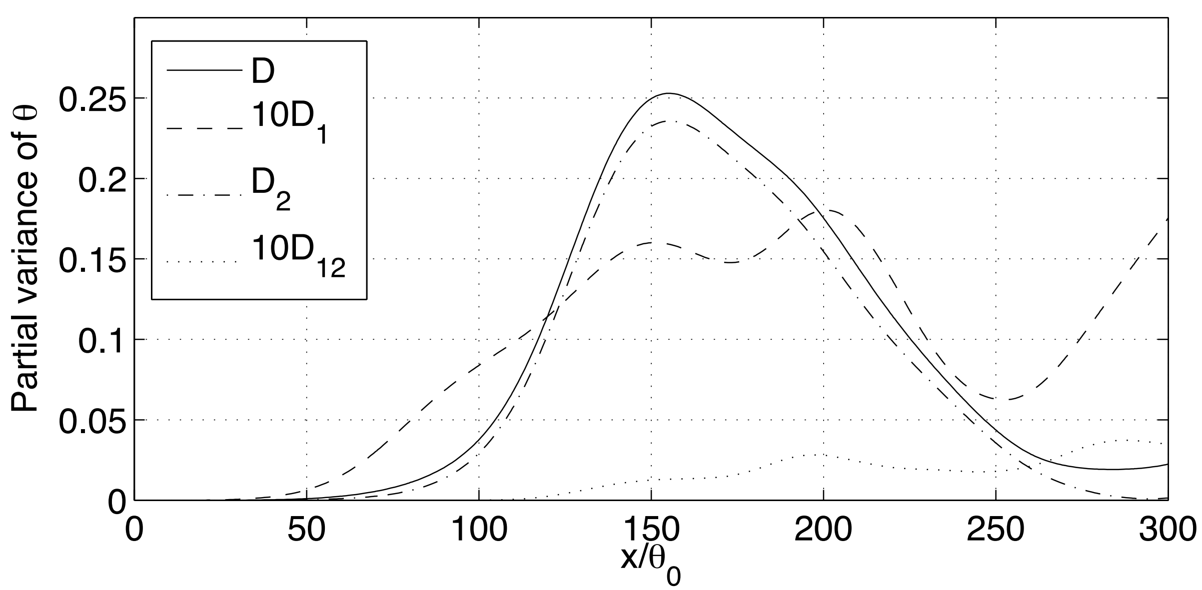
Time-averaged vorticity prediction
Tri-modal perturbation forcing

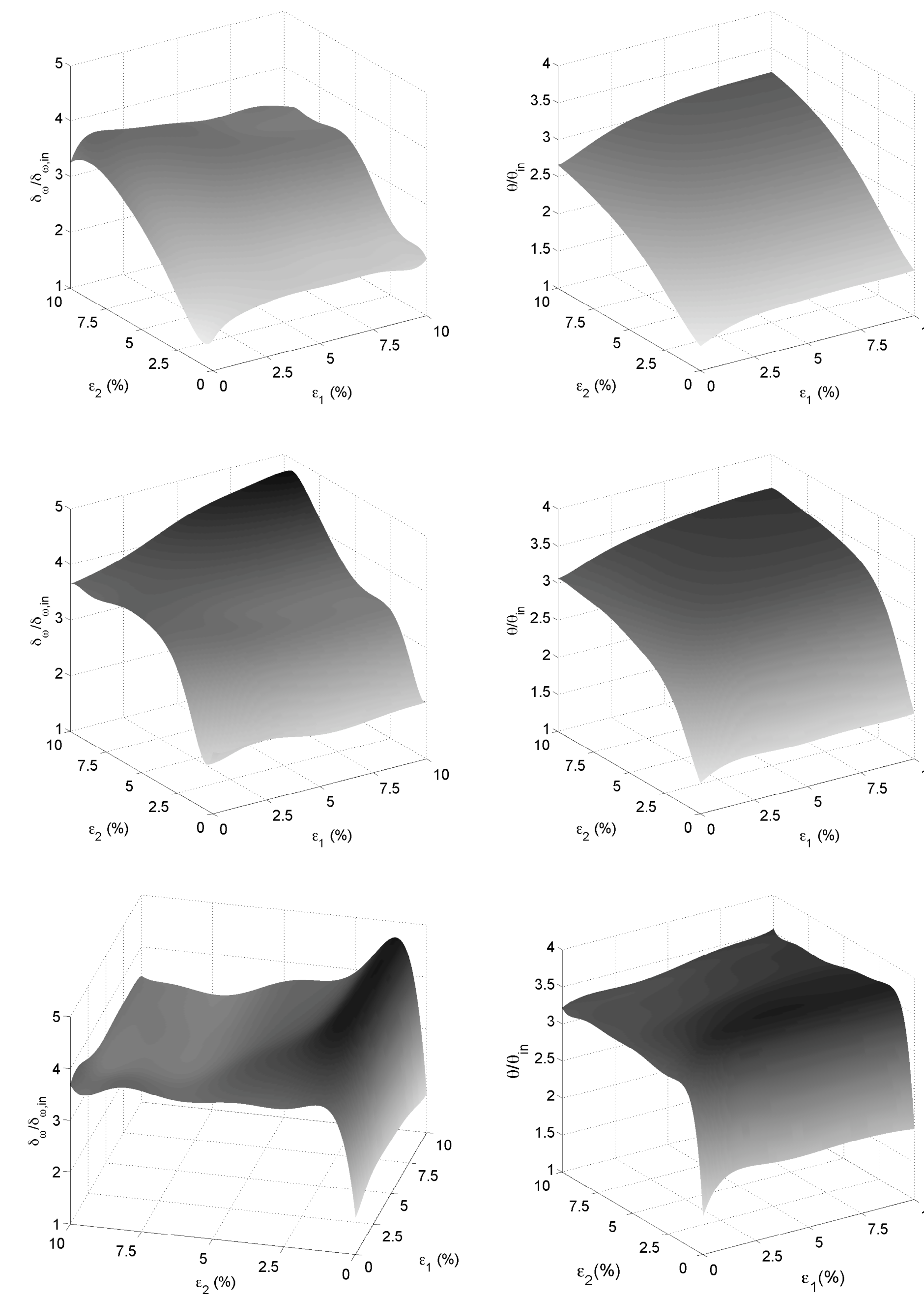




Sensitivity analysis
Statistical moments and surface responses

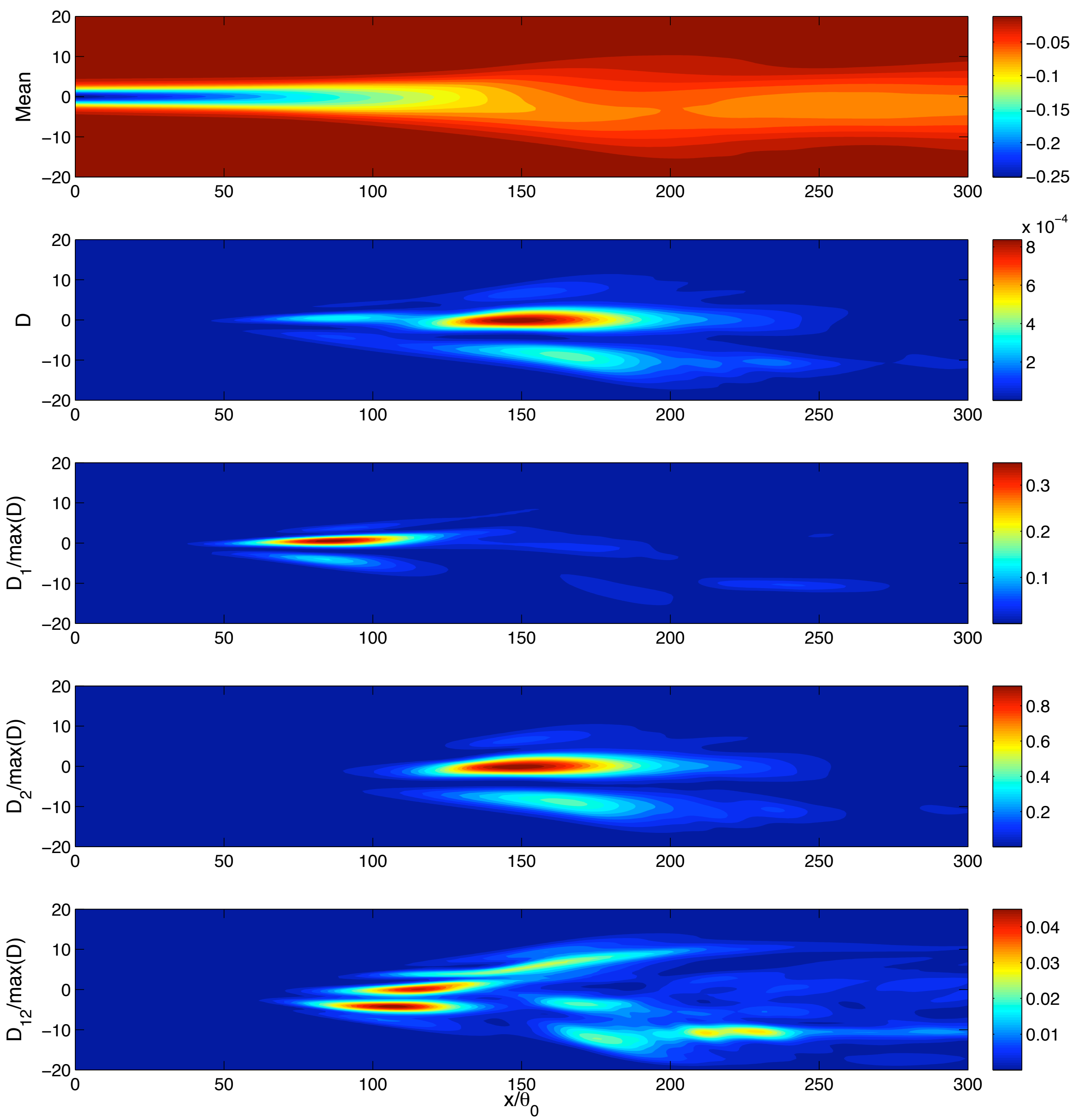




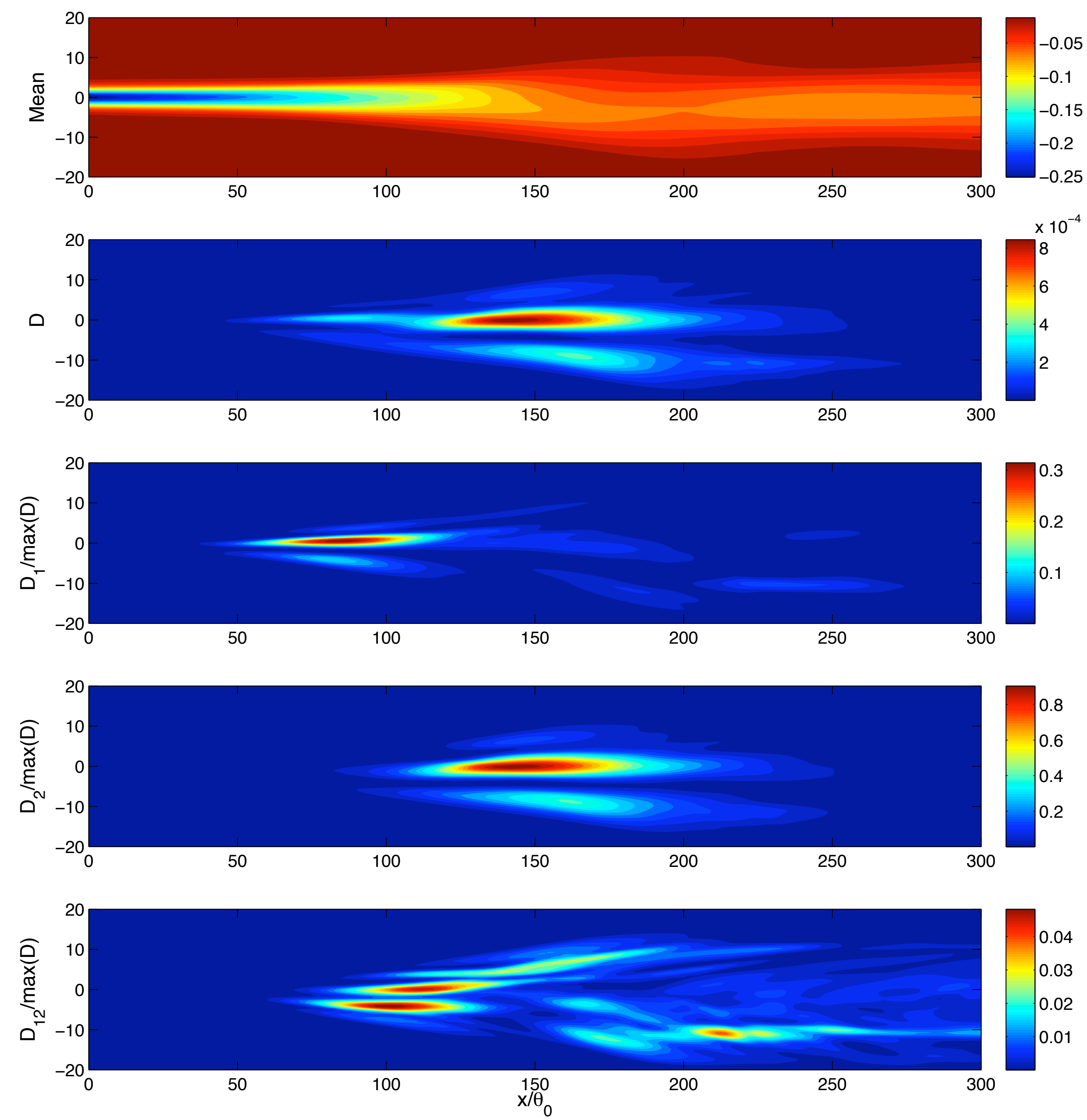


Spatial sensitivity analysis
Sobol coefficients

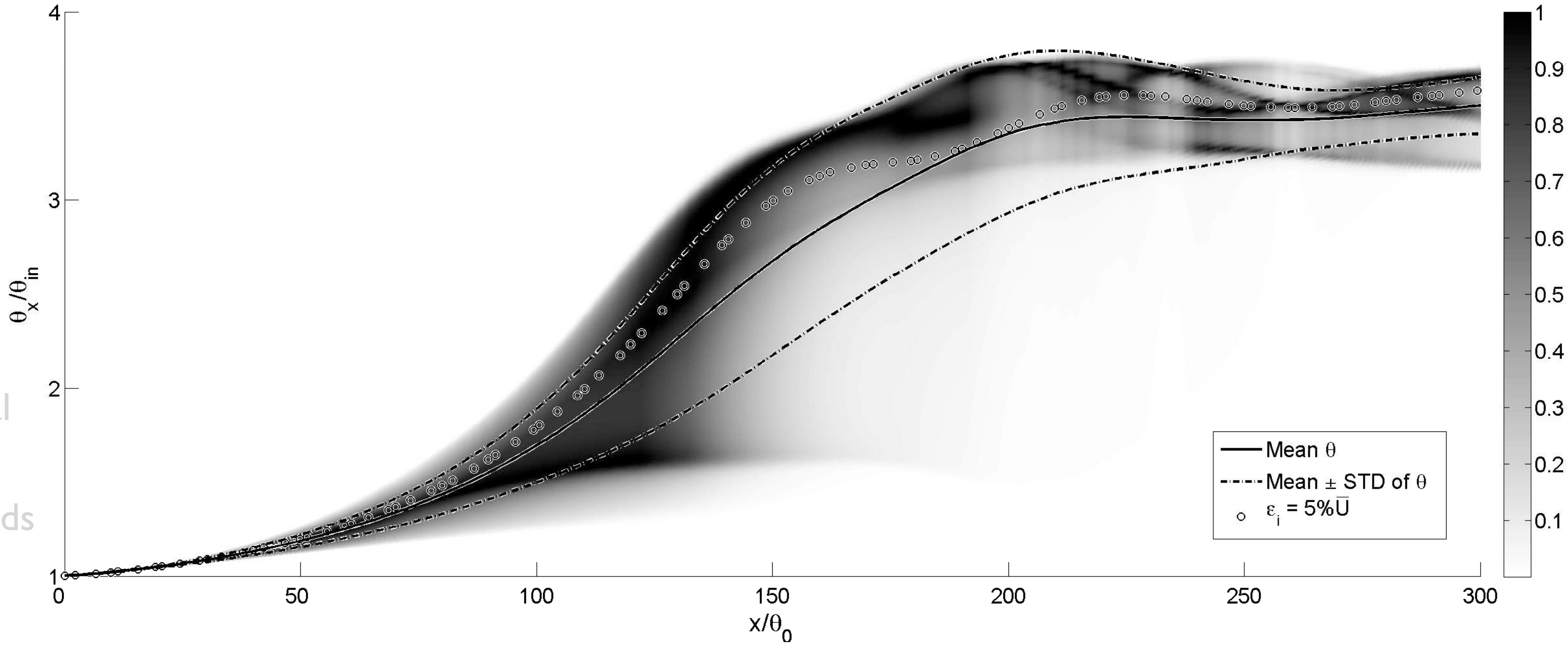
Gauss Quadrature

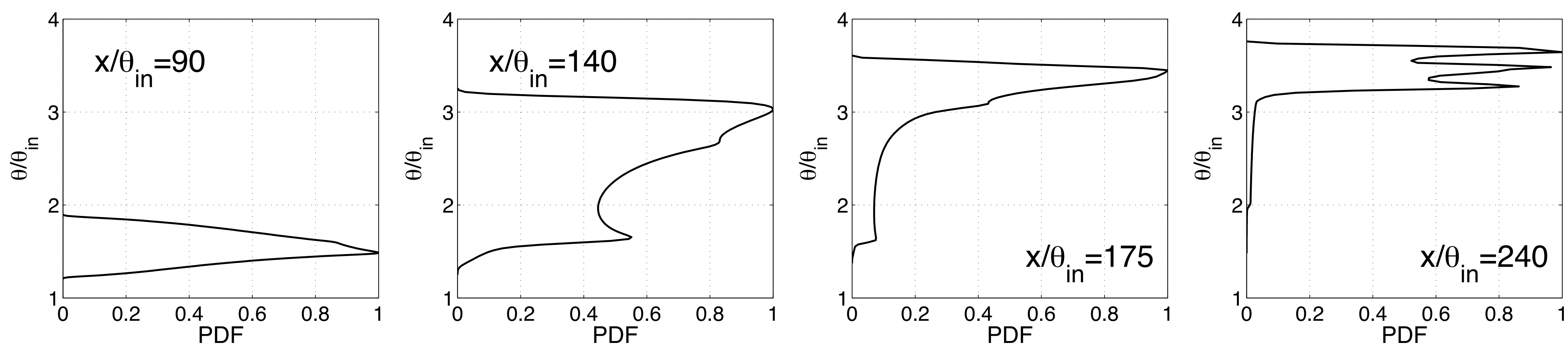


Sparse Quadrature

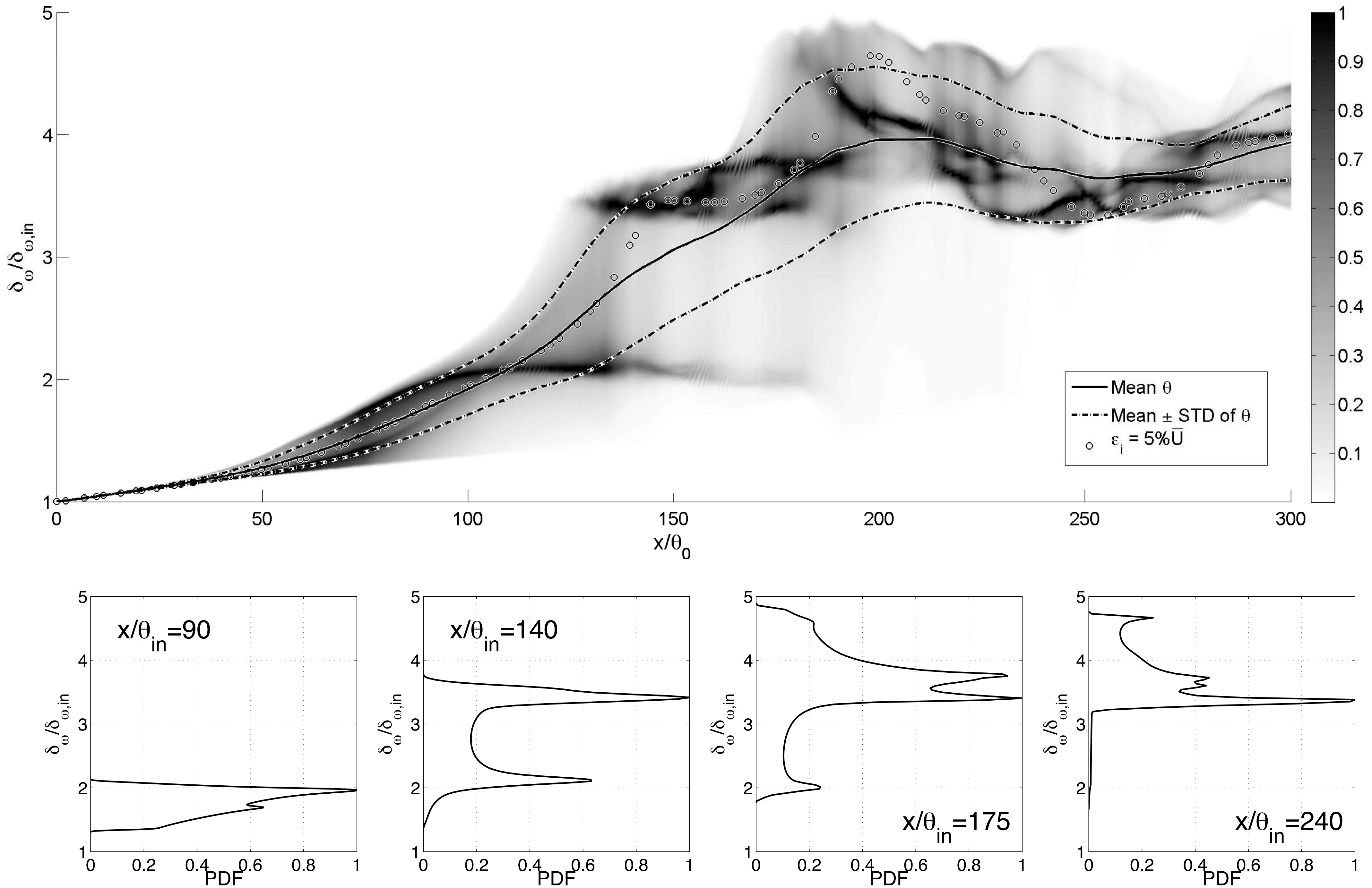


Downstream distribution of momentum thickness pdf
Bi-modal perturbation case





Downstream distribution of momentum thickness pdf
Bi-modal perturbation case



Conclusion

After seminal work of N.Wiener (1938), a long time passed until the work of Ghanem & Spanos (end of the 80s / beginning of the 90s) who pioneered the computational use of stochastic spectral representations.

- Method does not require high skills in prob. or statistics ⇒ seems to attract more the numerical analysis "deterministic" scientific community.
- Robust and accurate representation of second-order RPs expressed as functionals of a countable number of independent RVs, with known distributions.
- Not limited to small uncertainties with Gaussian distributions.
- Provide an explicit representation of the RP. Not only moments and/or pdf.
- Computational cost generally lower than sampling methods (Monte-Carlo type).
- High dimensions ⇒ many evaluation of the integrand. High CPU cost for large scale problems! Sparse basis or quadrature can alleviate this problem.
- Stability issues / convergence failure for discontinuous or non-smooth RPs ⇒ (multi-elements/multi-resolution) adaptive approaches.
- Choice between Galerkin or collocation method is problem-dependent. Collocation: advantage more noticeable for problems with more complicated forms of governing equations.