Introduction to uncertainty quantification (UQ).
With applications.

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OUTLINE

Introduction

Probability basics and Monte-Carlo

Orthogonal/orthonormal polynomials
Non-intrusive polynomial chaos methods in 1D
Intrusive polynomial chaos method in 1D

Extension to high dimensions

Examples of application

Conclusion
INTRODUCTION

Example I: drag minimization

- **Deterministic minimization of airplane cruise shape: define shape**
  - That minimizes total drag $C_d$ at $M=0.82$
  - Satisfying constraints on lift, pitching moment, inner volume...

- **Actually, variations of cruise flight Mach number**
  - Waiting for landing slot
  - Speeding up to cope with pilot maximum flight time
  - $\rightarrow$ Variable Mach number described by $D(M)$

- **Robust definition of airplane cruise shape**
  - Minimize $\int C_d(M)D(M)dM$, satisfying constraints for all values of $M$ present in $D(M)$
INTRODUCTION

Example II: Fan design

- Fan operational conditions subject to changes in wind conditions
- Manufacturing subject to tolerances
- Robust design accounts for
  - Variability of external parameters
  - Tolerances for internal parameters

Figure 1: Robust design (from cenaero.be)
INTRODUCTION

Example III: validation process

- **Unknown data in experiment**
  - Upwind Mach number not fully controlled in wind tunnels $dM = 0.001$

- **Unknown physical constant needed in numerical model**
  - Wall roughness constant (milled, brazed, eroded surface...)

- **Discrepancy in a computational/experimental validation process!**

- **Compute the mean and standard deviation of the output of interest due to the uncertain inputs**
INTRODUCTION
Definition of uncertain inputs

- **UNCERTAINTY QUANTIFICATION**: describe the stochastic behaviour of OUTPUTS of interest due to uncertain INPUTS

- **Overview of CFD actual uncertain INPUTS**:
  - Geometrical (manufacturing tolerance)
  - Operational: flow at boundaries (far field, injection...)
  - Reference:
    - *Proceedings of RTO-MP-AVT-147*
    - Evans T.P., Tattersall P. and Doherty J.J.: Identification and quantification of uncertainty sources in aircraft related CFD-computations - An industrial perspective

- **Stochastic behaviour of OUTPUTS. Presently, most often, mean and variance are calculated**
INTRODUCTION
Three issues in (UQ) – 1 terminology

- Lack of agreement on the definition of “error”, “uncertainty”...

- AIAA Guide G-077-1998 Uncertainty is a potential deficiency in any phase are activity of the modeling process that is due to the lack of knowledge. Error is a recognizable deficiency in any phase or activity of the modelling process that is not due to the lack of knowledge.

- ASME Guide V& V 20 (in its simpler version adopted for the Lisbon Workshops on CFD uncertainty). The validation comparison error is defined as the difference between the simulation value and the experimental data value. It is split in numerical, model, input and data errors (assumed to be independant). Numerical (resp. input, model, data) uncertainty is a bound of the absolute value of numerical (resp. input, model, data) error.
INTRODUCTION
Three issues in (UQ) – 2 (UQ) validation and verification

• (UQ) CFD-based exercise leads to a standard deviation on some outputs

• Compare this standard deviation to the numerical error
  □ Richardson method, GCI...
  □ Pierce et al. Venditti et al. adjoint based formulas for functional outputs

• Compare this standard deviation to the modeling error
  □ Run several (RANS) models
  □ Run better models than (RANS)

• Numerical (UQ) investigation only make sense if standard deviation due to uncertain inputs not much smaller than modelling or discretization error
INTRODUCTION

Three issues in (UQ) – 3 lack of shared well-defined problems

- Most often mean and variance of some outputs are computed in (UQ) exercises
  - □ as this is feasible with usual methods?
  - □ as this is actually required for applications?

- From EDF’s specialists point of view, three stochastic criteria of interest:
  - □ central dispersion (mean and variance of output)
  - □ range (min and max possible values of output)
  - □ probability of exceeding a threshold

- Get information from industry in order to define relevant (UQ) exercises
- Share mathematical industrial test cases and mathematical exercices to split the CFD influence / the one of (UQ) method
INTRODUCTION

Intrusive vs non-intrusive methods

- **Non-intrusive methods. No change in the analysis code**
  - Post-processing of deterministic simulations

- **Intrusive methods. Changes in the analysis code**
  - Stochastic expansion of state/primitive variables
  - Galerkin projections
  - Probably not feasible for large industrial codes
Introduction to uncertainty quantification

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Basics of probability (1)

A classical introduction to probability basics involves
- a sample space $\Omega$ (dice values, interval of Mach number values)
- events $\xi$ i.e. element of $\Omega$ or set of elements of $\Omega$ (even dice values, subinterval of Mach number values)
- event space $\mathcal{A}$, set of subsets of $\Omega$, stable by union, intersection, including null set $\emptyset$ and $\Omega$ (also called $\sigma$-algebra)

- [INPUT] a probability function $P$ on $\mathcal{A}$ such that $P(\Omega) = 1, P(\emptyset) = 0$, plus natural properties for complementary parts and union of disjoint parts (then denoted $D$ keeping "$P"$ for polynomials)

- [OUTPUT] random variables $X$ depending of the event $\xi$ (like $CDp$ or $CLp$ of an airfoil depending on the far-field Mach number through Navier-Stokes equations)
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Basics of probability (2)

Discrete example: regular 6-face Dice thrown once

- events $\xi = 1, 2, 3, 4, 5$ or 6
- sample space $\Omega = \{1, 2, 3, 4, 5, 6\}$
- probability space $\Omega = \emptyset$ plus all discrete sets of these numbers
  $\emptyset, \{1\}, \{2\}, \{3\}, \{4\}, \{5\}, \{6\}, \{1, 2\}, \{1, 3\}, \{1, 4\}, \{1, 5\}, \{1, 6\}, \{2, 3\}$
  $\ldots \{1, 2, 3, 4, 5, 6\}$
- probability function $P$ (later denoted $D$): $P(\emptyset) = 0$, $P(\{1\}) = 1/6$, $P(\{2\}) = 1/6$, $P(\{1, 2\}) = 1/3$, $P(\{1, 3\}) = 1/3$, $P(\{1, 4\}) = 1/3$, $P(\{1, 2, 3, 4, 5, 6\}) = 1$.
- random variables $X$, for example dice value to the power three...
**MONTE-CARLO**

**Basics of probability (3)**

**Discrete example : Mach number in [0.81,0.85]**

- events $\xi$ = a Mach number value in [0.81,0.85]
- sample space $\Omega = [0.81,0.85]$
- probability space $\Omega = $ all subparts of [0.81,0.85]
- probability function $P$ to be defined (later denoted $D$). For example from a beta distribution with power three:

$$P_\phi(\phi) = \frac{35}{32}(1 - \phi^2)^3 \quad \phi \in [-1, 1] \quad \phi = (\xi - 0.83)/0.02$$

$$P(\xi) = \frac{1}{0.02} P_\phi(\phi) = \frac{35}{32}(1 - \left(\frac{\xi - 0.83}{0.02}\right)^2)^3$$

- random variables $X$, aerodynamic pitching moment of a wing with variable Mach number $M_\infty$ ("event" $\xi$) in the farfield
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Set of probability density functions of $\beta$—distributions (on [0,+1] with the $\alpha - 1 \beta - 1$ convention for exponents)
Introduction to uncertainty quantification

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Basics of probability (4)

Allows to define probabilities for both discrete and continuous spaces

Quantities of interest = functions of the stochastic variables “random variables”
Example = pitching moment of wing $J$ (random variable) depending via NS equations of uncertain far-field Mach number (uncertain input/event)

Mean – Variance

$$E(J) = \int_{\Omega} J(\xi)D(\xi)d\xi$$

$$Var(J) = \int_{\Omega} (J(\xi) - E(J))^2 D(\xi)d\xi$$

Covariance of two random variables

$$Cov(J, G) = \int_{\Omega} (J(\xi) - E(J))(G(\xi) - E(G))D(\xi)d\xi$$
MONTE-CARLO
Basics

Monte-Carlo mimics the law of the event in a series of calculations

Reference method for all uncertainty propagation methods

- Generation of a sampling \((\xi_1, \xi_2, \ldots, \xi_p, \ldots, \xi_N)\) of the p.d.f \(D(\xi)\)

  *Example*: sampling for normal distribution. \(a^k, b^k\) indep. uniformly distributed in \([0., 1.]\)

  \[\xi^k = \sqrt{-2 \ln(a_k)} \cos(2\pi b_k)\]

- Computation of corresponding flow fields \(W(\xi^p), p \in [1, N]\)

- Computation of functional outputs \(J(\xi^p) = J(W(\xi^p), X(\xi^p))\)

- Estimation of following statistical quantities:

  \[
  E(J) = \int J(\xi)D(\xi)\,d\xi \approx \bar{J}_N = \frac{1}{N} \sum_{p=1}^{p=N} J(\xi^p)
  \]

  \[
  \sigma_J^2 = E((J - E(J))^2) \approx \sigma_{J_N}^2 = \frac{1}{N - 1} \sum_{p=1}^{p=N} (J(\xi^p) - \bar{J}_N)^2
  \]

Need to quantify accuracy of estimation
Introduction to uncertainty quantification

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Accuracy of estimation: mean (1)

Scalar case. variance $\sigma_J$ is known $\sqrt{N \frac{J_N - E(J)}{\sigma_J}} \sim \mathcal{N}(0, 1)$ (Normal distribution)

Reminders about $\mathcal{N}(0, 1)$

- Probability density function (p.d.f.) of $\mathcal{N}(0, 1)$- $D_{\mathcal{N}}(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}$
- Symmetric cumulative distribution function - $\Phi_{\mathcal{N}}(x) = \frac{1}{\sqrt{2\pi}} \int_{-x}^{x} e^{-\frac{t^2}{2}} dt$

With $\epsilon$ confidence:

$$E(J) \in [\bar{J}_N - u_{\epsilon} \frac{\sigma_J}{\sqrt{N}}, \bar{J}_N + u_{\epsilon} \frac{\sigma_J}{\sqrt{N}}]$$

$$\epsilon = \frac{1}{\sqrt{2\pi}} \int_{-u_{\epsilon}}^{u_{\epsilon}} e^{-\frac{t^2}{2}} dt$$

<table>
<thead>
<tr>
<th>$\epsilon$</th>
<th>0.5</th>
<th>0.9</th>
<th>0.95</th>
<th>0.99</th>
</tr>
</thead>
<tbody>
<tr>
<td>$u_{\epsilon}$</td>
<td>0.68</td>
<td>1.65</td>
<td>1.96</td>
<td>2.58</td>
</tr>
</tbody>
</table>

With 99% confidence:

$$E(J) \in [\bar{J}_N - 2.58 \frac{\sigma_J}{\sqrt{N}}, \bar{J}_N + 2.58 \frac{\sigma_J}{\sqrt{N}}]$$

(0.99 = $\frac{1}{\sqrt{2\pi}} \int_{-2.58}^{2.58} e^{-\frac{t^2}{2}} dt$)
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Accuracy of estimation: mean (2)

Scalar case: variance $\sigma_J$ is unknown - $\sqrt{N} \frac{\bar{J}_N - E(J)}{\sigma_J} \sim S(N - 1)$ (Student dist.)

With $\epsilon$ confidence:

$$E(J) \in [\bar{J}_N - u_{\epsilon(N-1)} \frac{\sigma_J}{\sqrt{N}}, \bar{J}_N + u_{\epsilon(N-1)} \frac{\sigma_J}{\sqrt{N}}]$$

$u_{\epsilon_N}$ as function of $\epsilon$ and $N$ found in tables

Student distribution converges to Normal distribution for large $N$

Tables for $u_{\epsilon N-1}$

<table>
<thead>
<tr>
<th>$\epsilon$</th>
<th>$N$</th>
<th>2</th>
<th>3</th>
<th>20</th>
<th>30</th>
<th>$\infty$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.95</td>
<td>12.7</td>
<td>4.30</td>
<td>2.09</td>
<td>2.04</td>
<td>1.96</td>
<td></td>
</tr>
<tr>
<td>0.99</td>
<td>63.7</td>
<td>9.93</td>
<td>2.86</td>
<td>2.75</td>
<td>2.58</td>
<td></td>
</tr>
</tbody>
</table>

Figure 3: Value of $u_{\epsilon(N-1)}$ for Student distribution $S(N - 1)$ $N \geq 2$
Introduction to uncertainty quantification

**MONTE-CARLO**

Accuracy of estimation: mean (3)

Scalar case: variance $\sigma_J$ is unknown - $\sqrt{N} \frac{\bar{J}_N - E(J)}{\sigma_J} \sim S(N - 1)$ (Student dist.)

With $\epsilon$ confidence:

$$E(J) \in [\bar{J}_N - u_{\epsilon (N-1)} \frac{\sigma_J}{\sqrt{N}}, \bar{J}_N + u_{\epsilon (N-1)} \frac{\sigma_J}{\sqrt{N}}]$$

- $u_{\epsilon N}$ as function of $\epsilon$ and $N$ found in tables
- $u_{\epsilon N}$ converges towards $u_\epsilon$ of normal law for large $N$

Density function of Student distribution $S(N)$

$$D_{S(N)}(x) = \frac{\Gamma \left( \frac{N+1}{2} \right)}{\Gamma \left( \frac{N}{2} \right) \sqrt{N} \pi} \left( 1 + \frac{x^2}{N} \right)^{-\frac{N+1}{2}}$$

Definition of $u_{\epsilon N}$

$$\epsilon = \int_{-u_{\epsilon N}}^{u_{\epsilon N}} D_{S(N)}(t) dt \quad (\epsilon \in ]0, 1.])$$
MONTE-CARLO

Accuracy of estimation: variance (1) (skpd)

Scalar case: mean $E_J$ is known

Notations

- $S_{J_N}^2 = \frac{1}{N} \sum_{i=1}^{i=N} (J(\xi^p) - E_J)^2$
- Chi-square $\chi^2_N$, probability distribution defined on $[0, \infty]$ with p.d.f.:
  $$D_{\chi^2_N}(x) = \frac{1}{\Gamma(N/2)2^{N/2}} x^{N/2-1} e^{-x/2}$$
- Chi-square cumulative d.f.:
  $$\Phi_{\chi^2_N}(x) = \int_0^x D_{\chi^2_N}(t) dt$$

Stochastic variable
$$N \frac{S_{J_N}^2}{\sigma_J^2} \sim \chi^2_N$$
MONTE-CARLO

Chi-square probabilistic density functions \( D_{\chi^2_N} \) and cumulative density functions \( \Phi_{\chi^2_N} \) (skpd)
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**Accuracy of estimation: variance (2) (skpd)**

Scalar case: mean $E(\mathcal{J})$ is known - $N\frac{S_{\mathcal{J}N}^2}{\sigma_{\mathcal{J}}^2} \sim \chi_N^2$

With $\epsilon = 1 - \alpha$ confidence:

$$\Phi_{\chi_N^2}^{-1}\left(\frac{\alpha}{2}\right) \leq N\frac{S_{\mathcal{J}N}^2}{\sigma_{\mathcal{J}}^2} \leq \Phi_{\chi_N^2}^{-1}\left(1 - \frac{\alpha}{2}\right)$$

With $\epsilon = 1 - \alpha$ confidence:

$$\sigma_{\mathcal{J}}^2 \in \left[N\Phi_{\chi_N^2}^{-1}\left(1 - \frac{\alpha}{2}\right), N\Phi_{\chi_N^2}^{-1}\left(\frac{\alpha}{2}\right)\right]$$

<table>
<thead>
<tr>
<th>$x$</th>
<th>$N$</th>
<th>2</th>
<th>20</th>
<th>30</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.005</td>
<td>10.597</td>
<td>39.997</td>
<td>53.672</td>
<td></td>
</tr>
<tr>
<td>0.995</td>
<td>0.0100</td>
<td>7.434</td>
<td>13.787</td>
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</tr>
</tbody>
</table>

Figure 4: Value of $\Phi_{\chi_N^2}^{-1}(x)$
MONTE-CARLO

Quality of estimation: variance - 99 % confidence

Application

\[ N = 2 \Rightarrow \sigma_J^2 \in [0.189 S_J^2, 200 S_J^2] \]
\[ N = 20 \Rightarrow \sigma_J^2 \in [0.500 S_J^{20}, 2.69 S_J^{20}] \]
\[ N = 30 \Rightarrow \sigma_J^2 \in [0.558 S_J^{30}, 2.17 S_J^{30}] \]
\[ N = 100 \Rightarrow \sigma_J^2 \in [0.713 S_J^{100}, 1.49 S_J^{100}] \]

Convergence speed of bounds towards 1.

\[ \Phi_{\chi^2_N}(x) \text{ can be expressed as } \Phi_{\chi^2_N}(x) = \frac{1}{\Gamma(N/2)} \int_0^{x/2} t^{N/2} e^{-t} dt = \frac{\gamma(N/2, x/2)}{\Gamma(N/2)} \] (\gamma lower incomplete \Gamma function)

Check properties of (the inverse of) \( \Phi_{\chi^2_N} \)

Check convergence speed of \( N/\Phi^{-1}_{\chi^2_N}(1 - \frac{\alpha}{2}) \) and \( N/\Phi^{-1}_{\chi^2_N}(\frac{\alpha}{2}) \)
MONTE-CARLO

Accuracy of estimation: variance (3) (skpd)

Scalar case: mean \( E(\mathcal{J}) \) is unknown - Stochastic variable 
\[
(N - 1) \frac{\sigma^2_{\mathcal{J}N}}{\sigma^2_{\mathcal{J}}} \sim \chi^2_{N-1}
\]

With \( \epsilon = (1 - \alpha) \) confidence :
\[
\sigma^2_{\mathcal{J}} \in \left[ (N - 1) \frac{\sigma^2_{\mathcal{J}N}}{\Phi_{\chi^2_{N-1}}^{-1} \left(1 - \frac{\alpha}{2}\right)}, (N - 1) \frac{\sigma^2_{\mathcal{J}N}}{\Phi_{\chi^2_{N-1}}^{-1} \left(\frac{\alpha}{2}\right)} \right]
\]

<table>
<thead>
<tr>
<th>( x )</th>
<th>( N )</th>
<th>3</th>
<th>4</th>
<th>20</th>
<th>30</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.005</td>
<td>10.597</td>
<td>12.838</td>
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<td>52.336</td>
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<td>0.995</td>
<td>0.0100</td>
<td>0.0717</td>
<td>6.844</td>
<td>13.121</td>
<td></td>
</tr>
</tbody>
</table>

Figure 5: Value of \( \Phi_{\chi^2_{N-1}}^{-1}(x) \)
MONTE-CARLO
Restriction for Monte-Carlo method. Meta-models

Convergence speed of Monte-Carlo for mean value estimation is \( \frac{1}{\sqrt{N}} \)

- Increasing precision of Monte-Carlo estimation by a factor of 10 requires multiplying the number of evaluations by a factor of 100

Not usable in the context of complex aeronautics simulation

- Cost of one evaluation very high (requires resolution of (RANS) equations)
- Aerodynamic function relatively smooth

⇒ replace flow field / aerodynamic function by a model built with a database of flow fields / function values
Introduction to uncertainty quantification

**METAMODEL BASED MONTE-CARLO**

Use meta-models with Monte-Carlo method

**Figure 6: Monte-Carlo method with meta-models**
Introduction to uncertainty quantification

METAMODEL BASED MONTE-CARLO  
Meta-models

Most often, approximation of a function of interest

Meta-models used at ONERA for CFD:
- Kriging, Radial Basis Function, Support Vector Regression

Other meta-models of specific interest for UQ:
- Adjoint based linear or quadratic Taylor expansion
- Discussed in more details in the extension to multi-dimension section

Influence of meta-model accuracy on mean and variance accuracy?
APPLICATION OF (METAMODEL BASED) MONTE-CARLO Presentation

Search confidence interval on aerodynamic function $C_L$ with uncertainty on AoA
Nominal configuration: NACA0012, $M = 0.73$, $Re = 6M$, AoA = $3^\circ$

$elsA^{(a)}$
(RANS+(k-w) Wilcox turbulence model) solver (Roe flux+Van Albada lim.)

Figure 7: Mesh

(a) The $elsA$ CFD software: input from research and feedback from industry Mechanics and Industry 14(3) L. Cambier, S. Heib, S. Plot
Introduction to uncertainty quantification

**APPLICATION OF (METAMODEL BASED) MONTE-CARLO**

Distribution of uncertainty

Beta distribution (parameters (2.,2.)) $[pdf_b(\xi) = \frac{15}{16} (1 - \xi)^2 (1 + \xi)^2]$ over [-1,1]

p.d.f of angle of attack AoA $[pdf_a(\alpha) = pdf_b(10.(\alpha - 3.))]$ over [2.9,3.1]

Figure 8: Beta distribution of AoA
APPLICATION OF (METAMODEL BASED) MONTE-CARLO

Monte-Carlo method: application on $C_L(1)$

Figure 9: Mean of $C_L$ coefficient and confidence interval
APPLICATION OF (METAMODEL BASED) MONTE-CARLO

Monte-Carlo method: application on $C_L(2)$

Figure 10: Variance of $C_L$ coefficient and confidence interval
APPLICATION OF (METAMODEL BASED) MONTE-CARLO
Monte-Carlo method with meta-models: learning sample

Use learning sample based on Tchebyshev polynomials

Figure 11: Tchebychev distribution (11 points)
APPLICATION OF (METAMODEL BASED) MONTE-CARLO
Monte-Carlo method with meta-models: reconstruction of $C_L$

Figure 12: $C_L$
APPLICATION OF (METAMODEL BASED) MONTE-CARLO

Monte-Carlo method with meta-models: application on $C_L(1)$

Figure 13: Mean of $C_L$ coefficient and confidence interval
APPLICATION OF (METAMODEL BASED) MONTE-CARLO
Monte-Carlo method with meta-models: application on $C_L(2)$

Figure 14: Variance of $C_L$ coefficient and confidence interval
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ORTHOGONAL POLYNOMIALS
Orthogonal/orthonormal polynomials

- **Polynomial/spectral expansion and stochastic post-processing**
  - Polynomials orthogonal for the product defined by p.d.f $D(\xi)$:
    \[ < P_l, P_m > = \int P_l(\xi)P_m(\xi)D(\xi)d\xi = \delta_{lm} \]

- **Basic references**
  - Orthogonal polynomials – Abramowitz and Stegun: Handbook of Mathematical functions. (1972). Chapter 22

- **Expand fields on this basis**
  - In non-intrusive PC method – fields of interest
  - In intrusive PC method – state/primitive variables
Introduction to uncertainty quantification

ORTHOGONAL POLYNOMIALS

Orthonormal polynomials (1/3)

- **Families of polynomials**
  - Normal distribution \( D_n(\xi) = \frac{1}{\sqrt{2\pi}} e^{-\frac{\xi^2}{2}} \) on \( \mathbb{R} \) → Hermitte polynomials
  - Gamma distribution \( D_g(\xi) = \exp(-\xi) \) on \( \mathbb{R}^+ \) → Laguerre polynomials
  - Uniform distribution \( D_u(\xi) = 0.5 \) on \([-1, 1]\) → Legendre polynomials
  - Chebyshev distribution \( D_{cf}(\xi) = \frac{1}{\Pi} \sqrt{1 - \xi^2} \) on \([-1, 1]\) → Chebyshev (first-kind) polynomials
  - Chebyshev distribution \( D_{cs}(\xi) = \sqrt{1 - \xi^2} \) on \([-1, 1]\) → Chebyshev (second-kind) polynomials
  - Beta distrib. \( D_\beta(\xi) = (1 - \xi)^\alpha (1 + \xi)^\beta / \int_{-1}^{1} (1 - u)^\alpha (1 + u)^\beta du \) \( \alpha > -1, \beta > -1 \) on \([-1, +1]\) → Jacobi polynomials (incl. Chebyshev polynomials)
  - Non-usual probabilistic density functions, \( D_l(\xi) \) computed by Gram-Schmidt orthogonalisation process.
ORTHOGONAL POLYNOMIALS

Orthonormal polynomials (2/3)

• Example: 1D problem. Hermite polynomials for normal law
  - Probability density function (p.d.f.) of $D_n(\xi) = \frac{1}{\sqrt{2\pi}} e^{-\frac{\xi^2}{2}}$

• Family of orthonormal polynomials for $\langle f, g \rangle = \int_{-\infty}^{+\infty} f(\xi)g(\xi)D_n(\xi)\,d\xi$
  - $PH_0(\xi) = 1$
  - $PH_1(\xi) = \xi$
  - $PH_2(\xi) = \xi^2 - 1$
  - $PH_3(\xi) = \xi^3 - 3\xi$
  - $PH_4(\xi) = \xi^4 - 6\xi^2 + 3$

• Normalization of Hermite polynomials $PH_j(\xi) = \frac{1}{\sqrt{j!(2\pi)^{(1/4)}}} \overline{PH_j}(\xi)$

• Orthonormality relation for $PH_j$:
  $$\langle PH_j, PH_k \rangle = \int_{-\infty}^{+\infty} PH_j(\xi)PH_k(\xi)D_n(\xi)\,d\xi = \delta_{jk}$$
ORTHOGONAL POLYNOMIALS

Orthonormal polynomials (3/3)

- Example: 1D problem on [-1,1]. First-kind Chebyshev polynomials
  - Probability density function (p.d.f.) of $D_{cf}(\xi) = \frac{1}{\Pi} \frac{1}{\sqrt{1-\xi^2}}$

- Family of orthonormal polynomials for $< f, g >= \int_{-1}^{1} f(t)g(t) D_{cf}(t) dt$
  - $T_0(\xi) = 1$
  - $T_1(\xi) = \xi$
  - $T_2(\xi) = 2\xi^2 - 1$
  - $T_3(\xi) = 4\xi^3 - 3\xi$
  - $T_4(\xi) = 8\xi^4 - 8\xi^2 + 1$

- Normalization of Chebyshev polynomials $T_0 = T_0 \ldots T_n = \sqrt{2} T_n \ (n \geq 1)$

- Orthonormality relation for $T_j$:
  $< T_j, T_k > = \int_{-\infty}^{+\infty} T_j(\xi)T_k(\xi) D_{cf}(\xi) d\xi = \delta_{jk}$

- Specific property $T_n(cos(\theta)) = cos(n\theta)$ (hence $||T_n||_\infty \leq 1$.
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GENERALIZED POLYNOMIAL CHAOS METHOD (N.-I.)

Basics

- Polynomial/spectral expansion and stochastic post-processing
  - Polynomials orthogonal for the product defined by p.d.f $D(\xi)$:
    $$< P_l, P_m > = \int P_l(\xi) P_m(\xi) D(\xi) d\xi = \delta_{lm}$$
  - Expand field of interest (entire flow field, flow field at the wall...). $i$ is the discrete space variable (mesh index).
  - Spectral expansion:
    $$W(i, \xi) \simeq PCW(i, \xi) = \sum_{l=0}^{M-1} C_l(i) P_l(\xi)$$
  - Stochastic post-processing for $PCW$ instead of $W$

- References [Wiener 1938][Ghanem et al. 1991]
GENERALIZED POLYNOMIAL CHAOS METHOD (N.-I.)

Stochastic post-processing

• Expansion of flow field on structured mesh depending on stochastic variable \( \xi \)
  
  \[
  W(i, \xi) \simeq PCW(i, \xi) = \sum_{l=0}^{M-1} C_l(i) P_l(\xi)
  \]

• Stochastic post-processing (mean and variance)
  
  \( \Box \) done for the expansion \( PCW \) instead of \( W \)
  
  \( \Box \) straightforward evaluation of mean value
  
  \[
  E(PCW(i, \xi)) = \int \sum_{l=0}^{M-1} C_l(i) P_l(\xi) D(\xi) d\xi = C_0(i)
  \]
  
  \[
  E(PCW(i, \xi)) = \langle PCW(i, \xi), 1 \rangle = C_0(i)
  \]

  \( \Box \) straightforward evaluation of variance
  
  \[
  E((PCW(i, \xi) - C_0(i))^2) = \int \left( \sum_{l=1}^{M-1} C_l(i) P_l(\xi) \right)^2 D(\xi) d\xi
  \]
  
  \[
  E((PCW(i, \xi) - C_0(i))^2) = \sum_{l=1}^{M-1} C_l(i)^2
  \]
GENERALIZED POLYNOMIAL CHAOS METHOD (N.-I.)

Accuracy of truncated spectral extension (1/3)

- General idea: the highest the regularity of the function of interest → the fastest the convergence of the truncated spectral expansion

- Discussed for Chebyshev first-kind polynomials

- Classical expansion of a continuous function over \([-1,1]\)
  \[
  f(\xi) = \sum_{n=0}^{\infty} C_n T_n(\xi)
  \]

- Definition of coefficients
  \[
  C_0 = \frac{1}{\Pi} \int_{-1}^{1} \frac{1}{\sqrt{1-\xi^2}} f(\xi) T_0(\xi) d\xi
  
  C_n = \frac{2}{\Pi} \int_{-1}^{1} \frac{1}{\sqrt{1-\xi^2}} f(\xi) T_n(\xi) d\xi \quad (n > 0)
  \]

- Convergence speed of truncated series
  \[
  f(\xi) = \sum_{n=0}^{N} C_n T_n(\xi)
  \]
GENERALIZED POLYNOMIAL CHAOS METHOD (N.-I.)

Accuracy of truncated spectral extension (2/3)

- **Cos Fourier series of** $g$ **periodic over** $[-\Pi, +\Pi] : g(\theta) = \sum_{n=0}^{\infty} A_n \cos(n\theta)$

  $$A_0 = \frac{1}{2\Pi} \int_{-\Pi}^{+\Pi} f(\theta) d\theta \quad A_n = \frac{1}{\Pi} \int_{-1}^{+1} g(\theta) \cos(n\theta) d\theta$$

- **Integration by part of** $A_n$ **for a** $C^k$ **function**

  $$A_n = -\frac{1}{n\Pi} \int_{-1}^{+1} g'(\theta) \sin(n\theta) d\theta$$

  $$A_n = -\frac{1}{n^2\Pi} \int_{-1}^{+1} g^{(2)}(\theta) \cos(n\theta) d\theta$$

  .................

  $$A_n = \frac{1}{n^k\Pi} \int_{-1}^{+1} g^{(k)}(\theta) \cos(n\theta + k\Pi/2) d\theta$$

- **Upper bound of the coefficients for a** $C^k$ **function**

  $$|A_n| \leq \frac{1}{n^k\Pi} \int_{-1}^{+1} |g^{(k)}(\theta)| d\theta \leq \frac{2}{n^k} \|g^{(k)}\|_\infty$$

- **Upper bound of the residual**

  $$|g(\theta) - \sum_{n=0}^{N} A_n \cos(n\theta)| \leq \sum_{n=N+1}^{\infty} |A_n| \leq \ldots$$

  $$\ldots \leq 2\|g^{(k)}\|_\infty \int_{N}^{\infty} \frac{1}{u^k} du \leq \frac{2\|g^{(k)}\|_\infty}{(k-1)N^{k-1}}$$
GENERALIZED POLYNOMIAL CHAOS METHOD (N.-I.)

Accuracy of truncated spectral extension (3/3)

- **Chebyshev expansion of a** $C^k$ **function** $f(\xi)$ **over** $[-1,1]$

  $$ f(\xi) = \sum_{k=0}^{\infty} A_k \overline{T}_k(\xi) $$

- **Change variable:** $\xi = \cos(\theta)$, $g = f \circ \cos$ **is** $C^k$ **over** $[-\Pi, \Pi]$

  $$ g(\theta) = f(\cos\theta) = \sum_{k=0}^{\infty} A_k \overline{T}_k(\cos(\theta)) $$
  $$ g(\theta) = \sum_{k=0}^{\infty} A_k \cos(k\theta) \text{ is a Fourier series!!!} $$

- **All results concerning Fourier series have a counterpart for Tchebyshev expansions**

  Express $\|g^{(k)}\|_{\infty}$ from $\|f^{(k)}\|_{\infty}$ ... $\|f'\|_{\infty}$

  Express the upper bound of $|A_k|$, use $\|\overline{T}_k\|_{\infty} = 1$.

  *Find the upper bound of truncation error of spectral expansion of $f$*

- **Extension to** $f(i, \xi) = \sum_{k=0}^{\infty} A_k(i) \overline{T}_k(\xi)$
GENERALIZED POLYNOMIAL CHAOS METHOD (N.-I.)
Coefficient computations (1/4)

- Expansion of flow field on structured mesh depending on stochastic variable $\xi$
  
  \[ W(i, \xi) \simeq PCW(i, \xi) = \sum_{l=0}^{M-1} C_l(i) P_l(\xi) \]

  - Straightforward stochastic post-processing for mean and variance (presented before)
  - Accuracy of ideal $PCW$ depending on degree and regularity - theory of spectral expansions (just discussed)

- Computation of $C_l$ coefficients?

- Accuracy of actual $PCW$ expansion? (articles on this topic?)
GENERALIZED POLYNOMIAL CHAOS METHOD (N.-I.)

Coefficients computation - Gaussian quadrature (2/4)

- Expansion of flow field on structured mesh depending on stochastic variable $\xi$
  
  $$W(i, \xi) \simeq PCW(i, \xi) = \sum_{l=0}^{M-1} C_l(i) P_l(\xi)$$
  
  From orthonormality property $C_l(i) = \langle PCW, P_l >$
  
  Under regularity assumptions $C_l(i) = \langle W, P_l >$

- Gaussian quadrature
  
  $$C_l(i) = \langle PCW, P_l > = \langle W, P_l > = \int W(i, \xi) P_l(\xi) D(\xi) d\xi$$

  □ Computation by Gaussian quadrature associated to $D$ with $G$ points.

  $$\int f(\xi) D(\xi) d\xi \simeq \sum_{k=1}^{G} w_k f(\xi_k)$$

  □ $(w_k, \xi_k)$ depend on $D(\xi)$

  □ Exact quadrature if $f(\xi)$ is a polynomial of degree $\leq (2G - 1)$.
    
    ◄ Polynomial chaos: $C_l(i)$ exact if $W(i, \xi) P_l(\xi)$ polynomial of

    $\xi$ of degree lower than/equal to $(2G - 1)$. 


GENERALIZED POLYNOMIAL CHAOS METHOD (N.-I.)

Coefficients computation - collocation (3/4)

- Other way: collocation - least-square collocation
  - Identify $W(i, \xi_l)$ and $PCW(i, \xi_l)$ for $M$ values of $\xi$. “Collocation”

$$W(i, \xi_k) = \sum_{l=0}^{l=M-1} C_l(i) P_l(\xi_k) \quad k \in \{1, M\} \text{ solved for } C_l(i)$$

- Solve least-square problem for more values of $W(i, \xi_l)$ than coefficients in the expansion

- Less general accuracy results than for Gauss quadrature
GENERALIZED POLYNOMIAL CHAOS METHOD (N.-I.)

Coefficients computation - collocation (4/4)

- Theoretical result for Chebyshev series (see Boyd pages 95-96). Expansion of a $C^k$ function $f(\xi)$ over $[-1,1]$ $f(\xi) = \sum_{k=0}^{\infty} A_k T_k(\xi)$

- Collocation at $x_k = -\cos\left(\frac{k\Pi}{M-1}\right)$ $k \in [0, M-1]$ (Chebyshev extrema)
  
  \[ P_{M-1}(\xi) = \sum_{k=0}^{M-1} \tilde{A}_k T_k(\xi) \]

- Collocation at $x_k = -\cos\left(\frac{(2k+1)\Pi}{2M}\right)$ $k \in [0, M-1]$ (Chebyshev roots)
  
  \[ Q_{M-1}(\xi) = \sum_{k=0}^{M-1} \tilde{A}_k T_k(\xi) \]

- Upper bounds of truncation error
  
  \[ |f(\xi) - \sum_{n=0}^{N} \tilde{A}_n T_n(\xi)| \leq 2 \sum_{N+1}^{\infty} |A_n| \leq \ldots \]
  \[ |f(\xi) - \sum_{n=0}^{N} \tilde{A}_n T_n(\xi)| \leq 2 \sum_{N+1}^{\infty} |A_n| \leq \ldots \]

- Factor TWO w.r.t. truncation of exact series
PROBABILISTIC COLLOCATION (N.-I.)

Basics (1/2)

- Another approach for non-intrusive polynomial chaos based on Lagrangian polynomial expansion. [Tatang 1995] [Xiu et al. 2005] [Loeven et al. 2007] for compressible CFD

- Presented for 1D problem (i is the discrete space variable – mesh index)

\[ W(i, \xi) \approx SCW(i, \xi) = \sum_{l=1}^{N} W_l(i) H_l(\xi) \]

\[ H_l(\xi) = \prod_{m=1, m

- Note that actually \( SCW(i, \xi_l) = W_l(i) \). \( \rightarrow \) no coefficient computation, define \( W_l(i) = W(i, \xi_l) \)

- Definition of \((\xi_1, \xi_2, ..., \xi_N)\) (most often, not absolutely necessary)

\( N \) points of the \( N \)-point quadrature associated to \( D(\xi) \)

\[ \int f(\xi) D(\xi) d\xi \approx \sum_{m=1}^{N} \omega_m f(\xi_m) \]
PROBABILISTIC COLLOCATION (N.-I.)
Basics (2/2)

- Expansion of flow field depending on stochastic variable $\xi$
- Stochastic post-processing (mean and variance)
  - done for the expansion $SCW$ instead of $W$
  - straightforward evaluation of mean value
    \[
    E(\text{SCW}(i, \xi)) = \langle \text{SCW}(i, \xi), 1 \rangle = \sum_{m=1}^{N} \omega_m W_m(i)
    \]
  - straightforward evaluation of variance
    \[
    E((\text{SCW}(i, \xi) - E(\text{SCW}(i)))^2) = \sum_{m=1}^{N} \omega_m W_m(i)^2
    - (\sum_{m=1}^{N} \omega_m W_m(i))^2
    \]
  - Both exact for $SCW$ as $N$-point Gaussian quadrature is exact for polynomial of degree up to $2N - 1$
PROBABILISTIC COLLOCATION (N.-I.)

Link between polynomial chaos and probabilistic collocation

- Two polynomial expansions
- Case when the methods merge
  - same degree \((M - 1)\) for both expansions
  - coefficients of chaos expansion computed by collocation
  - same set of \(M\) collocation points
  - polynomials of degree \((M - 1)\) having same values in \(M\) distinct abscissas
  - \(SCW = PCW\) (expressed in two different basis)
  - exact evaluation of mean and variance for and \(SCW\) and \(PCW\)
  - same evaluation of mean and variance by the two methods
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- Intrusive polynomial chaos method for the compressible Navier Stokes equations. Chris Lacor. Slides presented at ONERA Scientific Day on error approximation and uncertainty quantification. 3/12/2010 (available on ONERA’s web site)
INTRUSIVE POLYNOMIAL CHAOS

Principle

- Expand primitive variables (not state-variables! unless you get ratio of polynomial expansions) on PC basis
  \[ U(x, t, \xi) = \sum_{l=0}^{M-1} U_l(x, t) P_l(\xi) \]

- Input expansions in stochastic partial differential equations
- Do a Galerkin projection for all \( P_l \) (\( l \in [0, M - 1] \)):
  Multiply all equations by \( P_l(\xi) \) Apply the mean (in other words, multiply all equations by \( P_l(\xi) \times D(\xi) \) sum over \( \xi \) domain)
- Discretize resulting system of coupled partial differential equations
- Stochastic post-processing
Introduction to uncertainty quantification

INTRUSIVE POLYNOMIAL CHAOS
Example 1 (1/3)

- Steady incompressible flow. Continuity equation
- One uncertain parameter (angle of attack or...) following \( D_{cf}(\xi) = \frac{1}{\Pi} \frac{1}{\sqrt{1-\xi^2}} \)
- Order 2 expansion of primitive variables
  \[
  U(x, \xi) = \sum_{l=0}^{l=2} U_l(x) T_l(\xi) \quad p(x, \xi) = \sum_{l=0}^{l=2} p_l(x) T_l(\xi)
  \]
- reminder
  \[
  T_0(\xi) = 1 \quad T_1(\xi) = \sqrt{2} \xi \quad T_2(\xi) = \sqrt{2}(2\xi^2 - 1)
  \]
- Continuity equation
  \[
  \text{div} \left( U(x, \xi) \right) = \text{div} \left( \sum_{l=0}^{l=2} U_l(x) T_l(\xi) \right)
  \]
  \[
  \text{div} \left( U(x, \xi) \right) = \sum_{l=0}^{l=2} \text{div}(U_l(x)) T_l(\xi)
  \]
**INTRODUCTORY POLYNOMIAL CHAOS**

**Example 1 (2/3)**

- **Steady incompressible flow. Continuity equation.** One uncertain parameter (angle of attack or...) following $D_{cf}(\xi) = \frac{1}{\Pi} \frac{1}{\sqrt{1-\xi^2}}$

- **Continuity equation**

  $$\text{div} \ (U(x, \xi)) = \sum_{l=0}^{l=2} \text{div}(U_l(x))T_l(\xi) = 0$$

- **Galerkin projection for $T_0(\xi), T_1(\xi)$ and $T_2(\xi)$ (For $T_1$ for example)**

  $$\text{div} \ (U(x, \xi)) \ T_1(\xi) D_{cf}(\xi) = \sum_{l=0}^{l=2} \text{div}(U_l(x))T_l(\xi)T_1(\xi)D_{cf}(\xi) = 0$$

  $$A = \int_{-1}^{1} \text{div} \ (U(x, \xi)) \ T_1(\xi) D_{cf}(\xi) = 0$$
Introduction to uncertainty quantification

**INTRUSIVE POLYNOMIAL CHAOS**

Example 1 (3/3)

- **Steady incompressible flow. Continuity equation.** One uncertain parameter (angle of attack or...) following
  \[ D_{cf}(\xi) = \frac{1}{\Pi} \frac{1}{\sqrt{1-\xi^2}} \]

- **Continuity equation**
  \[ \text{div} \ (U(x, \xi)) = \sum_{l=0}^{l=2} \text{div}(U_l(x)) T_l(\xi) = 0 \]

- **Galerkin projection for** \( T_0(\xi), T_1(\xi) \) and \( T_2(\xi) \) (For \( T_1 \) for example)

  \[ A = \int_{-1}^{1} \sum_{l=0}^{l=2} \text{div}(U_l(x)) T_l(\xi) T_1(\xi) D_{cf}(\xi) d\xi = 0 \]

  \[ A = \sum_{l=0}^{l=2} \text{div}(U_l(x)) \int_{-1}^{1} T_l(\xi) T_1(\xi) D_{cf}(\xi) d\xi = \text{div}(U_1(x)) = 0 \]

Using orthonormality property: \( \text{div}(U_1(x)) = 0 \) (of course \( \text{div}(U_0(x)) \) and \( \text{div}(U_2(x)) \) are also proved to be equal to zero using corresponding Galerkin projection)
INTRUSIVE POLYNOMIAL CHAOS

Example 2 (1/3)

• Unsteady incompressible flow. Euler equations. Momentum equation. One uncertain parameter following $D_{cf}(\xi) = \frac{1}{\Pi} \frac{1}{\sqrt{1-\xi^2}}$

• Order 2 expansion of primitive variables ($\rightarrow$ final number of equations multiplied by three)

$$U(x, t, \xi) = \sum_{l=0}^{l=2} U_l(x, t) T_l(\xi) \quad p(x, t, \xi) = \sum_{l=0}^{l=2} p_l(x, t) T_l(\xi)$$

• Momentum equation

$$\frac{\partial U}{\partial t} + (U \cdot \nabla) U + \nabla p = 0$$

$$\frac{\partial}{\partial t} (\sum_{l=0}^{l=2} U_l(x, t) T_l(\xi)) + \sum_{l=0}^{l=2} \sum_{n=0}^{n=2} (U_l(x, t) \cdot \nabla) U_n(x, t) T_l(\xi) T_n(\xi) + \nabla \sum_{l=0}^{l=2} p_l(x, t) T_l(\xi) = 0$$
**INTRUSIVE POLYNOMIAL CHAOS**

**Example 2 (2/3)**

- **Steady incompressible flow. Euler equations. Momentum equation.** One uncertain parameter following 
  \[ D_{cf}(\xi) = \frac{1}{\Pi} \frac{1}{\sqrt{1-\xi^2}} \]

- **Momentum equation**
  \[
  \frac{\partial}{\partial t} \left( \sum_{l=0}^{l=2} U_l(x, t) T_l(\xi) \right) + \sum_{l=0}^{l=2} \sum_{n=0}^{n=2} (U_l(x, t) \cdot \nabla) U_n(x, t) T_l(\xi) T_n(\xi) + \nabla \sum_{l=0}^{l=2} p_l(x, t) T_l(\xi) = 0
  \]

- **Multiplying by** \( T_k \ \forall k \in [0, 2] \) **and taking the expected value for** \( D_{cf} \)
  \[
  \frac{\partial}{\partial t} \left( \sum_{l=0}^{l=2} U_l(x, t) \right) < T_l T_k > + \sum_{l=0}^{l=2} \sum_{n=0}^{n=2} (U_l(x, t) \cdot \nabla) U_n(x, t) < T_l T_n T_k > + \nabla \sum_{l=0}^{l=2} p_l(x, t) < T_l T_k >= 0
  \]
**INTRUSIVE POLYNOMIAL CHAOS**

Example 2 (3/3)

- Steady incompressible flow. Euler equations. Momentum equation. One uncertain parameter following $D_{cf}(\xi) = \frac{1}{\Pi} \frac{1}{\sqrt{1-\xi^2}}$

- Momentum equation

\[
\frac{\partial}{\partial t} \left( \sum_{l=0}^{l=2} U_l(x, t) \right) < T_l T_k > + \sum_{l=0}^{l=2} \sum_{n=0}^{n=2} (U_l(x, t) \cdot \nabla) U_n(x) < T_l T_n T_k > + \nabla \sum_{l=0}^{l=2} p_l(x, t) < T_l T_k > = 0
\]

- Using orthogonality property

\[
\frac{\partial}{\partial t} U_k(x, t) + \sum_{l, n=0}^{l, n=2} (U_l(x, t) \cdot \nabla) U_n(x, t) < T_l T_n T_k > + \nabla p_k(x, t) = 0
\]

- Set of p.d.e for $(p_0, p_1, p_2) (U_0, U_1, U_2)$. Coupling through momentum equation
INTRUSIVE POLYNOMIAL CHAOS

Stochastic post-processing

- Expand primitive variables on PC basis
  \[ U(x, t, \xi) = \sum_{l=0}^{M-1} U_l(x, t) P_l(\xi) \]

- Straightforward post-processing at continuous level
  \[
  E(U(x, t, \xi)) = U_0(x, t) \\
  E((U(x, t, \xi) - U_0(x, t))^2) = \sum_{l=1}^{M-1} U_l(x, t)^2
  \]

- Actual stochastic post-processing at discrete level
  *Use corresponding formulas at discrete level*
  *Derive mean and variance of (linearized) outputs of interest*
INTRUSIVE POLYNOMIAL CHAOS

Compressible Euler equations

- Including several technical details
  - Pseudo spectral approach for cubic terms
  - Truncation of higher order terms
  - Three applications

- Feasibility for large codes?
Introduction to uncertainty quantification

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**EXTENSION TO HIGH DIMENSIONS**

Basics of multidimensional probability (1)

- Several $\mathbb{R}$ values stochastic variables
  - a sample space $\Omega \in \mathbb{R}^d$
  - events i.e. element of $\Omega$ or set of elements of $\Omega$
  - elementary event $\xi \mathbb{R}^d$ valued vector
  - event space $\mathcal{A}$, set of subsets of $\Omega$, stable by union, intersection, including null set $\emptyset$ and $\Omega$ (also called $\sigma$-algebra)

- For the sake of simplicity $\Omega \in \mathbb{R}^2$
- Define, cumulative distribution of $(\xi_1, \xi_2)$, probability density function, marginal distributions, independance, covariance
EXTENSION TO HIGH DIMENSIONS

Basics of multidimensional probability (2)

- **Cumulative density function**

\[ \Phi(u_1, u_2) = P(\{\xi_1 \leq u_1\} \cap \{\xi_2 \leq u_2\}) \]

- **Probabilistic density function**

\[ D_{\xi}(\xi_1, \xi_2) = \frac{\partial^2 \Phi_{\xi}}{\partial x \partial y}(\xi_1, \xi_2) \]

Probability of \( \xi \in [\xi_1 - dx/2, \xi_1 + dx/2][\xi_2 - dy/2, \xi_2 + dy/2] \) is \( D_{\xi}(\xi_1, \xi_2)dx\,dy \)
EXTENSION TO HIGH DIMENSIONS

Basics of multidimensional probability (3)

- Marginal distribution w.r.t. the two variables

\[
\Phi_1(\xi_1) = \int_{-\infty}^{\xi_1} \left( \int_{-\infty}^{+\infty} D_\xi(x, y) dy \right) dx
\]

\[
\Phi_2(\xi_2) = \int_{-\infty}^{\xi_2} \left( \int_{-\infty}^{+\infty} D_\xi(x, y) dx \right) dy
\]

- Marginal probabilistic density function

\[
D_1(\xi_1) = \int_{-\infty}^{+\infty} D_\xi(\xi_1, y) dy
\]

\[
D_2(\xi_2) = \int_{-\infty}^{+\infty} D_\xi(x, \xi_2) dx
\]
EXTENSION TO HIGH DIMENSIONS
Basics of multidimensional probability (4)

- Independant $\xi_1$ and $\xi_2 = \text{one variable provides no information about the other :}$

$$\phi_\xi(\xi_1, \xi_2) = \Phi_1(\xi_1)\Phi_2(\xi_2)$$

$$D_\xi(\xi_1, \xi_2) = D_1(\xi_1)D_2(\xi_2)$$

- Null covariance is ensured for independant stochastic variable. Null covariance is (by far) a less stronger property than independance of stochastic variables

- Example : independant variables $\xi_1, \xi_2$ on $[-1, +1]^2$:

$$D_\xi(\xi_1, \xi_2) = \frac{35}{32}(1. - \xi_1^2)^3 \times \frac{15}{16}(1. - \xi_2^2)^2$$
EXTENSION TO HIGH DIMENSIONS
Basics of multidimensional probability (5)

- **Example**: independent variables $\xi_1, \xi_2$ on $[-1, +1]^2$:

$$D_\xi(\xi_1, \xi_2) = D_\xi(\xi_1, \xi_2) = \frac{35}{32} (1 - \xi_1^2)^3 \times \frac{15}{16} (1 - \xi_2^2)^2$$

- **Example = dependant variables** $\xi_1, \xi_2$ on $[-1, +1]^2$:

$$D^a_\xi(\xi_1, \xi_2) = D_\xi(\xi_1, \xi_2) = 3/4 (1 - 1/4 (\xi_1 - \xi_2)^2)$$
$$D^b_\xi(\xi_1, \xi_2) = D_\xi(\xi_1, \xi_2) = 3/4 (1 - 1/4 (\xi_1 + \xi_2)^2)$$

- **Exercise = calculate all previous quantities**:

$$D^a_{\xi_1}(\xi_1) = 3/4((5/6 - 1/2\xi_1^2) \quad D^a_{\xi_2}(\xi_2) = 3/4(5/6 - 1/2\xi_2^2)$$
$$D^b_{\xi_1}(\xi_1) = 3/4((5/6 - 1/2\xi_1^2) \quad D^b_{\xi_2}(\xi_2) = 3/4(5/6 - 1/2\xi_2^2)$$
$$E^a(\xi_1) = 0 \quad E^a(\xi_2) = 0 \quad E^b(\xi_1) = 0 \quad E^b(\xi_2) = 0$$
$$cov^a(\xi_1, \xi_2) = 1/6 \quad cov^b(\xi_1, \xi_2) = -1/6$$
EXTENSION TO HIGH DIMENSIONS
Changes from 1D to dimension $d$

- Several uncertainties considered simultaneously
  - $\xi$ is a vector $\xi = (\xi_1, \xi_2, \ldots, \xi_d)$
    - Caution: subscript = components <> exponent = number in a sampling

- What does not change:
  - Monte-Carlo method

- What does not change very much:
  - Monte-Carlo plus metamodel
  - Polynomial chaos method for independant uncertain $\xi_k$ and tensorial basis of polynomials. Size of polynomial basis (collocation grid) $G^d$

- What does change:
  - Polynomial chaos method for dependant uncertain $\xi_k$ or degree-$M$ multi-variate polynomials
INTRODUCTION TO UNCERTAINTY QUANTIFICATION

EXTENSION TO HIGH DIMENSIONS

Monte-Carlo method $\mathbb{R}^d$

- **Basic Monte-Carlo**
  - No difference between $\mathbb{R}$ and $\mathbb{R}^d$

- **Monte-Carlo plus Kriging, RBF, SVM/SVR...**
  - Number of inner parameters of the meta-model prop. to $d$
  - Cost of the definition of an accurate meta-model increasing with $d$

- **Monte-Carlo plus adjoint-based first or second order Taylor expansion**
  - First order: solve one adjoint equation to compute first-order derivative
  - Second order: solve $d$ direct equations plus one adjoint equation to compute first- and second-order derivatives
EXTENSION TO HIGH DIMENSIONS

Independant uncertain variables. Tensorial-product polynomial basis (1/2)

- \( D(\xi) = D_1(\xi_1)D_2(\xi_2) \)

- **For 2D problem** (\( i \) generic grid index)
  \[
  W(i, \xi) \simeq PCW(i, \xi) = \sum_{l_1=0, l_2=0}^{l_1=M, l_2=M} C_{l_1,l_2}(i) P_{l_1}(\xi_1)Q_{l_2}(\xi_2)
  \]
  - \( P \) orthonormal polynomials associated to \( D_1(\xi_1) \)
  - \( Q \) orthonormal polynomials associated to \( D_2(\xi_2) \)

- **Calculate** \( C_{l_1,l_2}(i) \) **by collocation**

- **Calculate** \( C_{l_1,l_2}(i) \) **by quadrature using** :
  \[
  C_{l_1,l_2}(i) = \langle PCW, P_{l_1}Q_{l_2} \rangle = \int PCW(i, \xi)P_{l_1}(\xi_1)Q_{l_2}(\xi_2)D_1(\xi_1)D_2(\xi_2)d\xi_1d\xi_2
  \]
  \[
  C_{l_1,l_2}(i) \simeq \langle W, P_{l_1}Q_{l_2} \rangle = \int W(i, \xi)P_{l_1}(\xi_1)Q_{l_2}(\xi_2)D_1(\xi_1)D_2(\xi_2)d\xi_1d\xi_2
  \]

using a \( G \times G \) grid based on Gaussian quadrature points
EXTENSION TO HIGH DIMENSIONS

Independent uncertain variables. Tensorial-product polynomial basis (2/2)

• **Accuracy issue.** How close is $W(i, \xi)P_{l_1}(\xi_1)Q_{l_2}(\xi_2)$ from a $(2G - 1)$ in $\xi_1$ times a $(2G - 1)$ polynomial in $\xi_2$?

• **Stochastic post-processing done for the expansion** $PCW$ instead of $W$
  - straightforward evaluation of mean value
    \[
    E(PCW(i, \xi)) = \langle PCW(i, \xi), 1 \rangle = C_{0,0}(i)
    \]
  - straightforward evaluation of variance
    \[
    E((PCW(i, \xi) - E(PCW(i)))^2) = \sum_{l_1=0, l_2=0}^{M, M} C_{l_1, l_2}(i)^2
    \]
EXTENSION TO HIGH DIMENSIONS

Independant uncertain variables. Tensorial-grid probabilistic collocation (1/2)

- \( D(\xi) = D_1(\xi_1)D_2(\xi_2) \)

- Lagrangian polynomial expansion

- For 2D problem

\[
W(i, \xi) \simeq SCW(i, \xi) = \sum_{l_1=1}^{N} \sum_{l_2=1}^{N} W_{l_1,l_2}(i) H_{l_1}(\xi_1) H_{l_2}(\xi_2)
\]

\[
H_l(\xi_j) = \Pi_{m=1}^{N} \frac{(\xi_j - \xi_{j,m})}{(\xi_j,l - \xi_{j,m})} \quad (j = 1 \text{ or } 2)
\]

- Note that actually \( SCW(i, \xi_{l_1}, \xi_{l_2}) = W_{l_1,l_2}(i) \). → no coefficient computation, define \( W_{l_1,l_2}(i) = W(i, \xi_{l_1}, \xi_{l_2}) \)

- Definition of \( (\xi_{j,1}, \xi_{j,2}, ..., \xi_{j,N}) \) (\( j = 1 \text{ or } 2 \)) (most often, not absolutely necessary)

\( N \) points of the \( N \)-point quadrature associated to \( D_j(\xi_j) \)
EXTENSION TO HIGH DIMENSIONS

Independant uncertain variables. Tensorial-grid probabilistic collocation (2/2)

- Stochastic post-processing (mean and variance)
  - done for the expansion $SCW$ instead of $W$
  - straightforward evaluation of mean value
    \[
    E(\text{SCW}(i, \xi)) = \langle \text{SCW}(i, \xi), 1 \rangle = \sum_{l_1=1}^{N_{l_1}} \sum_{l_2=1}^{N_{l_2}} \omega_{l_1} \omega_{l_2} W_{l_1, l_2}(i)
    \]

  - straightforward evaluation of variance
    \[
    E((\text{SCW}(i, \xi) - E(\text{SCW}(i)))^2) = \sum_{l_1=1}^{N_{l_1}} \sum_{l_2=1}^{N_{l_2}} \omega_{l_1} \omega_{l_2} W_{l_1, l_2}(i)^2
    - (\sum_{l_1=1}^{N_{l_1}} \sum_{l_2=1}^{N_{l_2}} \omega_{l_1} \omega_{l_2} W_{l_1, l_2}(i))^2
    \]
EXTENSION TO HIGH DIMENSIONS

Dependant uncertain variables. True degree $M$ polynomials in $\mathbb{R}^d$

- **Number of terms for a degree M polynomial in dimension d**
  \[
  \frac{(M+d)!}{M!d!}
  \]

- **Number of continuous equations for intrusive approach**
  - Multiplied by $\frac{(M+d)!}{M!d!}$ instead of $(M + 1)$

- **Computation of coefficients for non-intrusive approach**
  - Collocation: from at least $\frac{(M+d)!}{M!d!}$ flow computations
  - Exact quadrature for degree-M polynomial [Smolyak 1963]...
  - Define clever enrichment...
  - Huge interest the community. Huge literature...
  - ...Attend (UQ) course level two
Introduction to uncertainty quantification

OUTLINE

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Non-intrusive polynomial chaos methods in 1D
Intrusive polynomial chaos method in 1D

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Conclusion
Introduction to uncertainty quantification

Some outputs of NODESIM-CFD

M. Lazareff

- NODESIM-CFD = EU project 2007-2009

- Some important outputs of NODESIM-CFD
  
  - Split (UQ) issues and CFD analysis issues. Test (UQ) propagation method on well defined CFD test cases AND mathematical models
  
  - Compare standard deviation due to uncertainty to numerical errors and modelization errors
  
  - Need for accurate definition of the input p.d.f.
  
  - Actually, most often non intrusive methods for complex test cases
Introduction to uncertainty quantification

**RAE2822 profile**

**Configuration characteristics**

- **RAE2822 airfoil** \( Re = 6.5 \times 10^6, M = 0.734, \alpha = 2.79^\circ \)

- Classical test case of high-Re transonic CFD

- Complex flow with upper and lower shocks

- Strong dependance on turbulence model and mesh density
RAE2822 profile, $k - \omega$ model, $Re = 6.510^6$ around $M = 0.734, \alpha = 2.79^\circ$

TPS $C_L$ response surface with SST correction

medium CFD grid, low-density collocation (blue spheres)
Introduction to uncertainty quantification

**RAE2822 profile,** *k−ω* model, *Re = 6.510^6* around *M = 0.734, α = 2.79°*

TPS $C_L$ response surface without (transparent) and with (opaque, lower) SST correction
medium CFD grid, low-density collocation (white/blue spheres)
Introduction to uncertainty quantification

NASA Rotor37 compressor
Configuration characteristics

- Isolated rotor blade. Transonic flow. Subsonic outlet.

- Uncertainty propagation exercises
  - $\beta$ distribution (bounded support)
  - uncertainty on outlet static-pressure and tip-clearance
  - uncertainty quantification for several points of characteristic curve (several outlet static pressure $<>$ several mass flows)
  - polynomial chaos (gaussian quadrature) applied to functional outputs

- good quadrature convergence is observed
  - computed order-4 moments almost identical to order-3 ones

- use order-3 Jacobi polynomials (associated to $\beta$ distributions)
  - only 4 CFD points needed for near-complete characterisation
Introduction to uncertainty quantification

**NASA Rotor37 compressor**
Barplots for uncertainties on outlet pressure (left) and tip clearance (right) variations
Introduction to uncertainty quantification

NASA Rotor37 compressor

Tip clearance: order-1 (mean) moments for global quantities

Graphs showing the mass flow, total pressure ratio, total temperature ratio, and adiabatic efficiency for different orders.
Introduction to uncertainty quantification

NASA Rotor37 compressor

Tip clearance: order-2 (stdev) moments for global quantities

![Graph showing order-2 moments for global quantities](image)
Assessment of intrusive and non-intrusive non-deterministic CFD methodologies based on polynomial chaos expansions. [Dinsecu C, Smirnov S, Hirsch C, Lacor C. IJESMS 2 (2010)]

- Comparison between intrusive PC and probabilistic collocation
- NASA Rotor 37 (Compressor map)
- Uncertain parameters: outlet static pressure, height of tip clearance
- Output parameters: local static pressure (middle gridline, mid-span), pressure ratio, isentropic efficiency
- Very consistent results for mean and standard deviation
OUTLINE

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Conclusion

- **Uncertainty quantification**
  - more and more interest and projects (EU, RTO . . .)
  - get definition of industry relevant problems
  - “robust design” optimization process

- **Methods**
  - 1D definition
  - multi-D, sparsity, clever enrichment...

- **Challenges**
  - Get relevant p.d.f. for uncertain parameters
  - Deal efficiently with large number of uncertain parameters
  - Deal efficiently with geometrical uncertainties