

Méthodes d'estimation d'erreur et propagation des incertitudes en CFD

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Outline

- 1 Introduction. Need for Uncertainty Quantification (UQ)
- 2 Probability basics, Monte-Carlo, surrogate-based Monte-Carlo
- 3 Non-intrusive polynomial methods for 1D / tensorial n D propagation
- 4 Introduction to Smolyak's sparse quadratures
- 5 Examples of application
- 6 Conclusions

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Need for UQ

Example I: drag evaluation

- Deterministic drag of airplane in cruise
 - Total drag C_D at cruise nominal Mach number ($M=0.82$) $C_D(0.82)$
 - A/C shape satisfying constraints on lift, pitching moment, rolling moment...
 - Actually cruise flight Mach number M varies:
 - Waiting for landing slot;
 - Speeding up to cope with pilot maximum flight time;
- Variable Mach number described by $D(M)$.
- Robust calculation of airplane cruise drag: compute $\int C_D(M)D(M)dM$, instead of $C_D(0.82)$.

Need for UQ

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.

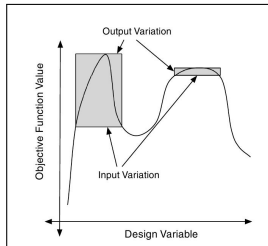


Figure: Robust design (from cenaero.be)

Need for UQ

Example III: validation process

- Unknown data in experiment
 - Upwind Mach number (equivalent to far-field Mach number in free-stream)
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(s) of interest due to the uncertain inputs

UQ inputs and outputs

Definition of uncertain inputs

- **UNCERTAINTY QUANTIFICATION:** describes 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: T. P. Evans, P. Tattersall, J. J. Doherty: Identification and quantification of uncertainty sources in aircraft related CFD computations—An industrial perspective. In *Proc. of NATO RTO-AVT-147 Symp. on Computational Uncertainty in Military Vehicle Design*, Paper #6. Athens, Greece, Dec. 3-6, 2007
- Stochastic behaviour of **OUTPUTS**
 - (Most often) mean and variance
 - Range = min and max possible values of outputs due to stochastic inputs
 - Probability that an output exceeds a threshold

Three issues with 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 or 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 modeling 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 error¹ 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.

¹Verification: solving the equations right, validation: solving the right equations

Three issues with UQ

2 – UQ validation and verification

- UQ CFD-based exercise leads to standard deviation of some outputs
- Compare this standard deviation to the discretization error
 - Richardson extrapolation method (1920's), Grid Convergence Index (GCI)...
 - Adjoint based formulas for functional outputs^{2,3}
- Compare this standard deviation to the modeling error
 - Run several Reynolds-Averaged Navier-Stokes (RANS) models
 - Run better models than RANS
- Numerical UQ investigation only makes sense if standard deviation due to uncertain inputs not much smaller than modelling or discretization error

²N. A. Pierce, M. B. Giles: Adjoint recovery of superconvergent functionals from PDE approximations. *SIAM Rev.* **42**(1), 247-264 (2000)

³D. A. Venditti, D. L. Darmofal: Adjoint error estimation and grid adaptation for functional outputs: application to quasi-one-dimensional flow. *J. Comput. Phys.* **164**(1), 204-227 (2000)

Three issues with UQ

3 – Lack of shared well-defined problems?

- Quite difficult to get information from industry in order to define relevant UQ exercises
- Quite difficult to understand when industry uses UQ and when industry uses multi-point analysis / optimization to deal with parameter variations
- Do not only common problems with in-house CFD and chosen UQ method. Also share
 - mathematical test cases with specific complexity
 - mathematical test cases derived from industrial cases (using surrogates)or it is difficult/impossible to split the influence of discrepancies in CFD methods and the one in UQ methods

Slides and lecture notes

- ONERA involved in EU projects, RTO project on UQ
- Provide accessible information for non-experts
- Examples, illustrations, explicit 2D formulas...
- Slides and lecture notes

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Basics of probability (1)

A classical introduction to probability basics involves

- event (one dice value, one Mach number value)
- a sample space Ω (all six dice values, interval of Mach number values)
- set of events space \mathcal{A} (σ -algebra) set of subsets of Ω , stable by union, intersection, complementation relative to Ω , including null set \emptyset and Ω
- 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

OUT random variables X depending on the event ξ (like C_{Dp} or C_{Lp} of an airfoil depending on the far-field Mach number through Navier-Stokes equations)

Basics of probability (2)

Discrete example: fair 6-face dice thrown once

- event $\xi = 1, 2, 3, 4, 5$ or 6 ;
- sample space $\Omega = \{1, 2, 3, 4, 5, 6\}$;
- set of events (σ -algebra) $\mathcal{F} = 2^\Omega =$ null set plus all discrete sets of these numbers $\{\emptyset, \{1\}, \{2\}, \{3\}, \{4\}, \{5\}, \{6\}, \{1, 2\}, \{1, 3\}, \{1, 4\}, \{1, 5\}, \{1, 6\}, \{2, 3\}, \dots \{1, 2, 3, 4, 5, 6\}\}$;
- probability function P : $P(\emptyset) = 0$, $P(\{1\}) = 1/6$, $P(\{2\}) = 1/6, \dots$
 $P(\{1, 2\}) = 1/3$, $P(\{1, 3\}) = 1/3$, $P(\{1, 4\}) = 1/3, \dots$
 $P(\{1, 2, 3, 4, 5, 6\}) = 1$.
- random variables X , for example, dice value to the power three...

Basics of probability (3)

Continuous example: far-field Mach number M_∞ in $[0.81, 0.85]$

- event ξ = a Mach number value in $[0.81, 0.85]$
- sample space $\Omega = [0.81, 0.85]$
- set of events (σ -algebra) $\mathcal{F} = 2^\Omega =$ all subparts of $[0.81, 0.85]$
- probability function P . Probability of (union of) intervals $I \in \mathcal{F}$ to be defined from a probability density function D , integrating D over I .

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

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

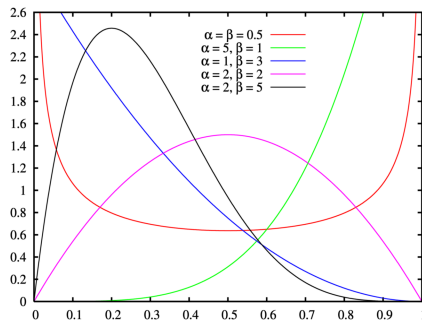
- possible random variables X = lift, drag, pitching moment of a wing... with variable Mach number M_∞ ("event" ξ) in the far-field

Basics of probability (4)

Example of probability density functions

Set of probability density functions of β_I distributions on $[0, 1]$ with the $\alpha - 1$ $\beta - 1$ convention for exponents

$$D_b(x) = \beta_I(x; \alpha, \beta) = \frac{x^{\alpha-1}(1-x)^{\beta-1}}{\int_0^1 t^{\alpha-1}(1-t)^{\beta-1} dt}, \quad x \in [0, 1]$$



Need for UQ

Intrusive vs non-intrusive methods

- Non-intrusive methods. No change in the analysis code
 - Post-processing of deterministic simulations
- Intrusive methods.^{4,5} Changes in the analysis code
 - Stochastic expansion of state/primitive variables
 - Galerkin projections. Larger set of equations
 - Probably not feasible for large industrial codes

⁴R. Ghanem, P. D. Spanos: *Stochastic Finite Elements: A Spectral Approach*. Springer, New York NY (1991)

⁵O. P. Le Maître, O. Knio: *Spectral Methods for Uncertainty Quantification. With Applications to Computational Fluid Dynamics*. Springer, Dordrecht (2010)

Monte-Carlo – 1

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

Reference method for all uncertainty propagation methods

- Generation of a N samples $(\xi^1, \xi^2, \dots, \xi^p, \dots, \xi^N)$ of the PDF $D(\xi)$
- Computation of corresponding flow fields $W(\xi^p), p \in \llbracket 1, N \rrbracket$
- Computation of functional outputs $\mathcal{J}(\xi^p) = J(W(\xi^p), X(\xi^p))$
- Discrete unbiased estimations of mean and variance:

$$\mathbb{E}(\mathcal{J}) = \int \mathcal{J}(\xi) D(\xi) d\xi \simeq \bar{\mathcal{J}}_N = \frac{1}{N} \sum_{p=1}^N \mathcal{J}(\xi^p)$$

$$\sigma_{\mathcal{J}}^2 = \mathbb{E}((\mathcal{J} - \mathbb{E}(\mathcal{J}))^2) = \int (\mathcal{J}(\xi) - \mathbb{E}(\mathcal{J}))^2 D(\xi) d\xi \simeq \sigma_{\mathcal{J}_N}^2 = \frac{1}{N-1} \sum_{p=1}^N (\mathcal{J}(\xi^p) - \bar{\mathcal{J}}_N)^2$$

- Need to quantify accuracy of estimation

Monte-Carlo – 2

Accuracy of mean

- Scalar case, variance $\sigma_{\mathcal{J}}$ is known, N sampling size, $\sqrt{N} \frac{\bar{\mathcal{J}}_N - \mathbb{E}(\mathcal{J})}{\sigma_{\mathcal{J}}} \rightsquigarrow \mathcal{N}(0, 1)$ (normal distribution)
- Probability density function (PDF) of $\mathcal{N}(0, 1)$: $D_n(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}$
- Symmetric cumulative distribution function (CDF): $\Phi_n(x) = \frac{1}{\sqrt{2\pi}} \int_{-x}^x e^{-\frac{t^2}{2}} dt$
- With ϵ confidence:

$$\mathbb{E}(\mathcal{J}) \in \left[\bar{\mathcal{J}}_N - u_{\epsilon} \frac{\sigma_{\mathcal{J}}}{\sqrt{N}}, \bar{\mathcal{J}}_N + u_{\epsilon} \frac{\sigma_{\mathcal{J}}}{\sqrt{N}} \right], \quad \epsilon = \frac{1}{\sqrt{2\pi}} \int_{-u_{\epsilon}}^{u_{\epsilon}} e^{-\frac{t^2}{2}} dt$$

ϵ	0.5	0.9	0.95	0.99
u_{ϵ}	0.674	1.645	1.960	2.576

- **Example:** with 99% confidence

$$\mathbb{E}(\mathcal{J}) \in \left[\bar{\mathcal{J}}_N - 2.576 \frac{\sigma_{\mathcal{J}}}{\sqrt{N}}, \bar{\mathcal{J}}_N + 2.576 \frac{\sigma_{\mathcal{J}}}{\sqrt{N}} \right] \quad \left(0.99 = \frac{1}{\sqrt{2\pi}} \int_{-2.576}^{2.576} e^{-\frac{t^2}{2}} dt \right)$$

Monte-Carlo – 3

Accuracy of mean

- Scalar case, variance $\sigma_{\mathcal{J}}$ is **unknown**, N sampling size, $\sqrt{N} \frac{\bar{\mathcal{J}}_N - \mathbb{E}(\mathcal{J})}{\sigma_{\mathcal{J}_N}} \rightsquigarrow \mathcal{S}(N-1)$ (Student distribution)
- With ϵ confidence:

$$\mathbb{E}(\mathcal{J}) \in \left[\bar{\mathcal{J}}_N - u_{\epsilon_{N-1}} \frac{\sigma_{\mathcal{J}_N}}{\sqrt{N}}, \bar{\mathcal{J}}_N + u_{\epsilon_{N-1}} \frac{\sigma_{\mathcal{J}_N}}{\sqrt{N}} \right]$$

- u_{ϵ_N} as function of ϵ and N found in tables. u_{ϵ_N} decreases with N increasing
- Student distribution converges to normal distribution for large N
- Tables for $u_{\epsilon_{N-1}}$

$\epsilon \backslash N-1$	1	2	20	30	∞
0.95	12.71	4.303	2.086	2.042	1.960
0.99	63.66	9.925	2.845	2.750	2.576

Table: Value of $u_{\epsilon_{N-1}}$ for Student distribution $\mathcal{S}(N-1)$, $N \geq 2$

Monte-Carlo – 4

Accuracy of mean

- Scalar case, variance $\sigma_{\mathcal{J}}$ is unknown, N sampling size, $\sqrt{N} \frac{\bar{\mathcal{J}}_N - \mathbb{E}(\mathcal{J})}{\sigma_{\mathcal{J}_N}} \rightsquigarrow \mathcal{S}(N-1)$ (Student distribution)
- Student distribution⁶ $\mathcal{S}(N)$ PDF:

$$D_{\mathcal{S}(N)}(x) = \frac{\Gamma(\frac{N+1}{2})}{\sqrt{N\pi} \Gamma(\frac{N}{2})} \left(1 + \frac{x^2}{N}\right)^{-\frac{N+1}{2}} \quad \left(\Gamma(u) = \int_0^{+\infty} t^{u-1} e^{-t} dt\right)$$

- With ϵ confidence ($\epsilon \in]0, 1[$):

$$\mathbb{E}(\mathcal{J}) \in \left[\bar{\mathcal{J}}_N - u_{\epsilon_{N-1}} \frac{\sigma_{\mathcal{J}_N}}{\sqrt{N}}, \bar{\mathcal{J}}_N + u_{\epsilon_{N-1}} \frac{\sigma_{\mathcal{J}_N}}{\sqrt{N}} \right] \quad \left(\epsilon = \int_{-u_{\epsilon_{N-1}}}^{u_{\epsilon_{N-1}}} D_{\mathcal{S}(N-1)}(t) dt \right)$$

⁶The random variable $T = \sqrt{\frac{N}{U}} G \sim \mathcal{S}(N)$ where $G \sim \mathcal{N}(0, 1)$ and $U \sim \chi_N^2$ independent from G follows the χ_N^2 law with N degrees of freedom ($N \geq 1$): $U = \sum_{n=1}^N G_n^2$ where $G_n \sim \mathcal{N}(0, 1)$ independent identically distributed (i.i.d.).

Monte-Carlo – 5

Accuracy of estimation: variance (1) [skp'd]

- Scalar case: mean $\mathbb{E}(\mathcal{J})$ is known
- Estimation of variance

$$\sigma_{\mathcal{J}_N}^2 = \frac{1}{N} \sum_{p=1}^N (\mathcal{J}(\xi^p) - \mathbb{E}(\mathcal{J}))^2$$

- Chi-square χ_N^2 probability distribution defined on $[0, \infty[$ with PDF:

$$D_{\chi_N^2}(x) = \frac{x^{\frac{N}{2}-1} e^{-\frac{x}{2}}}{2^{\frac{N}{2}} \Gamma(\frac{N}{2})}, \quad x \in \mathbb{R}_+$$

- Chi-square CDF:

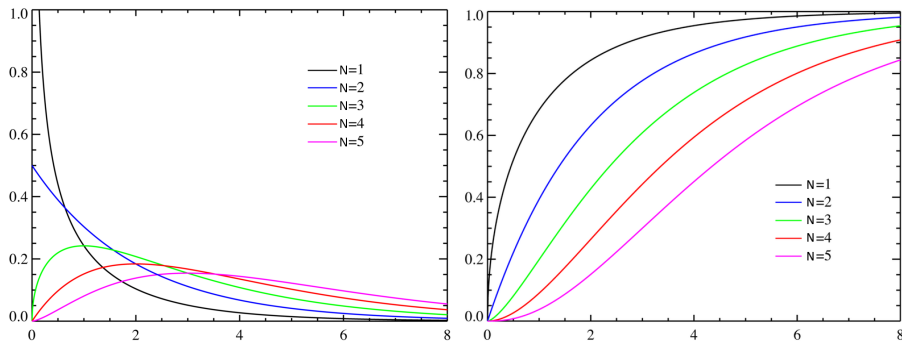
$$\Phi_{\chi_N^2}(x) = \int_0^x D_{\chi_N^2}(t) dt$$

- Stochastic variable

$$N \frac{\sigma_{\mathcal{J}_N}^2}{\sigma_{\mathcal{J}}^2} \rightsquigarrow \chi_N^2$$

Monte-Carlo – 6

Chi-square probabilistic density functions $D_{\chi_N^2}$ and cumulative density functions $\Phi_{\chi_N^2}$ [skp'd]



Monte-Carlo – 7

Accuracy of variance (2) [skp'd]

- Scalar case: mean $\mathbb{E}(\mathcal{J})$ is known, $N \frac{\sigma_{\mathcal{J}_N}^2}{\sigma_{\mathcal{J}}^2} \rightsquigarrow \chi_N^2$
- With $\epsilon = 1 - \alpha$ confidence:

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

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

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

$\epsilon \backslash N$	2	20	30
0.005	10.597	39.997	53.672
0.995	0.0100	7.434	13.787

Table: Value of $\Phi_{\chi_N^2}^{-1}(\epsilon)$

Monte-Carlo – 8

Accuracy of variance (3) [skp'd]

- Application. With 99% confidence, depending on N number of samples

$$\begin{aligned} N = 2 & \quad \sigma_{\mathcal{J}}^2 \in [0.189, 200] \times \sigma_{\mathcal{J}_2}^2 \\ N = 20 & \quad \sigma_{\mathcal{J}}^2 \in [0.500, 2.69] \times \sigma_{\mathcal{J}_{20}}^2 \\ N = 30 & \quad \sigma_{\mathcal{J}}^2 \in [0.559, 2.18] \times \sigma_{\mathcal{J}_{30}}^2 \\ N = 100 & \quad \sigma_{\mathcal{J}}^2 \in [0.713, 1.49] \times \sigma_{\mathcal{J}_{100}}^2 \end{aligned}$$

- Convergence speed of bounds towards 1.
- The cumulative distribution of the Chi-Square law $\Phi_N(x)$ can be expressed as

$$\Phi_{\chi_N^2}(x) = \frac{1}{\Gamma(N/2)} \int_0^{x/2} t^{N/2-1} e^{-t} dt = \frac{\gamma(N/2, x/2)}{\Gamma(N/2)}$$

where γ is the lower incomplete Γ function⁷

- Check properties of (the inverse of) $\Phi_{\chi_N^2}$
- Check convergence speed of $N/\Phi_{\chi_N^2}^{-1}(1 - \frac{\alpha}{2})$ and $N/\Phi_{\chi_N^2}^{-1}(\frac{\alpha}{2})$

⁷ $\gamma(s, x) = \int_0^x t^{s-1} e^{-t} dt$

Monte-Carlo – 9

Accuracy of variance (4) [skp'd]

- Scalar case: mean $\mathbb{E}(\mathcal{J})$ is unknown, stochastic variable $(N-1) \frac{\sigma_{\mathcal{J}_N}^2}{\sigma_{\mathcal{J}}^2} \rightsquigarrow \chi_{N-1}^2$
- With $\epsilon = 1 - \alpha$ confidence:

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

$\epsilon \backslash N$	3	4	20	30
0.005	10.597	12.838	38.582	52.336
0.995	0.0100	0.0717	6.844	13.121

Table: Value of $\Phi_{\chi_{N-1}^2}^{-1}(\epsilon)$

Monte-Carlo – 10

Cost issue. Regularity of outputs

- Typical realistic estimation of accuracy of mean estimated by Monte-Carlo is: with a N point sampling, with 99% confidence,

$$\mathbb{E}(\mathcal{J}) \in \left[\bar{\mathcal{J}}_N - u_{0.99,N-1} \frac{\sigma_{\mathcal{J}_N}}{\sqrt{N}}, \bar{\mathcal{J}}_N + u_{0.99,N-1} \frac{\sigma_{\mathcal{J}_N}}{\sqrt{N}} \right]$$

where $u_{0.99,1} = 63.66$, $u_{0.99,2} = 9.925$, $u_{0.99,3} = 5.841$, $u_{0.99,9} = 3.250$, $u_{0.99,19} = 2.861$, $u_{0.99,99} = 2.756$... decreasing with the number of samples N towards limiting value 2.576...

- 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

Extremely expensive if one evaluation requires numerical solution of Euler or RANS equations

- ... But Monte-Carlo is independent of the number of random inputs!

Monte-Carlo – 11

Cost issue. Regularity of outputs

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

Extremely expensive if one evaluation requires numerical solution of Euler or RANS equations

- Besides outputs of CFD calculations are often very regular functions of the parameters of interest

Take advantage of the regularity of (random) output variables seen as function of (stochastic/events) inputs variables

- Derive a surrogate of the output variables as function of the input variables using **specific stochastic surrogates** → next section
- Derive a surrogate of the output variables as function of the input variables using **general surrogates** → end of this section
- Calculate mean, variance, kurtosis, range, risk... for the surrogate

Meta-model based Monte-Carlo

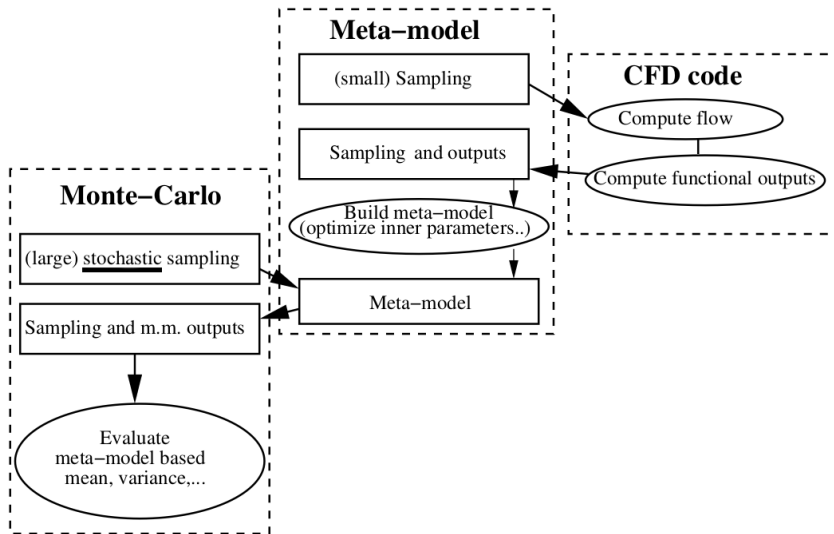


Figure: Monte-Carlo method with meta-models

Meta-models

- Restriction: approximation of a function of interest. What kind of surrogate can be used?
- 1 Classical metamodels: Kriging, Radial Basis Function, Support Vector Regression (used regularly at ONERA⁸).
 - 2 Other meta-models of specific interest for UQ: generalized polynomial Chaos (gPC), Stochastic Collocation (SC)
 - 3 Other model of specific interest for large dimensions: adjoint based linear or quadratic Taylor expansion
- Influence of meta-model accuracy on mean and variance accuracy?

⁸M. Bompard: *Modèles de substitution pour l'optimisation globale de forme en aérodynamique et méthode locale d'optimisation sans paramétrisation*. PhD Thesis, Université Nice – Sophia Antipolis, December 2011

Application of metamodel-based Monte-Carlo

- Confidence intervals on lift C_L with uncertainty on AoA
- Nominal configuration: NACA0012, $M = 0.73$, $Re = 6M$, $AoA = 3^\circ$
- ONERA *elsA* code⁹
- (RANS + $k-\omega$ Wilcox turbulence model) solver (Roe flux + Van Albada lim.)

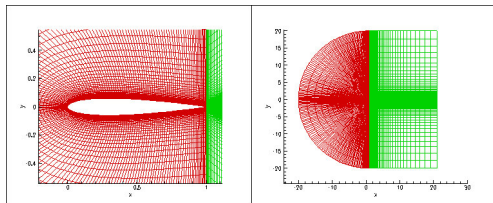


Figure: Mesh

⁹L. Cambier, S. Heib, S. Plot: The ONERA *elsA* CFD software: input from research and feedback from industry. *Mechanics & Industry* **14**(3), 159-174 (2013)

Distribution of uncertainty

- Beta distribution (parameters $(\alpha, \beta) = (3, 3)$) over $[-1, 1]$

$$D_b(\xi) = \frac{15}{16}(1 - \xi)^2(1 + \xi)^2 = \frac{15}{16}(1 - \xi^2)^2$$

- PDF of angle of attack AoA over $[2.9^\circ, 3.1^\circ]$

$$D_a(AoA) = 10D_b(10(AoA - 3))$$

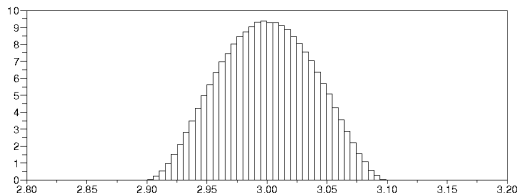


Figure: Beta distribution of AoA

Monte-Carlo method for C_L mean

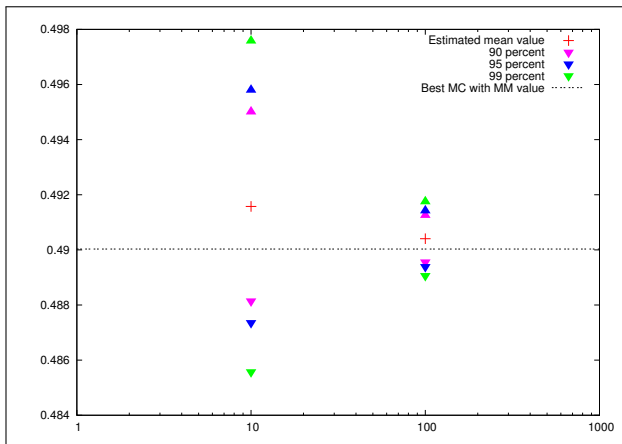


Figure: Mean of C_L coefficient and confidence interval

Monte-Carlo method for C_L variance

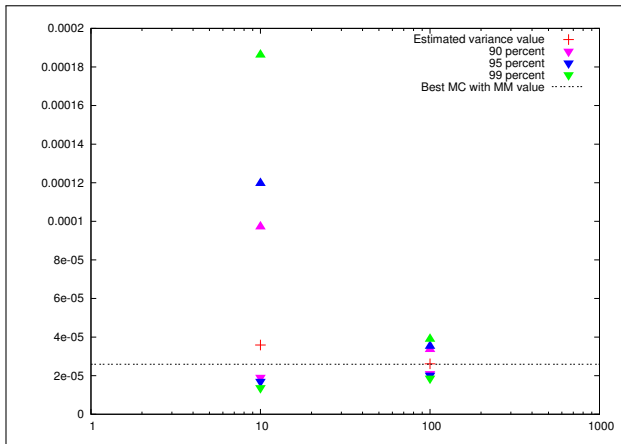


Figure: Variance of C_L coefficient and confidence interval

Metamodel based Monte-Carlo: learning sample

- Use learning sample based on roots of Chebyshev polynomials

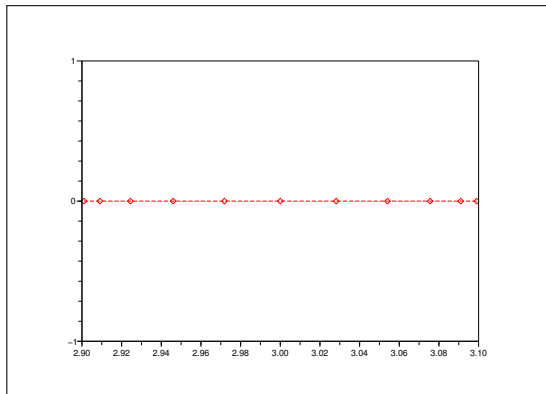


Figure: Chebyshev distribution (11 points)

Metamodel-based Monte-Carlo: reconstruction of C_L

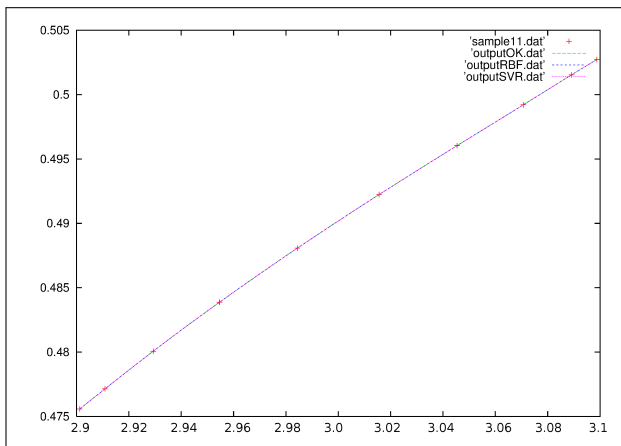


Figure: $AoA \mapsto mC_L(AoA)$

Metamodel-based Monte-Carlo for C_L mean

Calling metamodel instead of CFD code

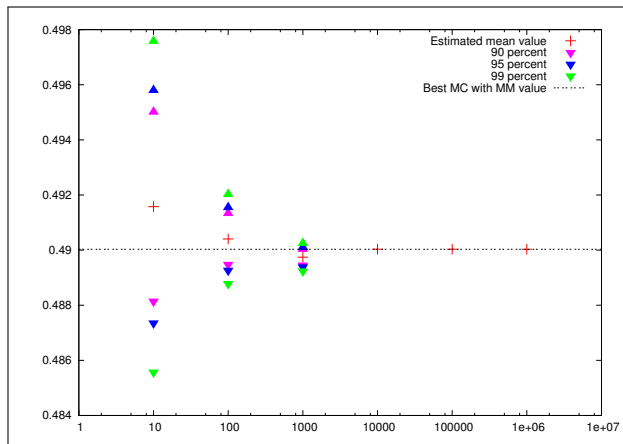


Figure: Mean of mC_L coefficient and confidence interval

Metamodel-based Monte-Carlo for C_L variance

Calling metamodel instead of CFD code

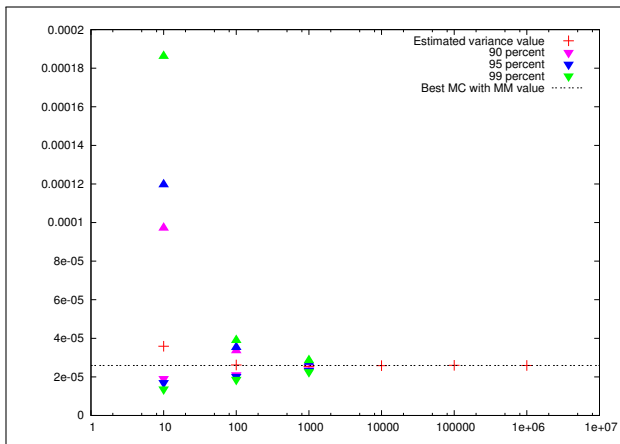


Figure: Variance of mC_L coefficient and confidence interval

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Two polynomial methods for UQ. 1D and n D tensorial

- **Stochastic specific polynomial surrogates**

- For all non-intrusive methods

- Presentation for one uncertain parameter ξ , probability density function $D(\xi)$
- Extension to a vector of two uncertain parameters $\xi = (\xi_1, \xi_2)$ under the restriction that

$$D(\xi) = D_1(\xi_1) \times D_2(\xi_2)$$

and no sparsity is sought for = extension of N -point evaluation method in 1D uses N^2 evaluations in dimension 2

- Extrapolation to d -D to discuss complexity and cost

- **Generalized polynomial chaos method**

- **Stochastic collocation method**

Generalized Polynomial Chaos (gPC) method – 1

- Polynomial expansion of the quantity of interest, scalar output or vector

$$F(\xi) \simeq gF(\xi) = \sum_{l=0}^M C_l P_l(\xi)$$

- Coefficients of the expansion computable by different methods (quadrature, collocation)
- Polynomial basis orthogonal for the dot product defined by the PDF $D(\xi)$

$$\langle P_l, P_m \rangle = \int P_l(\xi) P_m(\xi) D(\xi) d\xi = \delta_{lm}$$

- Straightforward calculation of mean and variance of the polynomial expansion (that approximates the quantity of interest)
- Orthogonal polynomials: M. Abramowitz, I. A. Stegun: *Handbook of Mathematical Functions*, chap. 22. National Bureau of Standards, Washington DC (1972).
- Spectral expansions: J. P. Boyd: *Chebyshev and Fourier Spectral Methods (2nd ed.)*. Dover, Mineola NY (2001).

Generalized Polynomial Chaos (gPC) method – 2

Families of orthogonal polynomials

- Normal distribution $D_n(\xi) = \frac{e^{-\frac{\xi^2}{2}}}{\sqrt{2\pi}}$ on $\mathbb{R} \rightarrow$ (Probabilists') Hermite polynomials
- Gamma distribution $D_g(\xi) = e^{-\xi}$ on $\mathbb{R}^+ \rightarrow$ Laguerre polynomials
- Uniform distribution $D_u(\xi) = 0.5$ on $[-1, 1] \rightarrow$ Legendre polynomials
- Chebyshev distribution $D_{cf}(\xi) = \frac{1}{\pi\sqrt{1-\xi^2}}$ on $[-1, 1] \rightarrow$ Chebyshev (first-kind) polynomials
- Chebyshev distribution $D_{cs}(\xi) = \sqrt{1-\xi^2}$ on $[-1, 1] \rightarrow$ Chebyshev (second-kind) polynomials
- Beta distribution $D_b(\xi) = \frac{1}{C_{\alpha\beta}}(1-\xi)^\alpha(1+\xi)^\beta$ on $[-1, 1]$ with $-1 < \alpha$, $-1 < \beta$, and normalization constant $C_{\alpha\beta} \equiv \int_{-1}^1 (1-u)^\alpha(1+u)^\beta du \rightarrow$ Jacobi polynomials (incl. Chebyshev and Legendre polynomials)
- Non-usual probabilistic density functions $D_l(\xi)$ computed by Gram-Schmidt orthogonalization process.

Generalized Polynomial Chaos (gPC) method – 3

Families of orthogonal polynomials

- Example: Stochastic variable in \mathbb{R} . Hermite polynomials for normal law $D_n(\xi) = \frac{e^{-\frac{\xi^2}{2}}}{\sqrt{2\pi}}$
- First polynomials
 - $\overline{PH}_0(\xi) = 1$
 - $\overline{PH}_1(\xi) = \xi$
 - $\overline{PH}_2(\xi) = \xi^2 - 1$
 - $\overline{PH}_3(\xi) = \xi^3 - 3\xi$
 - $\overline{PH}_4(\xi) = \xi^4 - 6\xi^2 + 3$
- Recursive definition
 - $\overline{PH}_0(\xi) = 1, \quad \overline{PH}_1(\xi) = \xi, \quad \overline{PH}_{n+1}(\xi) = \xi \overline{PH}_n(\xi) - n \overline{PH}_{n-1}(\xi)$
- Normalization $PH_j(\xi) = \frac{1}{\sqrt{j!}} \overline{PH}_j(\xi)$
- Orthonormality relation for PH

$$\langle PH_j, PH_k \rangle = \int_{\mathbb{R}} PH_j(\xi) PH_k(\xi) D_n(\xi) d\xi = \delta_{jk}$$

Generalized Polynomial Chaos (gPC) method – 4

Families of orthogonal polynomials

- Example: Stochastic variable in $[-1,1]$. First-kind Chebyshev polynomials for probability density function $D_{cf}(\xi) = \frac{1}{\pi} \frac{1}{\sqrt{1-\xi^2}}$
- Family of orthonormal polynomials for $\langle f, g \rangle = \int_{-1}^1 f(t)g(t)D_{cf}(t)dt$
 - $\bar{T}_0(\xi) = 1$
 - $\bar{T}_1(\xi) = \xi$
 - $\bar{T}_2(\xi) = 2\xi^2 - 1$
 - $\bar{T}_3(\xi) = 4\xi^3 - 3\xi$
- Recursive definition
 - $\bar{T}_0(\xi) = 1, \quad \bar{T}_1(\xi) = \xi, \quad \bar{T}_{n+1}(\xi) = 2\xi\bar{T}_n(\xi) - \bar{T}_{n-1}(\xi)$
- Normalization $T_0 = \bar{T}_0, \quad T_1 = \sqrt{2} \bar{T}_1, \dots, T_n = \sqrt{2} \bar{T}_n \quad (n \geq 1)$
- Orthonormality of the T_j

$$\langle T_j, T_k \rangle = \int_{-1}^1 T_j(\xi) T_k(\xi) D_{cf}(\xi) d\xi = \delta_{jk}$$

- Specific property $\bar{T}_n(\cos \theta) = \cos(n\theta)$ (hence $\|\bar{T}_n\|_\infty \leq 1$)

Generalized Polynomial Chaos (gPC) method – 5

Polynomial expansion

- Expansion of a functional output depending on stochastic variable ξ

$$F(\xi) \simeq gF(\xi) = \sum_{l=0}^M C_l P_l(\xi)$$

- Expansion of a field on part of the mesh depending on stochastic variable ξ (i is a generic index for a part of the mesh nodes like wall nodes)

$$W(i, \xi) \simeq gW(i, \xi) = \sum_{l=0}^M C_l(i) P_l(\xi)$$

- Accuracy of ideal gW depending on degree and regularity. Theory of spectral expansions
- Stochastic post-processing for gW (gF) instead of W (F)
- Straightforward calculation of gW (gF) mean and variance

Generalized Polynomial Chaos (gPC) method – 6

Coefficients computation (1/4) – Gaussian quadrature

- Expansion of part of flow field depending on stochastic variable ξ and generic mesh index i

$$W(i, \xi) \simeq gW(i, \xi) = \sum_{l=0}^M C_l(i) P_l(\xi)$$

- From orthonormality property $C_l(i) = \langle gW(i), P_l \rangle$. Under regularity assumptions $C_l(i) = \langle W(i), P_l \rangle$
- Proof:** Assume D is defined on an interval of \mathbb{R} and bounded. Assume uniform convergence of spectral expansion over its domain of definition

$$W(i, \xi) = \sum_{l=0}^{\infty} C_l(i) P_l(\xi)$$

Multiply by $P_n(\xi)D(\xi)$

$$W(i, \xi) P_n(\xi) D(\xi) = \sum_{l=0}^{\infty} C_l(i) P_l(\xi) P_n(\xi) D(\xi)$$

Integrating over domain of definition of $D(\xi)$ yields $C_n(i) = \langle W(i), P_n \rangle$

Generalized Polynomial Chaos (gPC) method – 7

Coefficients computation (2/4) – Gaussian quadrature

- Expansion of part of flow field depending on stochastic variable ξ and generic mesh index i

$$gW(i, \xi) = \sum_{l=0}^M C_l(i) P_l(\xi), \quad C_l(i) = \langle gW(i), P_l \rangle$$

- Gaussian quadrature for

$$C_l(i) = \langle W, P_l \rangle = \int W(i, \xi) P_l(\xi) D(\xi) d\xi$$

- Computation by Gaussian quadrature associated to PDF D with g points. Exact integration of polynomials up to degree $2g - 1$
- Example of criteria for definition of number of points g = enough points to recover orthogonality property at discrete level for all polynomials of the expansions

$$2M \leq 2g - 1$$

Generalized Polynomial Chaos (gPC) method – 8

Coefficients computation (3/4) – Gaussian quadrature

- Expansion of part of flow field depending on stochastic variable ξ and generic mesh index i

$$gW(i, \xi) = \sum_{l=0}^M C_l(i) P_l(\xi), \quad C_l(i) = \langle gW(i), P_l \rangle$$

- g -point Gaussian quadrature associated to D

$$\int h(\xi) D(\xi) d\xi \simeq \sum_{k=1}^g \omega_k h(\xi_k)$$

(ω_k, ξ_k) depend on $D(\xi)$. Exact for polynomials up to degree $2g - 1$

- Calculation of gPC coefficients

$$C_l(i) = \langle W, P_l \rangle = \int W(i, \xi) P_l(\xi) D(\xi) d\xi = \sum_{k=1}^g \omega_k W(i, \xi_k) P_l(\xi_k)$$

$C_l(i)$ exact if $W(i, \xi) P_l(\xi)$ polynomial of ξ of degree lower or equal to $2g - 1$

Generalized Polynomial Chaos (gPC) method – 9

Coefficients computation (4/4) – collocation

- Other way: collocation or least-square collocation
- NB: less accuracy results than for Gauss quadrature
- Identify $W(i, \xi_I)$ and $gW(i, \xi_I)$ for $M + 1$ values of ξ . Identify $F(\xi_I)$ and $gF(\xi_I)$ for $M + 1$ values of ξ .

$$\sum_{I=0}^M C_I P_I(\xi_k) = F(\xi_k) \quad \forall k \in \llbracket 1, M + 1 \rrbracket \quad \text{solved for } C_I$$

- 1 Number of F evaluations = number of coefficients. Linear system
 - 2 Number of F evaluations > number of coefficients. Solve least-square problem
 - 3 Number of F evaluations < number of coefficients. See later “sparsity-of-effects” & “compressed sensing”
- Matrix notation \mathbf{F} column vector of F values, \mathbf{C} column vector of unknown polynomial coefficients \mathbf{K} matrix $K_{kl} = P_l(\xi_k)$

$$\mathbf{KC} = \mathbf{F}$$

Generalized Polynomial Chaos (gPC) method – 10

Stochastic post-processing (1/3)

$$F(\xi) \simeq gF(\xi) = \sum_{l=0}^M C_l P_l(\xi)$$

- Stochastic post-processing (mean and variance) done for the expansion gF instead of F
 - straightforward evaluation of mean value

$$\mathbb{E}(gF(\xi)) = \int \left(\sum_{l=0}^M C_l P_l(\xi) \right) D(\xi) d\xi = C_0$$

- straightforward evaluation of variance

$$\mathbb{E}((gF(\xi) - C_0)^2) = \int \left(\sum_{l=1}^M C_l P_l(\xi) \right)^2 D(\xi) d\xi = \sum_{l=1}^M C_l^2$$

Generalized Polynomial Chaos (gPC) method – 11

Stochastic post-processing (2/3)

$$F(\xi) \simeq gF(\xi) = \sum_{l=0}^M C_l P_l(\xi)$$

- Stochastic post-processing (mean and variance) done for the expansion gF instead of F
 - Skewness

$$\mathbb{E} \left(\left(\frac{gF(\xi) - \mu}{\sigma} \right)^3 \right) = \frac{1}{(\sum_{l=1}^M C_l^2)^{3/2}} \int \left(\sum_{l=1}^M C_l P_l(\xi) \right)^3 D(\xi) d\xi$$

requires the knowledge/calculation of $\int P_l(\xi) P_n(\xi) P_p(\xi) D(\xi) d\xi$ integrals¹⁰

- Calculation of range. Sample ξ and evaluate $gF(\xi)$
- Probability of that F exceeds a threshold T . Sample ξ and evaluate $gF(\xi)$ for

$$\int \mathbf{1}_{\{gF(\xi) > T\}} D(\xi) d\xi$$

¹⁰É. Savin, B. Faverjon: Computation of higher-order moments of generalized polynomial chaos expansions. *Int. J. Num. Methods Engng.* **111**(12), 1192-1200 (2017). Codes: <https://github.com/ericsavin/LinCoef>

Generalized Polynomial Chaos (gPC) method – 12

Stochastic post-processing (3/3)

$$gW(i, \xi) = \sum_{l=0}^M C_l(i) P_l(\xi)$$

- For vectors as well, stochastic post-processing (mean and variance) done for the expansion gW instead of W
 - straightforward evaluation of mean value

$$\mathbb{E}(gW(i, \xi)) = \int \left(\sum_{l=0}^M C_l(i) P_l(\xi) \right) D(\xi) d\xi = C_0(i)$$

- straightforward evaluation of variance

$$\mathbb{E}((gW(i, \xi) - C_0(i))^2) = \int \left(\sum_{l=1}^M C_l(i) P_l(\xi) \right)^2 D(\xi) d\xi = \sum_{l=1}^M C_l(i)^2$$

- Estimation of skewness, kurtosis...
- Estimation of range
- Estimation of probability to exceed a threshold

2D tensorial extension of gPC method – 1

Definition

- 2 uncertain parameters $(\xi_1, \xi_2) \in I^1 \times I^2$

$$D(\xi_1, \xi_2) = D^\alpha(\xi_1)D^\beta(\xi_2)$$

- Families of orthogonal polynomials for $D^\alpha(\xi_1)$ and $D^\beta(\xi_2)$ are $(P_0^\alpha, P_1^\alpha, P_2^\alpha, \dots)$ and $(P_0^\beta, P_1^\beta, P_2^\beta, \dots)$
- Polynomial extension (output functional case)

$$F(\xi_1, \xi_2) \simeq gF(\xi_1, \xi_2) = \sum_{k \leq M^1, l \leq M^2} C_{kl} P_k^\alpha(\xi_1) P_l^\beta(\xi_2)$$

2D tensorial extension of gPC method – 2

Tensorial product of two quadrature rules

- Calculate the $(M^1 + 1) \times (M^2 + 1)$ coefficients by integration over interval $I^1 \times I^2$ as

$$C_{kl} = \int_{I^1 \times I^2} F(\xi_1, \xi_2) P_k^\alpha(\xi_1) P_l^\beta(\xi_2) D^\alpha(\xi_1) D^\beta(\xi_2) d\xi_1 d\xi_2$$

- Tensorial approach. First define the tensorial product of two 1D Gaussian rules for integration in directions ξ_1 and ξ_2 over I^1 and I^2

$$A[f] = \sum_{k=1}^{k=g^\alpha} \omega_k^\alpha f(\xi_k^\alpha) \quad \left(\text{approximating } \int_{I^1} f(u) D^\alpha(u) du \right)$$

$$B[g] = \sum_{l=1}^{l=g^\beta} \omega_l^\beta g(\xi_l^\beta) \quad \left(\text{approximating } \int_{I^2} g(v) D^\beta(v) dv \right)$$

- Tensorial quadrature $A \otimes B$ over $I^1 \times I^2$

$$A \otimes B[h] = \sum_{k \leq g^\alpha, l \leq g^\beta} \omega_k^\alpha \omega_l^\beta h(\xi_k^\alpha, \xi_l^\beta)$$

2D tensorial extension of gPC method – 3

Tensorial product of two quadrature rules

- Calculate the $(M^1 + 1) \times (M^2 + 1)$ coefficients by integration over interval $I^1 \times I^2$ as

$$C_{kl} = \int_{I^1 \times I^2} F(\xi_1, \xi_2) P_k^\alpha(\xi_1) P_l^\beta(\xi_2) D^\alpha(\xi_1) D^\beta(\xi_2) d\xi_1 d\xi_2$$

- Tensorial quadrature $A \otimes B$ over $I^1 \times I^2$

$$A \otimes B[h] = \sum_{k \leq g^\alpha, l \leq g^\beta} \omega_k^\alpha \omega_l^\beta h(\xi_k^\alpha, \xi_l^\beta)$$

(that is exact for $\xi_1^p \xi_2^q$ if $p \leq 2g^\alpha - 1$ and $q \leq 2g^\beta - 1$)

- Calculation of gPC coefficients

$$C_{kl} = \int_{I^1 \times I^2} F(\xi_1, \xi_2) D^\alpha(\xi_1) D^\beta(\xi_2) d\xi_1 d\xi_2 \simeq A \otimes B[F] = \sum_{k \leq g^\alpha, l \leq g^\beta} \omega_k^\alpha \omega_l^\beta F(\xi_k^\alpha, \xi_l^\beta)$$

2D tensorial extension of gPC method – 4

Calculation of coefficients using the tensor product of two quadrature rules

- Calculate the $M^1 \times M^2$ coefficients by integration over $I^1 \times I^2$ as

$$C_{kl} = \int F(\xi_1, \xi_2) P_k^\alpha(\xi_1) P_l^\beta(\xi_2) D^1(\xi_1) D^\beta(\xi_2) d\xi_1 d\xi_2$$

by tensorial quadrature rule

$$\int_{I^1 \times I^2} F(\xi_1, \xi_2) D^\alpha(\xi_1) D^\beta(\xi_2) d\xi_1 d\xi_2 \simeq \sum_{k \leq g^\alpha, l \leq g^\beta} \omega_k^\alpha \omega_l^\beta F(\xi_k^\alpha, \xi_l^\beta)$$

- Requires $g^\alpha \times g^\beta$ flow calculations and evaluations of F

2D tensorial extension of gPC method – 5

Calculation of coefficients using collocation

- Calculate the $(M^1 + 1) \times (M^2 + 1)$ coefficients of function expansion

$$F(\xi_1, \xi_2) \simeq gF(\xi_1, \xi_2) = \sum_{k \leq M^1, l \leq M^2} C_{kl} P_k^\alpha(\xi_1) P_l^\beta(\xi_2)$$

by collocation by identifying the spectral expansion for $(M^1 + 1) \times (M^2 + 1)$ points with exact evaluations

$$\sum_{k \leq M^1, l \leq M^2} C_{kl} P_k^\alpha(\xi_1^s) P_l^\beta(\xi_2^s) = F(\xi_1^s, \xi_2^s), \quad s \in \llbracket 1, 2, 3, \dots, (M^1 + 1) \times (M^2 + 1) \rrbracket$$

- Use least square approach if more sampling points than coefficients

2D tensorial extension of gPC method – 6

Stochastic post processing

- gPC 2D expansion

$$gF(\xi_1, \xi_2) = \sum_{k \leq M^1, l \leq M^2} C_{kl} P_k^\alpha(\xi_1) P_l^\beta(\xi_2)$$

- Calculation of mean

$$\mathbb{E}(gF) = \int \left(\sum_{k \leq M^1, l \leq M^2} C_{kl} P_k^\alpha(\xi_1) P_l^\beta(\xi_2) \right) d\xi_1 d\xi_2 = C_{00}$$

- straightforward evaluation of variance

$$\begin{aligned} \text{Var}(gF) &= \mathbb{E}((gF - C_{00})^2) \\ &= \int \left(\sum_{k \leq M^1, l \leq M^2} C_{kl} P_k^\alpha(\xi_1) P_l^\beta(\xi_2) D(\xi_1, \xi_2) d\xi_1 d\xi_2 - C_{00} \right)^2 D(\xi_1)^\alpha D(\xi_2)^\beta d\xi_1 d\xi_2 \\ &= \int \left(\sum_{1 \leq k \leq M^1, 1 \leq l \leq M^2} C_{kl} P_k^\alpha(\xi_1) P_l^\beta(\xi_2) \right)^2 D(\xi_1)^\alpha D(\xi_2)^\beta d\xi_1 d\xi_2 \\ &= \sum_{1 \leq k \leq M^1, 1 \leq l \leq M^2} C_{kl}^2 \end{aligned}$$

Stochastic collocation (SC) method – 1

Definition

- Another approach for non-intrusive polynomial chaos based on Lagrangian polynomial expansion.^{11,12,13}
- Dedicated stochastic polynomial expansion using Lagrangian polynomials (sum of polynomials of degree M)

$$W(i, \xi) \simeq scW(i, \xi) = \sum_{l=1}^{M+1} W_l(i) H_l(\xi), \quad H_l(\xi) = \prod_{m=1, m \neq l}^{M+1} \frac{(\xi - \xi_m)}{(\xi_l - \xi_m)}$$

- Note that $scW(i, \xi_l) = \sum_{l=1}^{M+1} W_l(i) H_l(\xi_l) = W_l(i) \rightarrow$ no coefficient calculation step
- Compute flows (and extract part of state variables fields) $W(i, \xi_l)$ corresponding to the ξ_l and substitute $W(i, \xi_l)$ to $W_l(i)$

$$scW(i, \xi) = \sum_{l=1}^{M+1} W(i, \xi_l) H_l(\xi)$$

¹¹M. A. Tatang, W. Pan, R. G. Prinn, G. J. McRae: An efficient method for parametric uncertainty analysis of numerical geophysical models. *J. Geophys. Res.* **102**(D18), 21925-21931 (1997)

¹²D. Xiu, J. S. Hesthaven: High-order collocation methods for differential equations with random inputs. *SIAM J. Sci. Comput.* **27**(3), 1118-1139 (2005)

¹³G. J. A. Loeven, J. A. S. Witteveen, H. Bijl: Probabilistic collocation: An efficient non-intrusive approach for arbitrarily distributed parametric uncertainties. AIAA Paper #2007-0317 (2007)

Stochastic collocation (SC) method – 2

Suitable set of points

- Polynomial expansion using Lagrangian polynomials

$$W(i, \xi) \simeq \text{sc}W(i, \xi) = \sum_{l=1}^{M+1} W(i, \xi_l) H_l(\xi)$$

- Definition of $(\xi_1, \xi_2, \dots, \xi_{M+1})$?

- $M + 1$ points of the $(M + 1)$ -point Gaussian quadrature associated to $D(\xi)$ (most often, not absolutely necessary)
- Any set of $(M + 1)$ distinct points
 - Calculate mean and variance using the $(M + 1)$ -point Gaussian quadrature associated to $D(\xi)$. Exact mean and variance. Not so simple formulas
 - Calculate mean and variance using interpolating quadrature associated to the nodes. Inexact mean and variance.

Stochastic collocation (SC) method – 3

Mean and variance evaluation 1/3

- Stochastic post-processing (mean and variance) done for the expansion scW instead of W – In case the interpolation points $(\xi_1, \xi_2, \dots, \xi_{M+1})$ are the $M + 1$ points of the $(M + 1)$ -point Gauss quadrature associated to $D(\xi)$, the weights being $(\omega_1, \omega_2, \dots, \omega_{M+1})$
- straightforward evaluation of mean value (degree M polynomial)

$$\mathbb{E}(scW(i, \xi)) = \int scW(i, \xi) D(\xi) d\xi = \sum_{m=1}^{M+1} \omega_m scW(i, \xi_m) = \sum_{m=1}^{M+1} \omega_m W(i, \xi_m)$$

- straightforward evaluation of variance (degree $2M$ polynomial)

$$\begin{aligned} \mathbb{E}((scW(i, \xi) - \mathbb{E}(scW(i, \xi)))^2) &= \mathbb{E}(scW(i, \xi)^2) - \mathbb{E}(scW(i, \xi))^2 \\ &= \int scW(i, \xi)^2 D(\xi) d\xi - \mathbb{E}(scW(i, \xi))^2 \\ &= \sum_{m=1}^{M+1} \omega_m scW(i, \xi_m)^2 - \mathbb{E}(scW(i, \xi))^2 \\ &= \sum_{m=1}^{M+1} \omega_m W(i, \xi_m)^2 - \left(\sum_{m=1}^{M+1} \omega_m W(i, \xi_m) \right)^2 \end{aligned}$$

- Both exact from quadrature polynomial exactness.

Stochastic collocation (SC) method – 4

Mean and variance evaluation 2/3

- Stochastic post-processing (mean and variance) done for the expansion scW instead of W – In case the interpolation points $(\xi_1, \xi_2, \dots, \xi_{M+1})$ are not the $M + 1$ points of the $(M + 1)$ -point quadrature associated to $D(\xi)$. Note these Gauss quadrature points $(\nu_1, \nu_2, \dots, \nu_{M+1})$ and the weights $(\omega_1, \omega_2, \dots, \omega_{M+1})$ (no flow have been calculated for the ν_m)
- This quadrature is used for evaluations of mean and variance
- Evaluation of mean value (degree M polynomial)

$$\mathbb{E}(scW(i, \xi)) = \int scW(i, \xi) D(\xi) d\xi = \sum_{m=1}^{M+1} \omega_m scW(i, \nu_m)$$

- Evaluation of variance (degree $2M$ polynomial)

$$\begin{aligned} \mathbb{E}((scW(i, \xi) - \mathbb{E}(scW(i, \xi)))^2) &= \mathbb{E}(scW(i, \xi)^2) - \mathbb{E}(scW(i, \xi))^2 \\ &= \int scW(i, \xi)^2 D(\xi) d\xi - \mathbb{E}(scW(i, \xi))^2 \\ &= \sum_{m=1}^{M+1} \omega_m scW(i, \nu_m)^2 - \left(\sum_{m=1}^{M+1} \omega_m scW(i, \nu_m) \right)^2 \end{aligned}$$

- Both exact from quadrature polynomial exactness. No simple expression for $scW(i, \nu_m)$

Stochastic collocation (SC) method – 5

Mean and variance evaluation 3/3 [skp'd]

- Stochastic post-processing (mean and variance) done for the expansion scW instead of W – In case the interpolation points $(\xi_1, \xi_2, \dots, \xi_{M+1})$ are not the $M+1$ points of the $(M+1)$ -point Gauss quadrature associated to $D(\xi)$
- Interpolating quadrature associated to the set is used (it is NOT associated to distribution D and D terms will remain). Weights are denoted $(\gamma_1, \gamma_2, \dots, \gamma_{M+1})$
- In general, inexact evaluation of mean value (due to D factor)

$$\mathbb{E}(scW(i, \xi)) = \int scW(i, \xi) D(\xi) d\xi \simeq \sum_{m=1}^{M+1} \gamma_m scW(i, \xi_m) D(\xi_m) = \sum_{m=1}^{M+1} \gamma_m W(i, \xi_m) D(\xi_m)$$

- In general, inexact evaluation of variance (due to D factor and polynomial degree)

$$\begin{aligned} \mathbb{E}((scW(i, \xi) - \mathbb{E}(scW(i, \xi)))^2) &= \mathbb{E}(scW(i, \xi)^2) - \mathbb{E}(scW(i, \xi))^2 \\ &= \int scW(i, \xi)^2 D(\xi) d\xi - \mathbb{E}(scW(i, \xi))^2 \\ &\simeq \sum_{m=1}^{M+1} \gamma_m W(i, \xi_m)^2 D(\xi_m) - \left(\sum_{m=1}^{M+1} \gamma_m W(i, \xi_m) D(\xi_m) \right)^2 \end{aligned}$$

2D tensorial extension of SC method – 1

Definition 1/2

- 2 uncertain parameters $(\xi_1, \xi_2) \in I^1 \times I^2$

$$D(\xi_1, \xi_2) = D^\alpha(\xi_1)D^\beta(\xi_2)$$

- For the sake of simplicity presented for a scalar output
- For the sake of simplicity, tensorial grid of $(M^1 + 1)$ and $(M^2 + 1)$ Gauss-points associated to D^α and D^β .

$$(\xi_1^\alpha, \xi_2^\alpha, \dots, \xi_{M^1+1}^\alpha) \otimes (\xi_1^\beta, \xi_2^\beta, \dots, \xi_{M^2+1}^\beta)$$

the weights being

$$(\omega_1^\alpha, \omega_2^\alpha, \dots, \omega_{M^1+1}^\alpha) \otimes (\omega_1^\beta, \omega_2^\beta, \dots, \omega_{M^2+1}^\beta)$$

- Lagrange polynomials associated to the two sets

$$H_k^\alpha(\xi_1) = \prod_{m=1, m \neq k}^{M^1+1} \frac{(\xi_1 - \xi_m^\alpha)}{(\xi_k^\alpha - \xi_m^\alpha)}, \quad H_l^\beta(\xi_2) = \prod_{m=1, m \neq l}^{M^2+1} \frac{(\xi_2 - \xi_m^\beta)}{(\xi_l^\beta - \xi_m^\beta)}$$

2D tensorial extension of SC method – 2

Definition 2/2

- 2 uncertain parameters $(\xi_1, \xi_2) \in I^1 \times I^2$

$$D(\xi_1, \xi_2) = D^\alpha(\xi_1)D^\beta(\xi_2)$$

- $H_k^\alpha(\xi_1)$, $H_l^\beta(\xi_2)$ Lagrange polynomials associated to the two sets of $(M^1 + 1)$ (resp. $(M^2 + 1)$) Gauss quadrature points associated to D^α (resp. D^β)
- Stochastic collocation 2D expansion

$$F(\xi_1, \xi_2) \simeq scF(\xi_1, \xi_2) = \sum_{k \leq M^1; l \leq M^2} d_{kl} H_k^\alpha(\xi_1) H_l^\beta(\xi_2)$$

- Identification of the coefficients $d_{kl} = F(\xi_k^\alpha, \xi_l^\beta)$

$$scF(\xi_1, \xi_2) = \sum_{k \leq M^1; l \leq M^2} F(\xi_k^\alpha, \xi_l^\beta) H_k^\alpha(\xi_1) H_l^\beta(\xi_2)$$

2D tensorial extension of SC method – 3

- The tensor product of the two Gaussian rules is

$$\int F(\xi_1, \xi_2) D^\alpha(\xi_1) D^\beta(\xi_2) d\xi_1 d\xi_2 = \sum_{k \leq M^1+1; l \leq M^2+1} \omega_k^\alpha \omega_l^\beta F(\xi_k^\alpha, \xi_l^\beta)$$

- It exactly integrates all monomials $\xi_1^p \xi_2^q$ such that $p \leq 2M^1 + 1$ and $q \leq 2M^2 + 1$
- Calculation of the mean of scF

$$\int scF(\xi_1, \xi_2) D^\alpha(\xi_1) D^\beta(\xi_2) d\xi_1 d\xi_2 = \sum_{k \leq M^1+1; l \leq M^2+1} \omega_k^\alpha \omega_l^\beta scF(\xi_k^\alpha, \xi_l^\beta)$$

but simply $scF(\xi_k^\alpha, \xi_l^\beta) = F(\xi_k^\alpha, \xi_l^\beta)$ and

$$\mathbb{E}(scF) = \int scF(\xi_1, \xi_2) D^\alpha(\xi_1) D^\beta(\xi_2) d\xi_1 d\xi_2 = \sum_{k \leq M^1+1; l \leq M^2+1} \omega_k^\alpha \omega_l^\beta F(\xi_k^\alpha, \xi_l^\beta)$$

2D tensorial extension of SC method – 4

- The tensor product of the two Gaussian quadratures

$$\int F(\xi_1, \xi_2) D^\alpha(\xi_1) D^\beta(\xi_2) d\xi_1 d\xi_2 = \sum_{k \leq M^1+1; l \leq M^2+1} \omega_k^\alpha \omega_l^\beta F(\xi_k^\alpha, \xi_l^\beta)$$

- Calculation of the mean of scF (exact due to polynomial degree)

$$\mathbb{E}(scF) = \int scF(\xi_1, \xi_2) D^\alpha(\xi_1) D^\beta(\xi_2) d\xi_1 d\xi_2 = \sum_{k \leq M^1+1; l \leq M^2+1} \omega_k^\alpha \omega_l^\beta F(\xi_k^\alpha, \xi_l^\beta)$$

- Calculation of the variance scF (exact due to polynomial degree)

$$\begin{aligned} \text{Var}(scF) &= \mathbb{E}((scF - \mathbb{E}(scF))^2) = \mathbb{E}(scF^2) - \mathbb{E}(scF)^2 \\ &= \int scF(\xi_1, \xi_2)^2 D^\alpha(\xi_1) D^\beta(\xi_2) d\xi_1 d\xi_2 - \mathbb{E}(scF)^2 \\ &= \sum_{k \leq M^1+1; l \leq M^2+1} \omega_k^\alpha \omega_l^\beta F(\xi_k^\alpha, \xi_l^\beta)^2 - \left(\sum_{k \leq M^1+1; l \leq M^2+1} \omega_k^\alpha \omega_l^\beta F(\xi_k^\alpha, \xi_l^\beta) \right)^2 \end{aligned}$$

d D tensorial generalized polynomial chaos (gPC) and stochastic collocation (SC) methods

- Assume same number of collocation or (Gaussian) quadrature points in all directions M
- Calculation of polynomial expansion in dimension d requires M^d CFD calculations
- Not sustainable if d is high. Example with 9 points per direction. Required number of simulations

$$9^2 = 81, \quad 9^4 = 6561, \quad 9^5 = 59,049, \quad 9^6 = 531,441, \\ 9^8 = 43,046,721, \quad 9^{10} = 3,486,784,401$$

feasible up to $d = 4$ or 5

- Introduction of **polynomial limited by total degree t** (straightforward)

Bound the total degree t of the polynomial instead of limiting the individual degree in each variable. Number of terms of the basis

$$Z = \binom{d+t}{t}$$

- Introduction of Smolyak's **sparse quadratures**¹⁴ often called sparse grids (not so simple)

¹⁴S. A. Smolyak: Quadrature and interpolation formulas for tensor products of certain classes of functions. *Soviet Math. Dokl.* **4**, 240-243 (1963)

Outline

- 1 Introduction. Need for Uncertainty Quantification (UQ)
- 2 Probability basics, Monte-Carlo, surrogate-based Monte-Carlo
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- 4 Introduction to Smolyak's sparse quadratures**
- 5 Examples of application
- 6 Conclusions

Smolyak sparse grids – 1

Tensorial product of two quadrature rules (Reminder)

- 2D case

$$A[f] = \sum_{i=1}^m a_i f(x_i), \quad B[f] = \sum_{i=1}^n b_i f(y_i),$$

$$A \otimes B[g] = \sum_{i=1}^m \sum_{j=1}^n a_i b_j g(x_i, y_j).$$

- Straightforward extension to d D

$$A_1 \otimes A_2 \otimes \cdots \otimes A_d[f] = \sum_{i_1=1}^{n_1} \sum_{i_2=1}^{n_2} \cdots \sum_{i_d=1}^{n_d} w_{1i_1} w_{2i_2} \cdots w_{di_d} f(x_{1i_1}, x_{2i_2}, \dots, x_{di_d})$$

Smolyak sparse grids – 2

Hierarchy of 1D quadratures. Difference of 1D quadratures

- 1D hierarchy of quadratures denotes Q_l with increasing number of points. Assumed to be used in all directions
- Nested (= quadrature points of points Q_l include the quadrature points of Q_{l-1}) or not nested
- Difference in successive quadratures

$$\begin{aligned}\Delta_k[f] &:= Q_k[f] - Q_{k-1}[f], \\ Q_0[f] &:= 0.\end{aligned}$$

- Rewriting of a tensor quadrature** (since $\sum_{k=1}^n \Delta_k[f] = Q_n[f]$)

$$Q_{l_1} \otimes \cdots \otimes Q_{l_d}[f] = \sum_{\mathbf{k} / 1 \leq k_j \leq l_j} \Delta_{k_1} \otimes \cdots \otimes \Delta_{k_d}[f]$$

2D illustration

$$\begin{aligned}Q_3 \otimes Q_2[f] &= (Q_3 - Q_2) \otimes (Q_2 - Q_1)[f] + (Q_3 - Q_2) \otimes (Q_1 - Q_0)[f] \\ &\quad + (Q_2 - Q_1) \otimes (Q_2 - Q_1)[f] + (Q_2 - Q_1) \otimes (Q_1 - Q_0)[f] \\ &\quad + (Q_1 - Q_0) \otimes (Q_2 - Q_1)[f] + (Q_1 - Q_0) \otimes (Q_1 - Q_0)[f]\end{aligned}$$

Smolyak sparse grids – 3

Smolyak sparse quadratures (1/2)

- Fundamental rewriting of a tensor quadrature

$$Q_{l_1} \otimes \cdots \otimes Q_{l_d}[f] = \sum_{\mathbf{k} / 1 \leq k_j \leq l_j} \Delta_{k_1} \otimes \cdots \otimes \Delta_{k_d}[f]$$

- Definition of **Smolyak's sparse quadrature of level l**

$$Q_l^d[f] = \sum_{|\mathbf{k}|_1 \leq l+d-1} \Delta_{k_1} \otimes \cdots \otimes \Delta_{k_d}[f]$$

- Very general construction referring to the **indices of the 1D quadratures in the hierarchy (not degree, not polynomial exactness...)**

Smolyak sparse grids – 4

Smolyak's sparse quadratures (2/2)

- Definition of **Smolyak's sparse quadrature of level l**

$$Q_l^d[f] = \sum_{|\mathbf{k}|_1 \leq l+d-1} \Delta_{k_1} \otimes \dots \otimes \Delta_{k_d}[f]$$

- Other expressions of Smolyak's sparse grids with difference of quadratures

$$Q_l^d[f] = \sum_{j=d}^{d+l-1} \sum_{\mathbf{k}/|\mathbf{k}|_1=j} \Delta_{k_1} \otimes \dots \otimes \Delta_{k_d}[f]$$

$$Q_{l+1}^d[f] = Q_l^d[f] + \sum_{\mathbf{k}/|\mathbf{k}|_1=d+l} \Delta_{k_1} \otimes \dots \otimes \Delta_{k_d}[f]$$

- Direct expressions of Smolyak's sparse grids with quadratures¹⁵

$$Q_l^d[f] = \sum_{\max(l,d) \leq |\mathbf{k}|_1 \leq l+d-1} (-1)^{l+d-|\mathbf{k}|_1-1} \binom{d-1}{|\mathbf{k}|_1-l} Q_{k_1} \otimes \dots \otimes Q_{k_d}[f]$$

¹⁵G. W. Wasilkowski, H. Woźniakowski: Explicit cost bounds of algorithms for multivariate tensor product problems. *J. Complexity* **11**(1), 1-56 (1995)

Smolyak sparse grids – 5

Polynomial exactness (1/2)

- Tensorial product of 1D polynomials

$$\bigotimes_{i=1}^d \mathbb{P}_{s_i}^1 = \left\{ \mathbb{R}^d \ni (x_1, \dots, x_d) \mapsto \prod_{i=1}^d p_i(x_i) \in \mathbb{R}, \quad p_i \in \mathcal{P}_{s_i}^1 \right\}$$

where $\mathcal{P}_{s_i}^1$ is the set of mono-variable polynomials of degree lower or equal to s_i

- The i -th quadrature of the 1D hierarchy Q_i is assumed to have polynomial exactness m_i such that $m_i \leq m_{i+1}$
- Smolyak's sparse grid quadrature

$$Q_l^d[f] = \sum_{|\mathbf{k}|_1 \leq l+d-1} \Delta_{k_1} \otimes \cdots \otimes \Delta_{k_d}[f]$$

is exact for all polynomials of the non classical space

$$\mathcal{V}(Q_l^d) = \text{Span}\{\mathcal{P}_{m_{k_1}}^1 \otimes \cdots \otimes \mathcal{P}_{m_{k_d}}^1; \quad |\mathbf{k}|_1 = l + d - 1\}$$

Smolyak sparse grids – 6

Polynomial exactness (2/2)

- Example: Series of nested (n to $n + 2$) rules U_1, U_2, U_3, U_4 involving $n_1 = 1, n_2 = 3, n_3 = 5, n_4 = 7$ points and having polynomial exactness $m_1 = 0, m_2 = 2, m_3 = 4, m_4 = 6$
- Polynomial exactness of Smolyak's sparse grid U_4^2

$$\begin{aligned}
 U_4^2[f] &= \sum_{j=2}^5 \sum_{\mathbf{k}/|\mathbf{k}|_1=j} \Delta_{k_1} \otimes \Delta_{k_2}[f] \\
 &= (U_4 \otimes U_1 + U_3 \otimes U_2 + U_2 \otimes U_3 + U_1 \otimes U_4 + \text{lower order})[f]
 \end{aligned}$$

- From previous slide, U_4^2 is exact for polynomial vector space $\mathcal{V}(U_4^2)$

$$\mathcal{V}(U_4^2) = \text{Span}\{\mathcal{P}_{m_4} \otimes \mathcal{P}_{m_1} + \mathcal{P}_{m_3} \otimes \mathcal{P}_{m_2} + \mathcal{P}_{m_2} \otimes \mathcal{P}_{m_3} + \mathcal{P}_{m_1} \otimes \mathcal{P}_{m_4}\},$$

that is

$$\mathcal{V}(U_4^2) = \text{Span}\{\mathcal{P}_6 \otimes \mathcal{P}_0 + \mathcal{P}_4 \otimes \mathcal{P}_2 + \mathcal{P}_2 \otimes \mathcal{P}_4 + \mathcal{P}_0 \otimes \mathcal{P}_6\}.$$

Smolyak sparse grids – 7

Number of evaluations, bounds for weights, error analysis

- Number of evaluations, bounds for weights, error analysis require analysis for each individual family of quadrature Q_l
- Classical results for Clenshaw-Curtis

$$\begin{cases} n_l = 2^{l-1} + 1, & l > 1, \\ n_1 = 1, \end{cases}$$

and $m_l = n_l - 1$.

- For fixed dimension d and $l \rightarrow \infty$ the number of points involved in Q_l^d , denoted by $n(Q_l^d)$, is equivalent (strong sense of limit of sequences being equal to 1) to:

$$n(Q_l^d) \simeq \frac{1}{(d-1)! 2^{d-1}} 2^{l-1} (l-1)^{d-1}$$

Maximum number of points along all axis (obtained for one k_j equal l all the other equal 1) equal $2^{l-1} + 1$. “Corresponding” tensorial number of points $(2^{l-1} + 1)^d$

- Error estimation depending on function regularity. See Novak-Ritter 1997 (possibly Dumont-Le Brazidec-Peter 2018)

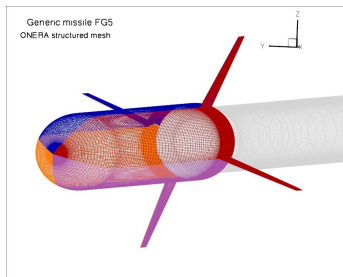
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FG5 generic missile – 3 uncertain parameters

Nominal mesh at the wall

- Generic missile FG5; joint ONERA, DLR, USAF exercise¹⁶
- ONERA experiments. RANS CFD
- 3 uncertain parameters exercise: angle of attack α , upper fin angle, upper fin position
- Three outputs of interest: side force (CYA), rolling moment (CLA), yawing moment (CNA)



¹⁶J. Peter, S. Görtz, R. E. Graves: Three-parameter uncertainty quantification for generic missile FG5. AIAA Paper #2017-1197 (2017)

FG5 generic missile – 3 uncertain parameters

Flow conditions. Uncertain parameters

- Nominal flow conditions: $M_\infty = 0.8$, $\alpha = 12^\circ$, $Re_D = 0.6 \cdot 10^6$
- Output of interest: rolling moment, yawing moment, side force
- Uncertain parameters
 - Angle of attack in $[10^\circ, 14^\circ]$ with PDF:

$$d\alpha' = (\alpha - 12)/2, \quad D^{s2}(d\alpha') = \frac{15}{16}(1 - d\alpha'^2)^2;$$

- Change in upper fin azimuthal position in $[-1^\circ, 1^\circ]$ with PDF:

$$d\phi = \phi - 22.5, \quad D^{s3}(d\phi) = \frac{35}{32}(1 - d\phi^2)^3;$$

- Upper fin angle in $[-1^\circ, 1^\circ]$ with PDF:

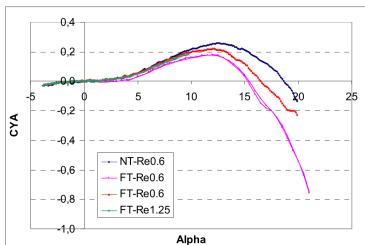
$$D^{s3}(\xi) = \frac{35}{32}(1 - \xi^2)^3.$$

- Joint probability of the three uncertain parameters:

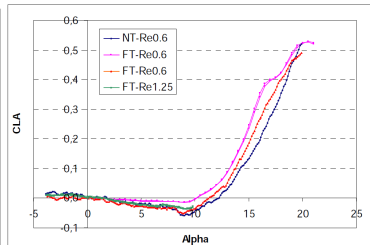
$$D(d\alpha', d\phi, \xi) = D^{s2}(d\alpha')D^{s3}(d\phi)D^{s3}(\xi) = \frac{15}{16} \frac{35^2}{32^2} (1 - d\alpha'^2)^2 (1 - d\phi^2)^3 (1 - \xi^2)^3$$

FG5 generic missile – 3 uncertain parameters

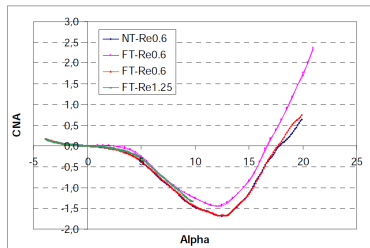
Outputs of interest as function AoA



Side Force



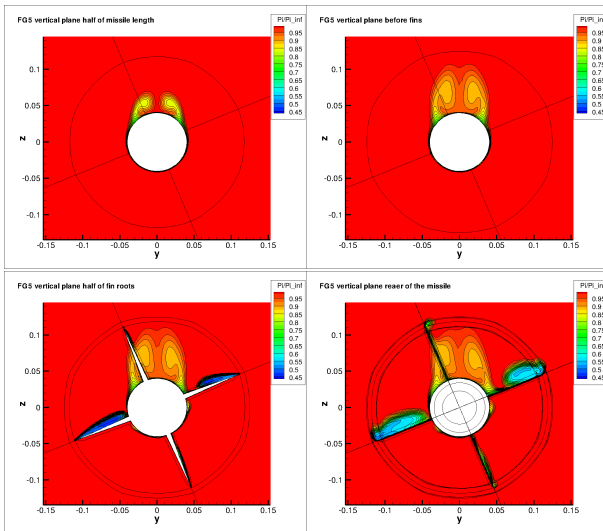
Rolling moment



yawing moment

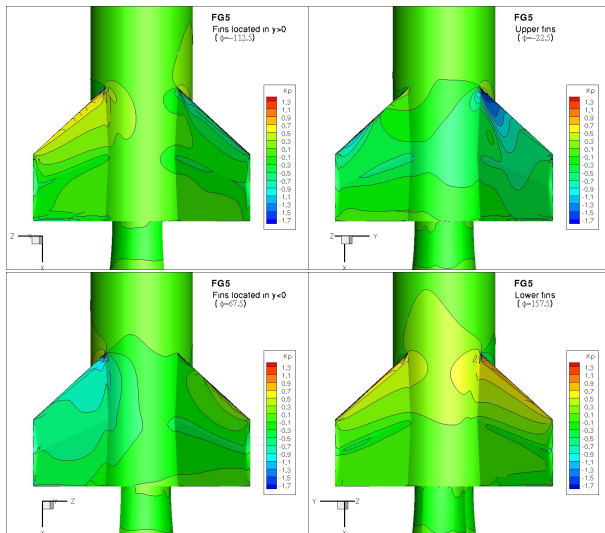
FG5 generic missile – 3 uncertain parameters

Nominal flow (1/2)



FG5 generic missile – 3 uncertain parameters

Nominal flow (2/2)



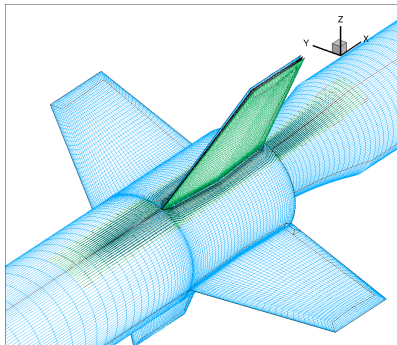
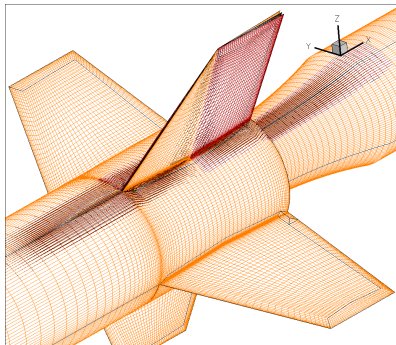
FG5 generic missile – 3 uncertain parameters

- Comparison of nominal flows
 - DLR Calculations with TAU, USAF calculations with AVUS, ONERA calculations with *e/sA*
 - Comparison of pressure coefficients K_p on the fins and rear part of the missile, comparison of stagnation pressure in vertical planes
 - The three flow solutions match well. Good starting point for UQ study
- Individual variation of outputs w.r.t. parameters
 - CYA, CLA, CNA non linear as function of α as in the experiment
 - CYA, CLA, CNA linear as function of fin angle
 - CYA, CLA, CNA linear as function of fin position

FG5 generic missile – 3 uncertain parameters

Fin deformation

(the two mesh deformations can be combined)



FG5 generic missile – 3 uncertain parameters

Strategies for UQ

• ONERA

- 3D quadrature = 31-point Smolyak sparse grid based on (1D) Féjer second rule.
- 31 flow calculations. Classical checks
- Quadrature exactly integrates degree 3 polynomials in dimension 3... but $D(d\alpha', d\phi, \xi)$ is a degree 16 polynomial
- Considered quadrature fails to correctly integrate $D(d\alpha', d\phi, \xi)$
- Kriging fitted to the 31 evaluations of CLA. Corresponding surrogates for CYA, CNA
- Calculation of mean value and variance based on Riemann sums for (surrogate $\times D(d\alpha', d\phi, \xi)$)

FG5 generic missile – 3 uncertain parameters

Strategies for UQ

- DLR

- 76 TAU simulations budget (actually 8, 16, 32, 64 then 76 performing intermediate statistics)
- Three Kriging surrogates fitted to the 8 then 16... then 76 CLA, CYA, CNA values
- One million Monte-Carlo sample built from the cumulative density functions of $D^{s^2}(d\alpha')$, $D^{s^3}(d\phi)$ and $D^{s^3}(\xi)$
- Monte-Carlo mean and variance for the Kriging surrogates based on the $D(d\alpha', d\phi, \xi)$ -consistent sampling
- (Visual) PDF of outputs

- ONERA - DLR

- Checking individual variations of CLA, CYA, CNA w.r.t. ONERA calculations showed differences in slopes → differences in variance expected.

FG5 generic missile – 3 uncertain parameters

Strategies for UQ

- USAF
 - 10 simulations budget
 - DoE = corners of the parameters domain plus two face centers
 - Quadratic surrogate
 - Analysis of variance based on the quadratic surrogate

FG5 generic missile – 3 uncertain parameters

More difference in standard deviation than in mean (than visually looking at Kp)

Aerodynamic coefficient	Deterministic, $\alpha=12^\circ$ Spalart-Allmaras	UQ, mean value Spalart-Allmaras	UQ, variance Spalart-Allmaras
CYA (side force)	0.151	0.147	1.93e-03
CLA (rolling moment)	-9.43e-03	-7.08e-03	1.09e-03
CNA (yawing moment)	-1.133	-1.105	1.03e-01

Aerodynamic coefficient	Deterministic, $\alpha=12^\circ$ Wilcox k- ω , central	UQ, mean value Wilcox k- ω , central	UQ, variance Wilcox k- ω , central
CYA (side force)	0.1330	0.1291	1.3053e-03
CLA (rolling moment)	0.0446	0.0455	3.0519e-05
CNA (yawing moment)	-0.9979	-0.9708	6.1329e-02

RAE2822 – 3 uncertain parameters

Nominal mesh at the wall

- RAE2822,¹⁷ UMRIDA EU project (www.umrida.eu)
- RAE experiments.
- Case 6. Flow conditions $\underline{M}_\infty = 0.725$, $\underline{\alpha} = 2.92^\circ$, $Re = 6.50 \cdot 10^6$
- RANS calculations. Outputs of interest C_D , C_L , C_M
- Uncertainties on free-stream Mach number \underline{M}_∞ , angle of attack $\underline{\alpha}$, thickness to chord ratio $\underline{r} = h/c$

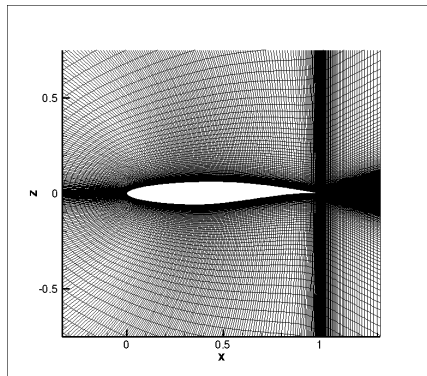
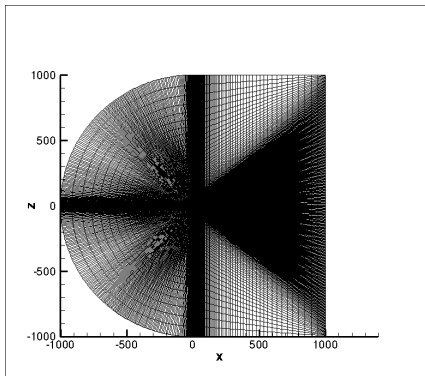
	$a = b$	X_m	X_M
ξ_1	4	$0.97 \times \underline{r}$	$1.03 \times \underline{r}$
ξ_2	4	$0.95 \times \underline{M}_\infty$	$1.05 \times \underline{M}_\infty$
ξ_3	4	$0.98 \times \underline{\alpha}$	$1.02 \times \underline{\alpha}$

$$\beta_I(x; a, b) = \mathbb{1}_{[X_m, X_M]}(x) \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} \frac{(x - X_m)^{a-1} (X_M - x)^{b-1}}{(X_M - X_m)^{a+b-1}}$$

¹⁷É. Savin, A. Resmini, J. Peter: Sparse polynomial surrogates for aerodynamic computations with random inputs. AIAA Paper #2016-0433 (2016)

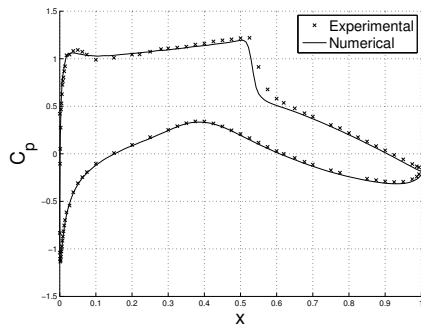
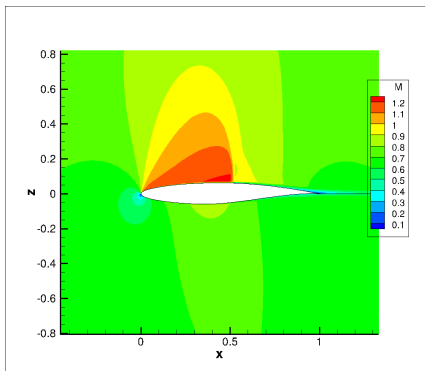
RAE2822 – 3 uncertain parameters

Mesh



RAE2822 – 3 uncertain parameters

Mesh



RAE2822 – 3 uncertain parameters

gPC expansion of outputs of interest [typo]

- gPC expansion. Normalized 1D Jacobi-polynomials ψ orthonormal for

$$\langle \psi_j, \psi_k \rangle = \int_{-1}^{+1} \psi_j(\xi) \psi_k(\xi) \frac{35}{32} (1 - \xi^2)^3 d\xi = \delta_{jk}$$

- Multivariate polynomials involved in the $\mathbb{R}^3 \rightarrow \mathbb{R}^1$ expansions of C_D , C_L , C_M

$$\psi_{\mathbf{j}}(\xi) = \prod_{d=1}^3 \psi_{j_d}(\xi_d), \quad |\mathbf{j}|_1 = j_1 + j_2 + j_3 \leq t$$

- Total degree is $t = 8$. Dimension is $d = 3$. Number of term in the polynomial expansion is

$$Z = \binom{t+d}{d} = \binom{8+3}{3} = \binom{11}{3} = 165$$

- C_D gPC expansion

$$gC_D(\xi_1, \xi_2, \xi_3) = \sum_{|\mathbf{j}|_1 = j_1 + j_2 + j_3 \leq 8} c_{\mathbf{j}} \psi_{j_1}(\xi_1) \psi_{j_2}(\xi_2) \psi_{j_3}(\xi_3)$$

RAE2822 – 3 uncertain parameters

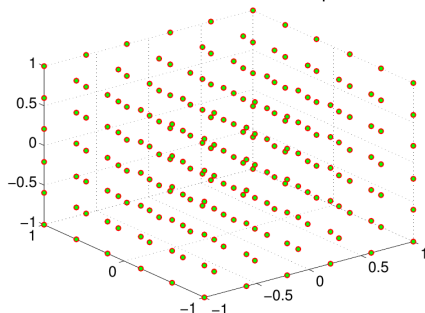
gPC expansion of outputs of interest

- 1D base-quadrature = p -point Gauss-Jacobi-Lobatto (GJL) quadrature.
Polynomial exactness degree $(2p - 3)$
- 3D quadratures
 - Tensorial grid = Tensorial product of the 10-point GJL quadrature.
Polynomial exactness up to degree 17 for each variable ξ_j . Exact integration of products of degree 8 polynomials. Exact variance of gPC expansions.
Number of points 1000 ($= 10^3$)
 - Smolyak sparse grid = 7-th level Smolyak sparse grid based on the family of GJL quadratures.
Number of points 201

RAE2822 – 3 uncertain parameters

Visualization of quadrature points

GJL 6-th level tensorized 3D-quadrature



GJL 7-th level sparse 3D-quadrature

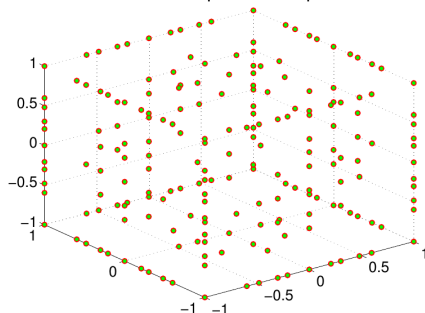


Figure: Visualization of 6-point tensorial GJL quadrature and 7-th level Smolyak quadrature based on GJL nodes—gPC coefficients are calculated with 10-point tensorial GJL quadrature and 7-th level Smolyak quadrature based on GJL nodes

RAE2822 – 3 uncertain parameters

gPC expansion of outputs of interest

- Calculation of the gPC coefficients as (for C_D)

$$\begin{aligned}
 c_j &= \int \psi_j(\xi) C_D(\xi) D(\xi) d\xi \\
 &= \int \psi_{j_1}(\xi_1) \psi_{j_2}(\xi_2) \psi_{j_3}(\xi_3) C_D(\xi_1, \xi_2, \xi_3) \frac{35^3}{32^3} (1 - \xi_1^2)^3 (1 - \xi_2^2)^3 (1 - \xi_3^2)^3 d\xi_1 d\xi_2 d\xi_3
 \end{aligned}$$

- First two moments of the aerodynamic coefficients computed by the 10–th level product rule (1000 points)

	μ	σ
C_D	133.37e-04	34.128e-04
C_L	72.274e-02	1.6695e-02
C_M	-453.99e-04	32.239e-04

- First two moments of the aerodynamic coefficients computed by the 7–th level sparse rule (201 points)

	μ	σ
C_D	133.38e-04	34.097e-04
C_L	72.269e-02	1.6729e-02
C_M	-453.96e-04	32.175e-04

RAE2822 – 3 uncertain parameters

gPC compressed sensing (1/4)

- Reminder: calculation of gPC coefficients by collocation.
- Presentation in case of a multi-variate polynomial of fixed total order

Identify $F(\xi)$ and $gF(\xi)$ for q values of ξ .

$$\sum_{|j|_1 \leq t} C_j P_j(\xi_k) = F(\xi_k), \quad \forall k \in \llbracket 1, q \rrbracket$$

- Matrix notation \mathbf{F} column vector of F values, \mathbf{C} column vector of unknown polynomial coefficients \mathbf{K} matrix $K_{ij} = P_j(\xi_i)$

$$\mathbf{K}\mathbf{C} = \mathbf{F}$$

- Square linear system if number of evaluations = dimension polynomial basis
- Least square system if number of evaluations $>$ dimension polynomial basis
- **Possible use of compressed sensing¹⁸ if number of evaluations $<$ dimension polynomial basis**

¹⁸E. J. Candès, M. B. Wakin: An introduction to compressive sampling. *IEEE Sig. Proc. Mag.* **25**(2), 21-30 (2008)

RAE2822 – 3 uncertain parameters

gPC compressed sensing (2/4)

Collocation linear system. Identify $F(\xi)$ and $gF(\xi)$ for q values of ξ .

$$F(\xi_k) = \sum_{|j|_1 \leq t} G_j P_j(\xi_k), \quad \forall k \in \llbracket 1, q \rrbracket$$

or in matrix notation

$$\mathbf{K}\mathbf{C} = \mathbf{F}$$

\mathbf{K} has q lines (number of evaluations) and Z columns (number of polynomials in the basis)

- May be solved with less information (evaluations) than unknowns (gPC coefficients) by **compressed sensing** provided
 - The actual *gPC* expansion that is looked for is sparse = has many coefficients very close to 0. This is often the case. This is called "**sparsity of effects.**" This is verified for the searched expansion
 - Requires a (random) **sampling incoherent with basis of polynomial** that is measured by the "mutual coherence"

$$\max_{\substack{1 \leq j, l \leq Z \\ j \neq l}} \frac{|K_j^T K_l|}{\|K_j\|_2 \|K_l\|_2}$$

that should have the lowest possible value

RAE2822 – 3 uncertain parameters

gPC compressed sensing (3/4)

- Collocation linear system. Identify $F(\xi)$ and $gF(\xi)$ for q values of ξ .

$$F(\xi_k) = \sum_{|\mathbf{j}|_1 \leq t} C_j P_j(\xi_k), \quad \forall k \in \llbracket 1, q \rrbracket$$

- In matrix notation

$$\mathbf{K}\mathbf{C} = \mathbf{F}$$

- The underdetermined problem is then solved by ℓ_1 minimization

$$\mathbf{C}^* = \arg \min_{\mathbf{h} \in \mathbb{R}^Z} \{ \|\mathbf{h}\|_1; \|\mathbf{K}\mathbf{h} - \mathbf{F}\|_2 \leq \epsilon \}$$

RAE2822 – 3 uncertain parameters

gPC compressed sensing (4/4)

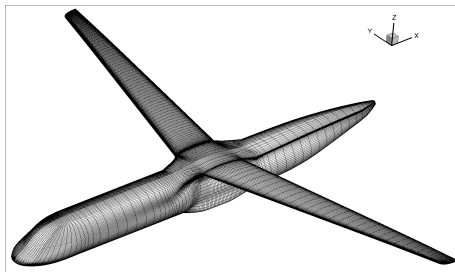
- 165 polynomials in the basis
- 80 random sampling points
- Mutual coherence equal 0.93
- Good recovery of mean and variance with compressed sensing gPC:

	μ	σ
C_D	133.33e-04	34.052e-04
C_L	72.271e-02	1.6703e-02
C_M	-453.95e-04	32.180e-04

ALBATROS¹⁹ flexible wing-fuselage configuration (3D)

Numerical model

- RANS + Spalart-Allmaras model, 9,008,512 cells:



- Implicit LU-SSOR phase; Jameson centered scheme with additional artificial viscosity outside of the boundary layers; Multigrid approach for the NS system over 3 grid levels; Backward Euler time integration scheme;
- Typical computational time: 6 hours on 60 cores.

¹⁹G. Carrier, O. Atinault, S. Dequand, J.-L. Hantrais-Gervois, C. Liauzun, B. Paluch, A.-M. Rodde, C. Toussaint. Investigation of a strut-braced wing configuration for future commercial transport. ICAS Paper 2012-1.10.2 (2012)

ALBATROS flexible wing-fuselage configuration (3D)

Definition of the uncertainties ($d = 10$)

- The Mach number $M \equiv \xi_1$, lift coefficient $C_L \equiv \xi_2$, 4 wing bending parameters ξ_3, \dots, ξ_6 , and 4 wing torsion parameters ξ_7, \dots, ξ_{10} are $d = 10$ variable parameters following uniform marginal probability laws.

	X_m	X_M
ξ_1	0.74	0.76
ξ_2	0.55	0.65
$\xi_3 \dots \xi_6$	$0.5 \times \underline{I}$	$2.0 \times \underline{I}$
$\xi_7 \dots \xi_{10}$	$0.02 \times \underline{J}$	$10.0 \times \underline{J}$

- Our aim is to construct polynomial surrogates for the angle of attack α , drag coefficients C_{Ds} and C_{Dv} computed at the wing skin and in the far-field, respectively, pitching moment coefficient C_M , wing tip bend U , and wing tip twist ϕ using PC adapted to the foregoing PDFs (Legendre polynomials).²⁰

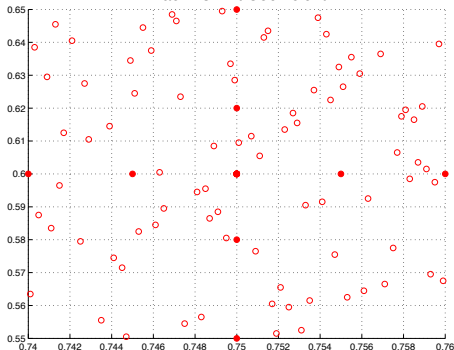
²⁰É. Savin, J.-L. Hantrais-Gervois. Sparse polynomial surrogates for non-intrusive, high-dimensional uncertainty quantification of aeroelastic computations. *Prob. Engng. Mech.* **59**, 103027 (2020).

ALBATROS flexible wing-fuselage configuration (3D)

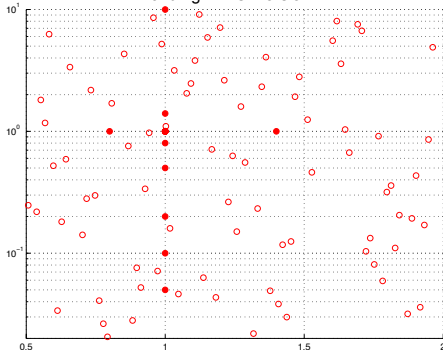
Sampling set (design of experiments DoE)

- The DoE is constituted by a combination of 18 manually generated sampling points (●) and 83 randomly generated sampling points (○) using Latin Hypercube Sampling (LHS).

Mach vs. Lift Coefficient



Bending #4 vs. Torsion #4



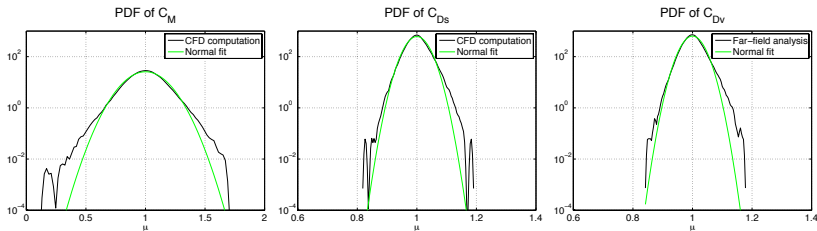
ALBATROS flexible wing-fuselage configuration (3D)

Output statistics by ℓ_1 -minimization ($t = 285$, $q = 101$)

- Mean, variance, root-mean square error, and Kullback-Leibler divergence from a Normal distribution \mathcal{N} :

	C_M	C_{Ds}	C_{Dv}	α	U	ϕ
μ	-11.63e-02	219.83e-04	218.69e-04	2.53	2.16	-6.10
σ	1.55e-02	6.53e-04	6.28e-04	0.20	0.26	0.80
e_2	4.70e-03	0.45e-03	0.35e-03	1.88e-03	1.65e-03	3.97e-03
$D_{KL}(\mathcal{P} \mathcal{N})$	1.10e-02	1.11e-02	1.39e-02	1.40e-02	0.50e-02	0.62e-02

- PDFs:



- Sensitivity to at most 2 or 3 parameters out of 10.

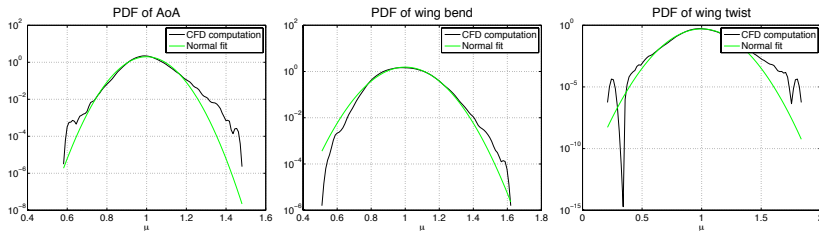
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- PDFs:



- Sensitivity to at most 2 or 3 parameters out of 10.

Outline

- 1 Introduction. Need for Uncertainty Quantification (UQ)
- 2 Probability basics, Monte-Carlo, surrogate-based Monte-Carlo
- 3 Non-intrusive polynomial methods for 1D / tensorial n D propagation
- 4 Introduction to Smolyak's sparse quadratures
- 5 Examples of application
- 6 Conclusions**

Way forward...

- Uncertainty quantification
 - needed for robust analysis, robust design, validation
 - more and more interest and projects (EU, RTO...)
- Way to proceed
 - Get precise definition of industry relevant problems
 - Use both mechanical and mathematical test cases
- Challenges
 - Deal with large numbers of uncertain parameters
 - Use sensitivity analysis (Sobol indices...)
 - Use sparsity of effects
 - Deal with geometrical uncertainties
- Free softwares: OpenTURNS (Airbus, EDF, Phimeca, ONERA ≥ 2018), UQLab (ETH Zürich), UQTK (Sandia National Laboratories), ChaosPy (U. of Oslo), PoCET (Technische Universität Chemnitz), UQit (KTH), PolyChaos (Karlsruhe Institute of Technology)...