# Generalized polynomial chaos and stochastic collocation methods for uncertainty quantification in aerodynamics

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[1] ONERA DAAA - DTIS

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# Outline

# Outline

# Need for (UQ)

## Example I : drag evaluation

- Deterministic drag of airplane in cruise
  - Total drag $Cd$ at cruise nominal Mach number ($M$=0.82) $Cd(0.82)$
  - a/c shape satisfying constraints on lift, pitching moment, rolling moment...
- Actually cruise flight Mach number varies
  - Waiting for landing slot
  - Speeding up to cope with pilot maximum flight time

  $\rightarrow$ Variable Mach number described by $D(M)$
- Robust calculation of airplane cruise drag
  - Compute $\int Cd(M)D(M)dM$, instead of $Cd(0.82)$

# 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

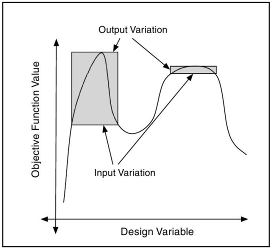



Figure: Robust design (from cenaero.be)

# Need for (UQ)

## Example III : validation process

- Unkown data in experiment
  - Upwind Mach number (equivalent to far-field Mach number in free-stream) not fully controled 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: *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. 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 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

# 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 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 makes sense if standard deviation due to uncertain inputs not much smaller than modelling or discretization error

# 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

# Outline

# Basics of probability (1)

A classical introduction to probability basics involves

- event (one dice value, one Mach number value)
- a sample space $\Omega$ (all six dice values, interval of Mach number values)
- set of events space $\mathcal{A}$ ($\sigma$-algebra) set of subsets of $\Omega$, stable by union, intersection, including null set $\emptyset$ and $\Omega$
- 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 $\xi$ (like *CDp* or *CLp* of an airfoil depending on the far-field Mach number through Navier-Stokes equations)

# Basics of probability (2)

**Discrete example : regular 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 ($\sigma$-algebra) $\mathcal{F}$ = null set plus all discrete sets of these numbers $\{\emptyset, \{1\}, \{2\}, \{3\}, \{4\}, \{5\}, \{6\}, \{1,2\}, \{1,3\}, \{1,4\}, \{1,5\}, \{1,6\}, \{2,3\}$ ... $\{1,2,3,4,5,6\}\}$
- probability function $P$ : $P(\emptyset) = 0$, $P(\{1\}) = 1./6.$, $P(\{2\}) = 1./6.$,... $P(\{1,2\}) = 1./3.$, $P(\{1,3\}) = 1./3$ , $P(\{1,4\}) = 1./3$.... $P(\{1,2,3,4,5,6\}) = 1.$
- random variables $X$, for example, dice value to the power three...

# Basics of probability (3)

**Continuous example : Far-field Mach number in [0.81,0.85]**

- event $\xi$ = a Mach number value in [0.81,0.85]
- sample space $\Omega$ = [0.81,0.85]
- set of events ($\sigma$-algebra) $\mathcal{F}$ = 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: $$D_\phi(\phi) = \frac{35}{32}(1. - \phi^2)^3 \quad \phi \in [-1,1] \qquad \phi = (\xi - 0.83)/0.02$$

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

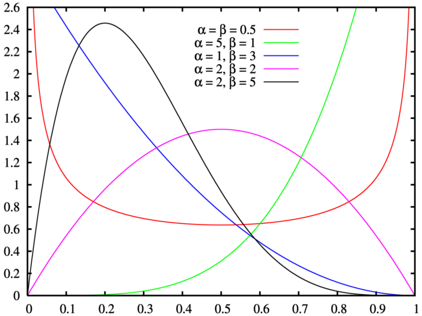
- possible random variables $X$ = lift, drag, pitching moment of a wing... with variable Mach number $M_\infty$("event" $\xi$) in the farfield

# Basics of probability (4)

## Example of probability density functions

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

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



# Need for (UQ)

## Intrusive vs non-intrusive methods

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

# 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 sampling $(\xi^1, \xi^2 ..., \xi^p ..., \xi^N ...)$ of the p.d.f $D(\xi)$
- Computation of corresponding flow fields $W(\xi^p), p \in [1, N]$
- Computation of functional outputs $\mathcal{J}(\xi^p) = J(W(\xi^p), X(\xi^p))$
- Discrete estimation of mean and variance:

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

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

- Need to quantify accuracy of estimation

# Monte-Carlo – 2

## Accuracy of mean

- Scalar case, variance $\sigma_{\mathcal{J}}$ is known, $N$ sampling size, $\sqrt{N}\frac{\bar{\mathcal{J}}_N - E(\mathcal{J})}{\sigma_{\mathcal{J}}} \rightsquigarrow \mathcal{N}(0,1)$ (Normal distribution)

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

| $\epsilon$ | 0.5 | 0.9 | 0.95 | 0.99 |
|---|---|---|---|---|
| $u_\epsilon$ | 0.674 | 1.645 | 1.960 | 2.576 |

- With 99% confidence :

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

# Monte-Carlo – 3

## Accuracy of mean

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

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

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

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

Figure: 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
  $\sqrt{N}\frac{\bar{\mathcal{J}}_N - E(\mathcal{J})}{\sigma_{\mathcal{J}_N}} \rightsquigarrow \mathcal{S}(N-1)$ – Student distribution

- Student distribution $\mathcal{S}(N)$ probability density function:

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

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

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

# Monte-Carlo – 5

Accuracy of estimation: variance (1) (skpd)

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

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

- 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. :

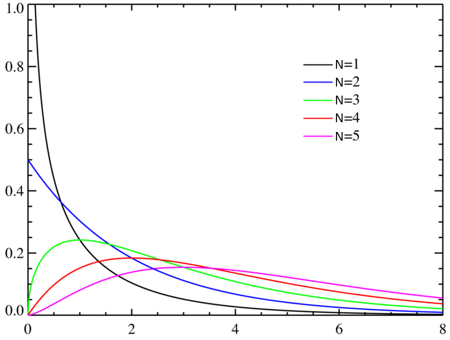
$$\Phi_{\chi^2_N}(x) = \int_0^x D_{\chi^2_N}(t)dt$$

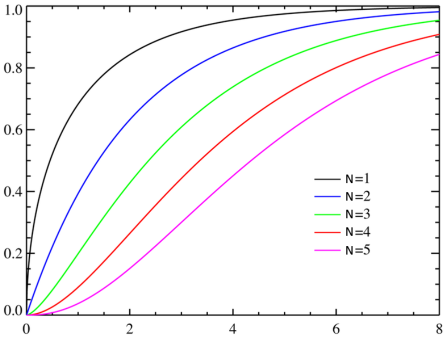
- Stochastic variable

$$N\frac{S^2_{\mathcal{J}_N}}{\sigma^2_{\mathcal{J}}} \rightsquigarrow \chi^2_N$$

# Monte-Carlo – 6

Chi-square probabilistic density functions $D_{\chi^2_N}$ and cumulative density functions $\Phi_{\chi^2_N}$ (skpd)



# Monte-Carlo – 7

## Accuracy of variance (2) (skpd)

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

$$\Phi^{-1}_{\chi^2_N}(\frac{\alpha}{2}) \leq N\frac{\sigma^2_{\mathcal{J}_N}}{\sigma^2_{\mathcal{J}}} \leq \Phi^{-1}_{\chi^2_N}(1. - \frac{\alpha}{2})$$

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

$$\sigma^2_{\mathcal{J}} \in [N\frac{\sigma^2_{\mathcal{J}_N}}{\Phi^{-1}_{\chi^2_N}(1 - \frac{\alpha}{2})}, N\frac{\sigma^2_{\mathcal{J}_N}}{\Phi^{-1}_{\chi^2_N}(\frac{\alpha}{2})}]$$

| $x$ $N$ | 2 | 20 | 30 |
|---|---|---|---|
| 0.005 | 10.597 | 39.997 | 53.672 |
| 0.995 | 0.0100 | 7.434 | 13.787 |

Figure: Value of $\Phi^{-1}_{\chi^2_N}(x)$

# Monte-Carlo – 8

## Accuracy of variance (3) (skpd)

- Application. With 99% confidence, depending on $N$ number of samples
  $N = 2 \Rightarrow \sigma^2_{\mathcal{J}} \in [0.189\ S^2_{\mathcal{J}_2},\ \ 200\ S^2_{\mathcal{J}_2}]$
  $N = 20 \Rightarrow \sigma^2_{\mathcal{J}} \in [0.500\ S^2_{\mathcal{J}_{20}},\ \ 2.69\ S^2_{\mathcal{J}_{20}}]$
  $N = 30 \Rightarrow \sigma^2_{\mathcal{J}} \in [0.559\ S^2_{\mathcal{J}_{30}},\ \ 2.18\ S^2_{\mathcal{J}_{30}}]$
  $N = 100 \Rightarrow \sigma^2_{\mathcal{J}} \in [0.713\ S^2_{\mathcal{J}_{100}},\ \ 1.49\ S^2_{\mathcal{J}_{100}}]$
- Convergence speed of bounds towards 1.
- The cumulative distribution of the Chi-Square law $\Phi_N(x)$ can be expressed as $\Phi_{\chi^2_N}(x) = \frac{1}{\Gamma(N/2)} \int_0^{x/2} t^{N/2} e^{-t} dt = \dfrac{\gamma(N/2, x/2)}{\Gamma(N/2)}$ ($\gamma$ 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 – 9

## Accuracy of variance (4) (skpd)

- Scalar case: mean $E(\mathcal{J})$ is unknown - Stochastic variable $(N-1)\frac{\sigma^2_{\mathcal{J}_N}}{\sigma^2_{\mathcal{J}}} \rightsquigarrow \chi^2_{N-1}$
- With $\epsilon = (1-\alpha)$ confidence :

$$\sigma^2_{\mathcal{J}} \in [(N-1)\frac{\sigma^2_{\mathcal{J}_N}}{\Phi^{-1}_{\chi^2_{N-1}}(1-\frac{\alpha}{2})}, (N-1)\frac{\sigma^2_{\mathcal{J}_N}}{\Phi^{-1}_{\chi^2_{N-1}}(\frac{\alpha}{2})}]$$

| $x$ $N$ | 3 | 4 | 20 | 30 |
|---|---|---|---|---|
| 0.005 | 10.597 | 12.838 | 38.582 | 52.336 |
| 0.995 | 0.0100 | 0.0717 | 6.844 | 13.121 |

Figure: Value of $\Phi^{-1}_{\chi^2_{N-1}}(x)$

# Monte-Carlo – 10

Cost issue. Regularity of output.

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

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

  with $u_{0.99,1} = 63.66$, $u_{0.99,2} = 9.925$, $u_{0.99,3} = 5.841$, $u_{0.99,9} = 3.250$, $u_{0.99,19} = 2.861$, $u_{0.99,19} = 2.756$,... 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**

# 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 ouputs 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** $\rightarrow$ next section

- Derive a surrogate of the output variables as function of the input variables using **general surrogates** $\rightarrow$ end of this section section

- Calculate mean, variance, kurtosis, range, risk... for the surrogate

# Meta-model based Monte-Carlo

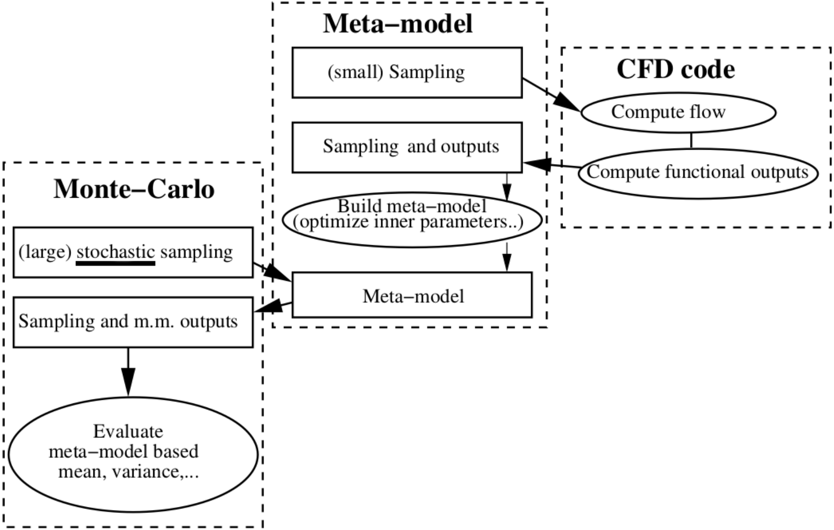



Figure: Monte-Carlo method with meta-models

# 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 ONERA [1])
2. Other meta-models of specific interest for UQ: generalized polynomial Chaos (gPC), Stochastic Colllocation (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 ?

[1] Modèles de substitution pour l'optimisation globale de forme en arodynamique et mthode locale d'optimisation sans paramtrisation. Manuel Bompard. PhD Thesis. December 2011

# Application of metamodel-based Monte-Carlo

- Confidence intervals on lift $C_L$ with uncertainty on AoA
- Nominal configuration: NACA0012, $M = 0.73$, $Re = 6M$, $AoA = 3°$
- ONERA *elsA*$^{(a)}$ code [2]
- (RANS+(k-w) Wilcox turbulence model) solver (Roe flux+Van Albada lim.)

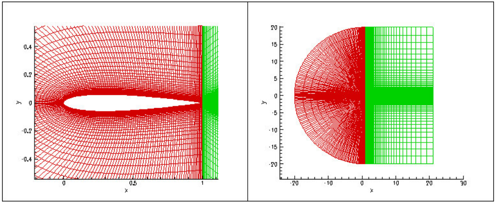


Figure: Mesh

[2] The *elsA* CFD software: input from research and feedback from industry *Mechanics and Industry 14(3)* L. Cambier, S. Heib, S. Plot. 2013

# Distribution of uncertainty

- Beta distribution (parameters (3.,3.))over [-1,1]

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

- p.d.f of angle of attack AoA over [2.9,3.1]

$$D_a(\alpha) = 10 D_b(10.(\alpha - 3.))$$

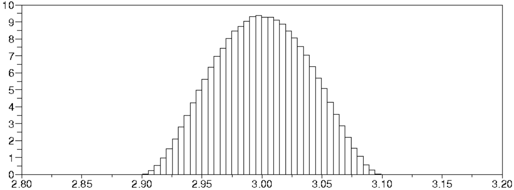



Figure: Beta distribution of AoA

# Monte-Carlo method for $C_L$ mean

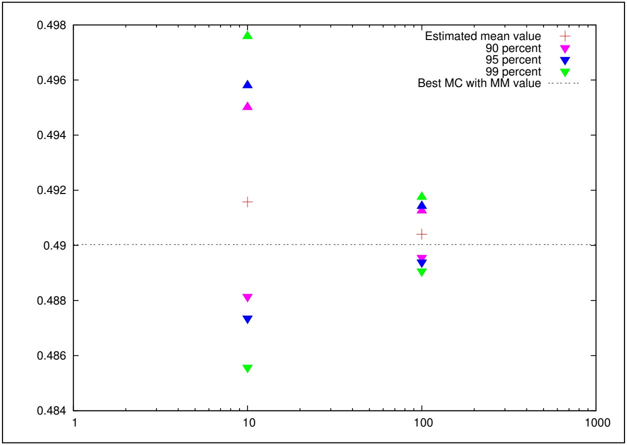



Figure: Mean of $C_L$ coefficient and confidence interval

# Monte-Carlo method for $C_L$ variance

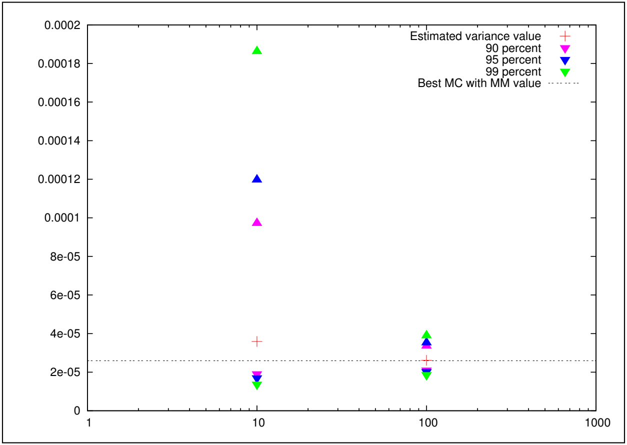



Figure: Variance of $C_L$ coefficient and confidence interval

# Metamodel based Monte-Carlo: learning sample

- Use learning sample based on roots of Tchebyshev polynomials

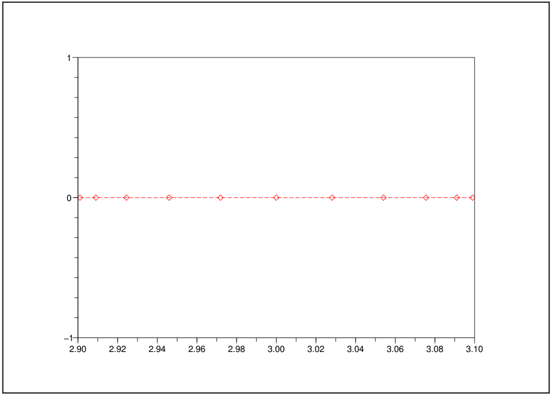



Figure: Tchebychev distribution (11 points)

# Metamodel-based Monte-Carlo: reconstruction of $C_L$

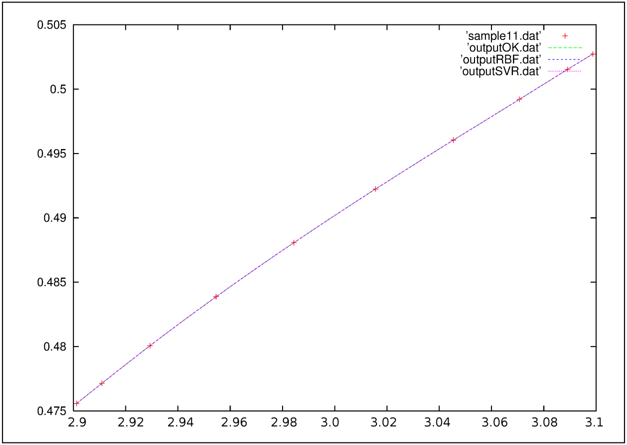



Figure: $C_L$

# Metamodel-based Monte-Carlo for $C_L$ mean

calling metamodel instead of CFD code

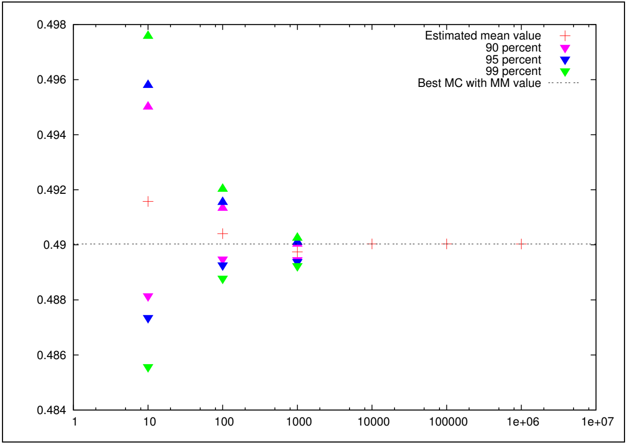



Figure: Mean of $C_L$ coefficient and confidence interval

# Metamodel-based Monte-Carlo for $C_L$ variance

calling metamodel instead of CFD code

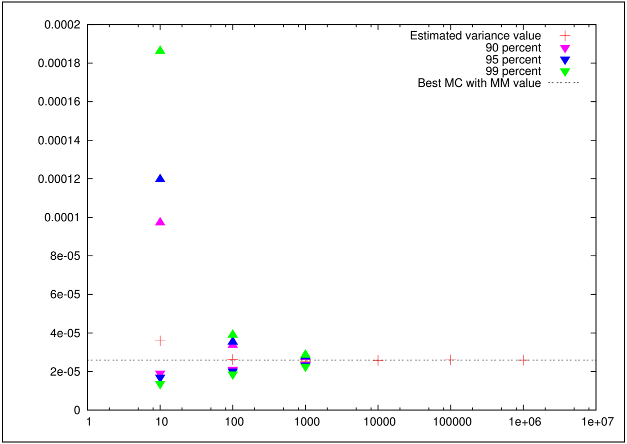



Figure: Variance of $C_L$ coefficient and confidence interval

# Outline

# Two polynomial methods for (UQ). 1D and nD tensorial

- **Stochastic specific polynomial surrogates**
- For all non-intrusive methods
  - Presentation for one uncertain parameter $\xi$, probability density function $D(\xi)$
  - Extention 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 Method (gPC) – 1

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

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

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

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

- Straightforward calculation of mean and variance of the polynomial expansion (that approximates the quantity of interest)

- Orthogonal polynomials – Abramowitz and Stegun: Handbook of Mathematical functions. (1972). Chapter 22
- Spectral expansions – J. P. Boyd: Chebyshef and Fourier spectral methods (2001)

# Generalized polynomial chaos Method (gPC) – 2

## Families of orthogonal polynomials

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

# Generalized polynomial chaos Method (gPC) – 3

## Families of orthogonal polynomials

- Example: Stochastic variable in $\mathbb{R}$. Hermite polynomials for normal law $D_n(\xi) = \frac{1}{\sqrt{2\Pi}} e^{-\frac{\xi^2}{2}}$
- 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
  - $\overline{PH}_0(\xi) = 1 \qquad \overline{PH}_1(\xi) = \xi \qquad \overline{PH}_{n+1}(\xi) = \xi\overline{PH}_n(\xi) - n\overline{PH}_{n-1}(\xi)$
- Normalization $PH_j(\xi) = \frac{1}{\sqrt{j!}}\overline{PH}_j(\xi)$
- Orthonormality relation for $PH$

$$< PH_j, PH_k >= \int_{-\infty}^{+\infty} PH_j(\xi)PH_k(\xi)D_n(\xi)d\xi = \delta_{jk}$$

# Generalized polynomial chaos Method (gPC) – 4

## Families of orthogonal polynomials

- Example: Stochastic variable in [-1,1]. First-kind Chebyshef polynomials for probability density function $D_{cf}(\xi) = \frac{1}{\Pi} \frac{1}{\sqrt{1-\xi^2}}$
- Family of orthonormal polynomials for $< f, g >= \int_{-1}^{1} f(t)g(t)D_{cf}(t)dt$
  - $\overline{T}_0(\xi) = 1$
  - $\overline{T}_1(\xi) = \xi$
  - $\overline{T}_2(\xi) = 2\xi^2 - 1$
  - $\overline{T}_3(\xi) = 4\xi^3 - 3\xi$
- Recursive definition
  - $\overline{T}_0(\xi) = 1 \quad \overline{T}_1(\xi) = \xi \qquad \overline{T}_{n+1}(\xi) = 2\xi\overline{T}_n(\xi) - \overline{T}_{n-1}(\xi)$
- Normalization $T_0 = \overline{T}_0 \quad T_1 = \sqrt{2}\ \overline{T}_1 \ldots \quad T_n = \sqrt{2}\ \overline{T}_n \quad (n \geq 1)$
- Orthonormality of the $T_j$,
  $< T_j, T_k >= \int_{-1}^{1} T_j(\xi)T_k(\xi)D_{cf}(\xi)d\xi = \delta_{jk}$
- Specific property $\overline{T}_n(cos(\theta)) = cos(n\theta)$ (hence $||\overline{T}_n||_\infty \leq 1$.)

# Generalized polynomial chaos Method (gPC) – 5

## Polynomial expansion

- Expansion of a functional output depending on stochastic variable $\xi$

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

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

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

- Accuracy of ideal $gW$ depending on degree and regularity. Theory of spectral expansions

- Stochastic post-processing for $gW$ ($gF$) instead of $W$ ($F$)
- Straighforward calculation of $gW$ ($gF$) mean and variance

# Generalized polynomial chaos Method (gPC) – 6

## Coefficients computation (1/4) - Gaussian quadrature

- Expansion of part of flow field depending on stochastic variable $\xi$ and generic mesh index $i$

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

- From orthonormality property $C_l(i) =< gW(i), P_l >$ Under regularity assumptions $C_l(i) =< W(i), P_l >$

- Proof Assume $D$ is defined on an interval of $\mathbb{R}$ and bounded. Assume uniform convergence of spectral expansion over its domain of definition

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

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

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

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

# Generalized polynomial chaos Method (gPC) – 7

## Coefficients computation (2/4) - Gaussian quadrature

- Expansion of part of flow field depending on stochastic variable $\xi$ and generic mesh index $i$

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

- Gaussian quadrature for

$$C_l(i) =< W, P_l >= \int W(i,\xi)P_l(\xi)D(\xi)d\xi$$

- Computation by Gaussian quadrature associated to p.d.f $D$ with $g$ points. Exact integration of poynomials 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 Method (gPC) – 8

## Coefficients computation (3/4) – Gaussian quadrature

- Expansion of part of flow field depending on stochastic variable $\xi$ and generic mesh index $i$

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

- $g$-point Gaussian quadrature associated to $D$

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

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

- Calculation of gPC coefficients

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

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

# Generalized polynomial chaos Method (gPC) – 9

## Coefficients computation (4/4) – collocation

- Other way : collocation or least-square collocation
- NB Less accuracy results than for Gauss quadrature

- Identify $W(i,\xi_l)$ and $gW(i,\xi_l)$ for $M+1$ values of $\xi$. Identify $F(\xi_l)$ and $gF(\xi_l)$ for $M+1$ values of $\xi$.

$$\sum_{l=0}^{l=M} C_l P_l(\xi_k) = F(\xi_k) \quad \forall\ k\ \in \{1, M+1\} \qquad \text{solved for} \quad C_l$$

1. Number of $F$ evaluations = number of coefficients. Linear system
2. Number of $F$ evaluations > number of coefficients. Solve least-square problem problem
3. Number of $F$ evaluations < number of coefficients. see later “sparsity-of-effects” & “compressed sensing”

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

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

# Generalized polynomial chaos Method (gPC) – 10

## Stochastic post-processing (1/3)

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

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

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

  - straightforward evaluation of variance

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

# Generalized polynomial chaos Method (gPC) – 11

## Stochastic post-processing (2/3)

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

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

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

    requires the knowledge/calculation of $\int P_l(\xi) P_n(\xi) P_p(\xi) D(\xi) d\xi$ integrals
  - Calculation of range. Sample $\xi$ and evaluate $gF(\xi)$
  - Probability of that $F$ exceeds a threshold $T$. Sample $\xi$ and evaluate $gF(\xi)$ for

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

# Generalized polynomial chaos Method (gPC) – 12

## Stochastic post-processing (3/3)

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

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

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

  - straightforward evaluation of variance

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

  - 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 $(\xi_1, \xi_2) \in \mathrm{I}^1 \times \mathrm{I}^2$

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

- Families of orthogonal polynomials for $D^\alpha(\xi_1)$ and $D^\beta(\xi_2)$ are $(P_0^\alpha, P_1^\alpha, P_2^\alpha, ...)$ and $(P_0^\beta, P_1^\beta, P_2^\beta, ...)$

- Polynomial extension (output functional case)

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

# 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 $\mathrm{I}^1\times\mathrm{I}^2$ as

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

- Tensorial approach. First define the tensorial product of two 1D Gaussian rules for integration in directions $\xi_1$ $\xi_2$ over $\mathrm{I}^1$ and $\mathrm{I}^2$

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

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

- Tensorial quadrature $(A\otimes B)$ over $\mathrm{I}^1\times\mathrm{I}^2$

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

# 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 $\mathrm{I}^1\times\,\mathrm{I}^2$ as

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

- Tensorial quadrature $(A\otimes B)$ over $\mathrm{I}^1\times\,\mathrm{I}^2$

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

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

- Calculation of gPC coefficient

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

# 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 $\mathrm{I}^1 \times \mathrm{I}^2$ as

$$C_{k,l} = \int F(\xi_1,\xi_2) P^{\alpha}_k(\xi_1) P^{\beta}_l(\xi_2) D^1(\xi_1) D^{\beta}(\xi_2) d\xi_1 d\xi_2$$

  by tensorial quadrature rule

$$\int_{\mathrm{I}^1 \times \mathrm{I}^2} F(\xi_1,\xi_2) D^{\alpha}(\xi^1) D^{\beta}(\xi^2) d\xi_1 d\xi_2 \simeq \sum_{k \le g^{\alpha}, l \le g^{\beta}} \omega^{\alpha}_k \omega^{\beta}_l F(\xi^{\alpha}_k, \xi^{\beta}_l)$$

- 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

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

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

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

- Use least square approach if more sampling points than coefficients

# 2D tensorial extension of (gPC) method – 6

## Stochastic post processing

- gPC 2D expansion

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

- Calculation of mean

$$E(gF) = \int \left( \sum_{k\le M^1, l\le M^2} C_{k,l} P_k^{\alpha}(\xi_1) P_l^{\beta}(\xi_2) \right) d\xi_1 d\xi_2 = C_{0,0}$$

- straightforward evaluation of variance

$$\begin{aligned}
V(gF) &= E((gF - C_{0,0})^2) \\
&= \int \left( \sum_{k\le M^1, l\le M^2} C_{k,l} P_k^{\alpha}(\xi_1) P_l^{\beta}(\xi_2) D(\xi_1,\xi_2) d\xi_1 d\xi_2 - C_{0,0} \right)^2 D(\xi_1)^{\alpha} D^{\beta}(\xi_2) d\xi_1 d\xi_2 \\
&= \int \left( \sum_{k\le M^1, l\le M^2 \ (k,l)\neq(0,0)} C_{k,l} P_k^{\alpha}(\xi_1) P_l^{\beta}(\xi_2) \right)^2 D(\xi_1)^{\alpha} D(\xi_2)^{\beta} d\xi_1 d\xi_2 \\
&= \sum_{k\le M^1, l\le M^2 \ (k,l)\neq(0,0)} C_{k,l}^2
\end{aligned}$$

# Stochastic collocation method – 1

## Definition

- 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
- Dedicated stochastic polynomial expansion using Lagrangian polynomials

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

(sum of polynomials of degree $M$)

- Note that

$$scW(i,\xi_l) = \sum_{l=1}^{l=N} W_l(i) H_l(\xi_l) = W_l(i)$$

$\rightarrow$ no coefficient calculation step. Compute flows (and extract part of state variables fields) $W(i,\xi_l)$ corresponding to the $\xi_l$ / substitute $W(i,\xi_l)$ to $W_l(i)$

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

# Stochastic collocation method – 2

## Suitable set of points

- Polynomial expansion using Lagrangian polynomials

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

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

1 $M+1$ points of the $(M+1)$-point Gaussian quadrature associated to $D(\xi)$ (most often, not absolutely necessary)

2 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 interpolatory quadrature associated to the nodes. Inexact mean and variance.

# Stochastic collocation 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 $(\xi_1, \xi_2, \ldots, \xi_{M+1})$ are the $M+1$ points of the $(M+1)$-point Gaussian quadrature associated to $D(\xi)$, the weights being $(\omega_1, \omega_2, \ldots, \omega_{M+1})$

- straightforward evaluation of mean value (degree $M$ polynomial)

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

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

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

- Both exact from quadrature polynomial exactness.

# Stochastic collocation 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 $(\xi_1, \xi_2, ..., \xi_{M+1})$ are not the $M+1$ points of the $(M+1)$-point quadrature associated to $D(\xi)$. Note these Gauss quadrature points $(\nu_1, \nu_2, ..., \nu_{M+1})$ and the weights $(\omega_1, \omega_2, ..., \omega_{M+1})$ (no flow have been calculated for the $\nu_m$)
- This quadrature is used for evaluations of mean and variance
- Evaluation of mean value (degree $M$ polynomial)

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

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

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

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

# Stochastic collocation method – 5

## Mean and variance evaluation 3/3 (skpd)

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

$$E(scW(i,\xi)) = \int scW(i,\xi)D(\xi)\xi \simeq \sum_{m=1}^{M+1} \gamma_l \; scW(i,\xi^l)D(\xi_l) = \sum_{m=1}^{M+1} \gamma_l \; W(i,\xi^l)D(\xi_l)$$

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

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

# 2D tensorial extension of (SC) method – 1

## Definition (1/2)

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

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

- 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 $D^\alpha$ and $D^\beta$.

$$(\xi_1^\alpha, \xi_2^\alpha, ..., \xi_{M^1+1}^\alpha) \times \quad (\xi_1^\beta, \xi_2^\beta, ..., \xi_{M^2+1}^\beta)$$

  the weights being

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

- Lagrange polynomials associated to the two sets

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

# 2D tensorial extension of (SC) method – 2

## Definition (2/2)

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

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

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

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

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

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

# 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 $p \leq 2M^1+1$ $q \leq 2M^2+1$
- 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

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

# 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)

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

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

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

# d-D tensorial generalized polynomial choas (gPC) and stochstic collocation (SC) method

- 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

  $9^2 = 81 \quad 9^4 = 6561 \quad 9^5 = 59049 \quad 9^6 = 531441 \quad 9^8 = 43.046721 \quad 9^{10} = 3.486.784401$

  feasible up to $d = 4$ or 5

- Introdution 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

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

- Introdution of Smolyak **sparse quadratures** often called sparse grids (not so simple)

# Outline

# Smolyak sparse grids – 1

## Tensorial product of two quadrature rules (Reminder)

- 2D case

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

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

- Straighforward extension to nD

$$A_1 \otimes A_2 \otimes ... \otimes A_d[f] = \sum_{i_1=1}^{n_1} ... \sum_{i_d=1}^{n_d} w_{1 i_1} ... w_{d i_d} \; f(x_{1 i_1}, ..., x_{d i_d})$$

# Smolyak sparse grids – 2

## Hierarchy of 1D qudratures. Difference of 1D quadratures

- 1D hierachy 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**

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

2D illustration

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

# Smolyak sparse grids – 3

## Smolyak sparse quadratures (1/2)

- Fundamental rewriting of a tensor quadrature

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

- Definition of **Smolyak sparse quadrature of level $l$**

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

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

# Smolyak sparse grids – 4

## Smolyak sparse quadratures (2/2)

- Definition of **Smolyak sparse quadrature of level $l$**

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

- Other expressions of Smolayk sparse grids with difference of quadratures

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

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

- Direct expressions of Smolayk sparse grids with quadratures

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

# Smolyak sparse grids – 5

## Polynomial exactness (1/2)

- Tensorial product of 1D polynomials

$$\bigotimes_{i=1}^{d} \mathbb{P}^1_{s_i} = \{(x_1, ..., x_d) \in \mathbb{R}^d \to \prod_{i=1}^{d} p_i(x_i) \in \mathbb{R},\ p_i \in \mathcal{P}^1_{s_i}\}$$

  where $\mathcal{P}^1_{s_i}$ 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 $m_i \leq m_{i+1}$

- The Smolyak sparse grid quadrature

$$Q^d_l[f] = \sum_{|\mathbf{k}|_1 \leq l+d-1} (\Delta_{k_1} \otimes ... \otimes \Delta_{k_d})[f]$$

  is exact for all polynomials of the non classical space

$$\mathcal{V}(Q^d_l) = Span\{\mathcal{P}^1_{m_{k_1}} \otimes ... \otimes \mathcal{P}^1_{m_{k_d}}\ /\ |\mathbf{k}|_1 = l + d - 1\}$$

# Smolyak sparse grids – 6

## Polynomial exactness (2/2)

- Example: Series $(n/n+2)$ nested 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 sparse grid $U_4^2$

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

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

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

that is

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

# 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 $Q_i$
- Classical results for Clenshaw-Curtis

$$n_1 = 1 \quad \text{then} \quad n_i = 2^{i-1} + 1 \;\; (i > 1) \quad \text{points} \quad m_i = n_i - 1$$

- For fixed dimension $d$ and $l \to \infty$ the number of points involved in $Q_l^d$, denoted $n_{(Q_l^d)}$, 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 $(2^{l-1}+1)^d$

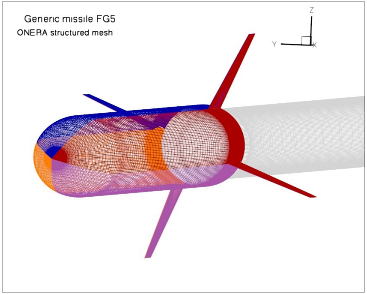
- Error estimation depending on function regularity. See Novak Ritter 1999 (possibly Dumont-Le Brazidec Peter 2018)

# Outline

# FG5 generic missile – 3 uncertain parameters

## Nominal mesh at the wall

- Generic missile FG5.
- ONERA experiments. RANS CFD
- 3 uncertain parameters exercise. Angle of attack $\alpha$, upper fin angle, upper fin position
- Three outputs of interest. Side force (CYA), rolling moment (CLA), yawing moment (CNA)
- Joint ONERA, DLR, USAF exercise. AIAA paper 2017-1197



# FG5 generic missile – 3 uncertain parameters

## Flow conditions. Uncertain parameters

- Nominal flow conditions $M = 0.8 \quad \alpha = 12^o \quad ReD = 0.6\ 10^6$
- Output of interest : rolling moment, yawing moment, side force
- Uncertain parameters
  - Angle of attack in $[10^o, 14^o]$

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

  - Change in upper fin azimutal position in $[-1^o, 1^o]$

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

  - Upper fin angle in $[-1^o, 1^o]$

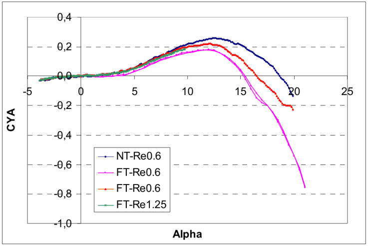
$$D^{s3}(\xi) = \frac{35}{32}(1 - \xi^2)^3$$

- Joint probability of the three uncertain parameters

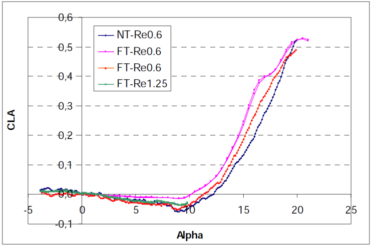
$$D(d\alpha', d\phi, \xi) = D^{s2}(d\alpha')D^{s3}(d\phi)D^{s3}(\xi) = \frac{15}{16}\frac{35^2}{32^2}(1-d\alpha'^2)^2(1-d\phi^2)^3(1-\xi^2)^3$$

# FG5 generic missile – 3 uncertain parameters

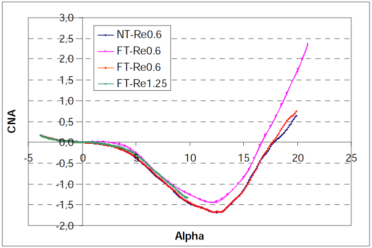
## Outputs of interest as function AoA




Side Force



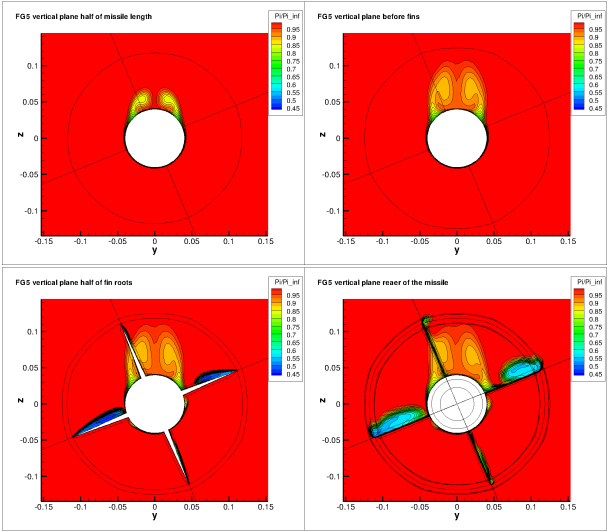

Rolling moment




yawing moment

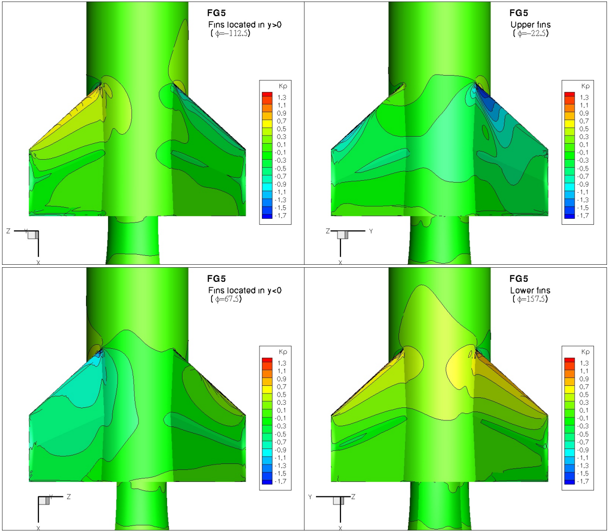
# FG5 generic missile – 3 uncertain parameters

## Nominal flow (1/2)



# FG5 generic missile – 3 uncertain parameters

## Nominal flow (2/2)



# FG5 generic missile – 3 uncertain parameters

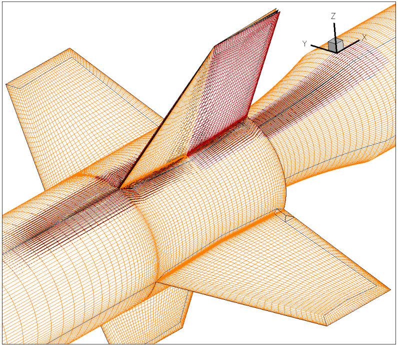
- Comparison of nominal flows
  - DLR Calculations with TAU, USAF caclulations with AVUS, ONERA calculations with elsA
  - Comparison of $Kp$ on the fins and rear part of the missile, comparison of stagnation pressure in vertical planes
  - The three flow solutions match well. Good starting point for (UQ) study

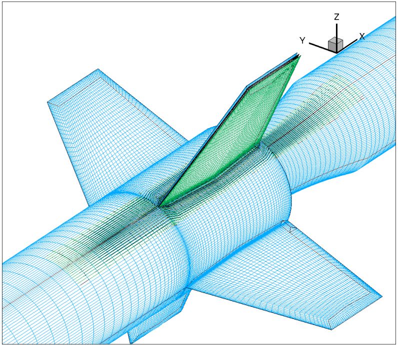
- Individual variation of outputs w.r.t. parameters
  - CYA, CLA, CNA non linear as function of $\alpha$ as in the experiment
  - CYA, CLA, CNA linear as function of fin angle
  - CYA, CLA, CNA linear as function of fin position

# 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 correctely 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, 32,88, 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 $D^{s2}(d\alpha')$, $D^{s3}(d\phi)$ and $D^{s3}(\xi)$
    - 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 $\rightarrow$ 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, α=12° 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, α=12° 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

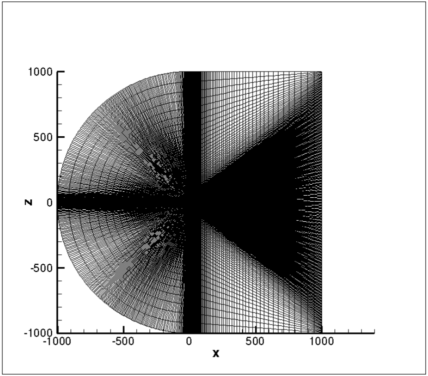
- RAE2822.
- RAE experiments.
- Case 6. Flow conditions $\underline{M}_\infty = 0.725$, $\underline{\alpha} = 2.92^o$, $Re = 6.50 \cdot 10^6$
- RANS calculations. Outputs of interest $C_D$, $C_L$, $C_M$
- Uncertainties on free-stream Mach number $\underline{M}_\infty$, angle of attack $\underline{\alpha}$, thickness to chord ratio $\underline{r} = h/c$
- AIAA Paper 2016-433 E. Savin et al.

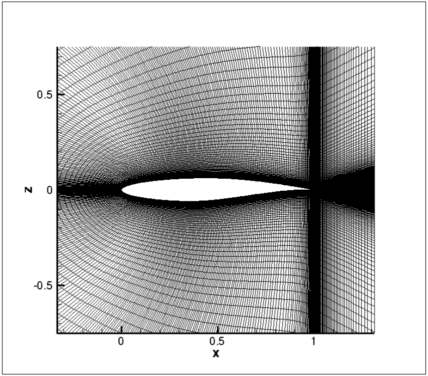
| | $a = b$ | $X_m$ | $X_M$ |
|---|---|---|---|
| $\xi_1$ | 4 | $0.97 \times \underline{r}$ | $1.03 \times \underline{r}$ |
| $\xi_2$ | 4 | $0.95 \times \underline{M}_\infty$ | $1.05 \times \underline{M}_\infty$ |
| $\xi_3$ | 4 | $0.98 \times \underline{\alpha}$ | $1.02 \times \underline{\alpha}$ |

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

# RAE2822 – 3 uncertain parameters

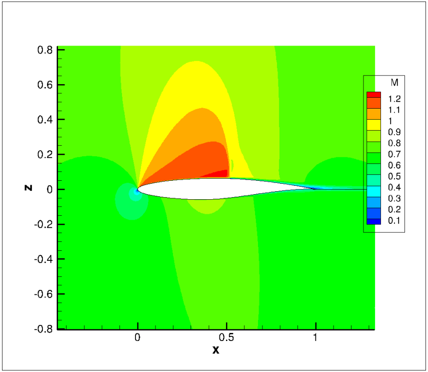
## Mesh

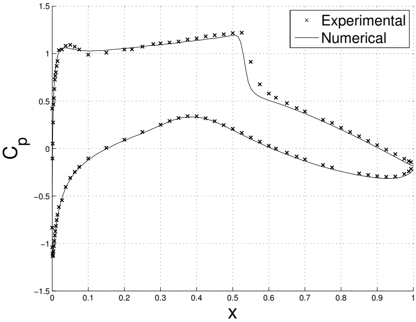


# RAE2822 – 3 uncertain parameters

## Mesh



# RAE2822 – 3 uncertain parameters

## gPC expansion of outputs of interest

- gPC expansion. Normalized 1D Jacobi-polynomials $\psi$ orthornormal for

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

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

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

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

# RAE2822 – 3 uncertain parameters

## Visualization of quadrature points

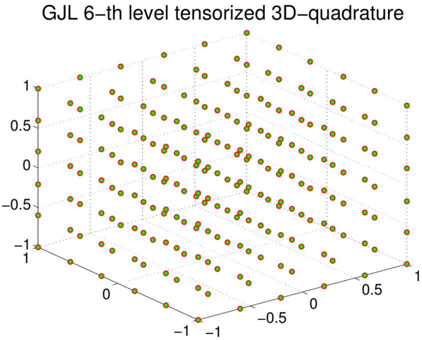



Figure: Visualization of 6-point tensorial Gauss-Jacobi-Lobatto quadrature and 7th level Smolyak quadrature based on Gauss-Jacobi-Lobatto quadratures – gPC coefficients are calculated with 10-point tensorial GJL and 7th level Smolyak quadrature based on GJL

# RAE2822 – 3 uncertain parameters

## gPC expansion of outputs of interest

- Calculation of the GPC coefficients as (for $c_D$)

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

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

| | $\mu$ | $\sigma$ |
|---|---|---|
| $C_D$ | 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)

| | $\mu$ | $\sigma$ |
|---|---|---|
| $C_D$ | 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 $\xi$.

$$\sum_{|\mathbf{j}|_1 \leq t} C_{\mathbf{j}} P_{\mathbf{j}}(\xi_k) = F(\xi_k) \quad \forall\ k\ \in \{1...q\}$$

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

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

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

# RAE2822 – 3 uncertain parameters

## gPC compressed sensing (2/4)

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

$$F(\xi_k) = \sum_{|\mathbf{j}|_1 \leq t} C_{\mathbf{j}} P_{\mathbf{j}}(\xi_k) \quad \forall\ k\ \in \{1...q\}$$

or in matrix notation

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

**K** has $q$ lines (number of evaluations) and $Z$ columns (number of polynomials in the basis)

- May be solved with less information (evaluations) than unkowns (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 verfied 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 $\xi$.

$$F(\xi_k) = \sum_{|\mathbf{j}|_1 \leq t} C_{\mathbf{j}} P_{\mathbf{j}}(\xi_k) \quad \forall\ k\ \in \{1...q\}$$

- In matrix notation

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

- The underdetermined problem is then solved by $L_1$ minimization

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

# RAE2822 – 3 uncertain parameters

## gPC compressed sensing (4/4)

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

| | $\mu$ | $\sigma$ |
|---|---|---|
| $C_D$ | 133.33e-04 | 34.052e-04 |
| $C_L$ | 72.271e-02 | 1.6703e-02 |
| $C_M$ | -453.95e-04 | 32.180e-04 |

# Outline

# 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