Un cadre mathématique pour la certification robuste sous incertitudes

(D'après Owhadi-Scovel-Sullivan-McKerns-Ortiz-Lucas ...)

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Uncertainty quantification vs. robust certification

- FP7 UMRIDA (2013-2016, PI C. Hirsch) :
  1. "Address major research challenges in both UQ and RDM to develop new methods able to **handle large numbers of simultaneous uncertainties** [...];"
  2. "Apply the UQ and RDM methods to representative industrial configurations. [...] A new generation of database, formed by industrial challenges, provided by the industrial partners, **with prescribed uncertainties**, is established."
- Optimization in terms of a **mean**, **nominal**, or **extreme** performance ("hero calculation").
- But the **probability** of deviating from that nominal performance may be non negligible!

Concentration-of-measure

- A real function $\boldsymbol{X} \mapsto F(\boldsymbol{X})$ oscillating about its mean $\mathbb{E}\{F\}$ without *a priori* knowledge of the PDFs of the random variables $\boldsymbol{X} = (X_1, \ldots X_d)^{\mathsf{T}} : \Omega \to \chi = \chi_1 \times \cdots \times \chi_d$.
- Assuming that the latter are independent, the following McDiarmid's inequality holds for all $\varepsilon > 0$:

$$P\left[|F(\boldsymbol{X}) - \mathbb{E}\{F(\boldsymbol{X})\}| \geq \varepsilon\right] \leq \exp\left(-2\frac{\varepsilon^2}{D_F^2}\right),$$

where $D_F = (\sum_{j=1}^{d} \mathrm{Osc}_j(F)^2)^{\frac{1}{2}}$ is the verification diameter of the function F, and for $1 \leq j \leq d$:

$$\mathrm{Osc}_j(F) = \sup_{\boldsymbol{x}\in\chi} \sup_{x_j'\in\chi_j} |F(x_1, \ldots x_{j-1}, x_j, x_{j+1}, \ldots x_d) - F(x_1, \ldots x_{j-1}, x_j', x_{j+1}, \ldots x_d)|.$$

S. Boucheron, G. Lugosi, P. Massart. *Concentration Inequalities*. Oxford University Press, Oxford (2013)
M. Ledoux. *The Concentration-of-Measure Phenomenon*. American Mathematical Society, Providence RI (2001)
https://terrytao.wordpress.com/2010/01/03/254a-notes-1-concentration-of-measure/

Examples

- Let $F(\boldsymbol{X}) = \frac{1}{d}\sum_{j=1}^{d} X_j$ and $\chi_j = [a_j, b_j]$. Then $\mathrm{Osc}_j(F) = \frac{1}{d}(b_j - a_j)$, and the following Hoeffding's inequality holds for all $\varepsilon > 0$:

$$P\left[|F(\boldsymbol{X}) - \mathbb{E}\{F(\boldsymbol{X})\}| \geq \varepsilon\right] \leq \exp\left(\frac{-2\varepsilon^2 d^2}{\sum_{j=1}^{d}(b_j - a_j)^2}\right) .$$

  Thus if $b_j - a_j = \Delta$ for all random inputs, one has:

$$P\left[|F(\boldsymbol{X}) - \mathbb{E}\{F(\boldsymbol{X})\}| \geq \varepsilon\right] \leq \exp\left(-2d\,\frac{\varepsilon^2}{\Delta^2}\right) ;$$

  the higher d is, the less $F(\boldsymbol{X})$ deviates from its mean $\mathbb{E}\{F(\boldsymbol{X})\}$.

- Markov's inequality for a non-negative r.v. X s.t. $\mathbb{E}\{X\} < +\infty$:

$$P\left[X \geq \varepsilon\right] \leq \frac{\mathbb{E}\{X\}}{\varepsilon} .$$

- Chebyshev's inequality for $x \mapsto F(x)$ monotonous, non-decreasing:

$$P\left[X \geq \varepsilon\right] \leq \frac{\mathbb{E}\{F(X)\}}{F(\varepsilon)} .$$

Application to certification

- **Performance measure**: assume $\boldsymbol{X} \mapsto F(\boldsymbol{X})$ is a performance measure of the system under consideration, such as a limit stress in structural design for which $\boldsymbol{X}$ are d varying geometrical parameters, physical parameters, operational conditions, numerical error sources, *etc.*
- Performance is formulated as the constraint $\{F(\boldsymbol{X}) \leq a\}$, where a: target threshold for the operation of the system.
- Then McDiarmid's inequality yields:

$$P\left[F(\boldsymbol{X}) \geq a\right] \leq \exp\left(-2\frac{(a - \mathbb{E}\{F(\boldsymbol{X})\})_+^2}{D_F^2}\right),$$

  where $x_+ := \max(0, x)$ (this cutting stems from the fact that if the mean performance is $\mathbb{E}\{F(\boldsymbol{X})\} \geq a$ then very little chance remains to certify the system).
- **Quantification of margins and uncertainties**: $(a - \mathbb{E}\{F(\boldsymbol{X})\})_+$ is the margin M, D_F is the uncertainty measure U, and $\delta = \frac{M}{U}$ is the confidence factor; therefore $P[F(\boldsymbol{X}) \geq a] \leq \varepsilon$ provided that the confidence factor $\delta > \sqrt{-\ln\sqrt{\varepsilon}}$.

L.J. Lucas, H. Owhadi, M. Ortiz. *Comput. Methods Appl. Mech. Engrg.* 197(51-52), 4591-4609 (2008)

Application to certification

- **Performance measures**: the analysis extends to multiple performance measures, formulated as *e.g.* the constraints $\{F_1(\boldsymbol{X}) \leq a_1\} \cap \{F_2(\boldsymbol{X}) \geq a_2\}$.
- Then McDiarmid's inequality yields:

$$P\left[\{F_1(\boldsymbol{X}) \geq a_1\} \cap \{F_2(\boldsymbol{X}) \leq a_2\}\right] \\ \leq \exp\left(-2\frac{(a_1 - \mathbb{E}\{F_1(\boldsymbol{X})\})_+^2}{D_1^2}\right) + \exp\left(-2\frac{(\mathbb{E}\{F_2(\boldsymbol{X})\} - a_2)_+^2}{D_2^2}\right).$$

L.J. Lucas, H. Owhadi, M. Ortiz. *Comput. Methods Appl. Mech. Engrg.* 197(51-52), 4591-4609 (2008)

Model-based certification

- The goal is to achieve rigorous certification with a maximum use of modeling and simulation and a minimum use of testing.
- Assume a (low-fidelity) model $\boldsymbol{X} \mapsto G(\boldsymbol{X})$ is used to assess the (high-fidelity) system response function, or performance $\boldsymbol{X} \mapsto F(\boldsymbol{X})$.
- Applying once again McDiarmid's inequality to F yields:

$$
\begin{aligned}
P\left[F(\boldsymbol{X}) \geq a\right] &\leq \exp\left(-2\frac{(a-\mathbb{E}\{F(\boldsymbol{X})\})_+^2}{D_F^2}\right) \\
&\leq \exp\left(-2\frac{(a-\mathbb{E}\{F(\boldsymbol{X})\})_+^2}{(D_G+D_{F-G})^2}\right),
\end{aligned}
$$

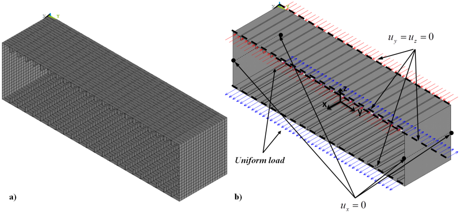
owing to the triangular inequality $D_F \leq D_G + D_{F-G}$.

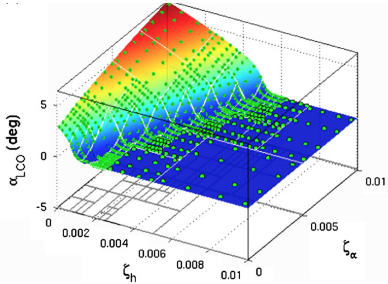
Model-based certification

- The mean performance $\mathbb{E}\{F(\boldsymbol{X})\}$ is assessed from legacy data, testing, or MDO for example;
- D_G is the predicted model diameter, *i.e.* a measure of the system uncertainty obtained by exerting the model without any testing;
- D_{F-G} is the model-error diameter, *i.e.* a quantitative measure of the model fidelity, or the discrepancy between model predictions and legacy data/experimental observations.
- One expects $D_{F-G} \ll D_F$ and $D_{F-G} \ll D_G$ for high-fidelity models, whence the number of tests required to compute D_{F-G} is minimized because (iterative) global optimization algorithms may converge rapidly.

Robust certification of aero-structural systems

- Composite structures, airfoil...
- Use of Machine Learning techniques to build a low-fidelity model $\boldsymbol{X} \mapsto G(\boldsymbol{X})$: replace a costly numerical simulation coming from fluid dynamics, structural mechanics, fluid-structure interaction... by a non-physical mathematical closed form expression (being used for fast and accurate evaluation within a design and optimization process).





$\boldsymbol{X} \mapsto F(\boldsymbol{X})$ $\qquad$ $\boldsymbol{X} \mapsto G(\boldsymbol{X})$

D. Bettebghor, N. Bartoli, S. Grihon, J. Morlier, M. Samuelides, *Struct. Multidisciplinary Optimization* 43(2), 243-259 (2011)
J.-C. Chassaing, D. Lucor, J. Trégon, *J. Sound Vib.* 331(2), 394-411 (2012)
M. Montemurro, A. Vincenti, P. Vannucci, *J. Optimization Theory Appl.* 155(1), 24-53 (2012)
É. Savin, A. Resmini, J. Peter, AIAA Paper 2016-0433 (2016)

Optimal Uncertainty Quantification

- One wants to certify $P[F(\boldsymbol{X}) \geq a] \leq \varepsilon$ BUT so far:
  1. F and P are not known exactly;
  2. One only knows $(F, P) \in \mathcal{A}$ where:

$$\mathcal{A} \subset \left\{ (f, \mu) \,\middle|\, \begin{array}{l} f : \chi \to \mathbb{R} \\ \mu \in \mathcal{P}(\chi) \end{array} \right\} .$$

- Alternatively one wants to compute optimal bounds:

$$\mathcal{U}(\mathcal{A}) = \sup_{(f,\mu)\in\mathcal{A}} \mu[f(\boldsymbol{X}) \geq a] \,,$$

$$\mathcal{L}(\mathcal{A}) = \inf_{(f,\mu)\in\mathcal{A}} \mu[f(\boldsymbol{X}) \geq a] \,,$$

such that $\mathcal{L}(\mathcal{A}) \leq P[F(\boldsymbol{X}) \geq a] \leq \mathcal{U}(\mathcal{A})$ and therefore:

- If $\mathcal{U}(\mathcal{A}) \leq \varepsilon$: the system is safe even in worst case;
- If $\mathcal{L}(\mathcal{A}) > \varepsilon$: the system is unsafe even in best case;
- If $\mathcal{L}(\mathcal{A}) \leq \varepsilon < \mathcal{U}(\mathcal{A})$: one cannot decide.

Owhadi *et al.* *SIAM Rev.* 55(2) 271 (2013)

Optimal Uncertainty Quantification

- **Reduction theorem**: let

$$\mathcal{A} = \left\{ (f,\mu) \;\middle|\; \begin{array}{c} f : \chi_1 \times \cdots \times \chi_d \to \mathbb{R} \\ \mu = \mu_1 \otimes \cdots \otimes \mu_d \\ \mathcal{C}_j(f,\mu) \leq 0\,,\; 1 \leq j \leq n_0 \\ \mathcal{C}_{j_k}(f,\mu_k) \leq 0\,,\; 1 \leq j_k \leq n_k \end{array} \right\};$$

  then $\mathcal{U}(\mathcal{A}) = \mathcal{U}(\mathcal{A}_\Delta)$ where:

$$\mathcal{A}_\Delta = \left\{ (f,\mu) \in \mathcal{A} \;\middle|\; \begin{array}{c} \mu_k = \sum_{i=0}^{n_0+n_k} \alpha_i \delta_{x_i} \\ \alpha_i \geq 0\,, \sum \alpha_i = 1 \end{array} \right\}.$$

- The solution is constructible: open-source `Mystic` optimization framework in Python, https://pypi.org/project/mystic/

Owhadi *et al.* *SIAM Rev.* 55(2) 271 (2013)

- **Example** (McDiarmid set): let

$$\mathcal{A}_{\mathrm{McD}} = \left\{ (f,\mu) \,\middle|\, \begin{array}{c} f : \chi_1 \times \cdots \times \chi_d \to \mathbb{R} \\ \mu = \mu_1 \otimes \cdots \otimes \mu_d \\ \mathbb{E}_\mu\{f(\boldsymbol{X})\} \leq 0 \\ \mathrm{Osc}_j(f) \leq D_j \,,\ 1 \leq j \leq d \end{array} \right\} ;$$

then for $d=2$ (the solution is explicit for $d=3$ as well):

$$\mathcal{U}(\mathcal{A}_{\mathrm{McD}}) = \begin{cases} 0 & \text{if } D_1 + D_2 \leq a \,, \\ \frac{(D_1+D_2-a)^2}{4D_1D_2} & \text{if } |D_1 - D_2| \leq a \leq D_1 + D_2 \,, \\ 1 - \frac{a}{\max(D_1,D_2)} & \text{if } 0 \leq a \leq |D_1 - D_2| \,, \end{cases}$$

where $\mathcal{U}(\mathcal{A}_{\mathrm{McD}}) = \sup\limits_{(f,\mu)\in\mathcal{A}} \mu[f(\boldsymbol{X}) \geq a]$.

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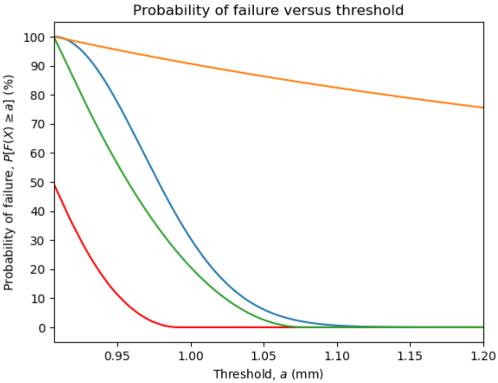
Example #1: deflection of a circular Euler-Bernoulli beam

- **Performance measure**: assume $\boldsymbol{X} \mapsto F(\boldsymbol{X})$ is the maximum deflection of the beam with $\boldsymbol{X} = (E, R)$, where E is its Young's modulus and R its radius.
- One wants to certify that the probability that the maximum deflection $F(\boldsymbol{X})$ exceeds the threshold a remains below a tolerance ε, *i.e.* $P[F(\boldsymbol{X}) \geq a] \leq \varepsilon$.



Probability of exceeding the threshold a for the deflection of a clamped beam. — Probability of failure given by Monte-Carlo method, — Optimal upper bound on the probability of failure, — Upper bound given by McDiarmid's inequality, — Upper bound given by Markov's inequality.

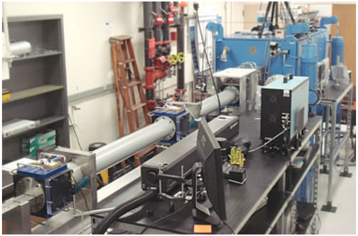
Example #2: hypervelocity impact

- **Performance measure**: assume $\boldsymbol{X} \mapsto F(\boldsymbol{X})$ is the perforation area (in mm^2) of a 440C steel plate with $\boldsymbol{X} = (h, \theta, v)$, where h is its thickness (in mm), v is the speed of the 440C steel ball of diameter $D_\mathrm{b} = 1.778$ mm, and θ is the obliquity vs. the plate normal:

$$F(h,\theta,v) = K\left(\frac{h}{D_\mathrm{b}}\right)^p (\cos\theta)^u \max\left(0, \tanh\left(\frac{v}{v_\mathrm{bl}} - 1\right)\right)^m, \quad v_\mathrm{bl} = H_0\left(\frac{h}{(\cos\theta)^n}\right)^s.$$

- v_bl is the ballistic limit velocity below which no perforation area occurs, and by least-squares fitting vs. 56 experimental data points:

$$H_0 = 0.5794\,\mathrm{km/s}, \quad s = 1.4004, \quad n = 0.4482, \quad K = 10.3936\,\mathrm{mm}^2,$$
$$p = 0.4757, \quad u = 1.0275, \quad m = 0.4682.$$



Caltech PSAAP Experimental Science Group, SPHIR (Small Paritcle Hypervelocity Impact Range) facility

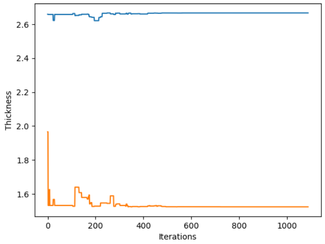
Example #2: hypervelocity impact

- **First admissible set**: F is known, $\boldsymbol{X} = (X_1, X_2, X_3) = (h, \theta, v)$ are independent random variables, and the mean perforation area lies in a prescribed range:

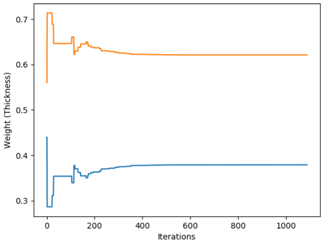
$$\mathcal{A}_F = \left\{ (F, \mu) \left| \begin{array}{c} F : \chi_1 \times \chi_2 \times \chi_3 \to \mathbb{R} \\ \mu = \mu_1 \otimes \mu_2 \otimes \mu_3 \\ \underline{F} \leq \mathbb{E}_\mu\{F(\boldsymbol{X})\} \leq \overline{F} \end{array} \right. \right\} .$$

- Then by the reduction theorem, $\mathcal{U}(\mathcal{A}_F) = \mathcal{U}(\mathcal{A}_\Delta)$ where:

$$\mathcal{A}_\Delta = \left\{ (F, \mu) \left| \begin{array}{c} \mu_j = \alpha_j \delta_{x_j} + (1 - \alpha_j)\delta_{y_j} \,,\; j = 1, 2, 3 \\ \alpha_j \geq 0 \,, x_j, y_j \in \chi_j \end{array} \right. \right\} .$$



Convergence for thickness x_1, y_1



Convergence for thickness weight α_1

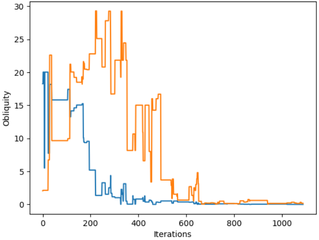
Example #2: hypervelocity impact

- **First admissible set**: F is known, $\boldsymbol{X} = (X_1, X_2, X_3) = (h, \theta, v)$ are independent random variables, and the mean perforation area lies in a prescribed range:

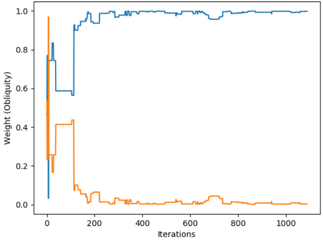
$$\mathcal{A}_F = \left\{ (F, \mu) \middle| \begin{array}{c} F : \chi_1 \times \chi_2 \times \chi_3 \to \mathbb{R} \\ \mu = \mu_1 \otimes \mu_2 \otimes \mu_3 \\ \underline{F} \leq \mathbb{E}_\mu\{F(\boldsymbol{X})\} \leq \overline{F} \end{array} \right\} .$$

- Then by the reduction theorem, $\mathcal{U}(\mathcal{A}_F) = \mathcal{U}(\mathcal{A}_\Delta)$ where:

$$\mathcal{A}_\Delta = \left\{ (F, \mu) \middle| \begin{array}{c} \mu_j = \alpha_j \delta_{x_j} + (1 - \alpha_j)\delta_{y_j} \, , \; j = 1, 2, 3 \\ \alpha_j \geq 0 \, , x_j, y_j \in \chi_j \end{array} \right\} .$$



Convergence for obliquity x_2, y_2



Convergence for obliquity weight α_2

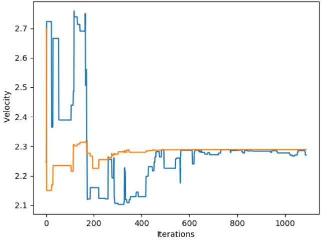
Example #2: hypervelocity impact

- **First admissible set**: F is known, $\boldsymbol{X} = (X_1, X_2, X_3) = (h, \theta, v)$ are independent random variables, and the mean perforation area lies in a prescribed range:

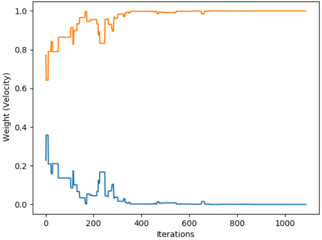
$$\mathcal{A}_F = \left\{ (F, \mu) \;\middle|\; \begin{array}{c} F : \chi_1 \times \chi_2 \times \chi_3 \to \mathbb{R} \\ \mu = \mu_1 \otimes \mu_2 \otimes \mu_3 \\ \underline{F} \leq \mathbb{E}_\mu\{F(\boldsymbol{X})\} \leq \overline{F} \end{array} \right\}.$$

- Then by the reduction theorem, $\mathcal{U}(\mathcal{A}_F) = \mathcal{U}(\mathcal{A}_\Delta)$ where:

$$\mathcal{A}_\Delta = \left\{ (F, \mu) \;\middle|\; \begin{array}{c} \mu_j = \alpha_j \delta_{x_j} + (1 - \alpha_j)\delta_{y_j} \,,\; j = 1, 2, 3 \\ \alpha_j \geq 0 \,, x_j, y_j \in \chi_j \end{array} \right\}.$$

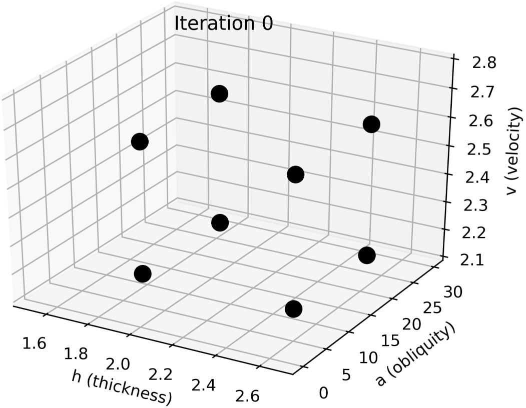


Convergence for velocity x_3, y_3



Convergence for velocity weight α_3

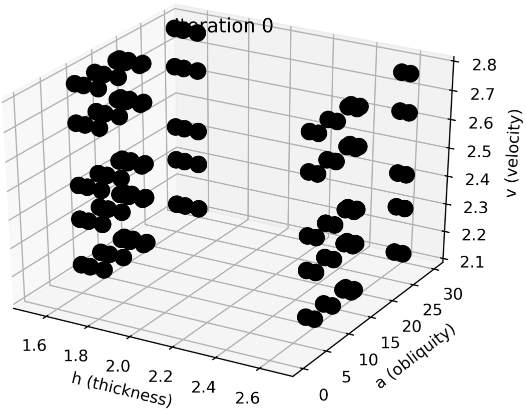
Example #2: hypervelocity impact



Evolution of the support of the reduced probability measure for $\#\mathrm{sup}\mu_j \leq 2$, $j = 1, 2, 3$.

M. McKerns *et al.* arXiv:1202.1055 **(2010)**
Owhadi *et al.* *SIAM Rev.* 55(2) 271 (2013)

Example #2: hypervelocity impact



Evolution of the support of the reduced probability measure for $\#\mathrm{supp}\mu_j \leq 5$, $j = 1, 2, 3$.

M. McKerns *et al.* arXiv:1202.1055 **(2010)**
Owhadi *et al.* *SIAM Rev.* 55(2) 271 (2013)

Example #2: hypervelocity impact

- **Second admissible set**: F is unknown, $\boldsymbol{X} = (X_1, X_2, X_3) = (h, \theta, v)$ are independent random variables, and the mean perforation area and its componentwise oscillations lie in prescribed ranges:

$$\mathcal{A}_{\mathrm{McD}} = \left\{ (f,\mu) \,\middle|\, \begin{array}{c} \mu = \mu_1 \otimes \mu_2 \otimes \mu_3 \\ \underline{F} \leq \mathbb{E}_\mu\{f(\boldsymbol{X})\} \leq \overline{F} \\ \mathrm{Osc}_j(f) \leq \mathrm{Osc}_j(F)\,,\ j = 1,2,3 \end{array} \right\}.$$

- Then by the reduction theorem for $d = 3$ one obtains the optimal upper bound on the probability of non perforation:

$$\begin{aligned} P[F=0] \leq \exp\left(-\frac{2\underline{F}^2}{\sum_{j=1}^3 \mathrm{Osc}_j(F)^2}\right) &= 66.4\% && \text{McDiarmid}\,, \\ P[F=0] \leq \mathcal{U}(\mathcal{A}_{\mathrm{McD}}) &= 43.7\% && \text{scenario \#2}\,, \\ P[F=0] \leq \mathcal{U}(\mathcal{A}_F) &= 37.9\% && \text{scenario \#1}\,, \end{aligned}$$

for $5.5\,\mathrm{mm}^2 \leq \mathbb{E}_\mu\{f(\boldsymbol{X})\} \leq 7.5\,\mathrm{mm}^2$ and:

$$\begin{array}{lll} h: & \chi_1 = [1.524, 2.667]\,\mathrm{mm} & \mathrm{Osc}_1(F) = 8.9\,\mathrm{mm}^2\,, \\ \theta: & \chi_2 = [0, \frac{\pi}{6}] & \mathrm{Osc}_2(F) = 4.2\,\mathrm{mm}^2\,, \\ v: & \chi_3 = [2.1, 2.8]\,\mathrm{km/s} & \mathrm{Osc}_3(F) = 7.2\,\mathrm{mm}^2\,. \end{array}$$

Example #3: RAE2822 (case #1: $\underline{M} = 0.676$, $\underline{\alpha} = 2.4^\circ$, Re $= 5.7\,10^6$)

- **Performance measure**: assume $\boldsymbol{X} \mapsto F(\boldsymbol{X})$ is the lift-to-drag ratio of an RAE2822 profile with $\boldsymbol{X} = (M, \alpha, r)$, where M is the Mach number, α is the angle of attack, and r is a geometrical parameter (thickness-to-chord ratio).
- **Admissible set**: F is computed using `MISES`, $\boldsymbol{X} = (X_1, X_2, X_3)$ are independent random variables, and the mean performance and its componentwise oscillations are prescribed:

$$\mathcal{A}_{\mathrm{McD}} = \left\{ (f, \mu) \,\middle|\, \begin{array}{c} \mu = \mu_1 \otimes \mu_2 \otimes \mu_3 \\ \mathbb{E}_\mu\{f(\boldsymbol{X})\} = \underline{F} \\ \mathrm{Osc}_j(f) \leq \mathrm{Osc}_j(F)\,,\ j = 1, 2, 3 \end{array} \right\} .$$

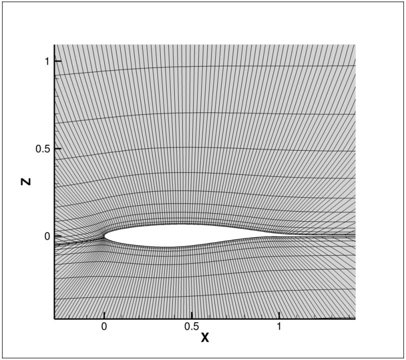
- Then by the reduction theorem for $d = 3$ one obtains the optimal upper bound on the probability of exceeding the threshold a given the nominal value $\underline{F} = 62.8$:

$$P\left[|F(\boldsymbol{X}) - \underline{F}| \geq a\right] \leq \mathcal{U}(\mathcal{A}_{\mathrm{McD}}) \leq \exp\left(- \frac{2a^2}{\sum_{j=1}^3 \mathrm{Osc}_j(F)^2} \right) ,$$

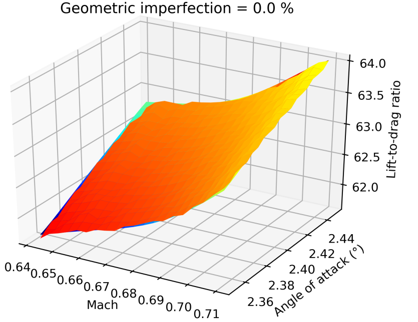
where:

$$\begin{array}{lll} M : & \chi_1 = [\underline{M} \pm 5\%] & \mathrm{Osc}_1(F) = 1.8\,, \\ \alpha : & \chi_2 = [\underline{\alpha} \pm 2\%] & \mathrm{Osc}_2(F) = 1.1\,, \\ r : & \chi_3 = [\underline{r} \pm 5\%] & \mathrm{Osc}_3(F) = 2.6\,. \end{array}$$

Example #3: RAE2822 (case #1: $\underline{M} = 0.676$, $\underline{\alpha} = 2.4^\circ$, $\mathrm{Re} = 5.7\,10^6$)



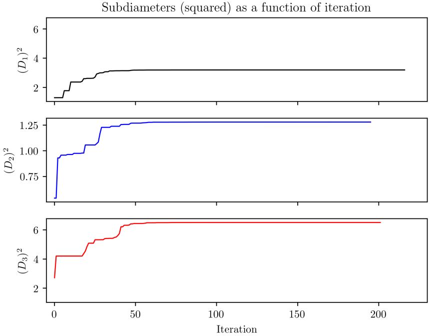
Mesh for LES computation.



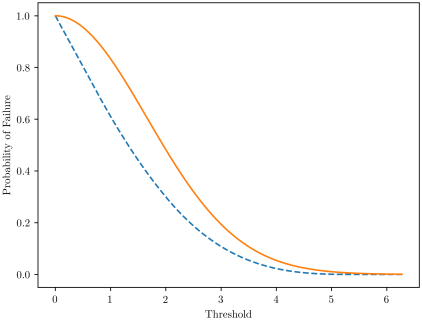
5–th order polynomial surrogate of $\boldsymbol{X} \mapsto F(\boldsymbol{X})$ and `MISES` computations.

M. B. Giles, M. Drela, *AIAA J.* 25(9) 1199 (1987)

Example #3: RAE2822 (case #1: $\underline{M} = 0.676$, $\underline{\alpha} = 2.4^\circ$, $\mathrm{Re} = 5.7\,10^6$)



Subdiameters $\mathrm{Osc}_j(F)$, $j = 1, 2, 3$.



Probability of exceeding the threshold a for the lift-to-drag ratio. ----- Optimal upper bound on the probability of failure, —— Upper bound given by McDiarmid's inequality.

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THANK YOU FOR YOUR ATTENTION! QUESTIONS?