



Overview of Combined Error and Uncertainty Estimates for CFD Problems¹

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¹British statistician George Box: *"All models are wrong but some are useful."*



CFD Vision 2030 Study



UQ and error topic findings from the *CFD Vision 2030* study by Slotnick *et al.*, 2014

- ▶ *“Errors in current CFD simulations are not well understood or well quantified, including errors due to spatial and temporal discretization, incomplete convergence, and the physical models and parameters they embody.”*
- ▶ *“Variability and uncertainty of inputs (boundary and initial conditions, parameters, etc.) to fluid dynamic problems are largely unquantified.”*
- ▶ *“Even if estimates are available and/or assumed, the propagation of these uncertainties poses a significant challenge due to the inherent cost, the lack of automation and robustness of the solution process, and the poor utilization of high performance computing.”*
- ▶ *“... the aerospace community, in particular, have had minimal investments to address these issues.”*



Introduction



- ▶ CFD codes often utilize finite-dimensional approximation (grids, basis functions, etc) thus incurring **CFD numerical errors**.
- ▶ Uncertainty propagation methods calculate uncertainty statistics for output quantities of interest using a numerical method (e.g. quadrature, kernel convolution, etc.) thus incurring **UQ numerical errors**.
- ▶ Given input sources of uncertainty, non-intrusive uncertainty propagation methods quantify the uncertainty in output quantities of interest by performing a finite number CFD realizations needed in the calculation of output statistics.

Unfortunately, the numerical errors associated with CFD realizations and statistics evaluation are generally not additive and the impact of this error on calculated output statistics is often non-intuitive.



Combined Uncertainty and Error Bounds



NASA T^3 project funded articles

- ▶ Barth, T.J., “Non-Intrusive Uncertainty Propagation with Error Bounds for Conservation Laws Containing Discontinuities”, **LCSE**, Vol. 92, 2013.
- ▶ Barth, T.J., *An Overview of Combined Uncertainty and A Posteriori Error Bound Estimates for CFD Calculations*, AIAA-2016-1062, 2016, (SciTech best paper in fluid dynamics).
- ▶ Barth, T.J., *On the Calculation of Moment Statistics with Error Bounds for CFD Calculations Containing Random Parameters and Fields*, **A Guide to Uncertainty Quantification and V&V**, Mehta *et al.* (Eds), Joint NASA/JANNAF TP-2016-219422, 2017.



A Combined Uncertainty and Error Bound Analysis Framework



For this analysis framework, we demand that

1. if the problem has no uncertainty, standard *a posteriori* error bound estimates for CFD realization error are obtained,
2. if the problem has no CFD realization error, standard uncertainty estimates are obtained,
3. if the problem has both CFD realization error and uncertainty, uncertainty estimates with error bound estimates are obtained.



A Combined Error and Uncertainty Framework



We also posit that a framework for combined uncertainty and error should answer the following questions:

1. How accurate is a computed output statistic?
2. How does the numerical error present in CFD realizations affect the accuracy of a computed output statistic?
3. How does numerical error incurred in evaluating statistics affect the accuracy of a computed output statistic?
4. To improve the accuracy of a computed statistic, should additional resources be devoted towards solving CFD realizations more accurately (e.g. finer mesh) or towards evaluating the statistics more accurately (e.g. more CFD realization evaluations)? Provide the computational tools for optimizing the selection of target realization errors and statistics errors (separate work).



Example Statistics



Expectation (mean), $E[\cdot]$

$$E[f] = \int f(x) p(x) dx$$

Variance (σ^2), $V[\cdot]$:

$$V[f] = \sigma^2[f] = \int (f(x) - E[f])^2 p(x) dx$$

Probability density function, p_f

$$Pr[a \leq f \leq b] = \int_a^b p_f(x) dx$$

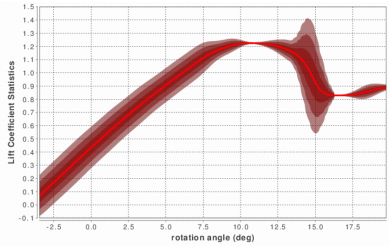
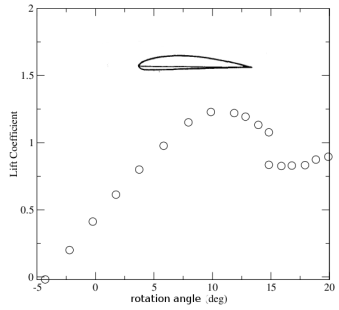
- ▶ Moment statistics such as expectation and variance are estimated using *numerical quadrature*.
- ▶ Probability density functions are estimated using a discrete kernel convolution. Histograms often not good enough.



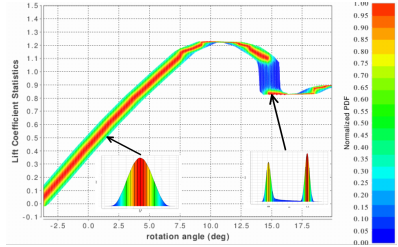
What Statistics Do Engineers Want or Need?



- ▶ Lowspeed NACA 4412 airfoil
- ▶ Uncertain angle-of-attack
- ▶ Angle of Attack
= Gaussian_{3σ}(0°, .5°)
- ▶ Airfoil rotated from -3° to 20°
- ▶ HYGAP uncertainty propagation.



Lift Curve Moment Statistics
(bands denote 1,2,3 std dev)



Lift Curve Normalized PDF
Statistics

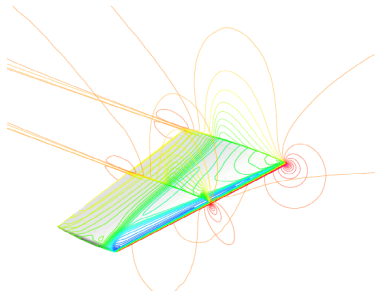


Preview Example: Uncertainty Calculation with Error Bounds

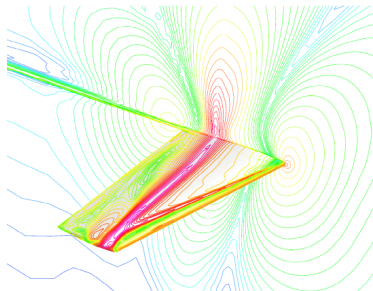


ONERA M6 wing calculation

- ▶ Compressible Navier-Stokes CFD calculation,
- ▶ Spalart-Allmaras turbulence model, Reynolds number 11.7×10^6 ,
- ▶ Inflow Mach number, $M_\infty = \text{Gaussian}_{3\sigma}(m = .84, \sigma = .012)$,
- ▶ Angle of Attack, $AOA = \text{Gaussian}_{3\sigma}(m = 3.06, \sigma = .075)$,
- ▶ Approximately 5 million mesh points.



expectation(density)



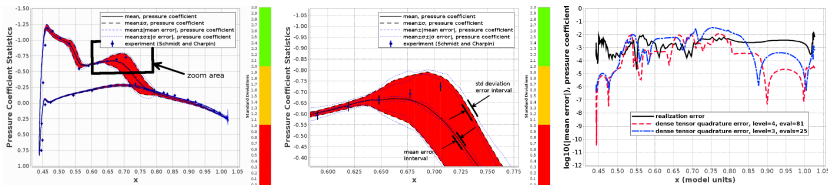
$\log_{10} \text{variance}(\text{density})$



Preview Example: Uncertainty Calculation with Error Bounds

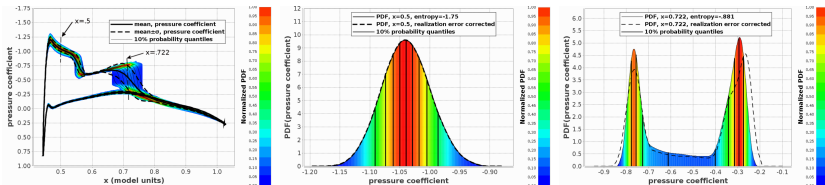


ONERA M6 wing surface pressure coefficient moment statistics at 65% wing span location.



Surface Pressure Statistics Closeup error bound intervals Error bound estimates

ONERA M6 wing surface pressure coefficient PDF statistics at 65% wing span location.



Surface Pressure Statistics PDF distribution, $x = .532$ PDF distribution, $x = .718$

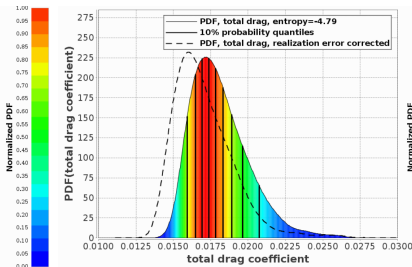
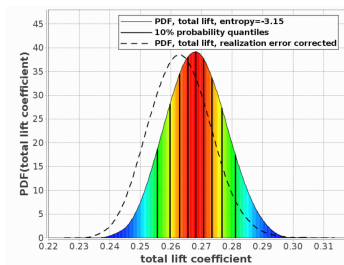




Preview Example: Uncertainty Calculation with Error Bounds



ONERA M6 Wing Lift and Drag PDF Statistics:





Output Quantities of Interests (QOI)



Let $\alpha \in \mathbf{R}^N$ denote a vector of N uncertain parameters, $u_h(x, t; \alpha)$ a numerical realization, and $u(x, t; \alpha)$ the exact infinite-dimensional counterpart.

Let $J(u_h; \alpha) \equiv J(u_h(x, t; \alpha); \alpha)$; denote an output quantity of interest (QOI)

- ▶ Functional such as space-time integrated forces and moments.
- ▶ Graph of derived quantities such as pressure or temperature along a space-time curve.
- ▶ Derived quantity from general space-time volume subsets.

The non-intrusive uncertainty propagation methods obtain estimates of QOI statistics and/or probability densities from M realization QOI outputs

$$\{J(u_h; \alpha^{(1)}), J(u_h; \alpha^{(2)}), \dots, J(u_h; \alpha^{(M)})\}$$



Numerical Quadrature



Let $I[f]$ denote the weighted **definite integral**

$$I[f] = \int_{\Xi} f(\xi) p(\xi) d\xi, \quad p(\xi) \geq 0$$

and $Q_M I[f]$ denote an M -point weighted **numerical quadrature**

$$Q_M I[f] = \sum_{i=1}^M w_i f(\xi_i)$$

with weights w_i with evaluation points ξ_i . Finally, define numerical **quadrature error** denoted by $R_M I[f]$, i.e.

$$R_M I[f] = I[f] - Q_M I[f].$$



Error Formulas for Moment Statistics-I



Given the QOI realization error magnitude

$$|\epsilon_h| \equiv |J(u; \alpha) - J(u_h; \alpha)|$$

and $|R_M I[\cdot]|$, we have the following bound estimates from Barth (2013):

Expectation Error Bound:

$$|E[J(u)] - Q_M E[J(u_h)]| \leq |Q_M E[|\epsilon_h|]| + |R_M E[|\epsilon_h|]| + |R_M E[J(u_h)]|$$

Variance Error Bound:

$$\begin{aligned} |V[J(u)] - Q_M V[J(u_h)]| &\leq 2 \left((|Q_M E[|\epsilon_h|^2]| + |R_M E[|\epsilon_h|^2]|) \right. \\ &\quad \left. \times (|Q_M V[J(u_h)]| + |R_M V[J(u_h)]|) \right)^{\frac{1}{2}} \\ &\quad + |Q_M E[|\epsilon_h|^2]| + |R_M E[|\epsilon_h|^2]| + |R_M V[J(u_h)]| \end{aligned}$$

- ▶ Red and magenta terms can be made smaller by decreasing realization error $\downarrow \epsilon_h$.
- ▶ Blue and magenta terms can be made smaller by decreasing quadrature error $\uparrow M$.



Error Formulas for Moment Statistics-II



When the *signed* QOI realization error

$$\epsilon_h \equiv J(u; \alpha) - J(u_h; \alpha)$$

and signed quadrature error $R_M[\cdot]$ are available, we have a much sharper estimate. Let $\tilde{J} \equiv J_h + \tilde{\epsilon}_h$

Expectation error estimate:

$$E[J] - Q_M E[J_h] \approx Q_M E[\tilde{J}] + R_M E[\tilde{J}] - Q_M E[J_h]$$

Variance error estimate:

$$V[J] - Q_M V[J_h] \approx Q_M E[\tilde{J}^2] + R_M E[\tilde{J}^2] - (Q_M E[\tilde{J}] + R_M E[\tilde{J}])^2 - (Q_M E[J_h^2] - Q_M^2 E[J_h])$$

- ▶ **Red** terms collectively can be made smaller via mutual cancellation by decreasing realization error $\downarrow \epsilon_h$.
- ▶ **Blue** terms can be made smaller by decreasing quadrature error $\uparrow M$.



Observation: Obtaining error bound estimates for expectation and variance then reduces to the tasks of

- ▶ estimating the realization error ϵ_h or realization error magnitude $|\epsilon_h|$,
- ▶ estimating the quadrature error $R_M I[\cdot]$ or quadrature error magnitude $|R_M I[\cdot]|$.



Calculation of Moment Statistics via Multi-level Quadrature

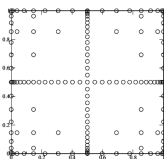


Let N denote the number of uncertainty (random variable) dimensions

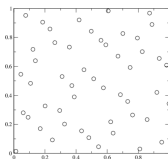
- ▶ **Multi-level dense tensorization methods** ($\#$ dimensions ≤ 4)
 - ▶ Multi-level Clenshaw-Curtis and Gauss-Patterson quadratures,
 - ▶ Hybrid Multi-level Clenshaw-Curtis and Adaptive Cubic Polynomial (HYGAP) quadrature, Barth (2011)
- ▶ **Multi-level sparse tensorization methods** ($\#$ dimensions ≤ 15)
 - ▶ Multi-level Clenshaw-Curtis and Gauss-Patterson sparse grids, Novak and Ritter (1996)
- ▶ **Multi-level sampling methods** ($\#$ dimensions large)
 - ▶ Optimal² multi-level MC sampling, Mishra and Schwab (2009)



Dense Tensor



Sparse Tensor



MC Sampling

²Subject to CFD order of accuracy constraints, $s < q(d + 1)$



Multi-level Quadrature Error Estimates



d -dimensional multi-level quadrature error estimates are of the form

- ▶ Dense tensor quadrature

$$\underbrace{R_L^{(d)}[f]}_{\text{quadrature error}} \equiv I^{(d)}[f] - Q_L^{(d)}[f] \approx \underbrace{\frac{1}{2^r - 1}}_{\text{regularity factor}} \underbrace{(Q_L^{(d)}[f] - Q_{L-1}^{(d)}[f])}_{\text{multi-level quadrature}}$$

- ▶ Sparse tensor quadrature

$$\underbrace{R_L^{(d)}[f]}_{\text{quadrature error}} \equiv I^{(d)}[f] - Q_L^{(d)}[f] \approx \underbrace{\frac{1}{\left(\frac{L-1}{L}\right)^{(d-1)(r+1)} 2^r - 1}}_{\text{regularity factor}} \underbrace{(Q_L^{(d)}[f] - Q_{L-1}^{(d)}[f])}_{\text{multi-level quadrature}}$$

- ▶ Monte Carlo quadrature given an M population of multi-level sampling evaluations

$$R_M^{(d)}[f] = \sqrt{V[f]/M}$$



Estimating QOI Realization Error



Estimate $\epsilon_h^{(i)} \equiv J(u; \alpha^{(i)}) - J(u_h; \alpha^{(i)})$ for each realization i .

- ▶ Richardson (2-level) and parameter-free Aitken (3-level) extrapolation using space-time grid hierarchies, e.g.

$$J(u; \alpha) - J(u_h; \alpha) \approx \frac{1}{2^q - 1} (J(u_h; \alpha) - J(u_{2h}; \alpha))$$

$$\text{with } 2^q = \frac{J(u_{2h}; \alpha) - J(u_{4h}; \alpha)}{J(u_h; \alpha) - J(u_{2h}; \alpha)}$$

- ▶ *A posteriori* error estimation of functionals using dual / adjoint problems, Becker and Rannacher (1996)

$$J(\mathbf{u}) - J(\mathbf{u}_h) = F(\Phi - \pi_h \Phi) - \mathcal{B}(\mathbf{u}_h, \Phi - \pi_h \Phi)$$

with $\mathcal{B}(\cdot, \cdot)$ the primal semi-linear form, $F(\cdot)$ the right-hand-side forcing, and Φ a linearized dual problem.

- ▶ Patch postprocessing techniques, Zienkiewicz-Zhu (1992), Bramble-Schatz (1998), Cockburn *et. al.* (2003), exploiting superconvergence.

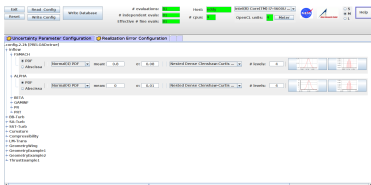


QUEST Software

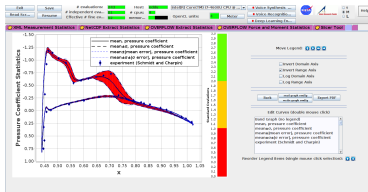


QUEST - Quantified Uncertainty with Error bound Software Toolkit

- ▶ status – beta testing with web launch in late spring



QUESTPrep preprocessor



QUESTPost postprocessor

Algorithm	# Dims	Moment Statistics	Hires PDFs	high	QOI Regularity high (piecewise)	low
CC dense tensor	small	✓	✓	✓	✗	✗
GP dense tensor	small	✓	✓	✓	✗	✗
HYGAP dense tensor	small	✓	✓	✓	✓	✗
CC sparse tensor	medium	✓	✓	✓	✗	✗
GP sparse tensor	medium	✓	✓	✓	✗	✗
M-L Sampling	large	✓	✗	✓	✓	✓*

CC - Clenshaw-Curtis, GP - Gauss-Patterson, HYGAP - Hybrid Global/Adaptive Polynomial

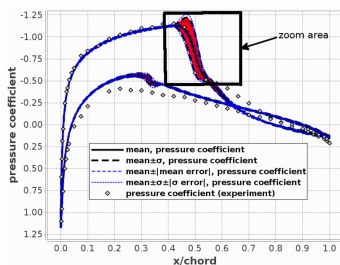


Turbulence Model Parameter Uncertainty

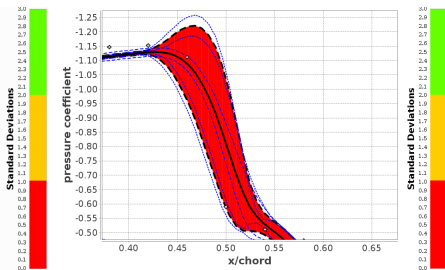


Uncertainty is imposed in 3 turbulence model parameters that are often observed to be most sensitive

- ▶ NACA 0012 airfoil, $M = 0.8$, $AOA=2.26^\circ$, $Re=9$ million,
- ▶ 513×65 mesh,
- ▶ Baldwin-Barth turbulence model with uncertainty,
- ▶ $c_\mu = \text{Uniform} [.081, .099]$,
- ▶ $c_{\epsilon_1} = \text{Uniform} [1.08, 1.32]$,
- ▶ $c_{\epsilon_2} = \text{Uniform} [1.8, 2.2]$.



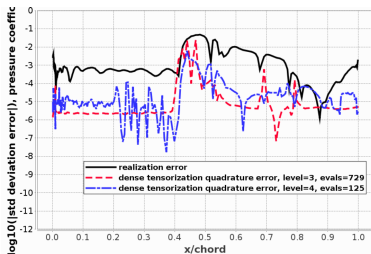
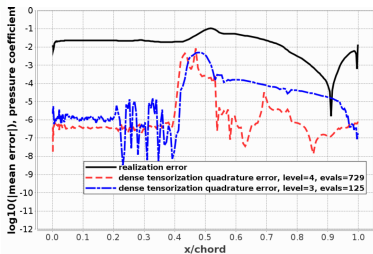
Surface pressure coefficient



Zoom closeup in shock region

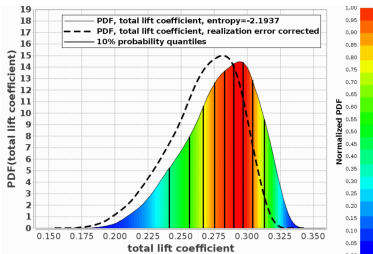


Turbulence Model Parameter Uncertainty

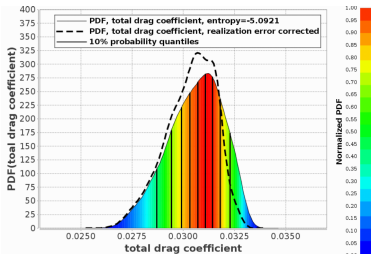


Expectation error on upper surface

Std deviation error on upper surface

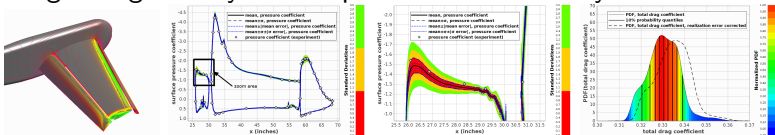


Lift probability density function

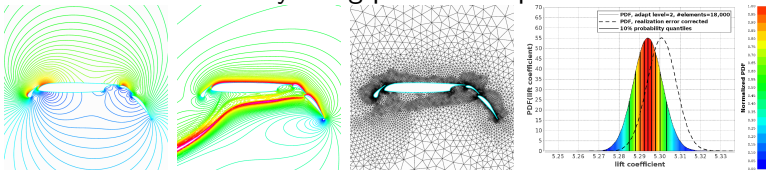


Drag probability density function

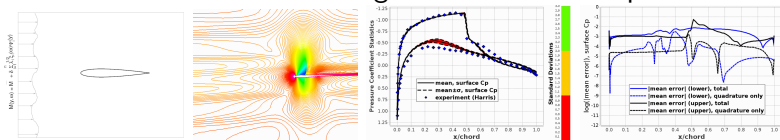
- High-lift geometry with flap and slat uncertainty



- Functional uncertainty using primal-dual problems



- Correlated random fields using Karhunen-Loeve representation





Concluding Remarks and Future Directions



Combined uncertainty and error bound estimates provide a quantitative guide when performing practical CFD calculations with uncertainty

1. quantifying the overall accuracy of computed statistics,
2. quantifying the impact of UQ numerical errors on computed statistics,
3. quantifying the impact of CFD numerical errors on computed statistics,
4. providing a systematic procedure for determining whether (and how much) additional resources, if needed, should be devoted to solving realizations more accurately (finer grids) or improving the accuracy of computed moment statistics quadratures (more parameter evaluations).

Current and future directions

1. methods for calculating high resolution PDFs with error bounds for high-dimensional problems, reduced regularity problems, inverse UQ problems, dynamical system problems,
2. dynamic adaptivity for both CFD and uncertainty statistics,
3. software beta testing
 - 3.1 Shashir Pandya (ongoing) - Normal surface flap blowing
 - 3.2 Jim Ross (initiated) - "Evaluation of CFD as a Surrogate for a Wind Tunnel at Mach 2.5-4.5"