Combined Error and Uncertainty Estimates for CFD Problems

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Non-Intrusive Uncertainty Propagation for CFD Calculations

Given input sources of uncertainty, non-intrusive uncertainty propagation methods quantify the uncertainty in output quantities of interest (QoI) by performing a finite number of CFD instance realizations needed in the calculation of output statistics. It is well known that this introduces multiple sources of error.

- CFD codes often utilize finite-dimensional approximation (grids, basis functions, etc) thus incurring **CFD numerical errors** often approximately reinterpreted as a statistical bias.
- Uncertainty propagation methods calculate uncertainty statistics for output quantities of interest using a numerical method (e.g. deterministic quadrature, sampling, etc.) thus incurring **UQ numerical errors**.

Importance of quantifying these errors in large scale scientific computing

- How accurate is an output statistic?
- How should additional computational resources be invested to further reduce the error in a statistic?

Fundamental Error Decomposition

- u infinite-dimensional aspirational "truth" solution,
- U infinite-dimension model solution,
- U_h finite-dimensional model solution,
- $J(\cdot)(x,t)$ output quantities of interest (QoI),
- $E[\cdot]$ statistics functional,
- $Q_M E[\cdot]$ M-evaluation approximated statistics functional.

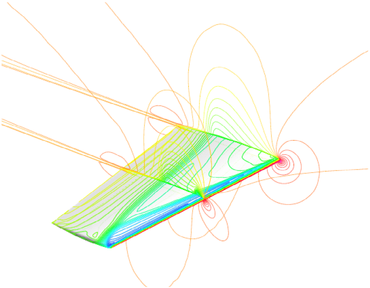
Statistics error

$$E[J(u)] - Q_M E[J(U_h)] = \underbrace{E[J(u)] - E[J(U)]}_{\text{stat model error}} + \underbrace{E[J(U)] - E[J(U_h)]}_{\text{stat CFD numerical error}} + \underbrace{E[J(U_h)] - Q_M E[J(U_h)]}_{\text{UQ numerical error}}$$

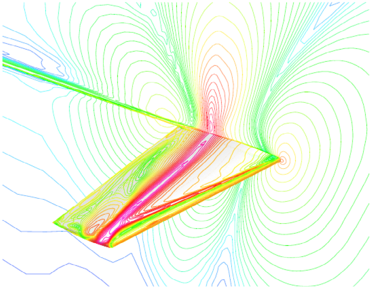
Preview Example: Uncertainty Calculation with Error Bounds - I

ONERA M6 wing calculation

- Compressible Reynolds-averaged Navier-Stokes CFD calculation,
- Spalart-Allmaras turbulence model, Reynolds number 11.7×10^6,
- $p = 1$ finite volume discretization (5 million mesh points),
- Inflow Mach number, $M_\infty \sim \mathrm{Normal}_{3\sigma}(m = .84, \sigma = .012)$,
- Angle of Attack, $AOA \sim \mathrm{Normal}_{3\sigma}(m = 3.06, \sigma = .075)$.



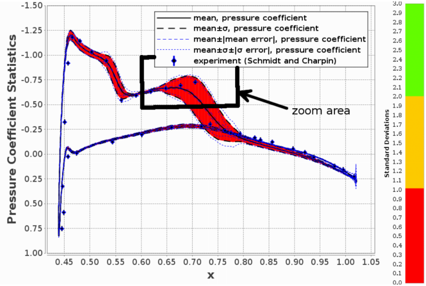
expectation(density)



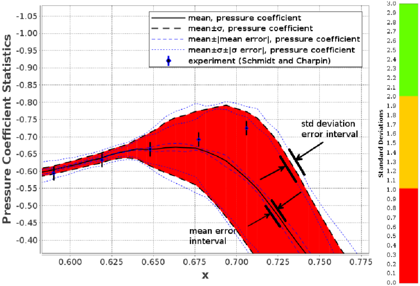
$\log_{10}$ *variance*(*density*)

Preview Example: Uncertainty Calculation with Error Bounds - II

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



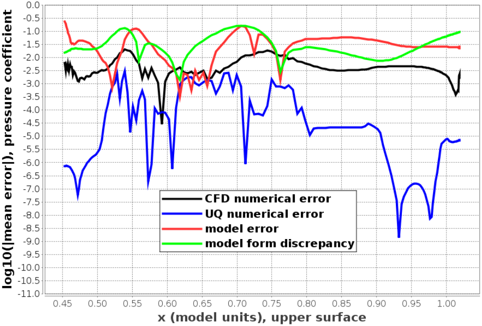
Surface Pressure Statistics



Closeup error bound intervals

Preview Example: Uncertainty Calculation with Error Bounds - III

ONERA M6 wing upper surface pressure coefficient expectation error at 65% wing span location.



$$E[J(u)] - Q_M E[J(U_h)] = \underbrace{E[J(u)] - E[J(U)]}_{\text{stat model error}} + \underbrace{E[J(U)] - E[J(U_h)]}_{\text{stat CFD numerical error}} + \underbrace{E[J(U_h)] - Q_M E[J(U_h)]}_{\text{UQ numerical error}}$$

Numerical Quadrature

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

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

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

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

with weights w_i and evaluation points $\boldsymbol{\xi}_i$ depending on $p(\boldsymbol{\xi})$. 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:

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

- Red and magenta terms can be made smaller by $\downarrow \epsilon_h$.
- Blue and magenta terms can be made smaller by $\uparrow M$.
- Issues: sharpness of variance estimate and regularity of integrands.

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 $R_M[\cdot]$ can be approximated, we have a sharp error representation. Let $\tilde{J} \equiv J_h + \tilde{\epsilon}_h$

Expectation error estimate:

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

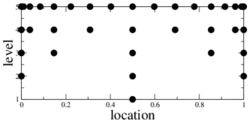
Variance error estimate:

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

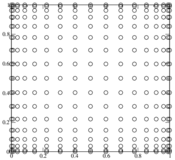
- Red terms collectively can be made smaller via mutual cancellation by decreasing realization error $\downarrow \tilde{\epsilon}_h$.
- Blue terms can be made smaller by decreasing quadrature error $\uparrow M$.

Calculation of Moment Statistics via Multi–level Quadrature

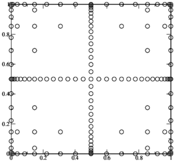
- **Multi-level dense product quadratures** (# dimensions ≤ 3)
  - Multi-level Clenshaw-Curtis and Gauss-Patterson quadratures,



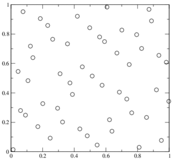
- **Multi-level sparse product quadratures** (# dimensions ≤ 12)
  - Multi-level Clenshaw-Curtis and Gauss-Patterson sparse grids, Novak and Ritter (1996)
- **Multi-level sampling methods** (# dimensions large)
  - Multi-level MC sampling, Mishra and Schwab (2009)



Dense Quadrature



Sparse Quadrature



MC Sampling

Multi–level Quadrature Error Estimates

d-dimensional *L*-level asymptotic quadrature error estimates

- Dense product quadrature

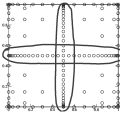
$$\underbrace{R_L^{(d)}[f]}_{quadrature\ \ error} \equiv I^{(d)}[f] - Q_L^{(d)}[f] \approx \underbrace{\frac{1}{2^r - 1}}_{regularity\ \ factor} \underbrace{\left(Q_L^{(d)}[f] - Q_{L-1}^{(d)}[f]\right)}_{multi-level\ \ quadrature}$$

$$2^r = \frac{Q_{L-1}^{(d)}[f] - Q_{L-2}^{(d)}[f]}{Q_L^{(d)}[f] - Q_{L-1}^{(d)}[f]}$$

- Sparse product quadrature, Novak and Ritter (1996)

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

$$2^r \approx \min_{i=1\ldots d} \frac{Q_{L-1}^{(1,i)}[f] - Q_{L-2}^{(1,i)}[f]}{Q_L^{(1,i)}[f] - Q_{L-1}^{(1,i)}[f]}$$



where $Q_L^{(1,i)}$ is an L-level one-dimensional quadrature in the i-th dimension.

Multi–level Monte Carlo–Finite Volume - I

Decompose the expectation (or the expectation of k-moments) as the sum of expectation increments computed on finite volume CFD mesh levels $\{0, \ldots, L\}$

$$E[U_L] = E[U_0] + \sum_{l=1}^{L} \Big(E[U_l] - E[U_{l-1}] \Big) = E[U_0] + \sum_{l=1}^{L} \Big(E[U_l - U_{l-1}] \Big)$$

Approximate the expectation at level l using M_l Monte Carlo samples

$$Q_{M_L} E[U_L] \approx Q_{M_0} E[U_0] + \sum_{l=1}^{L} Q_{M_l} E[U_l - U_{l-1}]$$

Optimize Monte Carlo sample size at each level M_l by asymptotic error balancing for an $\mathcal{O}(\Delta x^s)$ convergent FVM method (Mishra & Schwab (2009), Sukyis (2014))

$$M_l = C \, \Delta x_l^{2s} \; \Delta x_L^{-2s} = \mathcal{O}(2^{2s(L-l)})$$

- Largest # of MC samples, M_0, required for the coarsest CFD mesh,
- Smallest # of MC samples, M_L, required for the finest CFD mesh.

Computational work when $s \leq (d+1)/2$ is asymptotically the same as a single finite volume solve (modulo logarithmic factor).

Multi–level Monte Carlo–Finite Volume - II

Error estimate for multi-level MC-FVM (Mishra and Schwab (2009))

$$\|E[U(\cdot,t)] - Q_L E[U_L(\cdot,t)]\|_{L^2(\Omega,L^1(R^d))} = \mathcal{O}((L+2)\ 2^{-sL})$$

Output QoI variant of the multi-level Monte Carlo - finite volume method

$$Q_L E[J(U_L)] = Q_0 E[J(U_0)] + \sum_{l=1}^{L} \Big(Q_l E[J(U_l) - J(U_{l-1})] \Big)$$

Assume an asymptotic error ansatz for an unspecified rate constant q

$$|E[J(U)] - Q_L E[J(U_L)]| = \mathcal{O}((L+2)\ 2^{-qL})$$

Multi-level Monte Carlo-Finite Volume asymptotic error formula

$$\boxed{E[J(U)] - Q_L E[J(U_L)] = \frac{1}{\frac{L+1}{L+2}2^q - 1} \left(Q_L E[J(U_L)] - Q_{L-1} E[J(U_{L-1})] \right)}$$

$$2^q = \frac{(1+R)F(L) + \sqrt{(1+R)^2 F^2(L) - 4F(L)F(L-1)R}}{2F^2(L)F(L-1)}$$

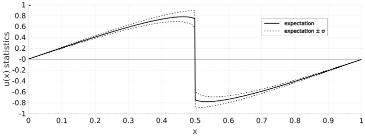
$$F(L) \equiv \frac{L+1}{L+2}, \quad R \equiv \frac{Q_{L-1}E[J(U_{L-1})] - Q_{L-2}E[J(U_{L-2})]}{Q_L E[J(U_L)] - Q_{L-1}E[J(U_{L-1})]}$$

Multi–level Monte Carlo–Finite Volume - III

Burgers equation with amplitude uncertain initial data

$$\begin{aligned} \partial_t u_{\mathbf{X}} + \partial_x u_{\mathbf{X}}^2/2 &= 0 \\ u_{\mathbf{X}}(x,0,\omega) &= \mathbf{X}(\omega)\sin(2\pi x) \end{aligned}$$

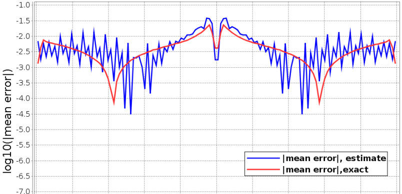
Random variable Burgers solution, $T = \frac{1}{4}$, $\mathbf{X}(\omega) \sim \mathcal{N}_3[m = .8, 0.1]$

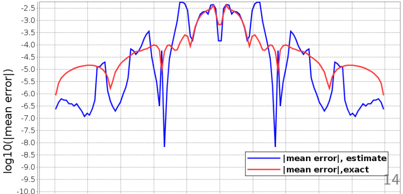


Output QoI functional

$$J(u)(x,t) = \int_{-w/2}^{w/2} u(x-\xi,t)\, d\,\xi$$

Estimated expectation $E[J(u)]$ error, $T = \frac{1}{4}$, $\Delta x = \frac{1}{128}$, $w = 5/256$, Sobol sampling,





Estimating CFD 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) asymptotic extrapolation using space-time grid hierarchies, e.g.

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

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

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

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

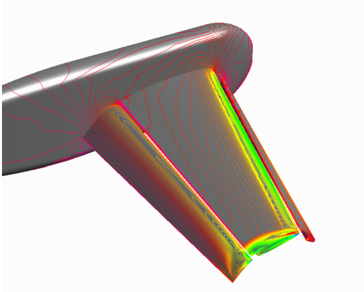
  with $\mathcal{B}(\cdot,\cdot)$ the primal semi-linear form, $F(\cdot)$ the right-hand-side forcing, and Φ a linearized dual problem.

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

Example: High-lift Wing-Body Flow with Geometric Uncertainty

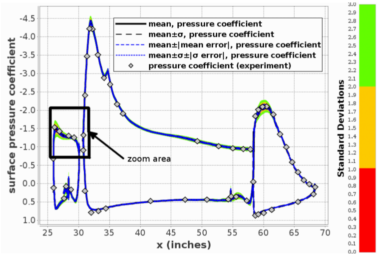
Wing-body flow with slat and flap angle uncertainty

- AIAA CFD High Lift Prediction Workshop test case,
- Reynolds-averaged Navier-Stokes equations, Spalart-Allmaras turbulence model,
- Mach=0.2, AOA=13°, $Re = 108,000$,
- 90 million mesh points,
- $\alpha_{\text{slat}} = 30° + \text{Gaussian}_{4\sigma}(m = 0.0°, \sigma = .75°)$,
- $\alpha_{\text{flap}} = 25° + \text{Gaussian}_{4\sigma}(m = 0.0°, \sigma = .75°)$.

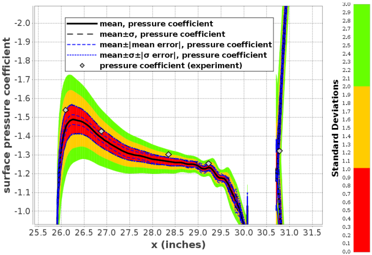


Example: High-lift Wing-Body Flow with Geometric Uncertainty

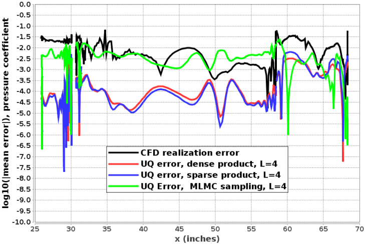
Surface pressure coefficient at 50% span



Surface pressure coefficient



Zoom closeup in slat region



Mean error on upper surface

- Dense product, $L = 4$, 81 evaluations,
- Sparse product, $L = 4$, 29 evaluations,
- MLMC sampling, $L = 4$, 56 effective fine resolution evaluations, $M_l = \{30, 120, 480, 1920\}$.

Concluding Remarks

Low cost quadratures with computable error estimates have been presented for the calculation of moment statistics

- Dense tensor product quadrature,
- Sparse tensor product quadrature,
- Multi-level Monte Carlo-Finite Volume sampling.

Combined uncertainty and error bound estimates

- quantify the overall accuracy of computed statistics,
- quantify the impact of UQ numerical errors on computed statistics,
- quantify the impact of CFD numerical errors on computed statistics,
- provide a guide for the allocation of computational resource when performing practical CFD calculations.

Ongoing work includes the extension of error bound techniques to the calculation of output probability densities, $pdf(J(u))(x,t)$