Combined Uncertainty and A-Posteriori Error Bound Estimates for General CFD Calculations: Theory and Software Implementation

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This workshop presentation discusses the design and implementation of numerical methods for the quantification of statistical uncertainty, including a-posteriori error bounds, for output quantities computed using CFD methods. Hydrodynamic realizations often contain numerical error arising from finite-dimensional approximation (e.g. numerical methods using grids, basis functions, particles) and statistical uncertainty arising from incomplete information and/or statistical characterization of model parameters and random fields. The first task at hand is to derive formal error bounds for statistics given realizations containing finite-dimensional numerical error [1]. The error in computed output statistics contains contributions from both realization error and the error resulting from the calculation of statistics integrals using a numerical method. A second task is to devise computable a-posteriori error bounds by numerically approximating all terms arising in the error bound estimates.

For the same reason that CFD calculations including error bounds but omitting uncertainty modeling are only of limited value, CFD calculations including uncertainty modeling but omitting error bounds are only of limited value. To gain maximum value from CFD calculations, a general software package for uncertainty quantification with quantified error bounds has been developed at NASA. The package provides implementations for a suite of numerical methods used in uncertainty quantification:

- Dense tensorization basis methods [3] and a subscale recovery variant [1] for non-smooth data,
- Sparse tensorization methods[2] utilizing node-nested hierarchies,

In addition, the software utilizes a high-performance OpenCL computation engine, multi-threaded parallel I/O, and a platform independent language implementation. The software provides the necessary tools and graphical user interface (GUI) for a user to rapidly pose uncertainty quantification problems to a CFD method and analyze the results of CFD computations.

Using this software package, Figure 1 shows uncertainty quantification results for transonic Navier-Stokes flow past an ONERA M6 wing with Gaussian distribution (mean=0.85, std dev=0.02) inflow Mach number and Gaussian distribution angle-of-attack (mean=3.06 deg, std dev=.075 deg). Fig. 1(a) shows statistics of the surface pressure coefficient profile at 65% wing span in terms of shaded probability distribution, quantiles of probability, mean statistic, and standard deviation envelope. All these uncertainty quantities have been calculated from the same set of CFD calculations. Experimental data with error bars provided by Schmidt and Charpin [5] are provided for comparison. Also graphed in this figure is an error bound estimate for the mean statistic (error bound estimates for the std deviation are also available but not shown here). An extreme closeup in the wing leading edge area shown in Fig. 1(b) reveals that the error in the mean statistic is quite large and comparable in magnitude to a standard deviation envelope. This raises doubt concerning the validity of computed uncertainty thus necessitating further error control and mesh refinement in CFD calculations.
The workshop presentation will discuss further aspects of error bound estimates for output statistics, provide further numerical examples, and provide a short demonstration of the numerical software.

Figure 1: ONERA M6 wing upper and lower surface pressure coefficient statistics at 65% wing span station for transonic Navier-Stoke flow with uncertain inflow Mach number and angle-of-attack. (a) Color shaded probability densities and quantiles lines of 10% probability at shown at \( x \) constant locations. Also graphed are mean statistics with error bound and a 1-standard deviation envelope. (b) Shows an extreme closeup in the wing leading edge region identifying an unacceptably large estimated mean statistic error resulting from inadequate mesh resolution in realizations.


