Suggestions for Making Useful the Uncertainty Quantification Results from CFD Applications

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• The focus of this presentation on what is a useful UQ product from the perspective of a consumer of the UQ results produced via CFD
• A kibitzer’s perception of the State-of-the-Practice of Aero UQ
• Two interpretations of probability
• Some examples from NASA uses of Aero UQ results
  – Wind Tunnel Data
  – Mars Entry, Descent and Landing
  – Launch Vehicles
• Suggestions
A Kibitzer’s Perception of the Aero UQ State-of-the-Practice
• NASA’s Wind Tunnel processes are now “under control” in the Statistical Process Control sense

• Wind Tunnel data variability is provided as an interval bound by a process similar to that in the ISO Guide to the Expression of Uncertainty in Measurement
  – Repeat runs in the same tunnel
  – Replication runs in different tunnels

• Wind Tunnel data bias
  – Standard instrument calibration
  – Various schemes for correcting for tunnel walls and model mounting mechanisms
• **CFD Discretization Error**
  – Estimated by Richardson extrapolation, e.g., grid-convergence index
  – Estimated via adjoint-based error “bounds”
    • these bounds are asymptotic or even heuristic
    • rigorous bounds are only provided by some classes of adjoint-based error analysis, and then only for smooth flows
  – The Drag Prediction Workshops have provided value quantitative data

• **CFD Iterative Convergence Error**
  – ???
• **Assessments focus on**
  - Turbulence model impact
  - Code-to-code variations
  - Surrogate model errors

• **Some sensitivity studies to transition location**

• **Little (no?) attention paid to UQ of**
  - Errors from lower-order CFD (Euler, potential, linear, boundary layer, etc.)
    • recall Mark Anderson’s Day 1 comments on the importance of multi-fidelity models in design
  - Transition region models (esp. important for hypersonic flows)
• Sensitivity analyses are rather rare
• CFD UQ in support of engineering decisions are almost always made using standard sampling techniques (e.g., Monte Carlo, Latin Hypercube) or moment methods
• There are few instances of engineering decisions based on CFD UQ using polynomial chaos
Uncertainty distributions are often just assumed

- Dependencies are often ignored
- Constructing a proper correlation matrix (which must be positive definite) becomes increasingly hard as the number of random variables increases
  - Some of the data may be lacking (completion problem)
  - Even when there are enough data noise may result in a non-positive definite matrix
Two Interpretations of Probability
Two Interpretations of Probability

• **Objective (Frequentist)**
  – The **limiting relative frequency** of the occurrence of the event (as the number of trials tends toward infinity)

• **Subjective (Bayesian)**
  – The **degree of belief** in the likelihood of the occurrence of the event
Frequentist Interpretation of Probability

- Intuitively, let $T_1, T_2, \ldots, T_N$ be “independent trials”, then
  \[ P(A) = \lim_{N \to \infty} \left( \frac{\text{# of occurrences of event } A \text{ in } N \text{ trials}}{N} \right) \]
- Mathematically rigorous (due to Kolmogoroff)
- The population parameters are constants; the sample points are random
- The notion of “confidence” in an uncertainty estimate makes sense
Subjective Interpretation of Probability

• An operational definition is based on an individual’s bet between two events (given some technical details)
• Mathematically rigorous (due to De Finetti & others in the 1920s-30s)
• The population parameters are random; the sample points are constants
• The notion of “confidence” in degree of belief makes no sense
Attitudes Towards Subjective Probability

• For many engineers, subjective probability is an unfamiliar concept
• For many of those who are aware of the concept, it is a highly suspect, perhaps even unscientific, one

• Nevertheless, in NASA applications
  – The frequentist interpretation of probability is largely confined to single discipline data
  – Applications of probability at the system level invariably make some use of subjective probability

• “The choice is not between using or not using expert judgment, but between using expert judgment well or using it badly” [Roger Cooke]
NASA Examples of Aero UQ
Typical Wind Tunnel Repeatability Data

- LaRC NTF data for Common Research Model
  - Wing-Body
  - Re=5 x 10^6
- Horizontal lines are 2-sigma bounds
  - Derived by a process similar to the GUM process
- See Rivers & Dittberner (AIAA-2010-4218)
The ISO Guide to the Expression of Uncertainty in Measurement (GUM) is an international standard.

It originated in the early 1990s.

Many organizations use a UQ process for experimental results that is similar to that of the GUM.

The most recent version is available at

Simplified GUM Process

• Let \((x_1,x_2, \ldots, x_n)\) be \(n\) measured values

• Compute the mean \(<x>\)

• Compute the standard deviation \(u\)

• Select a “coverage factor” \(k\)
  – A “level of confidence” can only be associated with \(k\) if the distribution is known (or assumed)

• Compute the expanded uncertainty: \(U = ku\)

• GUM uncertainty interval is \((<x>-U, <x>+U)\)
  – “an interval about the result of a measurement that may be expected to encompass a large fraction of the distribution of values that could reasonably be attributed to the measurand”

• In this simplified case, the GUM interval is equivalent to a confidence interval
The fraction of the distribution contained within a given multiple of the standard deviation depends strongly on the distribution.

A normal distribution contains much more of the distribution than an arbitrary or even a unimodal distribution.
A 95% confidence interval
- does not mean that there is a 95% probability that the true value lies in the interval
- does mean that if the process were repeated a large number of times, 95% of the confidence intervals would contain the true value

Experimental uncertainty intervals are not guaranteed to contain the true value

If thought of as a confidence interval then beware:
- “You can’t propagate a confidence interval” [Sankaran Mahadevan]

The GUM language is more suggestive of the subjective interpretation of probability than the frequentist one
• 2,000 Monte Carlo runs of the EDL simulation are typically performed to assess a variety of performance metrics

• Most uncertainties are treated by PDFs
  – The atmospheric variability is built into the Mars-GRAM atmospheric model using a first-order Markov model to represent spatial correlation

• Only simple Monte Carlo is used because of the atmospheric uncertainty description in Mars-GRAM
### PDFs Used for a Mars EDL Technology Study

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Nominal</th>
<th>Perturbation</th>
<th>Distribution</th>
<th>Rationale</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lift Coefficient Multiplier</td>
<td>1</td>
<td>±10 %</td>
<td>Normal</td>
<td>Larger than would be expected to provide sensitivity analysis. The sensitivity characteristics of the technology are important considerations. Also the aerodynamics are uncorrelated, to further magnify the sensitivities. Many technologies will look good at their design point – one major discriminator will be sensitivity.</td>
</tr>
<tr>
<td>Drag Coefficient Multiplier</td>
<td>1</td>
<td>±10 %</td>
<td>Normal</td>
<td>See Lift Coefficient Multiplier discussion.</td>
</tr>
<tr>
<td>Angle of Attack (deg)</td>
<td>55</td>
<td>±5</td>
<td>Normal</td>
<td>Angle of attack will vary the ballistic coefficient, and will amplify the ratio of Mass/CL to Mass/CD, to provide sensitivity analysis.</td>
</tr>
<tr>
<td>Engine Isp (sec)</td>
<td>369</td>
<td>±2.5 %</td>
<td>Normal</td>
<td>This was an estimate for LOX/CH4 engines which have not been built. This parameter is expected to be a secondary sensitivity parameter for most of the technologies to be considered. If it becomes a primary driver, this will be reevaluated.</td>
</tr>
<tr>
<td>Deorbit ΔV (m/s)</td>
<td>14.978167</td>
<td>±0.279*</td>
<td>Normal</td>
<td>In lieu of having initial states generated for this study (time and resources that would not be a driver in selecting technologies), this parameter is used as an analog to provide the entry g’s and heat pulse variation that would be expected from this type of mission.</td>
</tr>
<tr>
<td>Atm Random #</td>
<td>1</td>
<td>1-29999</td>
<td>Integer Uniform</td>
<td>In lieu of having initial states generated for this study (time and resources that would not be a driver in selecting technologies), this parameter is used as an analog to provide the entry g’s and heat pulse variation that would be expected from this type of mission.</td>
</tr>
<tr>
<td>Dusttau</td>
<td>0.7</td>
<td>0.1:0.9</td>
<td>Uniform</td>
<td>This determines the dust loading and thus the density and wind profiles that the vehicle will experience. This range provides large variability, but would not include dust storms.</td>
</tr>
</tbody>
</table>

**Notes**

* ΔV perturbation selected to produce a +/- 0.25 deg variation in entry Flight Path Angle

- **The above table is taken from the 2008-2010 EDL Systems Analysis Study to determine technology needs for human missions to Mars [NASA/TM-2010-216720]**
• The EDL engineers are interested in the uncertainties relevant to the flight vehicle
  – The only frequentist aero data is for the wind tunnel and ballistic range tests, which are not exact models of the actual vehicle
• No Mars EDL flight data exist for past missions
  – MSL was the first mission to take aero & TPS data during EDL
• Only one flight will be made for this particular design
• The EDL engineers use the language of subjective probability when discussing the distributions
Ares 1-X Aerodynamics

- Aerodynamics provided databases for
  - Forces & moments
  - Aerodynamic loads
- Forces impact performance (e.g., payload to orbit)
- Forces & moments impact GN&C and trajectory (6 DoF simulations)
- Loads impact structures
- Aero databases fused wind tunnel, high-fidelity CFD, and low-fidelity aero results
- Uncertainties were used for a variety of Monte Carlo simulations to verify Ares I-X system requirements

Ares I-X Flight Test
Oct. 28, 2009
Separation Re-contact Requirement

- **Requirement Statement (from System Requirements Document)**
  - The FTV [Flight Test Vehicle] shall achieve all separations without re-contact

- **Verification Plan (from Verification Requirements Document)**

<table>
<thead>
<tr>
<th>FTV SRD Requirement to be Verified</th>
</tr>
</thead>
<tbody>
<tr>
<td>Verification Number:</td>
</tr>
<tr>
<td>VR-FTV-027</td>
</tr>
</tbody>
</table>

**Requirement Title:** Separation Re-contact

**Verification Requirements**

**Verification method:** Verification that the FTV will separate without re-contact shall be verified by *Analysis*.

**Description of verification activities to be performed:** The Ares I-X ID&A Trajectory Team shall perform a separation and recontact analysis to determine the relative position and orientation time history between the First Stage and Upper Stage. The analysis shall be done using a NASA approved 6-DOF non-linear flight dynamics model of the individual stages. The analysis shall be done using Monte Carlo simulations that vary input parameters that model vehicle performance, loads and environmental conditions with up to worst case (3-sigma) dispersions.

The SE&I GN&C Team shall conduct a near-field recontact analysis covering the first three seconds after separation, before the booster tumble motors ignite. The SE&I Trajectory Team shall conduct a far-field recontact analysis beginning at booster tumble motor ignition and extending until 30 seconds after separation.

Both recontact analyses shall be peer reviewed by a panel that includes one or more independent experts.

**Success Criterion:** The verification shall be considered successful when the analysis results show that the FTV first stage and upper stage have a recontact probability less than 0.13%.

**Rationale:** Because of the wide variation of possible inputs and because of lack of access to the flight-like mission environment, analysis with an accredited simulation is appropriate for this verification.
Role of Aerodynamics

- NASA Trajectory and GN&C teams traditionally do Monte Carlo simulations with normal distributions for the uncertain variables.
- The numerical criterion for verification (less than 0.13% failure) was based on this heritage approach.
- The aerodynamic force and moment database is one of many inputs to this (and many other) higher level requirements.
- Other inputs to the GN&C simulations were:
  - Structural properties
  - "Environmental" properties
• The Ares I-X was a one-of-a-kind system
• The aero uncertainties that mattered were the uncertainties on the vehicle during its one-and-only flight test
  – Not the uncertainties on the wind tunnel data
  – Not the uncertainties on the CFD data
• The GN&C Lead desired
  – A distribution, not an interval
  – The “degree of belief” on the uncertainties for flight
• For the Ares I design, the Aero Team specified interval uncertainty bounds
  – GN&C needed a distribution
  – Aero specified that if a distribution were used, it should be a uniform distribution
  – This led to what was in all likelihood a very conservative vehicle design (with reduced payload performance) due to the large number of failure cases arising in the GN&C simulations due to the fat tail
Suggestions for CFD UQ Applications
Suggestions 1: Working with the Customer

- Use technically precise language in describing uncertainty estimates
  - See, e.g., T. Zang, On the expression of uncertainty intervals in engineering, TCFD, 2012

- Give the customer the kind of UQ representation that is useful to him
Suggestions 2: Input Distributions

- **Use credible input distributions**
  - Without credible input distributions, many will just dismiss the UQ results as “garbage-in/garbage-out”
  - Developing input distributions needs relatively more UQ resources and developing advanced UQ propagation algorithms needs relatively less

- **Estimate dependencies amongst the uncertain variables**
  - Techniques exist for addressing the noisy data and incomplete data problems
  - See, e.g., Kurowicka & Cooke, Uncertainty Analysis with High Dimensional Dependence Modeling, Wiley, 2006
Suggestions 3: Uncertainty Analysis

- Do a broad sensitivity analysis to identify which parameters matter the most and then do the UQ on the small set that matters.
- Collect data and develop a process for converting estimates of discretization error, iterative convergence error and model form error into subjective probability distributions.
- Use subjective probability for UQ of wind tunnel data bias.
Suggestions 4: Resource Allocation

- Balance the precision of the CFD UQ outputs with those of the input distributions.
- Balance the precision of the CFD UQ outputs with those from the other contributing disciplines in system applications.
Suggestions 5: “Confidence” Assessment

- The desire for “confidence/trust/reliability” in CFD results occurred frequently in Day 1, but only in a vague sense.
- The NASA Standards for Models and Simulations (NASA-STD-7009) includes a “Credibility Assessment Scale” that may be useful for judging “confidence” in CFD results.
- The criteria were informed by interviews with Engineering Directors and project Chief Engineers at all centers.
- This represents the consensus of a team representing 9 NASA centers and many different disciplines.