Breakout_A-4 (What are the obstacles to community developed software for uncertainty quantification)

Issue: https://github.com/CFDSI/Kickoff_Workshop/issues/#
Related Issues:

Issue Statement: What are the obstacles to community developed software for uncertainty quantification?
Discussion topic:
Moderator: Mike Park
Note taker: Daniel Appelo
Reporter: Mike Park
Group Members: Bob Moser, Alireza Doostan, Omar Knio, Ryan King, Max Gunzburger, Lorena Barba, Mike Park, Daniel Appelo, Kurt Maute.
-
-

Please address these topics in your discussion (moderators please make sure that there is enough time to cover all three before the session ends).

1. Describe the problem:

- Obstacles: expensive function evals (solve PDE).
- Robustness at tail cases.
- Sparse and under resolved is outside comfort zone for traditional methods.
- Difficult to know appropriate inputs and outputs for process.
- Accounting for truncation errors and uncertainties at the same time.
- Added cost of incorporating UQ may deter its use.
- Aid user in choosing QOI.
- How to map to input files.
- Underappreciation of difficulty with repeatability in experiments (single or multiple).
- Multi Fidelity can have different uncertainties at different levels.
- Answer the question: when is results good enough to be new science?
- Reporting is traditionally limited (by page limits). This may have created a tradition of under reporting.

2. What are potential solutions?

- Infrastructure to support surrogates for reduced cost & robustness.
- Experiments are expensive, software should inform for optimal experimental design.
- CFD using UQ intrusive or non-intrusive.
- Software that enables model to model comparison.

3. What can CFDSI do to help?

- Standards and guidelines (at least minimal) for codes and experiments. Maybe different tiers of requirements (incremental)?
- Provide experimental/simulation datasets with extensive information on its provenance.
- Building a software (CDFSI) stack should include UQ hooks from the start.
- Aid user in managing uncertain inputs: multi fidelity different inputs/output are each level, reconstruction/interpolation/extrapolation for common comparison

4. Misc ideas so they don't get lost (e.g., Did you find new issues? If yes, create the issues on GitHub!):

-

5. Summary for report-back (Alternatively, just bold the key points above):

- Expensive function evaluations with interesting case in the tails where the tools are not robust, verified, or validated
- Samples are sparse and resolution is needed outside comfort zone
- Knowing the sensitive features of the system
- Simultaneous modeling and discretization errors
- Reporting provenance for simulation and experiments
- When is knowledge gained? Significance?
- Should UQ be embedded in simulation or simulation tools be adapted to interact with UQ frameworks
- Output verification for visualization
- Error bars need error bars
- Aid user in managing uncertain inputs: multi fidelity different inputs/output are each level, reconstruction/interpolation/extrapolation for common comparison