Some Research Directions in Uncertainty Quantification for Large-scale Multi-physics Applications

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Uncertainty Quantification: needs & challenges

- Our multi-physics codes have many UQ needs
  - Calculate margin and uncertainty (QMU)
  - Identify important physics/algorithmic issues (prioritize research)
  - Validate model against experimental data
  - Calibrate model parameters to fit data
  - Explore parameter space (conceptual validation)
  - Design optimization, inverse UQ, phenomenological studies
- Our multi-physics applications are characterized by
  - High computational cost (2D low resolution: hrs on 100’s procs)
  - Nonlinear input-output relationships, complex interactions
  - Correlated input (e.g. inequality constraints)
  - Many uncertain parameters (currently up to ~70)
  - Need non-intrusive UQ
- These are high-consequence applications
  - Need efficient and robust UQ methods
  - Need to validate our UQ methods

We found the following global sensitivity analysis methodology useful

Uncertain parameter list
Outputs and diagnostics
Model assumptions (e.g. linearity)

→ **Problem definition**

Derive credible ranges
Shape and forms (e.g. normal)
Critical: may be time-consuming
(recursive)

→ **Uncertain parameter setup**

For large parameter space
Coarse sampling

→ **Screening for most sensitive Uncertain parameters**

Low dimension function approximation

→ **Create response surfaces**

On reduced parameter space
Variance decomposition
Parameter interactions

→ **Quantify parameter sensitivity**

Set research priorities/reduce parameter uncertainties

Lessons learned from applying the methodology

- **The process is as important as the results (a good tool for conceptual validation).**
- **The process is manageable: easy to understand, yet effective.**
- **Concern 1 : We should spend time thinking about each simulation and do not let machines take over human thinking.**
  - **The screening design exhibits a pattern, anomalies can easily be spotted, & each calculation forces us to ask physics questions.**
- **Concern 2 : UQ should have people in mind (social element).**
  - **Screening promotes communication between designers, analysts, and mathematicians/statisticians.**
- **Setup ! Setup ! Setup !**
  - **Need a systematic way of job launching and postprocessing**
  - **Need an UQ-friendly job queuing system**
  - **Need to be able to examine each calculation**
  - **Need good graphical tools to display results**

R&D Issues

- **More defensible screening methods:**
  - **Type II errors (quantified confidence in down-select)**
  - **Separation of nonlinearities and interactions (confounded)**
  - **Non-orthogonal inputs (may need many additional simulations)**
- **More defensible response surface methods**
  - **Good coverage not of the whole space but also the boundaries**
  - **Validation methods (need more rigorous mathematical theory)**
  - **More efficient sampling (adaptive, machine learning)**
- **More defensible quantitative analysis**
  - **Need more robust self-validation schemes**
  - **Need to deal with complex input and output constraints**
- **Others:**
  - **Large scale numerical optimization**
  - **Inverse UQ with multiple constrained outputs**
  - **Good UQ framework (design, experiment, analysis)**

We are seeking academic/industrial collaborators to work on these issues