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Uncertainty Quantification and Multiscale Mathematics

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Outline of talk

- Context and Characterization
- Propagation
- Application

Uncertainty is …

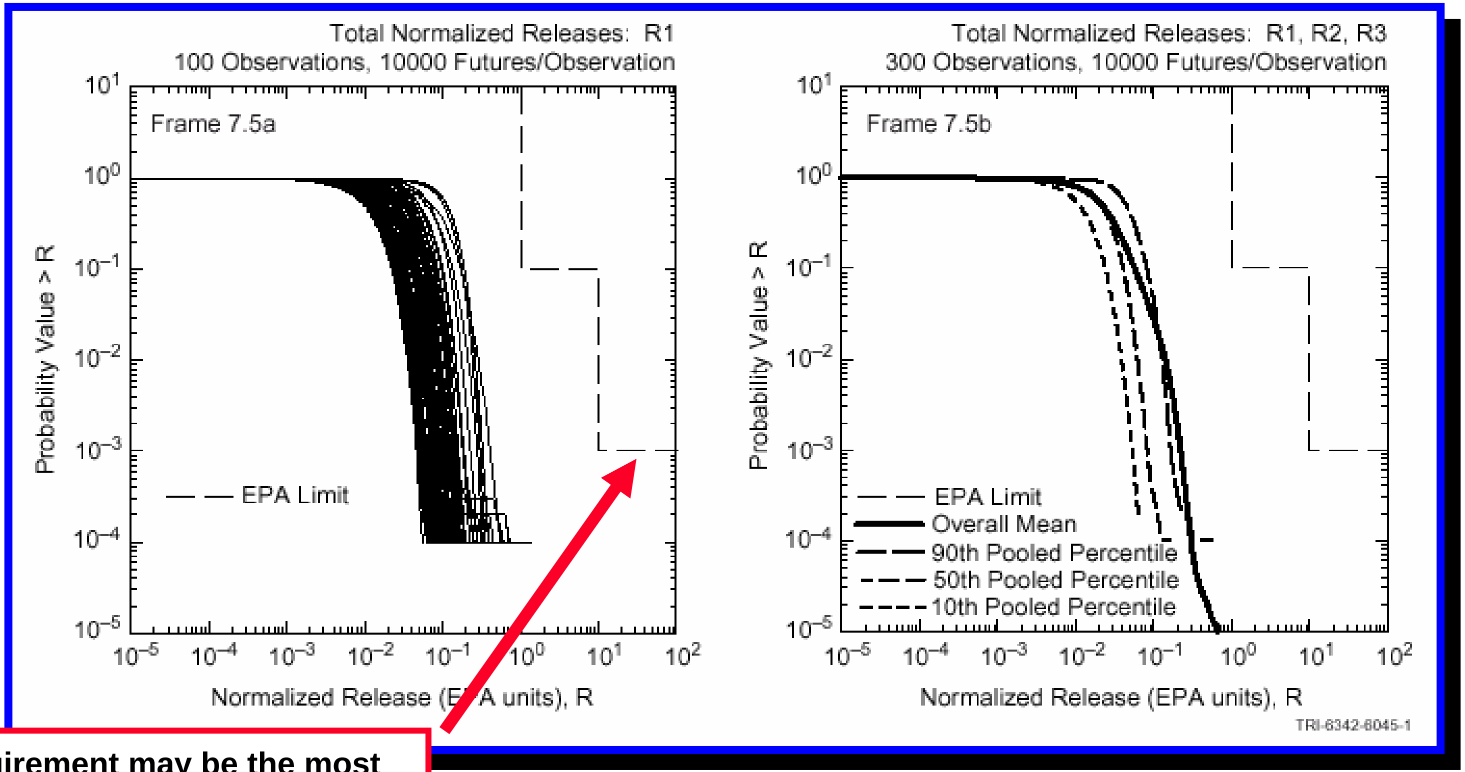
- Aleatory (irreducible) uncertainty is probabilistic variability.
  - Increasing knowledge will not eliminate variability
  - Think of drawing balls from an urn
  - Random variables represent variability
- Epistemic (reducible) uncertainty is lack of knowledge.
  - (Subjective) probability can represent epistemic uncertainty
  - Increasing knowledge does reduce subjective uncertainty
  - Think of uncertainty about numerical error
  - GIF (Generalized Information Theory – fuzzy sets; evidence theory; possibility theory) can also represent epistemic uncertainty. (Won't discuss here.)

Comments

- I'm not going to worry about Bayesian versus frequensic probability interpretations here. We feel comfortable with both, depending on how and when they are used.
- It is important to emphasize that probability distribution functions (pdf's) based on poor data have subjective uncertainty.
  - This means that we should worry a lot about the uncertainty underlying frequensic characterizations of pdf's when we propagate uncertainty.

"The Probability of Frequency"

Example of accounting for uncertainty in the probability distributions:



The requirement may be the most uncertain element on this plot.

Uncertainty in computational models arises from myriad sources

- **Initial conditions**
- **Boundary conditions**
- **Numerical procedures**
- **Fidelity of physics and associated equations**
- **Software quality**
- **Application**

A notation I will use is:

$$\boxed{D_{(\vec{x},t)}\left[\vec{u},\vec{a}\right]=0}$$

Think of this as a system of PDEs, a code, or a model. Here, *u* is the vector of dependent variables, α a vector of (possibly) time and space dependent parameters.

Uncertainty Quantification:

- Uncertainty quantification (UQ) is a foundation for predictability.
  – To the extent uncertainty is present in calculations, we are talking about uncertain prediction.
- UQ emphasizes how we look at the solution of a mathematical problem for purposes of applying it.

  "Indeed there is a general absence of accepted frameworks for quantifying and controlling uncertainties from underlying sources of error in estimates, computations, and analysis." (Banks, 2001)
- UQ aims at Best Estimate Plus Uncertainty

Probability can be used without focusing on UQ: regularization

- For example, we can regularize highly variable (or stochastic) equations via an averaging principle, roughly like:

$$\boxed{\begin{aligned} &D_{(\vec{x},t)}\left[\vec{u},\vec{a}\right]=0 \quad \Rightarrow \bar{D}_{(\vec{x},t)}\left[\vec{u},\vec{a}\right]=0 \\ &\Rightarrow \quad \sim D^{Closure}_{(\vec{x},t)}\left[\bar{\vec{u}},\bar{\vec{a}}\right]=0 \end{aligned}}$$

- The overbar denotes some kind of "averaging;" "closure" denotes a renormalization and closure, which may further involve asymptotic, rather than convergent, expansions.
- Goal is to eliminate variability, sensitive dependence on data, etc in straightforward way by calculating the approximation $\bar{u}$.

Probability can be used without focusing on UQ: regularization cont

- Add a probabilistic interpretation to the regularization by assuming that the parameters are stochastic. For example, we might seek:

$$\boxed{\begin{gathered}\text{Expectation} \equiv \operatorname{Exp}\left[\vec{u}\right] = F_1\left(\vec{x},t;\vec{\alpha}\right)\\ \text{Variance} \equiv \operatorname{Var}\left[\vec{u}\right] = F_2\left(\vec{x},t;\vec{\alpha}\right)\\ \vdots\end{gathered}}$$

- But the easy way out doesn't work in general:

$$\boxed{\begin{gathered}D_{\left(\vec{x},t\right)}\left[\operatorname{Exp}\left(\vec{u}\right),\operatorname{Exp}\left(\vec{\alpha}\right)\right] \neq 0\\ D_{\left(\vec{x},t\right)}\left[\operatorname{Var}\left(\vec{u}\right),\operatorname{Var}\left(\vec{\alpha}\right)\right] \neq 0\end{gathered}}$$

Majda et al is a on-steroids version of this kind of regularization.

- They start with a model:

$$\boxed{D_{(\vec{x},t)}\left[\vec{u},\vec{\alpha}\right]=0}$$

- They introduce a regularization roughly in the form (^ is macro, ~ is micro):

$$\boxed{\begin{aligned}\hat{D}_{(\vec{x},t)}\left[\hat{\vec{u}},\vec{\alpha}\right]&=0\\ \tilde{D}_{(\vec{x},t)}\left[\hat{\vec{u}},\tilde{\vec{u}},\vec{\alpha}\right]&=0\end{aligned}}$$

with the most singular self-interaction term at the small scale regularized with a noise model.

Majda et al :

- This regularization then allows statements like (?)

$$\boxed{\mathrm{Exp}\left(Q\left[\hat{\vec{u}},\tilde{\vec{u}}\right]\right) \approx \mathrm{Exp}\left(Q\left[\hat{\vec{u}},\tilde{\vec{u}}_{nominal}\right]\right)}$$

  in the (singular) limit of infinite scale separation.
- *Q* is some function(al) of the dependent variables of interest.
- I claim approximation in the above to emphasize that scale separation is never infinite in a real application, so application of the result only yields an approximation.
- <u>Uncertainty is not quantified in this work</u>.

Probability can be used without focusing on UQ: ROM

- Chorin has suggested a procedure for defining an optimal reduced order model (ROM) under specific assumptions about the form of the model *D*. For example:
  - D is a Hamiltonian system
  - Treat *u* as an *n* component random vector
  - Project the Hamiltonian to an $m<n$ component subset of *u* via a conditional expectation (with respect to the joint pdf of u) in this subset.
  - This is called 1st order optimal prediction
  - The technical issue is how to actually calculate the conditional expectation in specific cases.
- <u>Uncertainty is not quantified in this work</u>.

Uncertainty Quantification: Characterization

- All UQ starts with identifying and quantifying uncertainties underlying the particular model, code, calculation one is interested in.
- We call this uncertainty characterization.
- Poorly performed characterization introduces further uncertainty (for example, frequensic distributions can become epistemic uncertainties).
- Improving an initial uncertainty characterization may result from a forward/backward uncertainty analysis (see comment below).

Uncertainty Quantification: Propagation I

The uncertainty is in the parameters.

$$D_{(\vec{x},t)}\left[\vec{u},\vec{\alpha}\right]=0,$$

$$\vec{\alpha} \sim f_{\vec{\alpha}}$$

$$\Rightarrow \qquad \vec{u} \sim f_{\vec{u}}$$

$$\Rightarrow \qquad \mathrm{Exp}\left(\vec{u}\right),\mathrm{Var}\left(\vec{u}\right)$$

Uncertainty Quantification: Propagation I

- For example, BE + U then is:

$$\boxed{\mathrm{Exp}\left(\vec{u}\right) \pm \mathrm{Var}\left(\vec{u}\right)}$$

- Dominant approach is sampling-based:
  – Monte Carlo (yuk!)
  – LHS and improvements (common but still painful)
  – Voronoi tesselation (rocket science?) – of great interest
- Implication is that resulting distribution for the dependent variables is an empirical distribution.
  – How accurate are the resulting statistics?
  – Bad news if the dependent variables end up with multimodal, or tail heavy distributions: you'll likely never see this?
- Because of computational expense this is a BIG PROBLEM.
  – Note that introducing ROMs (i.e. less accurate calculations) does not *necessarily* help because of the potential for introducing further uncertainty.
  – In fact – this is an *attractive area* for investigation (including use of response surfaces) (See Santner, et al, 2003)
- How to get by with sampling remains very important and complex problem that occupies most of the community.

Uncertainty Quantification: Propagation II

Why not cut to the chase? Let's just solve SDE's!

$$\boxed{D_{(\vec{x},t)}\left[\vec{u},\vec{\alpha}+"d\vec{w}"\right]=0}$$

This theoretically maps parameter pdf's (in a HIGHLY RESTRICTED FORM) to dependent variable pdf's.

- **First of all – HORRORS!!! even if this thing is somehow well defined.**
- **Second, is it really going to be sensible?**

Uncertainty Quantification: Propagation II

- It seems highly unlikely that this object will be well defined with all this nasty noise, especially in a multi-scale problem.
- For example, simply introduce internal state variables for a good laboratory:

$$\boxed{\begin{aligned} &D^{macro}_{(\vec{x},t)}\left[\vec{u},\vec{\alpha}_1,\vec{\alpha}_2\right]=0 \\ &D^{micro}_{(\vec{x},t)}\left[\vec{\alpha}_2\right]=0 \end{aligned}} \longrightarrow \boxed{\begin{aligned} &D^{macro}_{(\vec{x},t)}\left[\vec{u},\vec{\alpha}_1+''d\vec{w}'',\vec{\alpha}_2+''d\vec{w}''\right]=0 \\ &D^{micro}_{(\vec{x},t)}\left[\vec{\alpha}_2+''d\vec{w}''\right]=0 \end{aligned}}$$

- The singularity of the Wiener process and complex nonlinearities present above are worrisome, let alone calculable.

Uncertainty Quantification: Propagation II

- It is also worth emphasizing that the uncertainty characterizations we care about typically don't result in "parameter plus noise."
  - Usually the parameters are assigned standard distributions such as uniform, normal, lognormal, etc.
- Regarding SDE's:

  "One generally requires very specific types of noise (additive, initial data, white noise, etc) to obtain a rigorous theory. Stochastic parameters (such as rate constants, delays, nonlinearities) not in a special class are generally not amenable to a theoretical treatment." (Banks, 2001)

Uncertainty Quantification: Propagation III

- An important area of work that goes well beyond sampling, and stops short of dealing with the horrible SDEs, is polynomial chaos expansions (and related stochastic finite element methods).
- This is centered on spectral representation of the dependent variables and stochastic parameters in appropriate bases, with coefficients calculated by a Galerkin procedure from the given differential equations.
- Recent work suggests that multiscale structure in the basic problem can be reflected in the procedures through appropriate bases (such as wavelets). See the work of Najm and colleagues (Le Maitre, et al 2004a,b); also Xiu and Karniadakis (2002).
- Going beyond brute force sampling for uncertainty propagation is of mandatory, in my opinion, so this kind of work is very important.
- Tools will need to be developed and deployed for production environments (e.g. Sandia engineering) to take full advantage of this work.
- (There is also ongoing work at Sandia with stochastic finite element implementations for structural mechanics by Red-Horse and Ghanem.)

Uncertainty Propagation: Backwards

- Propagation of uncertainty, plus comparison with one or more benchmarks, allows "improvement" of the model, for example through calibration (tuning parameters) or through Bayesian updating (to improve the original uncertainty characterization).
- An interesting example of this process that represents a probabilistic downscaling method is the work of Glimm et al (2000, 2001), which roughly does the following:

  Prior permeability (micro) →

  propagation →

  comparison with oil production benchmarks (macro) →

  Bayesian updating →

  Posterior permeability (micro)

  (Loop)
- These authors also produce a very rich probabilistic prediction (a result with statistical confidence intervals).

Uncertainty Propagation: Caution

- **The result of a calibration is sometimes simply reported as:**

$$\boxed{D_{(\vec{x},t)}\left[\vec{u},\vec{\alpha}_{optimal}\right]=0}$$

- **This is not in the form of Best Estimate Plus Uncertainty.**
- **Standard calibration reflects uncertainty in the calibration data and assumed uncertainty characterization of the parameters, but NOT in the model (*D* above).**
  - **This is an important limitation and has been under study (see Kennedy and O'Hagan, 2001, for an approach incorporating model uncertainty in a Bayesian framework). Concern goes back considerably further.**
  - **We call this Calibration Under Uncertainty (CUU).**
  - **It is not clear what it buys us (yet).**
  - **The standard Markov Chain Monte Carlo relied upon for Bayesian updating is (hopelessly) impractical for computational physics models.**

Applications – I.e. Decisions

- High risk decisions (economic forecasting, finance, climate, reactor safety, waste repository performance, chemical facility performance, stockpile stewardship, etc) require:

  Best Estimate Plus Uncertainty

  (Helton, 1994 discusses the surrounding issues.)

The decision to use the model depends on model credibility (V&V)

Partial Differential Equations

Numerical Solution Required

Algorithms

Software Required

Code

Code Input (including mesh) required

Infrastructure required

Calculations

<u>Verification</u>: Mathematically sound? Accurate? No bugs?

<u>Validation</u>: Physically accurate? Predictive credibility?

<u>Accreditation</u>: Should the code be used?

Evaluation:

Comparison with benchmarks

Results applied?

Uncertainty in Verification

- "Numerical error is an uncertainty." (Trucano)
- What is the basis for this statement?
  - Empirical evidence: Nobody apparently knows or reports solution errors (read an issue of Physics of Plasmas, for example).
  - Software reliability theory (highly unlikely our codes and algorithms are bug free) (Singpurwalla and Wilson, 1999)
- What solution error?

  ~~Convergence?~~ ~~A Posteriori Error Estimates?~~
- I'm not the only one who has noticed this:
  - "When quantifying uncertainty, one cannot make errors small and then neglect them, as is the goal of classical numerical analysis; rather we must of necessity study and model these errors."
  - "…most simulations of key problems will continue to be under resolved, and consequently useful models of solution errors must be applicable in such circumstances."
  - "…an uncertain input parameter will lead not only to an uncertain solution but to an uncertain solution error as well."

  B. DeVolder et al. (2001)

Uncertainty in Validation

- **Validation metrics:**

  Experimental data have uncertainty and this dominates inferences drawn from comparing calculations with experiments.

- **Maybe you don't <u>need to</u> validate multiscale simulations:**

  "The important aspect of nanoscale systems that makes them such a TMS challenge is that the characterization of uncertainty will often have to be done in the absence of experimental data, since many of the property measurement experiments one would like to perform on nanoscale systems are impossible in many cases or unlikely to be done in cases where they are possible. Hence, the concept of self-validating TMS methods arises as a significant challenge in nanoscience. By self-validating TMS methods we mean that a coarser-grained description (whether it be atomistic molecular dynamics or mesoscale modeling, for example) is always validated against more detailed calculations (e.g., electronic structure calculations in the case of atomistic molecular dynamics, and atomistic molecular dynamics in the case of mesoscale modeling). (DOE, 2002)

Maybe you can't validate multiscale simulations?

"Groundwater models cannot be validated"

Title of article by Konikov and Bredehoeft.

(They recommend doing BE+U instead…!)

Decision to use the calculation:

<u>"Don't use our software for anything important!"</u>

- **Actually, what they really said was -**

  > **"We make no warranties, express or implied, that the programs contained in this volume are FREE OF ERROR, or are consistent with any particular merchantability, or that they will meet your requirements for any particular application. THEY SHOULD NOT BE RELIED UPON FOR SOLVING A PROBLEM WHOSE SOLUTION COULD RESULT IN INJURY TO A PERSON OR LOSS OF PROPERTY…" [Emphasis Mine] (from <u>Numerical Recipes in Fortran</u>, Press, Teukolsky, Vetterling, and Flannery)**

  but I'm hard pressed to see the difference. (Similar warnings come along with Sandia codes and everybody else's codes for that matter.)

- **Who actually uses computational physics software to make decisions?**

Needs

- How does a multiscale mathematical formalism imprint sampling methodologies for uncertainty propagation? Ditto for chaos expansions?
- Advances in sampling and chaos expansions.
  - How do we optimally compute? (Gunzburger's multi-everything should be important here. We're currently only scratching the surface of multi-fidelity, multi-physics UQ.)
- Can we really solve complicated, probably singular SDE's with non-classical noise?
- How can a multiscale math/computation framework best encompass UQ?
- How do you V&V the calculations? If you can't what do you do next?
- The connection between ROM's and UQ:
  - Uncertainty created by ROM's
  - Selection of ROM's
- Tools for doing UQ (especially managing the resulting information).

Epilogue – “Scientization”

“…policy makers call for more study to reduce uncertainties in an attempt to settle debates. But when the research is done, new uncertainties frequently emerge, and controversial questions are rarely settled…”

John Fleck, ABQ Journal, Sunday, December 12; regarding the local debate over the Sandia National Labs mixed waste landfill on Kirtland AFB.

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