What is UQ?

Clint Scovel, CCS-3; Houman Owhadi, Tim Sullivan, Mike McKerns, Michael Ortiz, California Institute of Technology

We describe how Uncertainty Quantification (UQ) is currently ill-posed. We then describe the LANL and CalTech opening gambit, Optimal Uncertainty Quantification (OUQ), to resolve this situation and develop a science of UQ. When applied to a problem of seismic safety of structures, we show how the OUQ framework produces rigorous guarantees on the probability of failure of the structure as a function of the magnitude of the earthquake size. Finally, we mention that this framework can be used to develop a framework for UQ for modeling, which, along with a theory of validation, certification, and extrapolation, produces a rigorous scientific theory of certification without testing.

While everyone agrees that Uncertainty Quantification (UQ) is a fundamental component of objective science, it appears not only that there is no universally accepted notion of the objectives of UQ, there is also no universally accepted framework for the communication of UQ results. In particular, most people do not understand what UQ is, and among those that do, there is much disagreement. This dilemma has its origins, in part, in the fact that UQ, as it currently stands, has all the symptoms of an ill-posed problem–e.g. Oreskes et al. [1] assert that validation is impossible, and [2,3] describe rigorous methods for it. Moreover, often the appropriate problem is not validation but certification–using a model to assess the performance of a physical system.

Indeed, it appears that UQ is currently at the stage where probability theory was before its rigorous formalization by Kolmogorov. In an effort to resolve this situation we seek foundations for UQ. For example, in linear algebra we have vector spaces, linear transformations, the Jordan form, the spectral theorem, and the QR algorithm. Calculus has integrals and derivatives and the fundamental theorem of calculus. Linear Programming has linear programming problems and the fundamental theorems of linear programming, giving rise to the simplex algorithm. If UQ is going to be a science, then the following questions naturally come to mind:

- What are the fundamental objects of UQ?
- What are the fundamental theorems of UQ?

One important application of these ideas for the modeling community is: "What are the fundamental theorems of validation and certification?"

In an effort to resolve this situation, LANL has teamed with the Predictive Science Academic Alliance Program (PSAAP) at CalTech in an opening gambit. Our approach, which we call Optimal Uncertainty Quantification (OUQ), is very simple and follows John Dewey's [4] assertions that "a problem well formulated is half solved" and "without a problem, there is blind groping in the dark." That is, quantitatively express the problem to be solved, while quantitatively stating the assumptions being made. The main results of [5] describe OUQ optimization problems that, if solved, provide rigorous optimal solutions to UQ problems. Moreover, we describe finite dimensional reductions for a large class of these OUQ Optimization Problems. With the advent of ever more powerful computing platforms, such as the upcoming exascale systems, solutions to many of these OUQ problems may now be within our reach. Nick Hengartner at LANL tells us that this situation is similar to that experienced by the Bayesians. Namely, the Bayesian framework was not used until computers were powerful enough to compute the posteriors.

Let us apply the OUQ framework to the problem of the Seismic Safety Assessment of the structure in Fig. 1. As is standard in the seismic engineering community, we say that the structure is safe if the displacements of all the members of the truss system are less than the corresponding yield strains. Moreover, we use a standard model of the response of the truss system to ground acceleration and assume this model to be a correct representation of reality. When an earthquake hits at a fixed distance R and magnitude M on the Richter

For more information contact Clint Scovel at jcs@lanl.gov

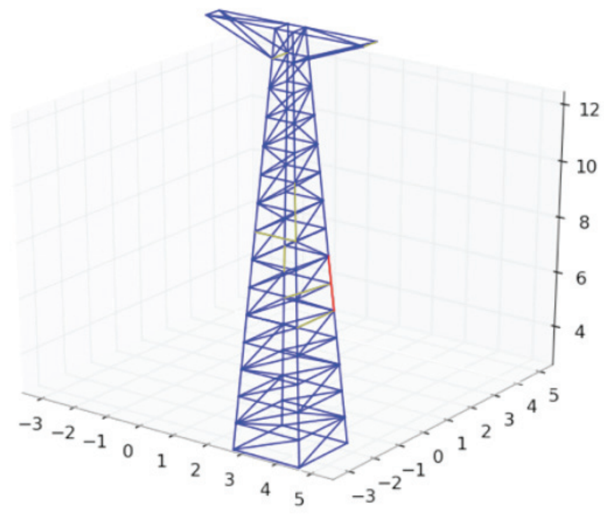

Fig. 1. *Truss structure*

scale, we represent the impulse structure of the earthquake in a standard way as a series of boxcar impulses with the magnitudes and timings of the boxcars being random variables. Moreover, the transfer function, defined by the structure of the earth, is also defined by some random components. The result of the earthquake is that the truss structure responds according to the response model, with the ground acceleration as input; the ground acceleration is determined by the random transfer function convolved with the random impulse model of the earthquake. So far, this is the standard methodology. Where our approach differs is that in the standard approach the random components are specified in terms of a large set of well-recognized distributions, such as Gaussians, by specifying their means and variances. We instead specify an independence structure and some simple bounds on the ranges and first moments of these random inputs. Figure 2 describes the optimal probability of failure as a function of the magnitude M for such an assumption set. The curve does not represent the probability of failure of the system, but an optimal upper bound on the probability of failure given this simple set of assumptions. Namely, there is a random model that satisfies these same assumptions but for which its probability of failure is at the value of this curve. The lower optimal bound is identically zero.

Now you may say "I don't like your assumptions!"—tell me what assumptions you do like and we will input them into our methodology and provide you with an optimal estimate of the probability of failure.

So how does this affect the modeling community? In [6] we are using this methodology to develop a comprehensive framework for uncertainty quantification for modeling, which includes, in addition to a comprehensive framework for validation, certification, and extrapolation, a scientifically rigorous approach to the problem of certification without testing.

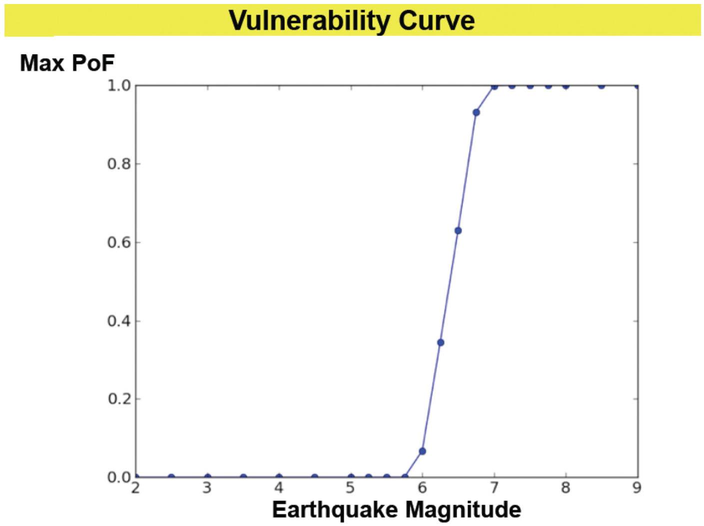

Fig. 2. Optimal upper bound on probability of failure –given the assumptions

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[2] Lucas, L.J. et al., *Comput Meth Appl Mech Eng* **197,** 4591; http://dx.doi.org/10.1016/j.cma.2008.06.008 (2008).
[3] Scovel, C. and I. Steinwart, LANL Technical Report LA-UR-10-02355; *J Complex* **26**, 641 (2010).
[4] Dewey, J., *Logic-Theory of Inquiry,* Henry Holt and Company (1938).
[5] Owhadi, H. et al., "Optimal Uncertainty Quantification," *SIAM Review*, resubmittal under review; http://arxiv.org/pdf/1009.0679v2 (2011).
[6] Scovel, C., "Uncertainty Quantification for Modeling," unpublished results (2012).

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