Optimal Uncertainty Quantification and Certification of Material Response

Tim Sullivan

tjs@caltech.edu

with D. Balzani, M. McKerns, M. Ortiz, H. Owhadi & C. Scovel

California Institute of Technology, Universität Duisburg-Essen
& Los Alamos National Laboratory

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Outline

Why Bother with Uncertainty Quantification? Being overly conservative may lead to huge economic losses, but being overly optimistic may lead to loss of life, environmental damage *& c.*

↑ Space Shuttle *Columbia*, 1 February 2003

↓ Eyjafjallajökull, Iceland, 27 March 2010

↓ Deepwater Horizon, 21 April 2010

Four Phases of Design

1. Just build it!
2. Build as best you can, or according to rules of thumb.
3. Build to meet/exceed the *deterministic* worst case scenario.
   e.g. Elishakoff & Ohsaki, *Optimization and Anti-Optimization of Structures Under Uncertainty* (2010)
4. Build with a quantitative probabilistic understanding of the uncertainties.
   Owhadi, Scovel, Sullivan, McKerns & Ortiz, "Optimal Uncertainty Quantification" (preprint, 2010)

The optimization problems that we consider can involve huge numbers of model evaluations; in practical applications they will rely upon — and stimulate — developments in parallel computing.

Types of Uncertainty

- Uncertainties are often divided into two types: epistemic and aleatoric uncertainties.
- An epistemic uncertainty is one that stems from a fundamental lack of knowledge — we don't know the rules that govern the problem. Epistemic uncertainties are potentially very hard to deal with.
- An aleatoric uncertainty is one that stems from intrinsic randomness in the system — a "roll of the dice". Aleatoric uncertainties are nicer than epistemic ones since we can, in principle, bring the tools of probability theory to bear.
- In practice, many apparently aleatoric uncertainties are epistemic: you know that some parameter X is randomly distributed in some set, but you don't know its probability distribution exactly.

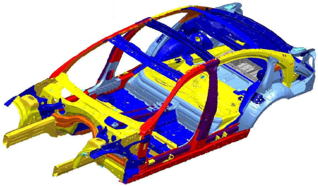
Example: Design of Multiphase Steels

Advanced High-Strength Steels (AHSS) offer many advantages in *e.g.* automobile construction:

- light-weight construction;
- enhanced crash safety.

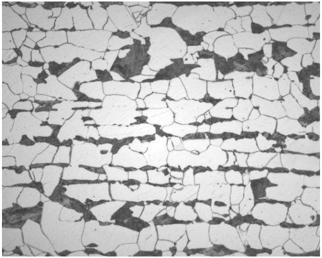
AHSS have complex microstructure, involving two or more phases, leading to a complex macroscopic response (anisotropy, kinematic hardening, *& c.*). Significant sources of uncertainty include:

- microstructure morphology;
- material properties of individual phases.



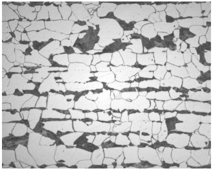
↑ From www.bmw.de

↓ Micrograph of DP steel



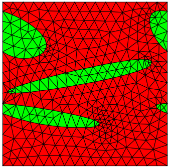
Description of the Material Problem

- We use a micro-macro approach: a microscopic BVP is solved at each macroscopic Gauss point; the microscopic BVP is posed on a statistically similar representative volume element (SSRVE).
- For simplicity, we will assume that there is no error in this model except for the statistical accuracy of the SSRVE.
  - Generalization → validation distance between computational code and physical reality.



↑ Micrograph

↑ SSRVE



↑ Meshed SSRVE

Description of the Material Problem

- Ferrite matrix phase with material parameters $\boldsymbol{y}_{\mathsf{mat}}$.
- Perlite or austenite inclusion phase with material parameters $\boldsymbol{y}_{\mathsf{inc}}$.
- Inclusion morphology described by a parameter γ.
  - Matrix-inclusion interface described by a collection of splines.
  - The number of splines, and their control points, are part of the parameter γ.
- By "statistical similarity", we mean that the simulated microstructure matches certain statistics of the real microstructure as seen in a scanned micrograph:
  - known ranges/mean values for the parameters $\boldsymbol{y}$ and γ;
  - known range/mean value for volume fraction $\mathcal{P}_V$ occupied by the inclusion phase;
  - higher-order probability functions.

Reliability and Certification

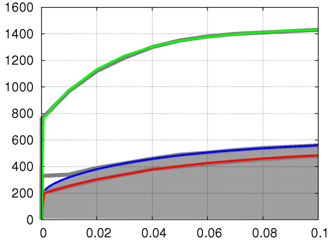
For simplicity, we choose a single scalar performance measure: the area under the (macroscopic) stress-strain curve in a uniaxial tension test:

$$G(\boldsymbol{\gamma}, \boldsymbol{y}) := \int_0^{1/10} \sigma(\epsilon, \boldsymbol{\gamma}, \boldsymbol{y}) \, \mathrm{d}\epsilon.$$

Given a performance threshold θ, we want to certify that the probability of failure

$$\mathbb{P}[G(\boldsymbol{\gamma}, \boldsymbol{y}) \leq \theta]$$

is acceptably small, with respect to the random variable $(\boldsymbol{\gamma}, \boldsymbol{y})$.



↑ Uniaxial test stress-strain curves for several different realizations of the microstructure parameters

Monte Carlo Certification

- Why not simply certify the probability of failure using a Monte Carlo method? That is, take a large number of samples, and see if the proportion of samples that fail is acceptably small?
- The problem is that if one wishes to certify that the probability of failure is it most p (and it is actually that small), then this method takes of the order of $\frac{1}{p^2} \log \frac{1}{p}$ samples — this clearly impractical if p is small.
  - For seismic safety of nuclear power plants, $p = 0$.
    Esteva (1970), Drenick, Wang, Yun & Philippacopoulos (1980)
  - In the aviation industry, the maximum acceptable probability of catastrophic failure per flight hour is 10^{-9}.
    Soekkha (1997), Boeing (2010)
  - US environmental standards for acceptable increased lifetime chance of developing cancer due to lifetime exposure to a substance: 10^{-6}.
    Mantel & Bryan (1961), Kelly (1993)

Optimal Uncertainty Quantification (OUQ)

The Optimal Uncertainty Quantification (OUQ) framework takes a different approach: we try to give the sharpest bounds on the probability of failure given what we know about the uncertainties.

- Generalized system of interest: an unknown function G of random inputs X, which have an unknown probability distribution $\mathbb{P}$.
- Write down all the information that you have about the uncertainties, be they aleatoric or epistemic. *E.g.* for $G(X_1, X_2)$
  - X_1 and X_2 are independent;
  - $X_1 \in [0, 1]$, $X_2 \geq 0$;
  - G is smooth and $\|\nabla G\| \leq 2$;
  - $\mathbb{E}[G(X_1, X_2)] = 3$.
- Now optimize (minimize and maximize) the probability of failure over the collection $\mathcal{A}$ of all admissible scenarios (f, μ) that are consistent with this information about $(G, \mathbb{P})$ *i.e.* any $(f, \mu) \in \mathcal{A}$ could be $(G, \mathbb{P})$.

OUQ for the Material Problem

- For simplicty, we'll assume that our computational model is exact.
- Let $\mathcal{A}$ denote the set of all measures μ on pairs $(\boldsymbol{\gamma}, \boldsymbol{y})$ that are consistent with all given information about the real microstructure.
- We ask, what are the minimum and maximum probabilities of failure

$$\mu[G(\boldsymbol{\gamma}, \boldsymbol{y}) \leq \theta] \text{ with respect to } \mu \in \mathcal{A}?$$

- Hence, we obtain the double inequality

$$\inf_{\mu \in \mathcal{A}} \mu[G(\boldsymbol{\gamma}, \boldsymbol{y}) \leq \theta] \leq \mathbb{P}[G(\boldsymbol{\gamma}, \boldsymbol{y}) \leq \theta] \leq \sup_{\mu \in \mathcal{A}} \mu[G(\boldsymbol{\gamma}, \boldsymbol{y}) \leq \theta],$$

  which is the sharpest possible conservative bound on the probability of failure given the information encoded in $\mathcal{A}$.
- Note that more information $\implies$ more constraints $\implies$ a smaller feasible set $\mathcal{A}$ $\implies$ sharper bounds.

$\mathcal{A}$ for the Material Problem

- Bounds constraints for basic variables:

$$\boldsymbol{\gamma} \in [\boldsymbol{\gamma}^-, \boldsymbol{\gamma}^+],$$
$$\boldsymbol{y}_{\mathsf{inc}} \in [\boldsymbol{y}_{\mathsf{inc}}^-, \boldsymbol{y}_{\mathsf{inc}}^+],$$
$$\boldsymbol{y}_{\mathsf{mat}} \in [\boldsymbol{y}_{\mathsf{mat}}^-, \boldsymbol{y}_{\mathsf{mat}}^+].$$

- Bounds constraints for microstructure statistics:

volume fraction of inclusion phase: $\mathcal{P}_V(\boldsymbol{\gamma}, \boldsymbol{y}) \in [\mathcal{P}_V^-, \mathcal{P}_V^+]$.

- Mean constraint for microstructure statistics:

volume fraction of inclusion phase: $\mathbb{E}_\mu[\mathcal{P}_V(\boldsymbol{\gamma}, \boldsymbol{y})] = \overline{\mathcal{P}_V}$.

- Additional technical constraints:

the individual inclusion phases are not allowed to intersect each other.

Reduction of OUQ Problems

OUQ optimization problems are made tractable by reduction theorems like the following: Owhadi *& al.* (2010)

Theorem

Suppose that $\mathcal{A}$ is given by n linear inequalities on generalized moments of μ: for some $h_1, \dots, h_n \colon \Gamma \times Y \to \mathbb{R}$,

$$\mathcal{A} := \left\{ \mu \,\middle|\, \mathbb{E}_\mu[h_1(\boldsymbol{\gamma}, \boldsymbol{y})] \leq 0, \dots, \mathbb{E}_\mu[h_n(\boldsymbol{\gamma}, \boldsymbol{y})] \leq 0 \right\}.$$

Let

$$\mathcal{A}_\Delta := \left\{ \mu \in \mathcal{A} \,\middle|\, \begin{array}{c} \mu = \sum_{i=0}^{n} \alpha_i \delta_{(\boldsymbol{\gamma}_i, \boldsymbol{y}_i)} \\ \text{for some } \alpha_i \geq 0, (\boldsymbol{\gamma}_i, \boldsymbol{y}_i) \in \Gamma \times Y, \\ \sum_{i=0}^{n} \alpha_i = 1 \end{array} \right\}.$$

Then

$$\sup_{\mu \in \mathcal{A}} \mu[G(\boldsymbol{\gamma}, \boldsymbol{y}) \leq \theta] = \sup_{\mu \in \mathcal{A}_\Delta} \mu[G(\boldsymbol{\gamma}, \boldsymbol{y}) \leq \theta].$$

Reduction of OUQ Problems

The moral of the reduction theorem is

> *"If your random variables are constrained by n linear inequalities on moments, then you can pretend that they're discrete random variables with at most $n + 1$ values."*

- This is great news, because such variables have a finite-dimensional parametrization, and the probability of failure, mean performance *& c.* are very easy to calculate.
- In contrast to deterministic worst-case design, in which we seek a single worst-case scenario $(\boldsymbol{\gamma}_0, \boldsymbol{y}_0)$, we seek a worst-case ensemble of scenarios $(\boldsymbol{\gamma}_0, \boldsymbol{y}_0)$, . . . , $(\boldsymbol{\gamma}_n, \boldsymbol{y}_n)$ with probabilities α_0, . . . , α_n that sum to unity and obey the given constraints in a statistical sense.

The Fruits of OUQ

- The (approximate) extremizers of OUQ problems are very singular, but they capture very important information: they illustrate the critical vulnerabilities of the system given your current state of knowledge.
- Traditional UQ methods often make strong assumptions about the structure of the problem (*e.g.* known priors, rapid spectral decay, sub-Gaussian tails, . . .) and it can be very difficult to "play" with those assumptions to see if your conclusions are robust with respct to them.
- Contrarily, by placing information/assumptions/constraints at the centre of the problem, OUQ is very amenable to this kind of robustness analysis.

Hypervelocity Impact Example

- We *expect* that the multiphase steel example with have similar features to a hypervelocity impact example that has been studied extensively using the OUQ method.
- In this example, the variables are the speed of the incoming projectile, the thickness of the target plate, and the obliquity of the impact.
- Again, the constraints are bounds constraints on the three variables, and a mean constraint (the mean perforation area); failure is non-perforation.
- In the following graphics, note that the key uncertainty is the plate thickness, not velocity nor obliquity.

Convergence of Reduced Optimization Variables

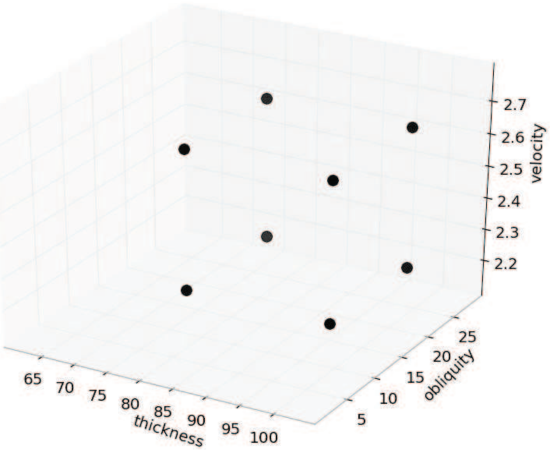


Figure: Support of the $2 \times 2 \times 2$-point measure μ at iteration 0.

Convergence of Reduced Optimization Variables

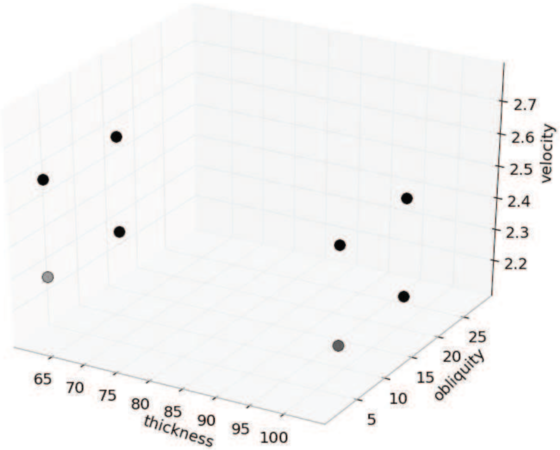


Figure: Support of the $2 \times 2 \times 2$-point measure μ at iteration 150.

Convergence of Reduced Optimization Variables

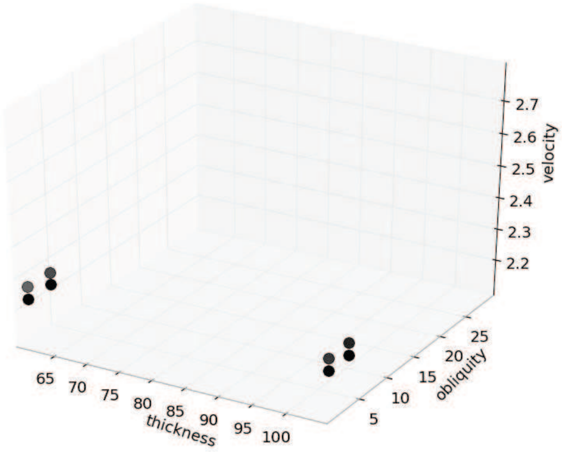


Figure: Support of the $2 \times 2 \times 2$-point measure μ at iteration 200.

Convergence of Reduced Optimization Variables

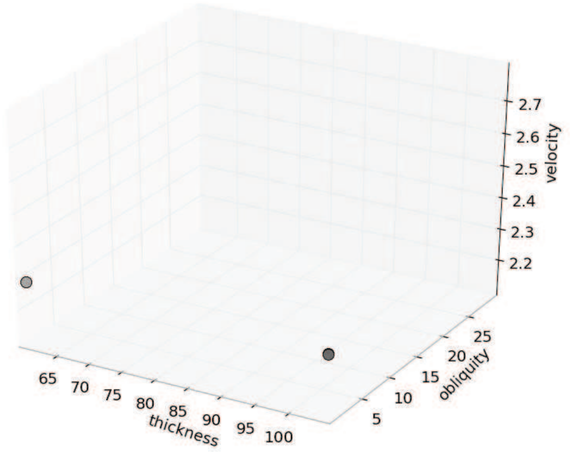
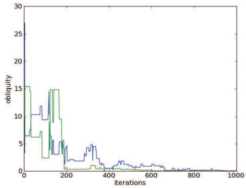
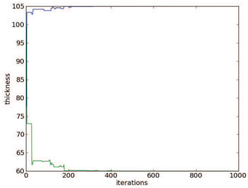


Figure: Support of the $2 \times 2 \times 2$-point measure μ at iteration 1000.

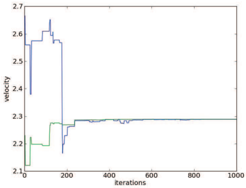
Numerical Convergence



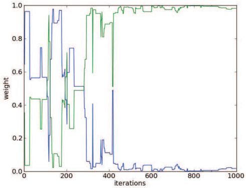
(a) oblquity positions



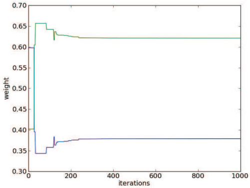
(b) thickness positions



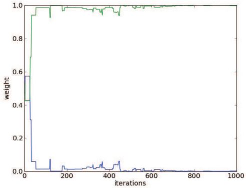
(c) velocity positions



(d) obliquity masses



(e) thickness masses



(f) velocity masses

Application to Earthquake Engineering

- We consider the elastic response of a truss structure to a random earthquake. The material properties of the structure are assumed to be known, but could also be part of an extended OUQ analysis.
- The key ingredient is the information on the ground motion acceleration, which is the time convolution of the earthquake source s with a (perhaps known, perhaps not) transfer function ψ. How to represent these?
- We assume that s is a sum of boxcar time impulses (step functions) of indepenendent durations $\tau_{\min} \leq \tau_i \leq \tau_{\max}$, independent unit directions in $\mathbb{R}^3$, and independent magnitudes $0 \leq X_i \leq a_{\max}$ — use *e.g.* Esteva (1970)'s semi-empirical law

$$a_{\max} := \frac{a_0 e^{\lambda M_{\mathsf{Richter}}}}{(R_0 + R)^2}$$

Application to Earthquake Engineering

- Similarly, express the transfer function ψ in a Fourier/wavelet expansion with coefficients that are free to vary according to whatever information is known — *e.g.* total duration, corellations between nearby coefficients, *& c.*
- Note that, in the absence of strong enough constraints, the OUQ solution will coincide with deterministic worst-case analysis.
  - Drenick (1973): a seismic design based on critical excitation could be "far too pessimistic to be practical".
- With more information (interaction among experts, $\mathcal{A}$, and the OUQ results), we identify the "worst" structures, earthquakes, and transfer functions.

Conclusions

- Optimal UQ is a new UQ method that places information at the centre of the UQ problem.
- By doing so, we can obtain rigorous and sharp bounds on probabilities of failure, in a way that is very robust with respect to rare events and with easily perturbed assumptions.
- The computation of these extrema is facilitated by powerful reduction theorems. The (reduced) extrema carry important information about the vulnerabilities of the system.

Outlook

- How can statistical information of a higher order than the volume fraction (*e.g.* 2-point probability functions, lineal path functions, spectra) be incorporated, while keeping the optimization problems relatively inexpensive?
- Other OUQ applications now under investigation:
  - hypervelocity impact;
  - safety of structures under earthquakes;
  - inverse problems for random media;
  - data-on-demand *vs* legacy data.
- UQ in general, and OUQ in particular, should be seen as a "wrapper" to put around any problem of interest, especially high-consequence ones.