Optimal Uncertainty Quantification

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The Quantification of Margins and Uncertainties (QMU) Paradigm

• Aim: *Predict mean performance and uncertainty in the behavior of complex physical/engineered systems*

• *Paradigm shift* in experimental science, modeling and simulation, scientific computing (*predictive science*):
  – Deterministic → Non-deterministic systems
  – Mean performance → Mean performance + Uncertainty
What is QMU?: Certification view

- Certification: PoF of the system below tolerance,

\[ \mathbb{P}[\text{failure}] = \mathbb{P}[y \notin A] \leq \varepsilon \]

- Exact probability of failure:

\[ \mathbb{P}[\text{failure}] = \int \left\{ \begin{array}{ll} 0, & \text{if } f(x) \in A \\ 1, & \text{if } f(x) \notin A \end{array} \right\} d\mu(x) \]
QMU – A simple truss example

- System input: Applied force \( (P) \)
- System output: Tip deflection \( (\delta) \)
- Response function \((f)\): Energy minimization, static equilibrium
- Failure criterion: \( \delta > \text{threshold} \)
- To compute: 

\[
P[\text{failure}] = \int \left\{ \begin{array}{ll} 0, & \text{if } \delta < \delta_{\text{max}} \\ 1, & \text{if } \delta \geq \delta_{\text{max}} \end{array} \right\} d\mu(P)
\]
QMU – A simple truss example

- Assume: Deterministic response, known probability distribution of inputs

\[ \delta = f(P) \]

1-PoF
QMU – A simple truss example

• Assume: Stochastic response function, known probability distribution of inputs

\[
\text{PoF} = \int \text{PoF}(\omega) d\nu(\omega)
\]

\[
\delta = f(P, \omega)
\]

unknown unknowns!
Certification: PoF of the system below tolerance,

\[ P[\text{failure}] = P[y \not\in A] \leq \epsilon \]

Exact probability of failure:

\[ P[\text{failure}] = \int \left\{ \begin{array}{ll} 0, & \text{if } f(x) \in A \\ 1, & \text{if } f(x) \not\in A \end{array} \right\} d\mu(x) \]
QMU – Essential difficulties

- Input space of high dimension, unknown unknowns
- Probability distribution of inputs not known in general
- System response stochastic, not known in general
- Models are inaccurate, partially verified & validated
- System performance cannot be tested on demand
- Legacy data incomplete, inconsistent, and noisy
- Failure events rare, high consequence decisions…
QMU – Conservative certification

- Conservative certification: **Upper bound** on the PoF of the system below tolerance,

\[
P[\text{failure}] = P[y \notin A] \leq \text{upper bound} \leq \epsilon
\]

- **Problem**: Obtain **tight** (optimal?) PoF upper bounds from all information known about the system...
Optimal Uncertainty Quantification

- **Wanted**: $\mathbb{P}[^{\text{failure}}] = E_\mu[\{f \in A\}]$
- **Assume information about** $(\mu, f)$: Data, models...
- **Admissible set**: $A = \{(\mu, f) \text{ compatible with info}\}$
- **Optimal PoF bounds given** $A$:
  $$\inf_{(\mu,f) \in A} E_\mu[\{f \in A\}] \leq \text{PoF} \leq \sup_{(\mu,f) \in A} E_\mu[\{f \in A\}]$$

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Theorem [Owhadi et al. (2011)] Suppose that
\[ A = \left\{ (\mu, f) \mid \text{some conditions on } f \text{ alone} \right\} \]
\[ \mathbb{E}_\mu[\varphi_1] \leq 0, \ldots, \mathbb{E}_\mu[\varphi_n] \leq 0 \}

Let:
\[ A_{\text{red}} = \left\{ (\mu, f) \in A \mid \mu = \sum_{i=1}^n \alpha_i \delta_{x_i}, \alpha_i \geq 0, \sum_{i=1}^n \alpha_i = 1 \right\} \]

Then:
\[ \inf_{(\mu, f) \in A} \mathbb{E}_\mu[\{f \in A\}] = \inf_{(\mu, f) \in A_{\text{red}}} \mathbb{E}_\mu[\{f \in A\}] \]
\[ \sup_{(\mu, f) \in A} \mathbb{E}_\mu[\{f \in A\}] = \sup_{(\mu, f) \in A_{\text{red}}} \mathbb{E}_\mu[\{f \in A\}] \]

• OUQ problem is reduced to optimization over finite-dimensional space of measures: Program feasible!

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Example – Certifying lethality in terminal ballistics

- Thickness ($h$)
- Obliquity ($\theta$)
- Impact velocity ($v$)
- Impactor material (steel, nylon…)
- Target material (Al, Fe, Ta…)

system output

f

system inputs

Caltech’s SPHIR facility

perforation area (profilometry)

threshold

failure

perforation area

ballistic limit

impact velocity

$$f(h, \theta, v) = K \left(\frac{h}{D}\right)^p \cos^q(\theta) \tanh^r \left(\frac{v}{v_0} - 1\right)$$

$$v_0 = V_0 \left(\frac{h}{D}\right)^m \cos^n(\theta)$$

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Example – Certifying lethality

\( f \quad (h, \theta, v) \in \mathcal{X} \equiv \mathcal{X}_1 \times \mathcal{X}_2 \times \mathcal{X}_3 \)

\( h \in \mathcal{X}_1 \equiv [1.524, 2.667] \text{ mm} \)

\( \theta \in \mathcal{X}_2 \equiv [0, \frac{\pi}{6}] \)

\( v \in \mathcal{X}_3 \equiv [2.1, 2.8] \text{ km s}^{-1} \)

- **Admissible set:**
  \[ \mathcal{A} \equiv \left\{ (f, \mu) \left| \begin{array}{c}
  f \text{ known exactly, } \\
  \mu = \mu_1 \otimes \mu_2 \otimes \mu_3, \\
  5.5 \text{mm}^2 \leq \mathbb{E}_\mu[f] \leq 7.5 \text{mm}^2
\end{array} \right. \right\} \]

- **Reduced admissible set:**
  \[ \mathcal{A}_{\text{red}} \equiv \left\{ (f, \mu) \left| \begin{array}{c}
  f \text{ known exactly, } \\
  \mu = \mu_1 \otimes \mu_2 \otimes \mu_3, \\
  \mu_i = \alpha_i \delta_{a_i} + (1 - \alpha_i) \delta_{b_i}, \quad i = 1, 2, 3, \\
  5.5 \text{mm}^2 \leq \mathbb{E}_\mu[f] \leq 7.5 \text{mm}^2
\end{array} \right. \right\} \]
Example – Certifying lethality

- Evolution of support of reduced probability measure:
Example – Certifying lethality

Caltech’s SPHIR facility

\( (h, \theta, v) \in \mathcal{X} \equiv \mathcal{X}_1 \times \mathcal{X}_2 \times \mathcal{X}_3 \)

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- Reduced admissible set:

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  5.5 \text{mm}^2 \leq \mathbb{E}_\mu[f] \leq 7.5 \text{mm}^2
\end{array} \right\}
\]

- Optimal PoF upper bound:

\[
\sup_{(\mu, f) \in \mathcal{A}} \mathbb{E}_\mu[\{f = 0\}] = \sup_{(\mu, f) \in \mathcal{A}_{\text{red}}} \mathbb{E}_\mu[\{f = 0\}] = 37.9\%
\]

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Example – Seismic risk assessment

Simulation of seismic waves from rupture initiating at Parkfield, central California, and propagating over Los Angeles basin (http://krishnan.caltech.edu/krishnan/res.html)

3D truss structure of power-line tower
Example – Seismic risk assessment

• Ground motion acceleration:
  \[ \ddot{u}_0(t) = (\psi \ast s)(t) \]
  where: \( s(t) \equiv \) Source activity
  \( \psi(t) \equiv \) Transfer function

• Structural response:
  \[ M\ddot{u} + C\dot{u} + Ku = -MT\ddot{u}_0(t) \]

• Failure criterion: \( f \leq 0 \), where
  \[ f = \min_{i \in \text{members}} \left\{ \sigma_y - \max_{t \geq 0} |\sigma_i(t)| \right\} \]
Example – Seismic risk assessment

- Assumptions on source term \( s(t) \):
  - Piecewise constant (boxcar) in time
  - Random amplitudes in \([-a_{\text{max}}, a_{\text{max}}]\) (given by Richter magnitude \( M \)) with zero mean
  - Random time interval durations with bounded mean

- Assumptions on transfer function \( \psi(t) \):
  - Piecewise linear in time
  - Random amplitudes with zero mean, bounded \( L^2 \) norm

- Reduced OUQ problem: Global optimization in 179 dimensions

- One PoF calculation takes \( O(24 \text{ hrs}) \) on \( O(1000) \) AMD opteron cluster
Optimal PoF upper and lower bounds for steel tower vs. Richter scale magnitude $M$ at hypocentral distance $R=25$ km, $(a_{\text{max}}$ given by Esteva's semi-empirical expression as a function of $M$)
OUQ with diameter data

- Question: How is $\mathcal{A}$ to be defined? What type of data on system response leads to effective UQ?

- Oscillation of a function of one variable:
  \[
  \text{osc}(f, E) = \sup_{x \in E} f(x) - \inf_{x \in E} f(x) = \sup_{x, x' \in E} |f(x) - f(x')|
  \]

- Function subdiameters:
  \[
  f : E \subset \mathbb{R}^N \rightarrow \mathbb{R}, \quad D_i(f, E) = \sup_{\hat{x}_i \in \mathbb{R}^{N-1}} \text{osc}(f, E \cap \{\hat{x}_i\}), \quad \hat{x}_i = \{x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_N\}
  \]

possibly unknown unknowns! global optimization!

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OUQ with diameter data

- Admissible set for diameter data with scatter:

\[
A \equiv \left\{ (f, \mu) \mid \begin{array}{l}
D_i(f, x) \leq D_i, \ i = 1, \ldots, n \\
\mu = \mu_1 \otimes \cdots \otimes \mu_n,
\end{array}
\right\}
\]

\[
\begin{align*}
& m_1 \leq \mathbb{E}_\mu[f] \leq m_2 \\
& D_z \leq D_i(f, x) - \mathbb{E}_\mu[f], \ i = 1, \ldots, n
\end{align*}
\]
OUQ with diameter data

- **OUQ problem explicitly solvable in low dimension!**

- **For** $n = 2$: 
  
  $$
  \sup_{(\mu, f) \in A} \mathbb{E}_\mu[\{f \leq 0\}] =
  \begin{cases}
  0, & \text{if } D_1 + D_2 \leq \mathbb{E}_\mu[f] \\
  \frac{(D_1 + D_2 - \mathbb{E}_\mu[f])^2}{4D_1D_2}, & \text{if } |D_1 - D_2| \leq \mathbb{E}_\mu[f] \leq D_1 + D_2 \\
  1 - \frac{\mathbb{E}_\mu[f]}{\max(D_1, D_2)}, & \text{if } 0 \leq \mathbb{E}_\mu[f] \leq |D_1 - D_2|
  \end{cases}
  $$
Model-based OUQ with diameter data

system inputs $x_1$  

unknown unknowns! $z$

system (black box) $f, g$

system outputs $y_1$  

$y_2$

Probability $(\mu)$

- Diameters $D_i(f)$ define seminorms of $f$.
- From the triangular inequality,

$$D_i(f) \leq D_i(g) + D_i(f - g)$$

- model diameter
- modeling error

safe set $A$
Model-based QMU – McDiarmid

- Working assumptions:
  - $f-g$ far more regular than $f$ or $g$ alone
  - Global optimization for $D(f-g)$ converges fast
  - Evaluation of $D(f-g)$ requires few experiments
Model-based QMU – McDiarmid

- Calculation of $D(f)$ requires exercising model only
- Uncertainty Quantification burden mostly shifted to modeling and simulation!

- Evaluation of $D(f-g)$ requires few experiments
- Rigorous certification not achievable by modeling and simulation alone!
Case Study – Steel/Al ballistics

- Target/projectile materials:
  - Target: Al 6061-T6 plates (6”x 6”)
  - Projectile: S2 Tool steel balls (5/16”)
- Model input parameters ($x$):
  - Plate thickness (0.032”-0.063”)
  - Impact velocity (200-400 m/s)
Case Study – Steel/Al ballistics

Perforation area vs. impact velocity (note small data scatter!)

- System output (y): **Perforation area**!
- Certification criterion: \( y > 0 \) (lethality)
Lagrangian solver: Optimal-Transportation Meshfree (OTM)

• Time integration (OT):
  – Optimal transportation methods:
    • Geometrically exact, discrete Lagrangians
  – Discrete mechanics, variational time integrators:
    • Symplecticity, exact conservation properties
  – Variational material updates, inelasticity:
    • Incremental variational structure

• Spatial discretization (M):
  – Max-ent meshfree nodal interpolation:
    • Kronecker-delta property at boundary
  – Material-point sampling:
    • Numerical quadrature, material history
  – Dynamic reconnection, ‘on-the-fly’ adaptivity
Case Study – OTM modeling error

Measured vs. computed perforation area

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Case study – Terminal ballistics

Model diameter $D(g)$

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>thickness</td>
<td>4.33 mm²</td>
</tr>
<tr>
<td>velocity</td>
<td>4.49 mm²</td>
</tr>
<tr>
<td>RMS</td>
<td>6.24 mm²</td>
</tr>
</tbody>
</table>

Modeling error $D(f-g)$

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>thickness</td>
<td>4.96 mm²</td>
</tr>
<tr>
<td>velocity</td>
<td>2.16 mm²</td>
</tr>
<tr>
<td>RMS</td>
<td>5.41 mm²</td>
</tr>
</tbody>
</table>

Uncertainty $D(g) + D(f-g)$

- 11.65 mm²

Empirical mean $E[f]$

- 47.77 mm²

- Perforation can be certified with 99.9% confidence!
- Total number of experiments ~ 50 → Approach feasible!
Concluding remarks…

• Rigorous and conservative certification can be achieved by means of PoF upper bounds!

• PoF bounds ‘fold in’ all information available on the system (experimental data, V&V’d physics models…)

• PoF bounds are similar in spirit to bounds on effective moduli of elastic composites (which cannot be obtained exactly in general from existing data on the composite)

• However: Bounds can be suboptimal (e.g., Voigt, Reuss…) and result in excessive conservatism

• It possible to compute optimal PoF bounds (for given information about the system): Optimal Uncertainty Quantification! (OUQ)
Concluding remarks – Systems view of Computational Mechanics…

Orchestration

QMU

Solvers (FE, CFD)

Material Points


Assembly

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Concluding remarks – Disciplinary view of QMU and Predictive Science
Concluding remarks...

Thank you!