Optimal Uncertainty Quantification

M. Ortiz
California Institute of Technology

Advanced Computational Engineering Workshop
Oberwolfach (Germany) Feb 12-18, 2012

ASC/PSAAP Centers

CALTECH PSAAP

STANFORD UNIVERSITY PSAAP

California Institute of Technology 1891

PRISM
NNSA Center for Prediction of Reliability, Integrity and Survivability of Microsystems

PURDUE UNIVERSITY

CALTECH PSAAP

Center for Radiative Shock Hydrodynamics

MICHIGAN

ICES
The Institute for Computational Engineering and Sciences

THE UNIVERSITY OF TEXAS AT AUSTIN

M. Ortiz

PSAAP: Predictive Science Academic Alliance Program

Caltech Center Team

CALTECH PSAAP

Experimental

A. Rosakis
G. Ravichandran
M. Adams
J. Mihaly
J. Brown
L. Bodelot
A. Kidane
K. John

Software

M. Aivazis
M. Stalzer
M. McKerns
S. Brunett
J. Cummings
J. Lindheim
S. Lombeyda
B. Li
L. Strand

Management

M. Ortiz
M. Stalzer

UQ

H. Owhadi
T. J. Sullivan
M. McKerns
B. Li
C. Scovel (LANL)

Fluids

D. Meiron
D. Pullin
P. Barton
J. Cummings
G. Ward
A. L. Ortega

Solids

M. Ortiz
K. Bhattacharya
W. A. Goddard III
A. van de Walle
A. Pandolfi
A. Jaramillo-Botero
J. Amelang
L. Djodom Fokuoa
A. Kowalski
X. Wang
A. Richards
L. Miljacic
B. Li
A. Bompadre
S. Demers
P. Theofanis
J. Tahir-Kheli
P. Cesana
L. Perotti
D. Kochmann

The Quantification of Margins and Uncertainties (QMU) Paradigm

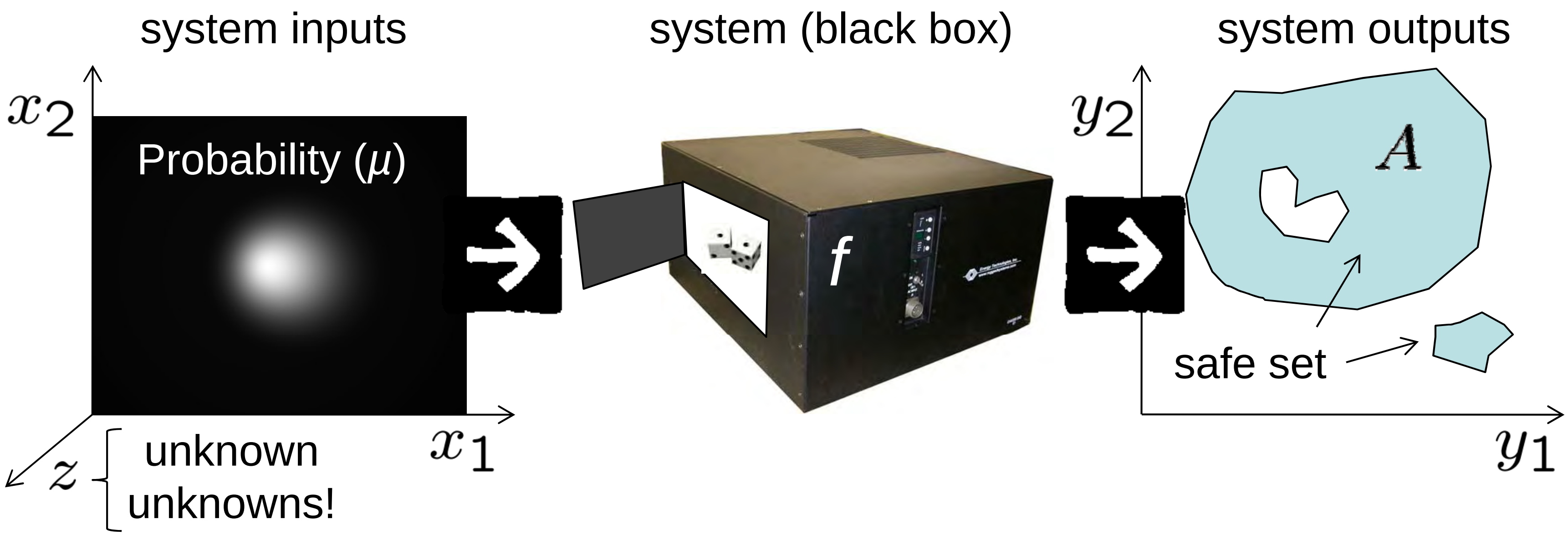
CALTECH PSAAP

- 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

Old single-calculation paradigm

New ensemble-of-calculations paradigm (QMU)

What is QMU?: Certification view



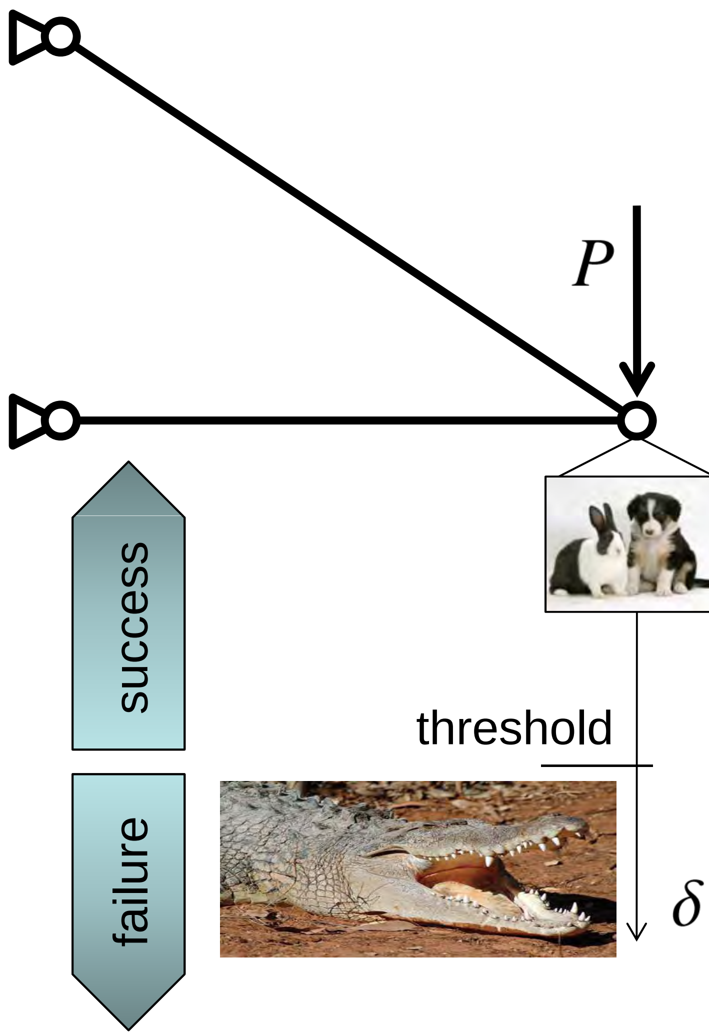
- Certification: PoF of the system below tolerance,

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

- 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



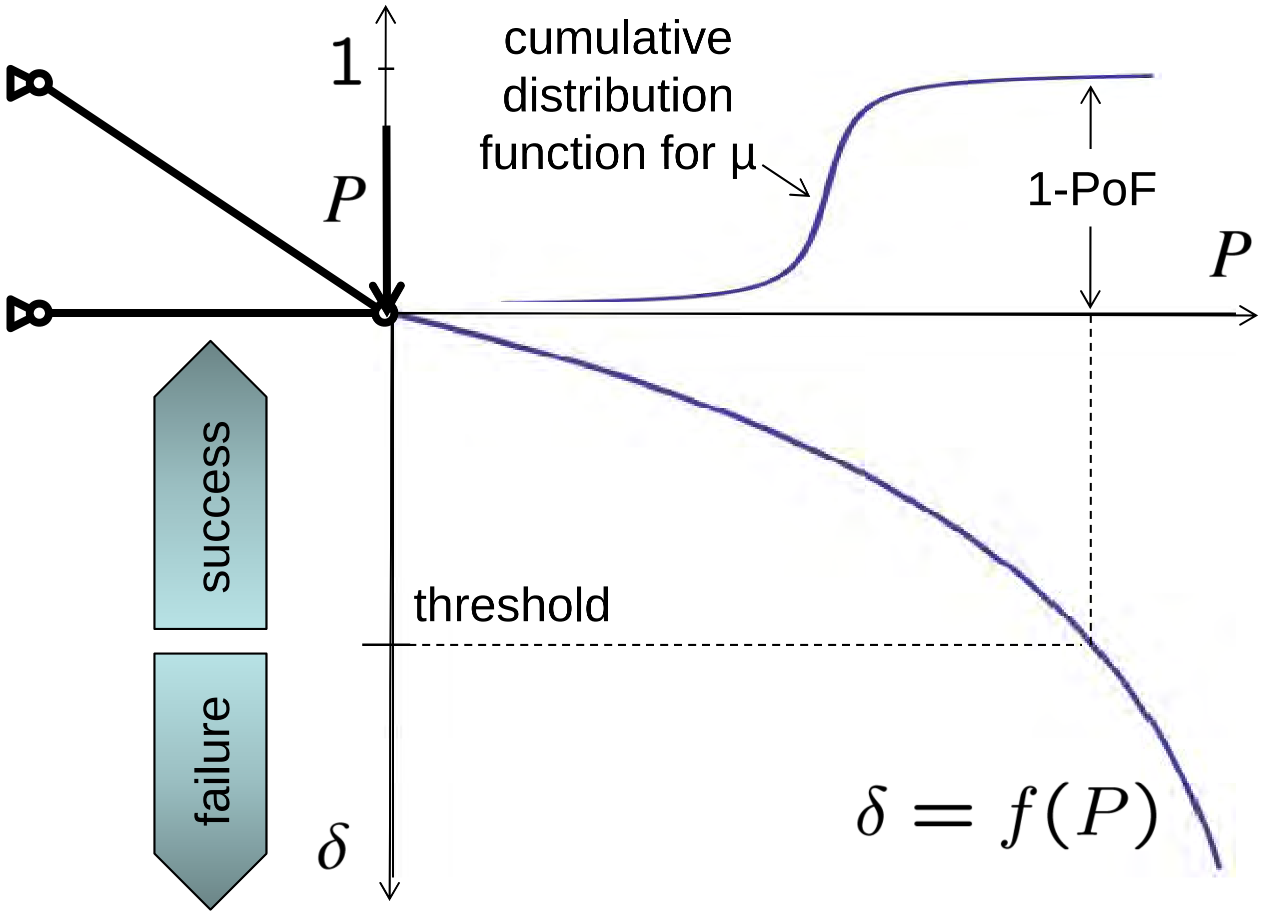
- System input: Applied force (*P)*
- System output: Tip deflection (*δ*)
- Response function (*f*): Energy minimization, static equilibrium
- Failure criterion: *δ* > threshold
- To compute: $\mathbb{P}[\text{failure}] =$

$$\int \left\{ \begin{array}{ll} 0, & \text{if } \delta < \delta_{\text{max}} \\ 1, & \text{if } \delta \geq \delta_{\text{max}} \end{array} \right\} d\mu(P)$$

M. Ortiz

QMU – A simple truss example

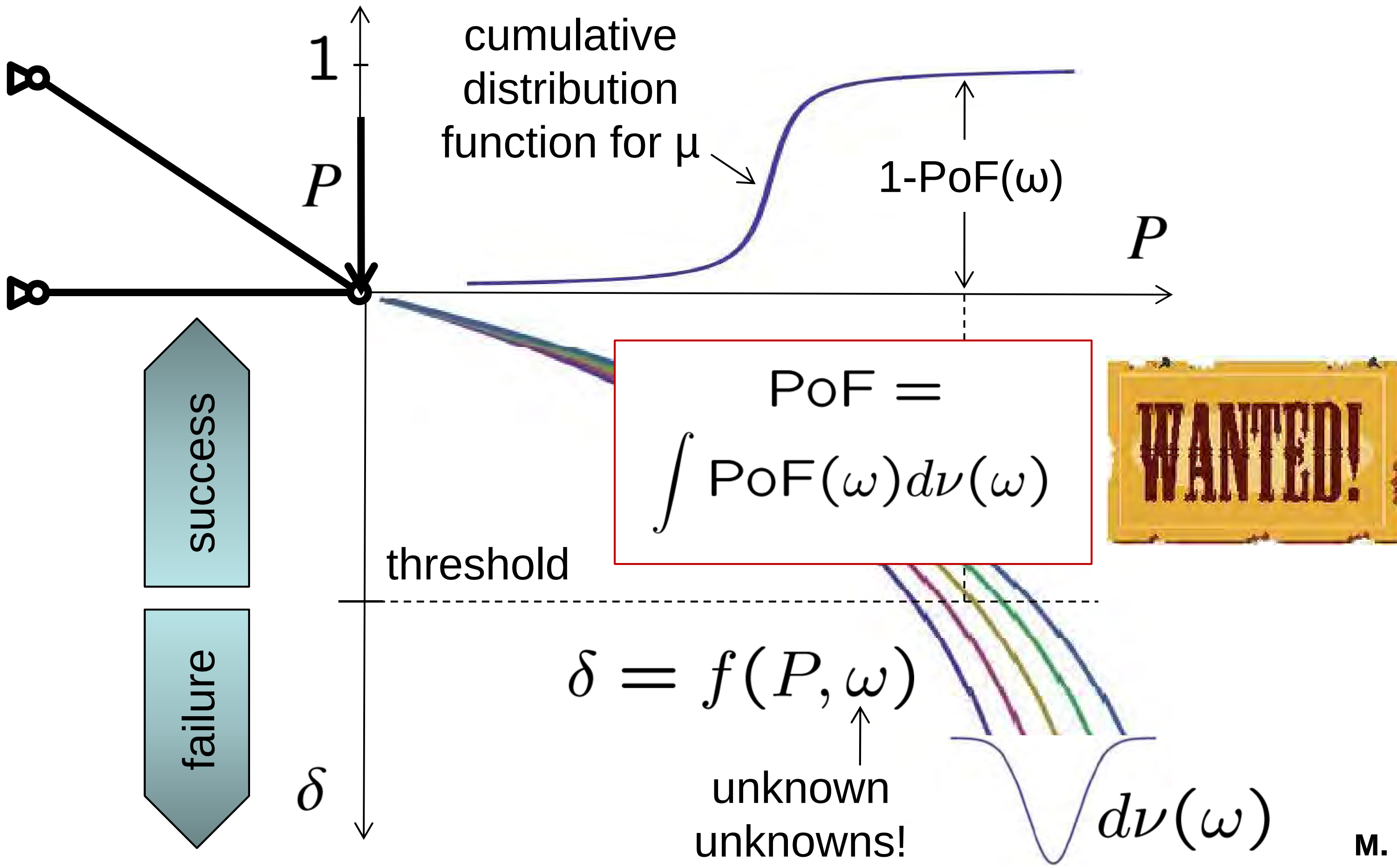
- Assume: Deterministic response, known probability distribution of inputs



QMU – A simple truss example

CALTECH PSAAP

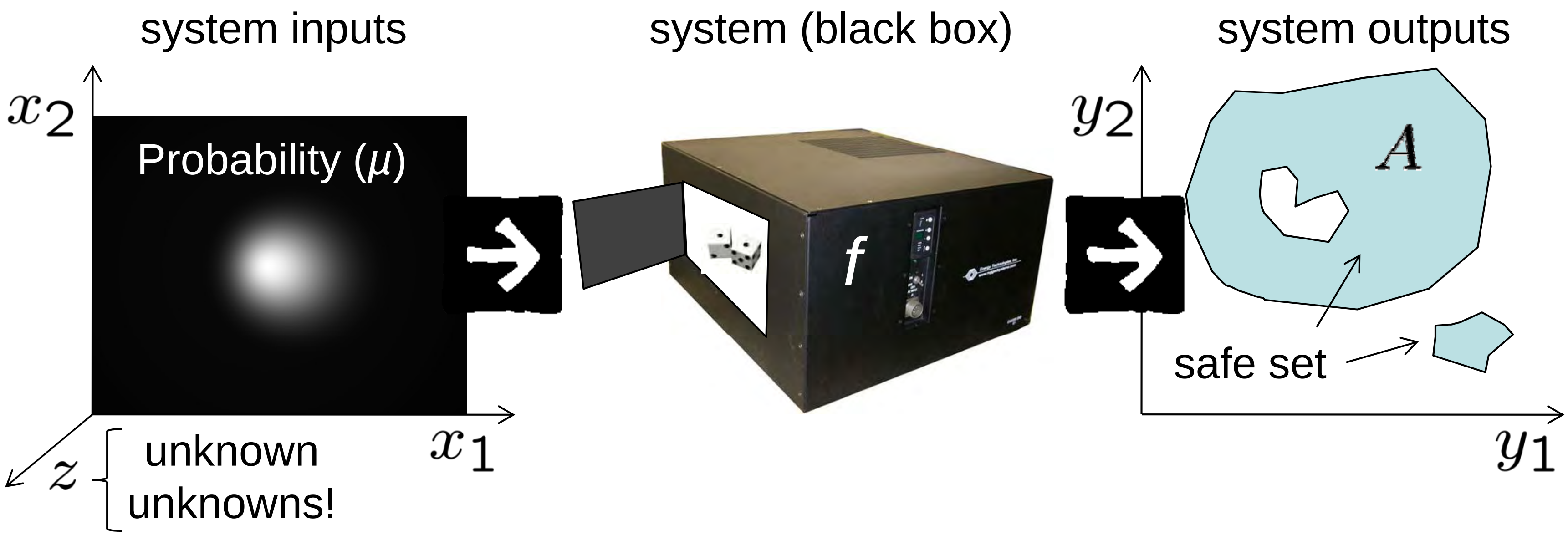
- Assume: Stochastic response function, known probability distribution of inputs



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

M. Ortiz

QMU – Certification view



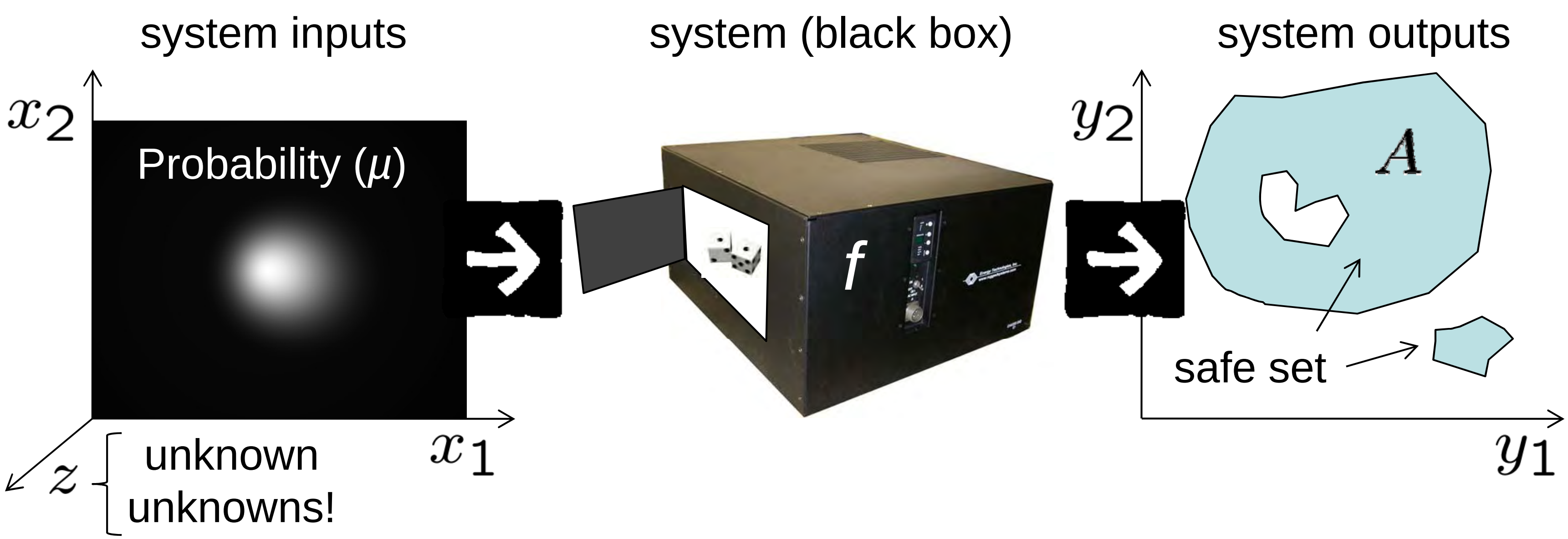
- Certification: PoF of the system below tolerance,

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

- Exact probability of failure:

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

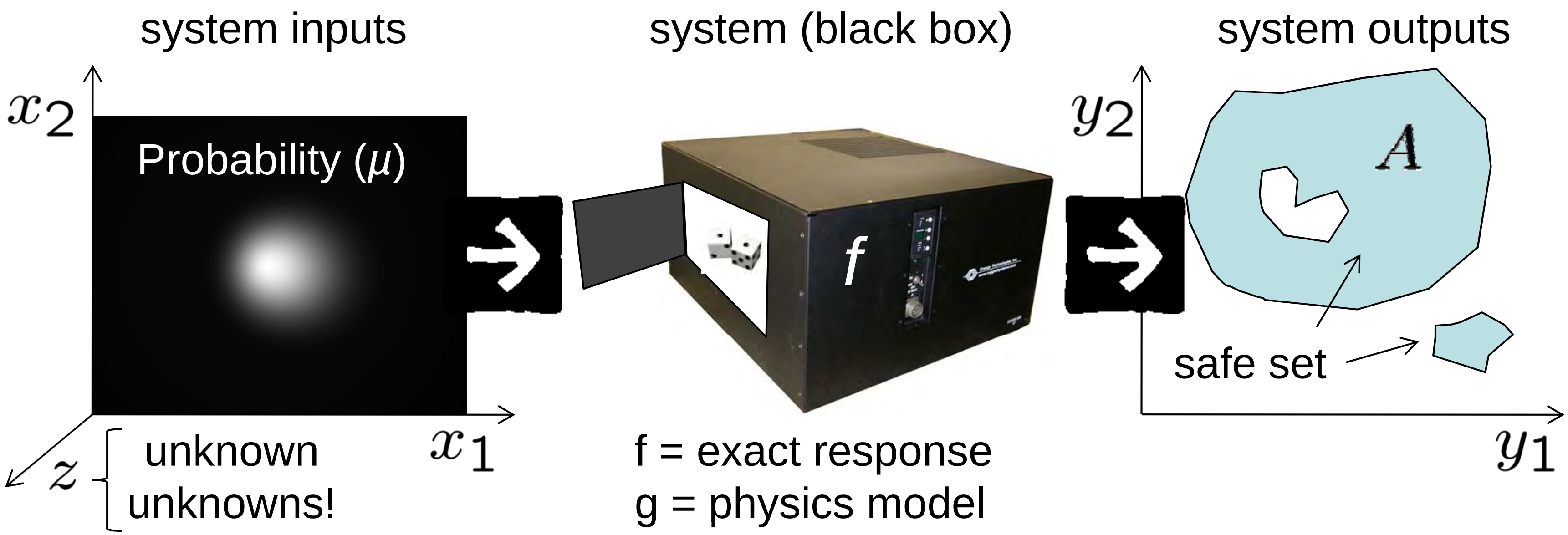
QMU – Essential difficulties



- 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…

M. Ortiz

QMU – Conservative certification



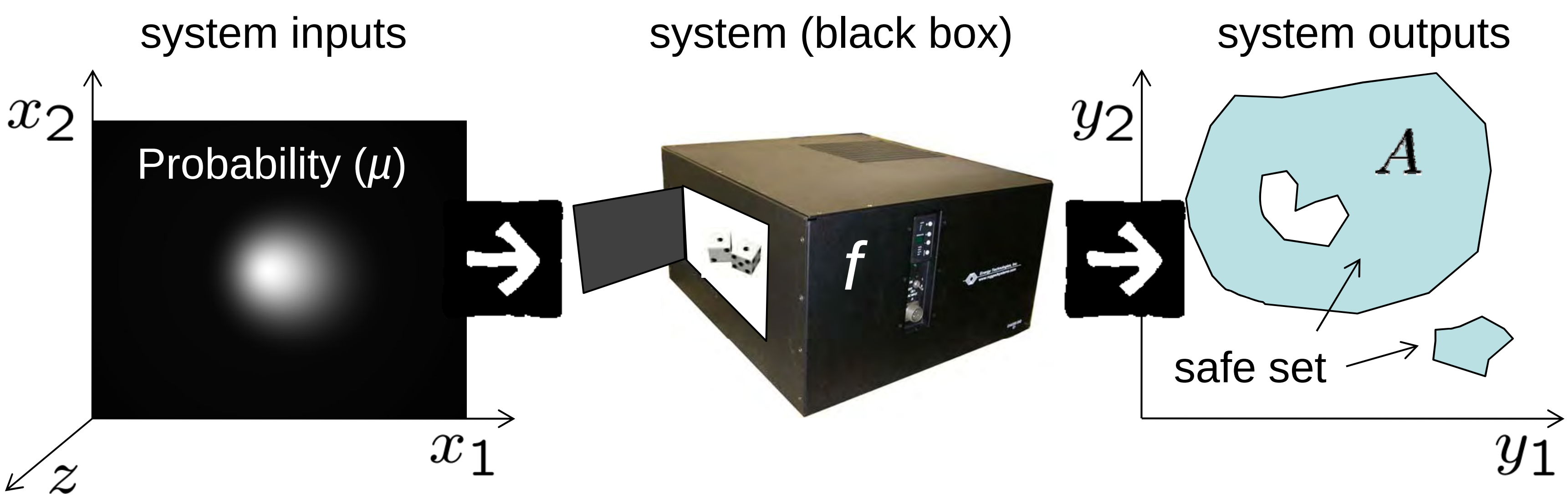
- Conservative certification: **Upper bound** on the PoF of the system below tolerance,

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

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

M. Ortiz

Optimal Uncertainty Quantification



- Wanted: $\mathbb{P}[\text{failure}] = \mathbb{E}_\mu[\{f \in A\}]$
- Assume information about (μ, f): Data, models...
- Admissible set: $\mathcal{A} = \{(\mu, f) \text{ compatible with info}\}$
- Optimal PoF bounds given $\mathcal{A}$:

$$\inf_{(\mu,f)\in\mathcal{A}} \mathbb{E}_\mu[\{f \in A\}] \leq \text{PoF} \leq \sup_{(\mu,f)\in\mathcal{A}} \mathbb{E}_\mu[\{f \in A\}]$$

OUQ – The Reduction Theorem

CALTECH PSAAP

Theorem [Owhadi *et al.* (2011)] Suppose that

$$\mathcal{A} = \left\{ (\mu, f) \middle| \begin{array}{c} \langle \text{some conditions on } f \text{ alone} \rangle \\ \mathbb{E}_\mu[\varphi_1] \le 0, \dots \mathbb{E}_\mu[\varphi_n] \le 0 \end{array} \right\}. \text{ Let:}$$

$$\mathcal{A}_{\text{red}} = \left\{ (\mu, f) \in \mathcal{A} \middle| \mu = \sum_{i=1}^{n} \alpha_i \delta_{x_i},\ \alpha_i \ge 0,\ \sum_{i=1}^{n} \alpha_i = 1 \right\}$$

Then:

$$\inf_{(\mu,f)\in\mathcal{A}} \mathbb{E}_\mu[\{f \in A\}] = \inf_{(\mu,f)\in\underline{\mathcal{A}_{\text{red}}}} \mathbb{E}_\mu[\{f \in A\}]$$

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

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

M. Ortiz

Example – Certifying lethality in terminal ballistics

CALTECH PSAAP

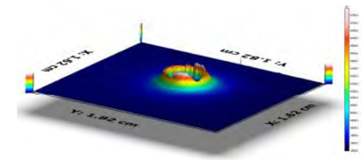
system inputs (x_1, x_2, z):

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

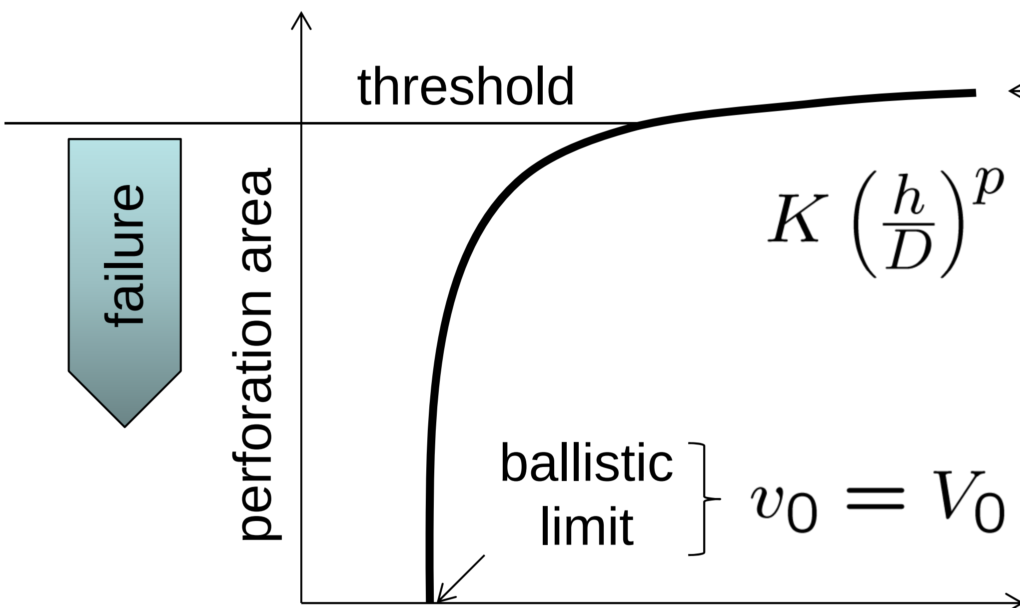
→ f →

Caltech's SPHIR facility

system output (y_1, y_2):



perforation area (profilometry)



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

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

Example – Certifying lethality

CALTECH PSAAP

Caltech's SPHIR facility

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

$$h \in \mathcal{X}_1 \equiv [1.524, 2.667]\,\mathrm{mm}$$

$$\theta \in \mathcal{X}_2 \equiv [0, \tfrac{\pi}{6}]$$

$$v \in \mathcal{X}_3 \equiv [2.1, 2.8]\,\mathrm{km\,s}^{-1}$$

- Admissible set:

$$\mathcal{A} \equiv \left\{ (f, \mu) \;\middle|\; \begin{array}{c} f \text{ known exactly}, \\ \mu = \mu_1 \otimes \mu_2 \otimes \mu_3, \\ 5.5\mathrm{mm}^2 \leq \mathbb{E}_\mu[f] \leq 7.5\mathrm{mm}^2 \end{array} \right\}$$

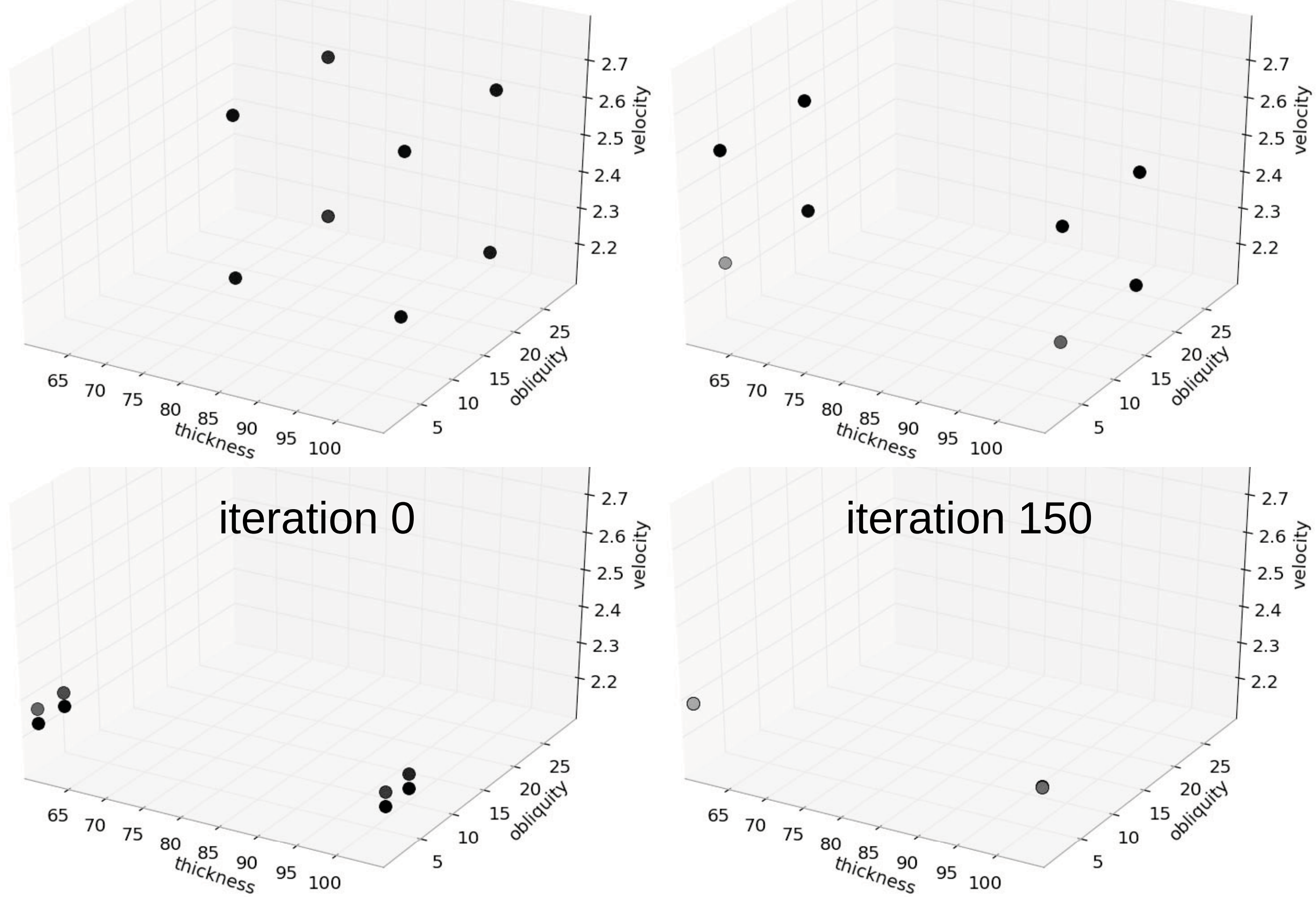
- Reduced admissible set:

$$\mathcal{A}_{\mathrm{red}} \equiv \left\{ (f, \mu) \;\middle|\; \begin{array}{c} f \text{ known exactly}, \\ \mu = \mu_1 \otimes \mu_2 \otimes \mu_3, \\ \mu_i = \alpha_i \delta_{a_i} + (1 - \alpha_i)\delta_{b_i},\; i = 1, 2, 3, \\ 5.5\mathrm{mm}^2 \leq \mathbb{E}_\mu[f] \leq 7.5\mathrm{mm}^2 \end{array} \right\}$$

Example – Certifying lethality

CALTECH PSAAP

- Evolution of support of reduced probability measure:



iteration 0

iteration 150

iteration 200

iteration 1000

M. Ortiz

Example – Certifying lethality

CALTECH PSAAP

Caltech's SPHIR facility

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

$$h \in \mathcal{X}_1 \equiv [1.524, 2.667]\,\mathrm{mm}$$

$$\theta \in \mathcal{X}_2 \equiv [0, \tfrac{\pi}{6}]$$

$$v \in \mathcal{X}_3 \equiv [2.1, 2.8]\,\mathrm{km\,s^{-1}}$$

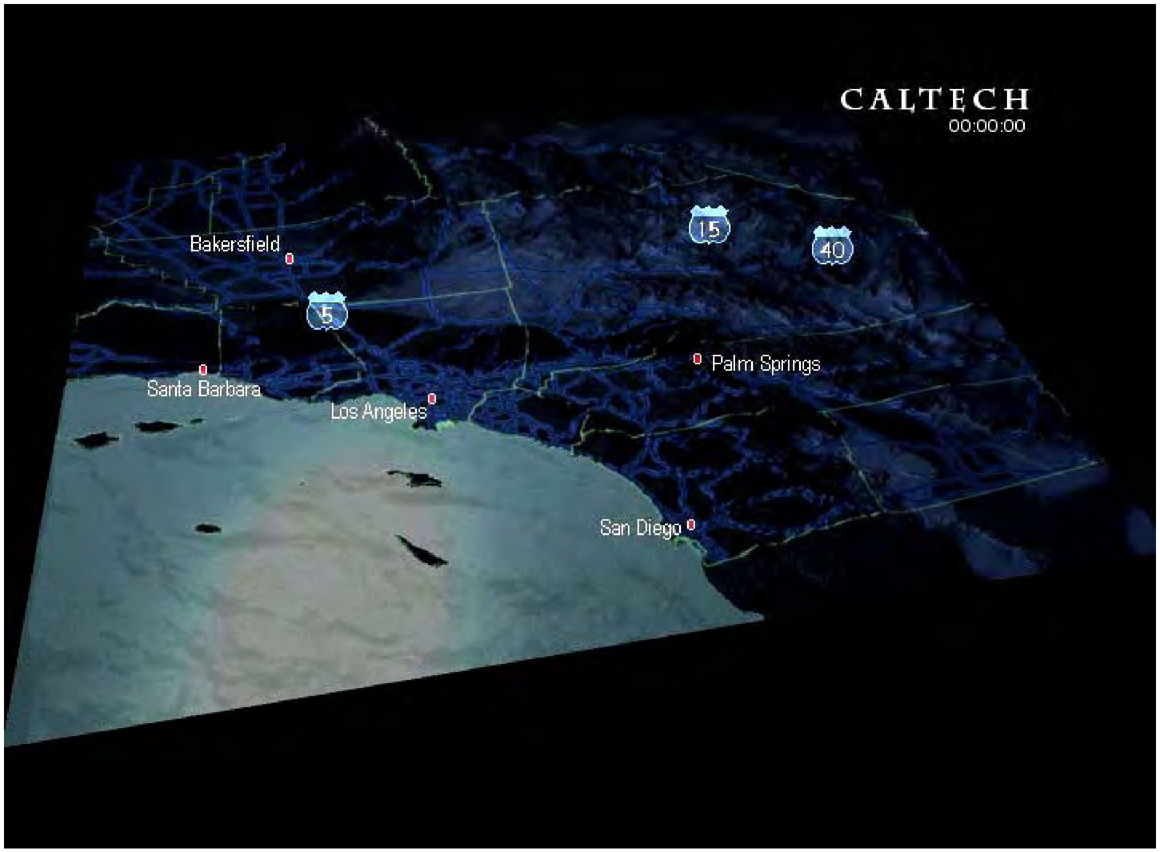
- Reduced admissible set:

$$\mathcal{A}_{\mathrm{red}} \equiv \left\{ (f, \mu) \;\middle|\; \begin{array}{c} f \text{ known exactly}, \\ \mu = \mu_1 \otimes \mu_2 \otimes \mu_3, \\ \mu_i = \alpha_i \delta_{a_i} + (1 - \alpha_i)\delta_{b_i},\ i = 1, 2, 3, \\ 5.5\mathrm{mm}^2 \leq \mathbb{E}_\mu[f] \leq 7.5\mathrm{mm}^2 \end{array} \right\}$$

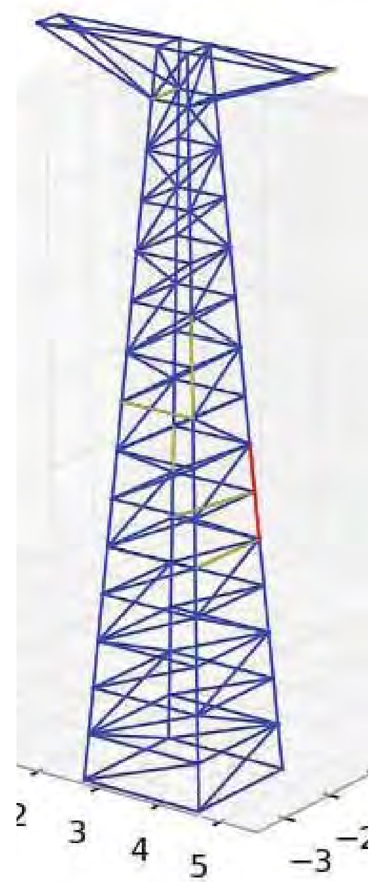
- Optimal PoF upper bound:

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

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

M. Ortiz

Example – Seismic risk assessment

CALTECH PSAAP

- Ground motion acceleration:

$$\ddot{u}_0(t) = (\psi * s)(t)$$

where: $s(t) \equiv$ Source activity

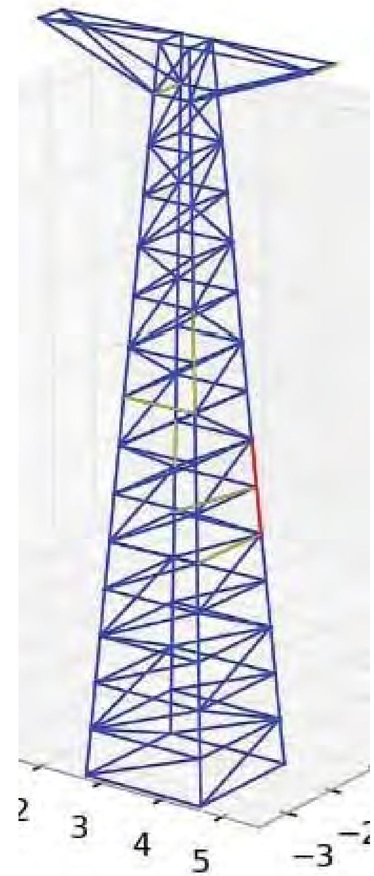
$\psi(t) \equiv$ Transfer function

- Structural response:

$$M\ddot{u} + C\dot{u} + Ku = -MT\ddot{u}_0(t)$$

- Failure criterion: $f \leq 0$, where

$$f = \min_{i \in \text{members}} \left\{ \sigma_{\text{y}} - \max_{t \geq 0} |\sigma_i(t)| \right\}$$

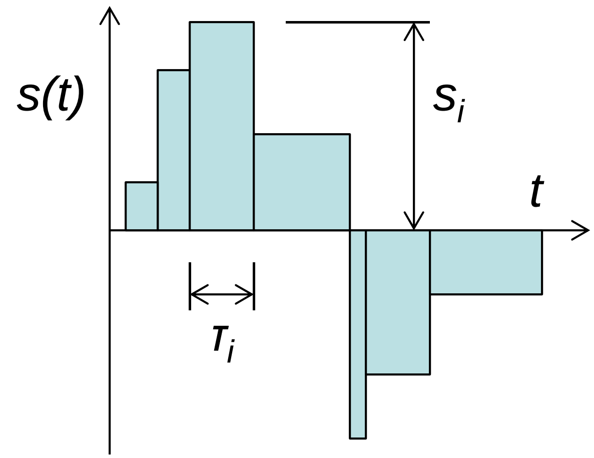


3D truss structure
of power-line tower

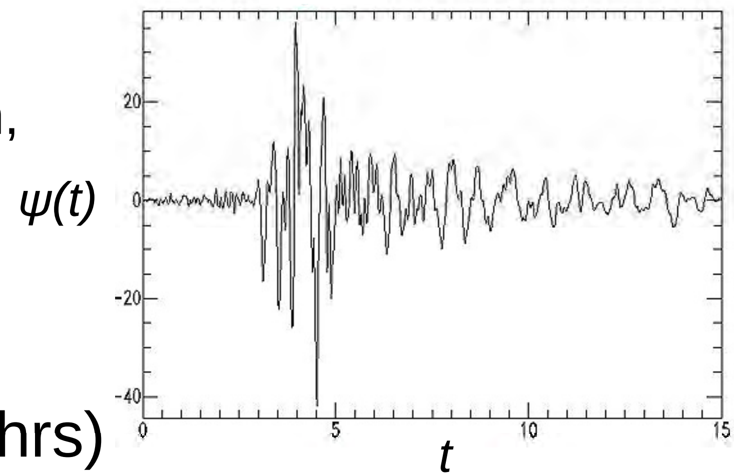
Example – Seismic risk assessment

CALTECH PSAAP

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



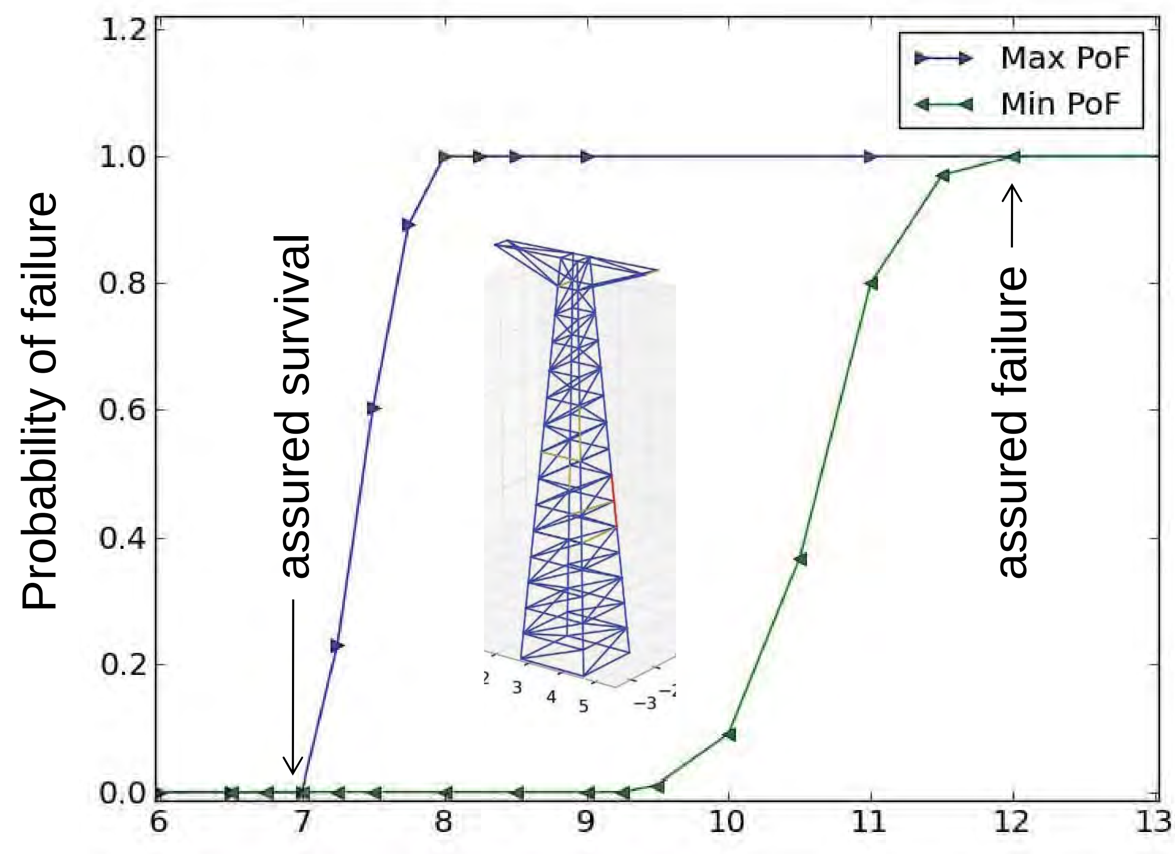
- Assumptions on transfer function *ψ(t)*:
  - Piecewise linear in time
  - Random amplitudes with zero mean, bounded L^2 norm
- Reduced OUQ problem: Global optimization in 179 dimensions
- One PoF calculation takes O(24 hrs) on O(1000) AMD opteron cluster



M. Ortiz

Example – Seismic risk assessment

CALTECH PSAAP



Richter-scale local magnitude M

Optimal PoF upper and lower bounds for steel tower vs. Richter scale magnitude M at hypocentral distance R=25 km, (a_{max} given by Esteva's semi-empirical expression as a function of M)

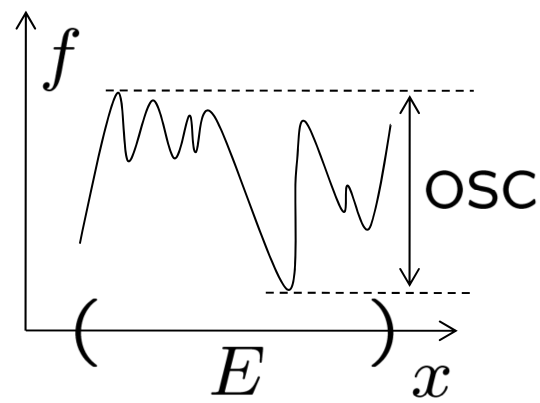
M. Ortiz

OUQ with diameter data

CALTECH PSAAP

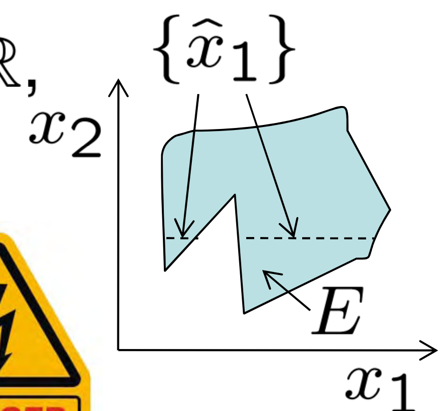
- Question: How is $\mathcal{A}$ to be defined? What type of data on system response leads to effective UQ?

- 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: $f : E \subset \mathbb{R}^N \to \mathbb{R}$,

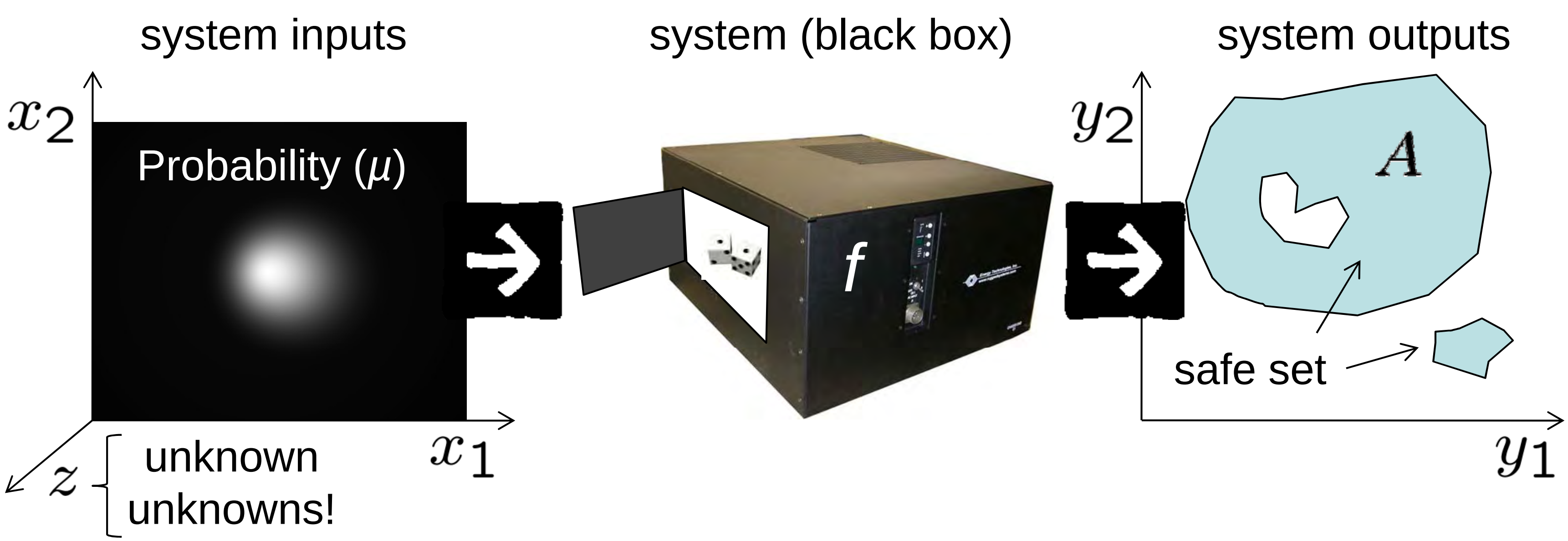


$$D_i(f, E) = \sup_{\widehat{x}_i \in \mathbb{R}^{N-1}} \text{osc}(f, E \cap \{\widehat{x}_i\}),$$
$$\widehat{x}_i = \{x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_N\}$$

possibly unknown unknowns!

global optimization!

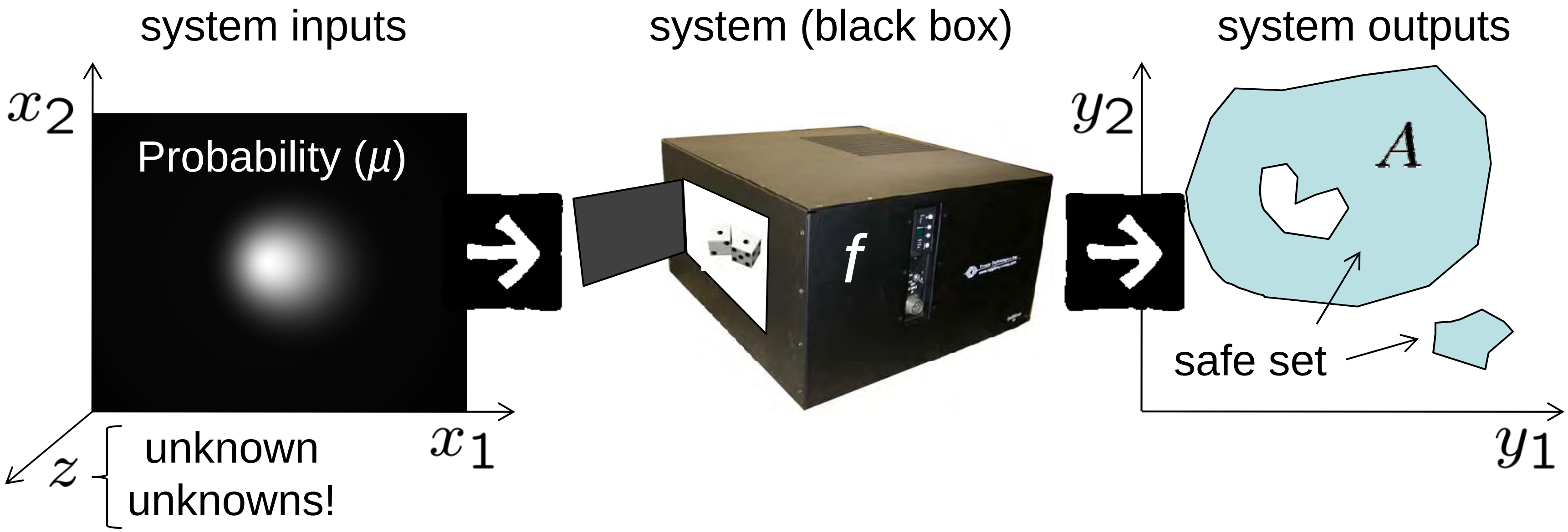
OUQ with diameter data



- Admissible set for diameter data with scatter:

$$\mathcal{A} \equiv \left\{ (f, \mu) \middle| \begin{array}{c} D_i(f, \mathcal{X}) \leq D_i, \; i = 1, \dots, n \\ \mu = \mu_1 \otimes \cdots \otimes \mu_n, \\ m_1 \leq \mathbb{E}_\mu[f] \leq m_2 \\ D_z \leq D_i(f, \mathcal{X}) - \mathbb{E}_\mu[f], \; i = 1, \dots, n \end{array} \right\}$$

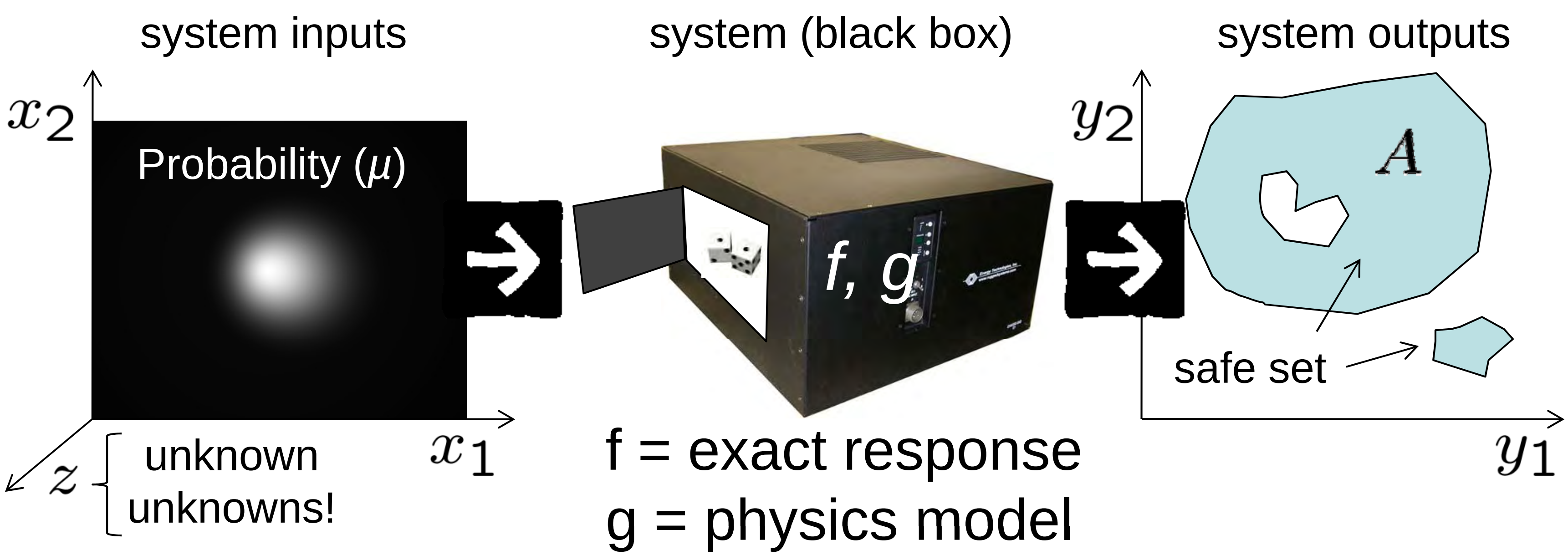
OUQ with diameter data



- OUQ problem explicitly solvable in low dimension!
- For $n = 2$: $\sup_{(\mu,f)\in\mathcal{A}} \mathbb{E}_\mu[\{f \le 0\}] =$

$$\begin{cases} 0, & \text{if } D_1 + D_2 \le \mathbb{E}_\mu[f] \\ \frac{(D_1+D_2-\mathbb{E}_\mu[f])^2}{4D_1D_2}, & \text{if } |D_1 - D_2| \le \mathbb{E}_\mu[f] \le D_1 + D_2 \\ 1 - \frac{\mathbb{E}_\mu[f]}{\max(D_1,D_2)}, & \text{if } 0 \le \mathbb{E}_\mu[f] \le |D_1 - D_2| \end{cases}$$

Model-based OUQ with diameter data

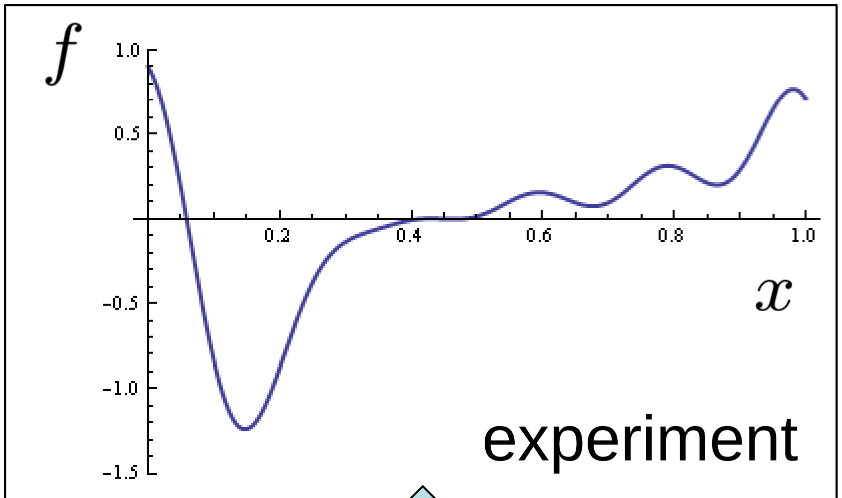


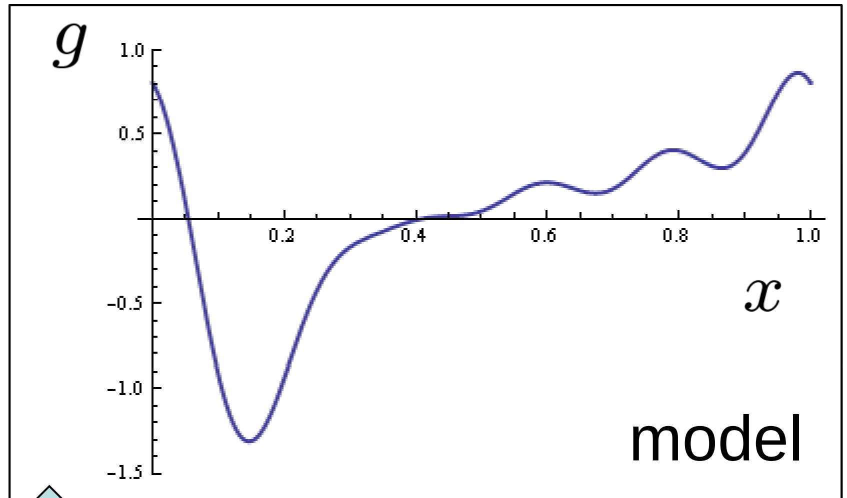
f = exact response
g = physics model

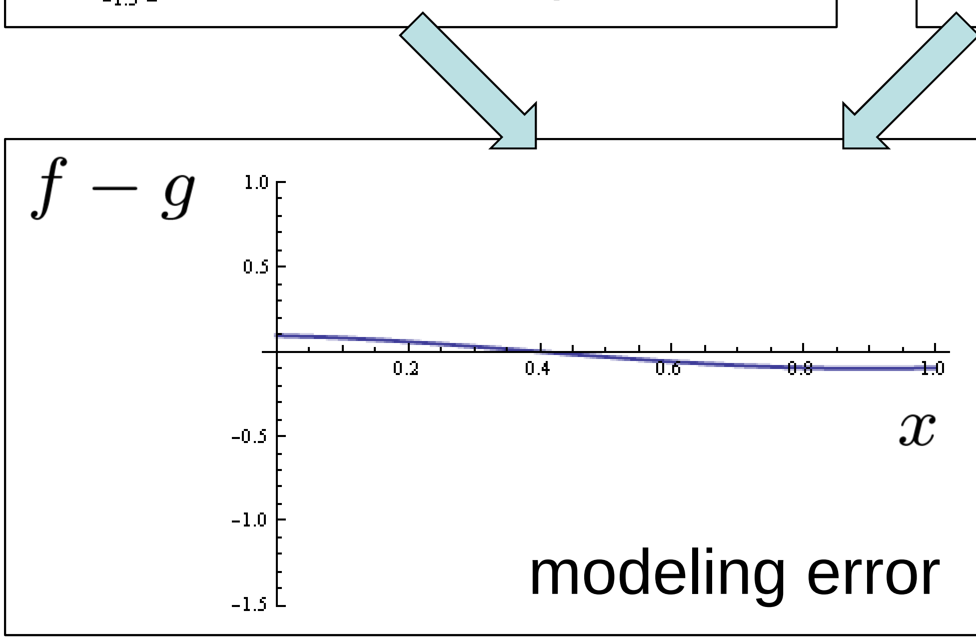
- Diameters $D_i(f)$ define seminorms of f.
- From the triangular inequality,

$$D_i(f) \leq \underbrace{D_i(g)}_{\text{model diameter}} + \underbrace{D_i(f-g)}_{\text{modeling error}}$$

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

M. Ortiz

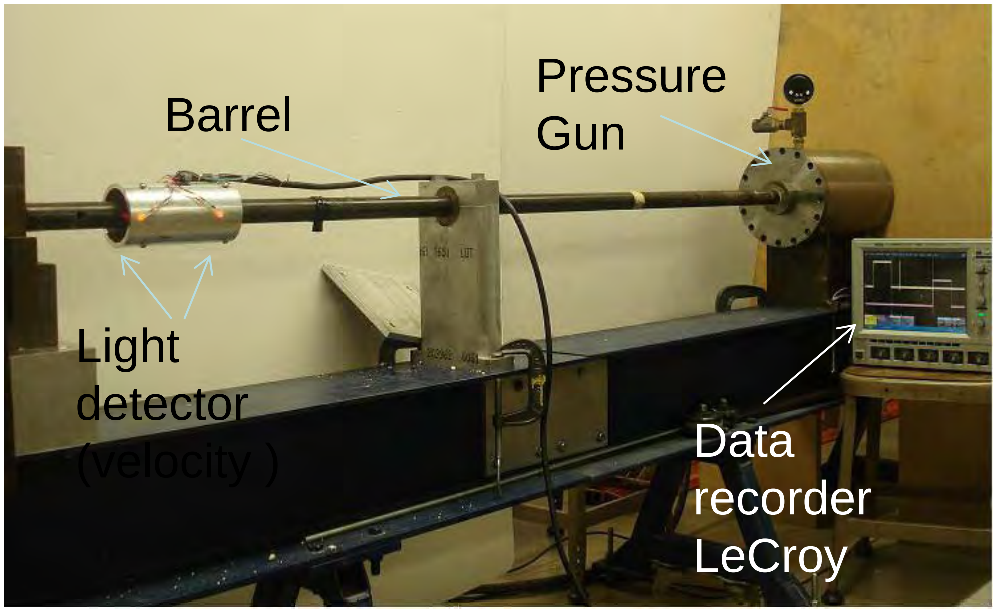
Model-based QMU – McDiarmid

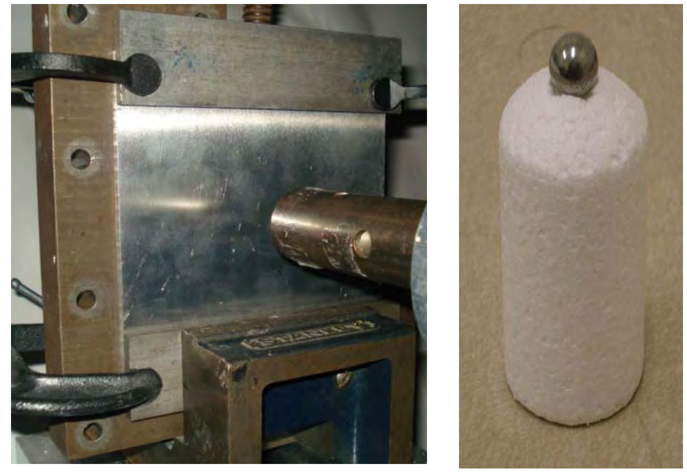
- Calculation of *D(f)* requires exercising model only
- Uncertainty Quantification burden mostly shifted to modeling and simulation!

- Evaluation of *D(f-g)* requires few experiments
- Rigorous certification not achievable by modeling and simulation alone!

Case Study – Steel/Al ballistics

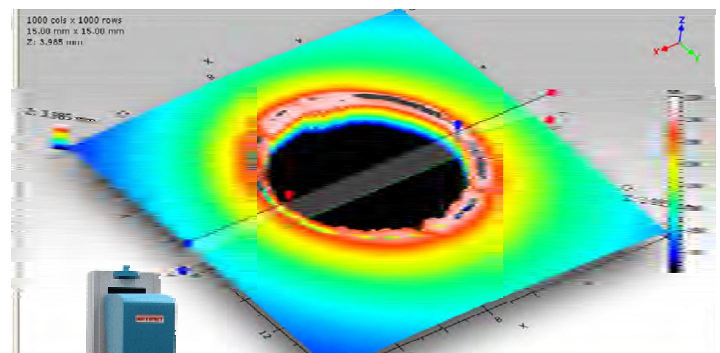
CALTECH PSAAP





Target and projectile

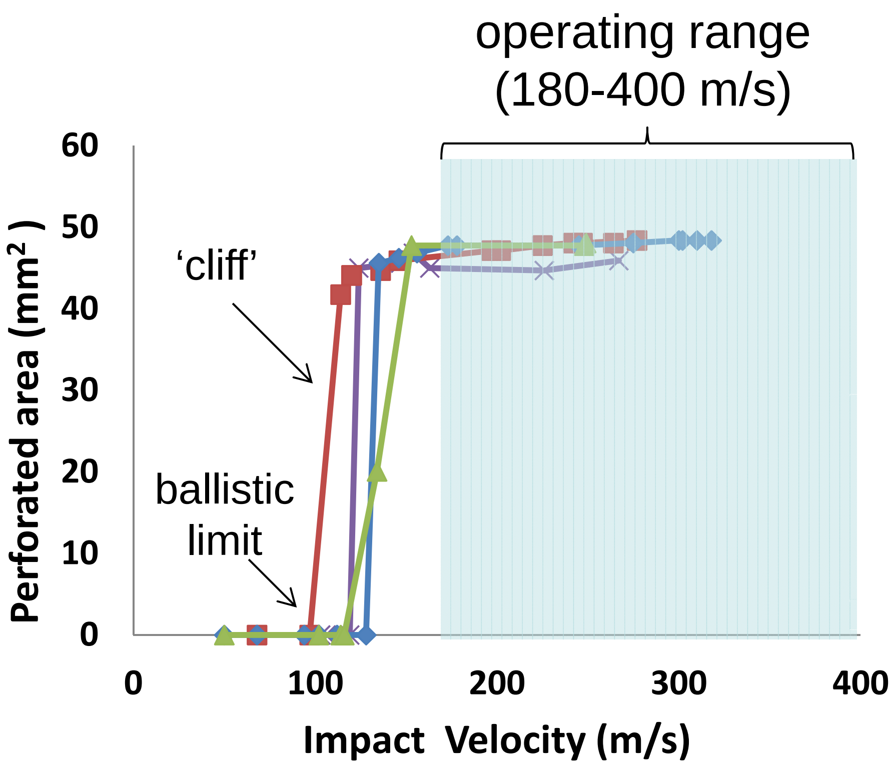
- Target/projectile materials:
  - Target: Al 6061-T6 plates (6”x 6”)
  - Projectile: S2 Tool steel balls (5/16”)
- Model input parameters (*x*):
  - Plate thickness (0.032’’-0.063’’)
  - Impact velocity (200-400 m/s)



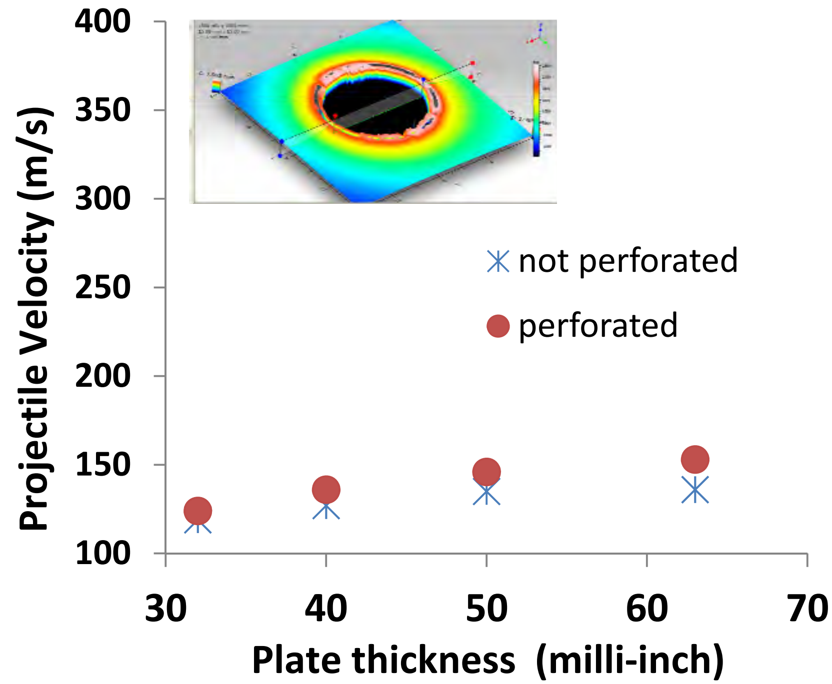
Optimet MiniConoscan 3000

M. Ortiz

Case Study – Steel/Al ballistics



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



Perforation/non-perforation boundary

- System output (y): ***Perforation area!***
- Certification criterion: y>0 (lethality)

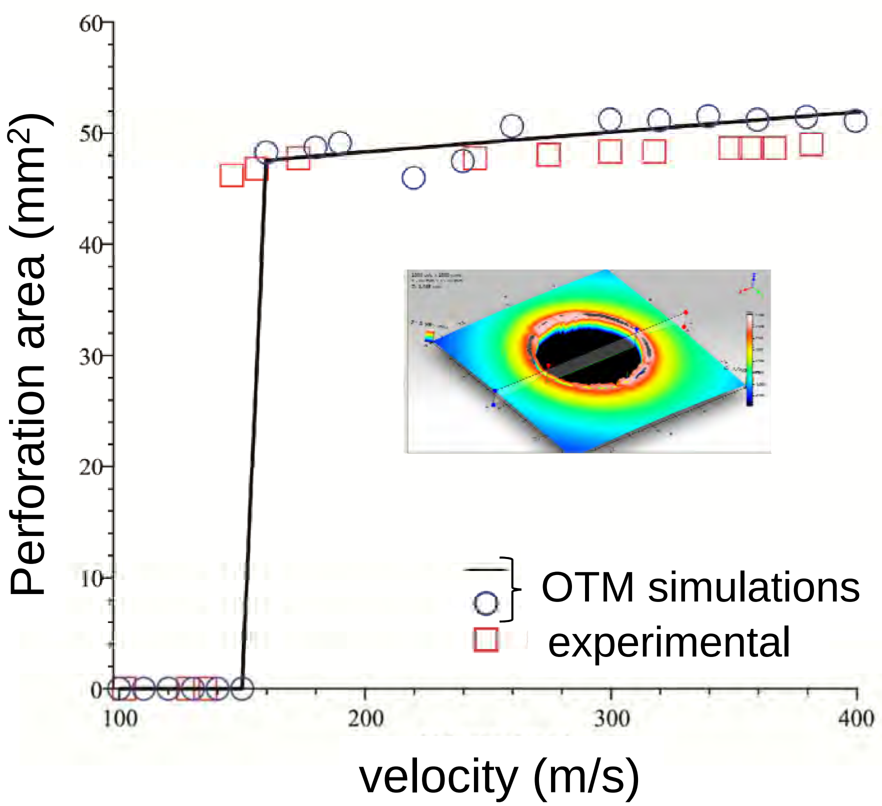
M. Ortiz

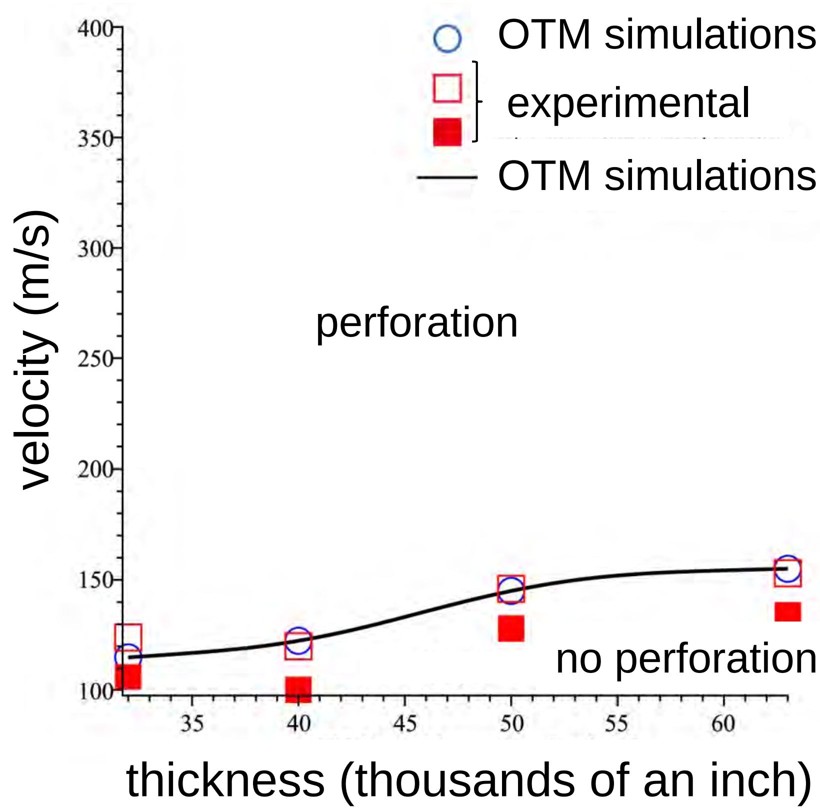
Lagrangian solver: Optimal-Transportation Meshfree (OTM)

- 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

CALTECH PSAAP



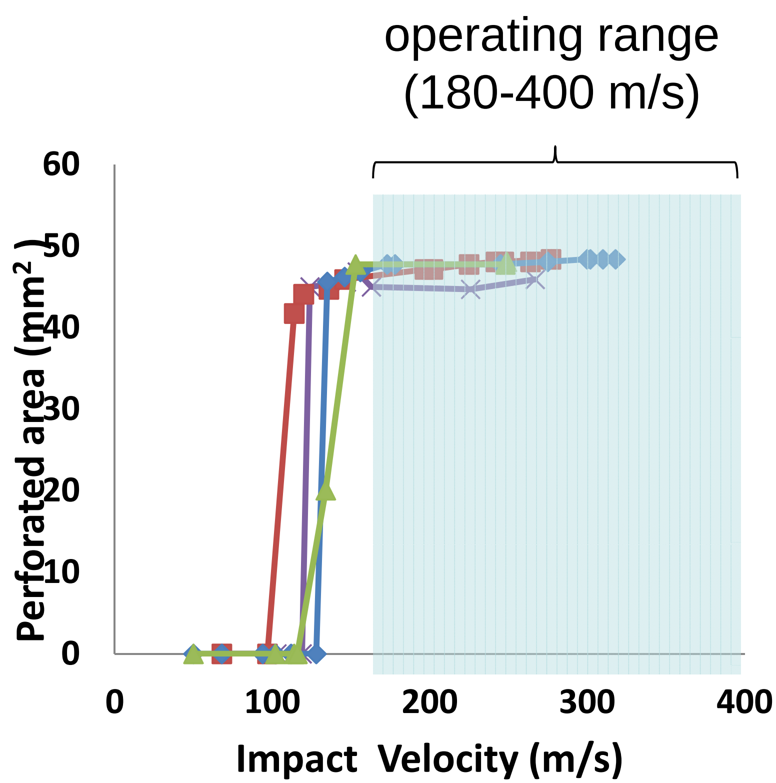


Measured *vs*. computed perforation area

Case study – Terminal ballistics

CALTECH PSAAP

Model diameter *D(g)*	thickness	4.33 mm^2
	velocity	4.49 mm^2
	RMS	6.24 mm^2
Modeling error *D(f-g)*	thickness	4.96 mm^2
	velocity	2.16 mm^2
	RMS	5.41 mm^2
Uncertainty *D(g)+ D(f-g)*		11.65 mm^2
Empirical mean *E[f]*		47.77 mm^2



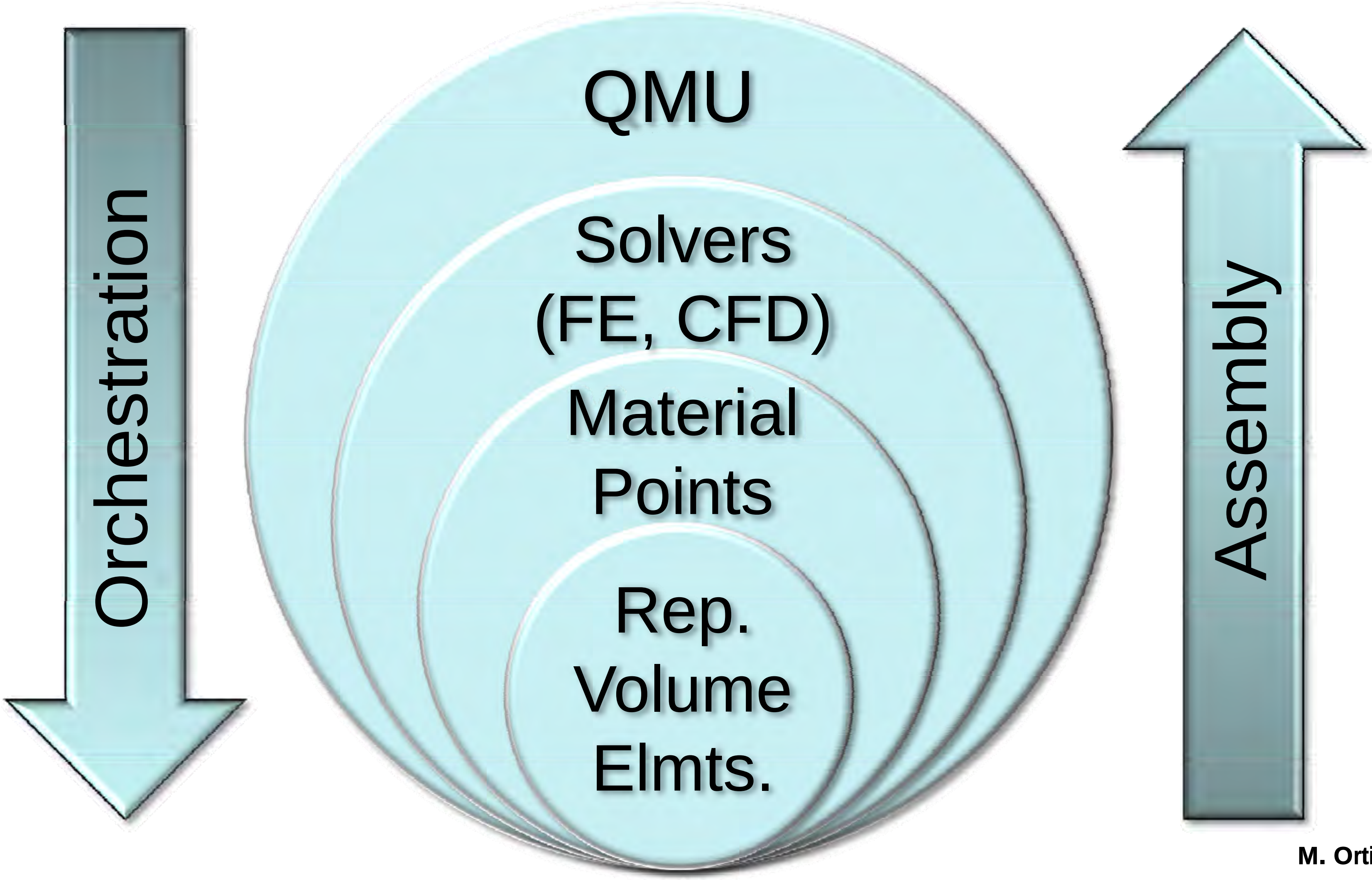
- Perforation can be certified with 99.9% confidence!
- Total number of experiments ~ 50 → Approach feasible!

M. Ortiz

Concluding remarks…

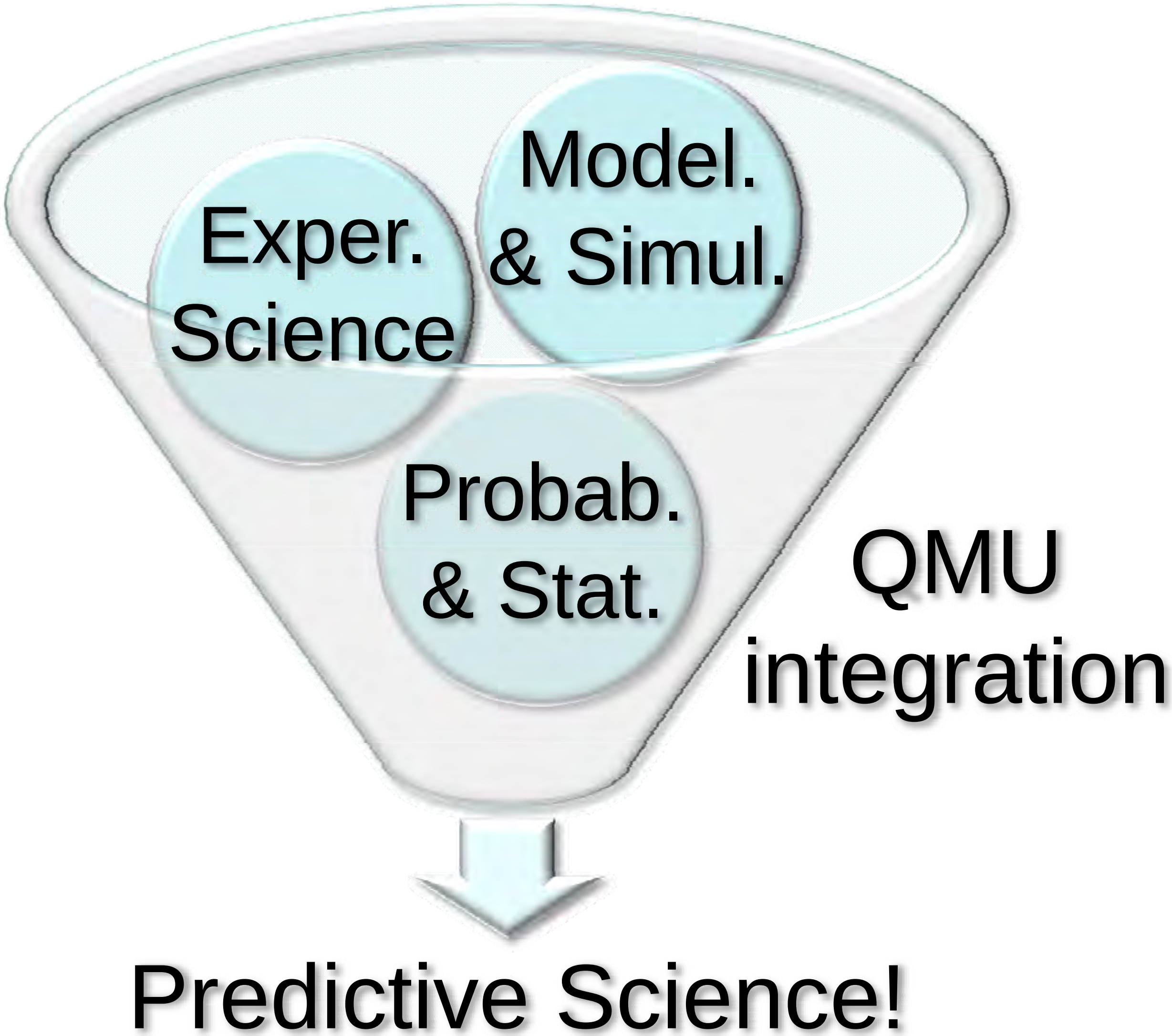
- Rigorous and conservative certification can be achieved by means of PoF upper bounds!
- PoF bounds ‘fold in’ all information available on the system (experimental data, V&V’d physics models…)
- PoF bounds are similar in spirit to bounds on effective moduli of elastic composites (which cannot be obtained 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…



Concluding remarks – Disciplinary view of QMU and Predictive Science

CALTECH PSAAP



M. Ortiz

Concluding remarks…

CALTECH PSAAP

Thank you!

M. Ortiz