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Model-Based Rigorous Uncertainty Quantification in Complex Systems

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ASC/PSAAP Centers

PSAAP: Predictive Science Academic Alliance Program

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The Quantification of Margins and Uncertainties (QMU) Paradigm

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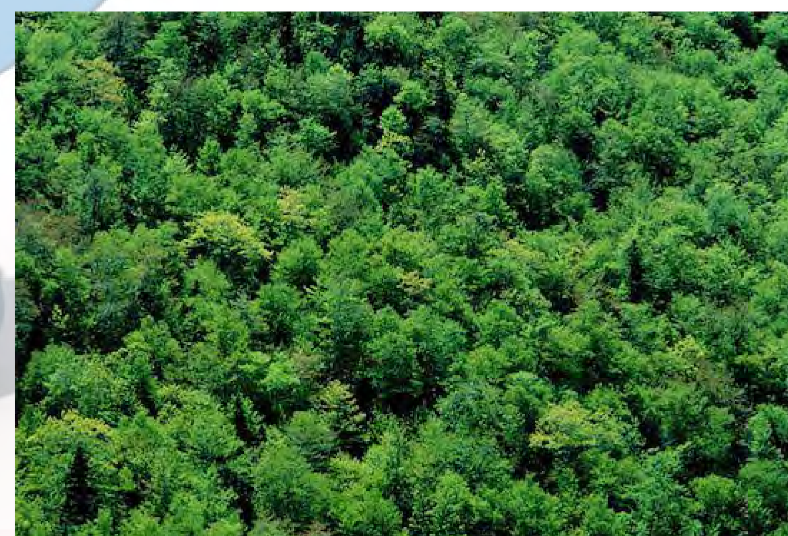
- Aim: *Predict mean performance and* ***uncertainty*** *in the behavior of complex physical/engineered systems*
- ***Paradigm shift*** in experimental science, modeling and simulation, scientific computing (***predictive science***):
  - Deterministic → Non-deterministic systems
  - Mean performance → Mean performance + Uncertainty

Old single-calculation paradigm



New ensemble-of-calculations paradigm (QMU)

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:

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

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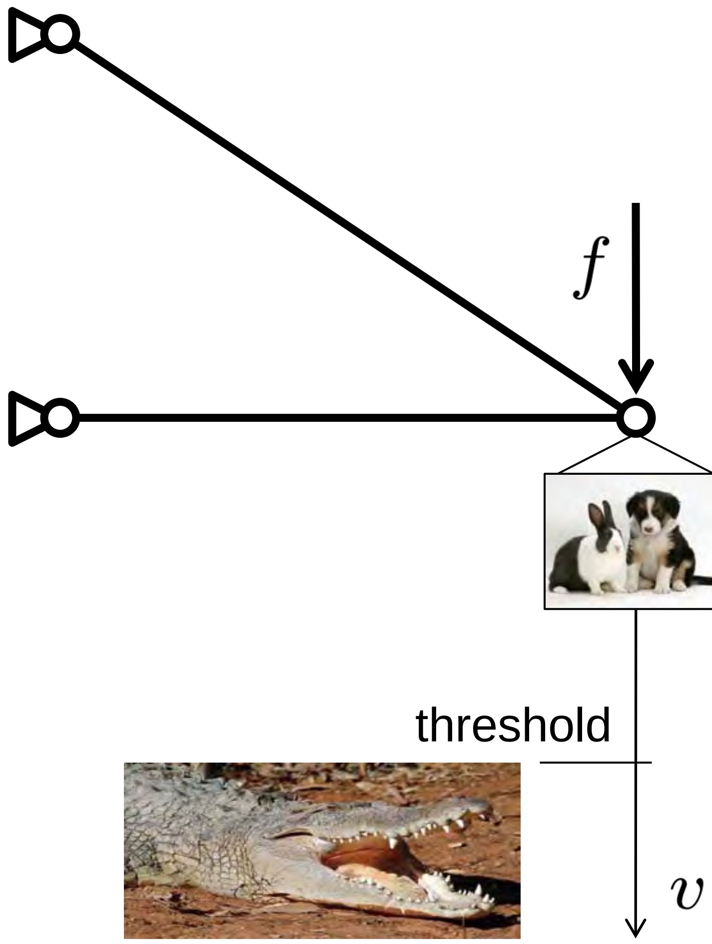
QMU – A simple truss example



- System input: Applied force (*f*)
- System output: Tip deflection (*v*)
- Response function (*G*): Energy minimization, static equilibrium
- Model (*F*): Energy minimization with approximate strain-energy density function *W*
- Failure criterion: *v* > threshold
- To compute: $\mathbb{P}[\text{failure}] =$

$$\int \begin{Bmatrix} 0, & \text{if } v < v\text{max} \\ 1, & \text{if } v \geq v\text{max} \end{Bmatrix} d\mu(f)$$

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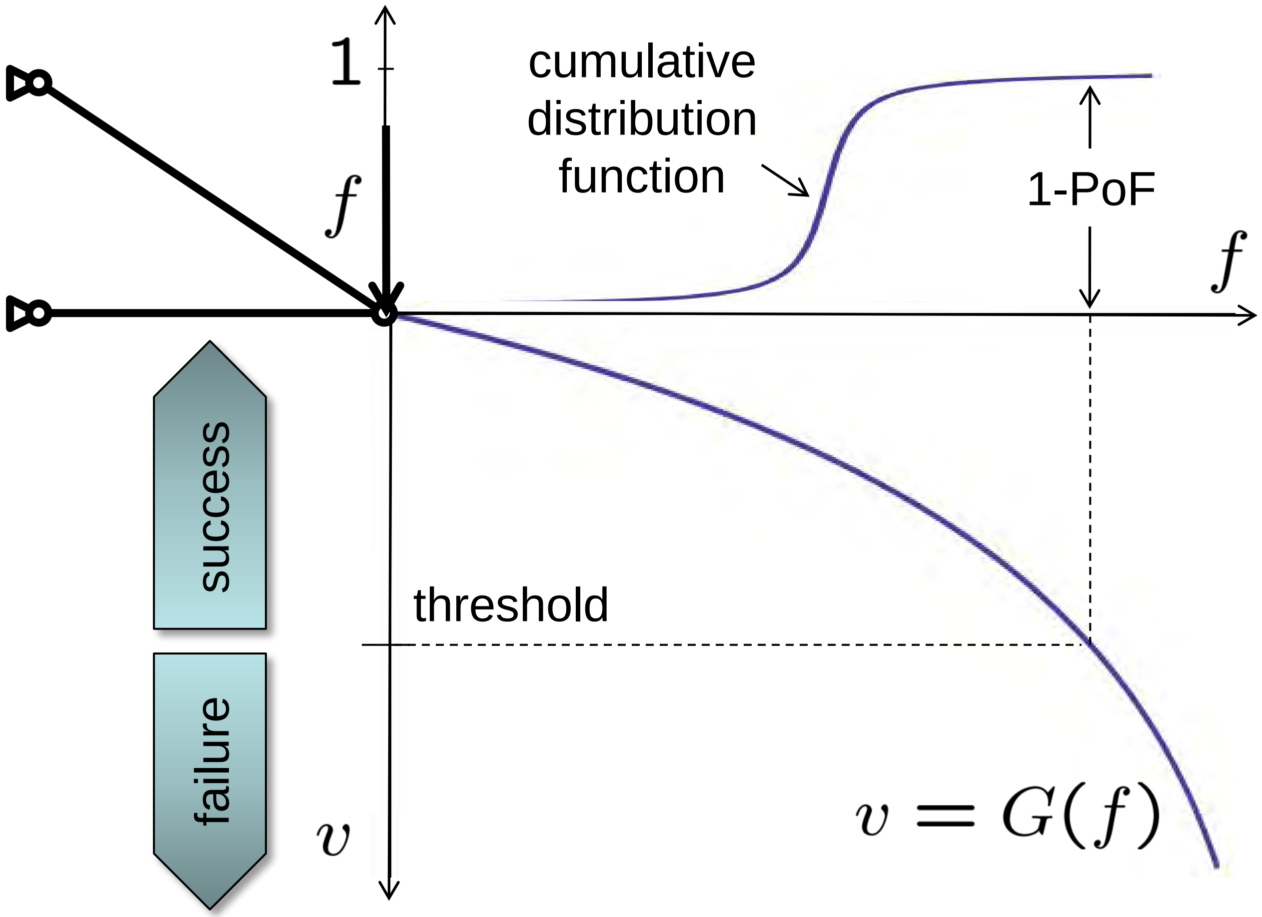
QMU – A simple truss example

- Assume: Deterministic response, known probability distribution of inputs



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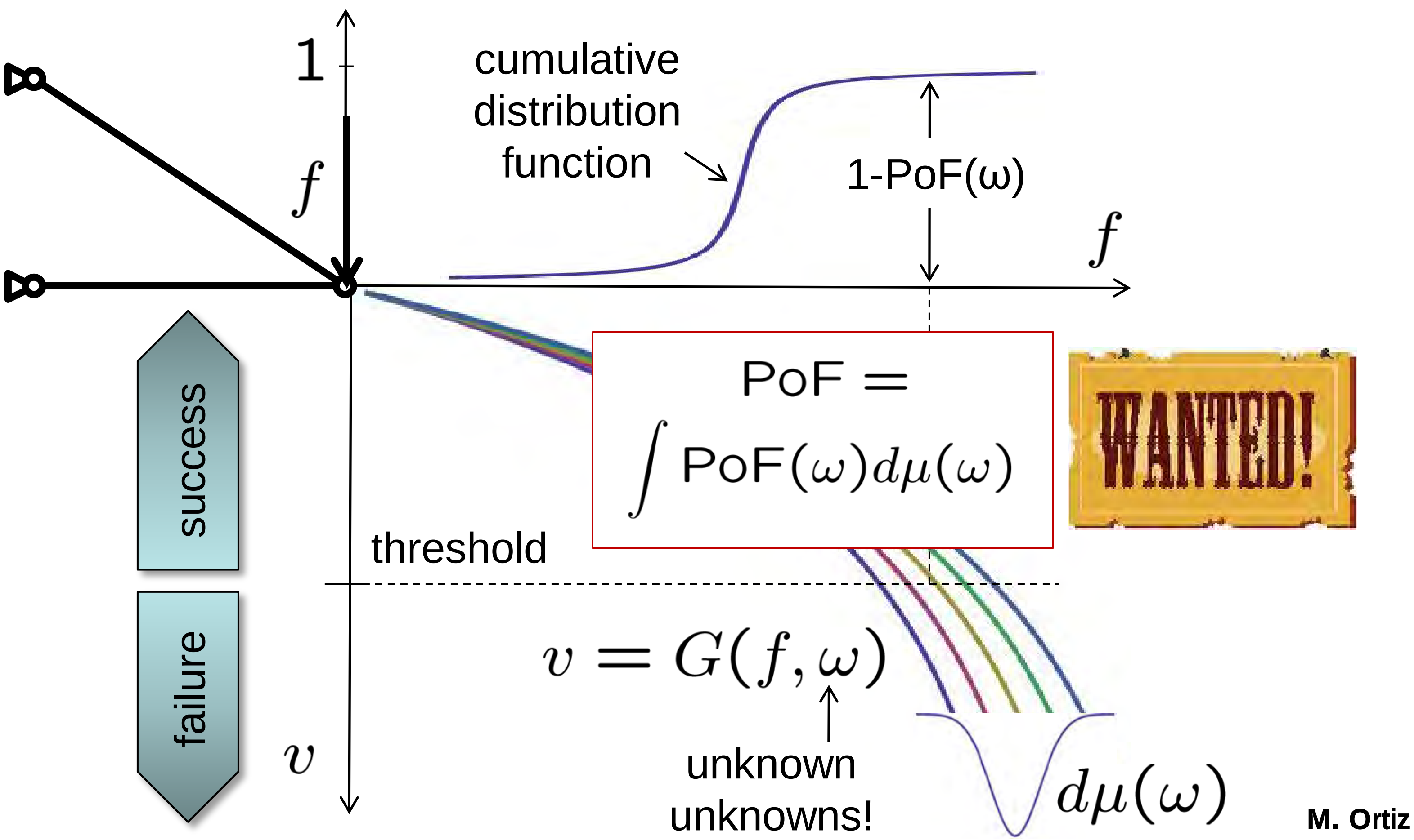
QMU – A simple truss example

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



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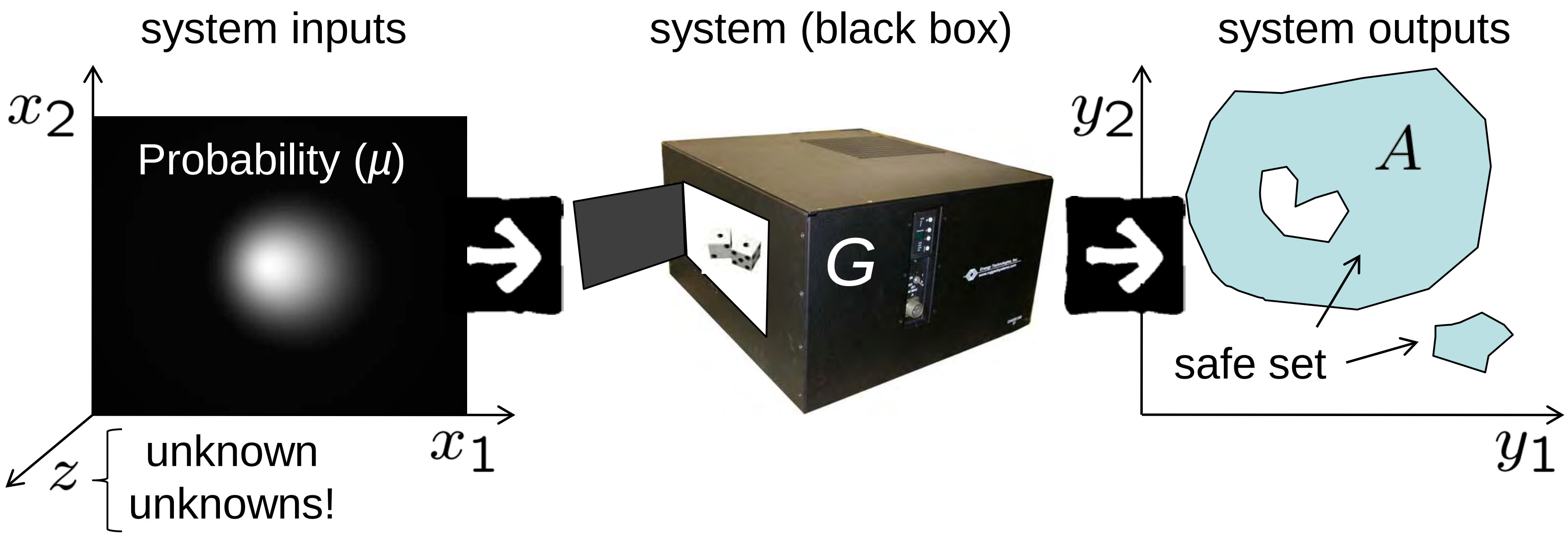
QMU – Certification view



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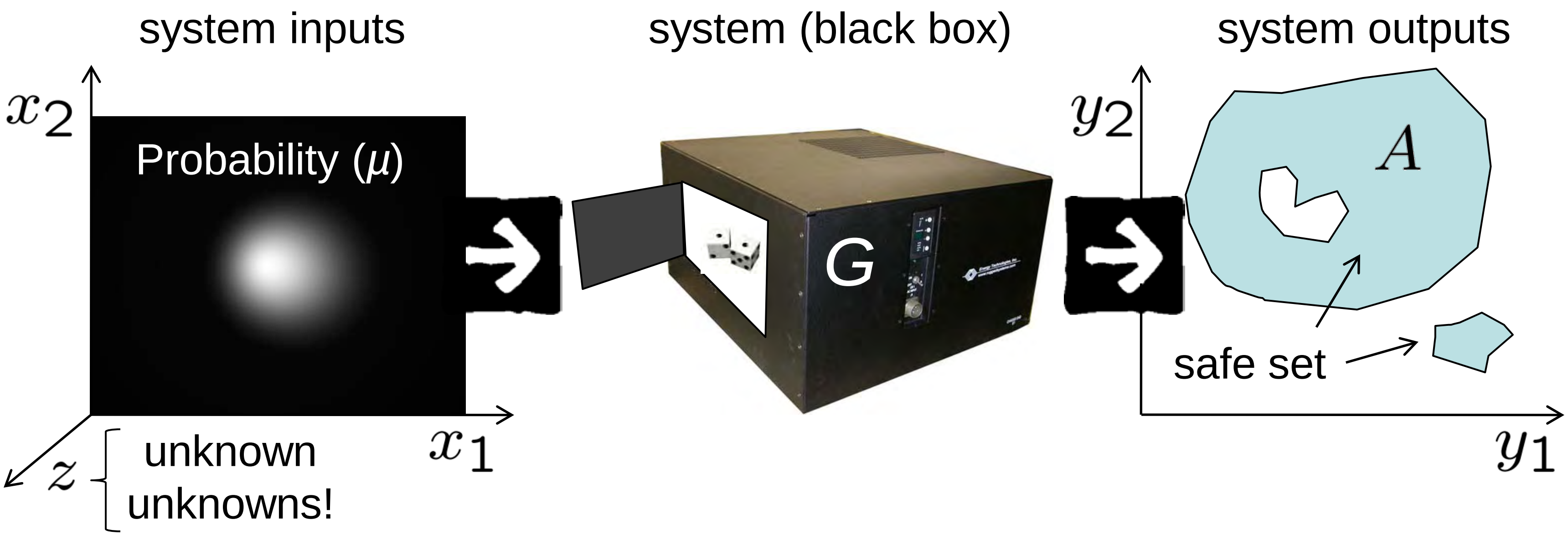
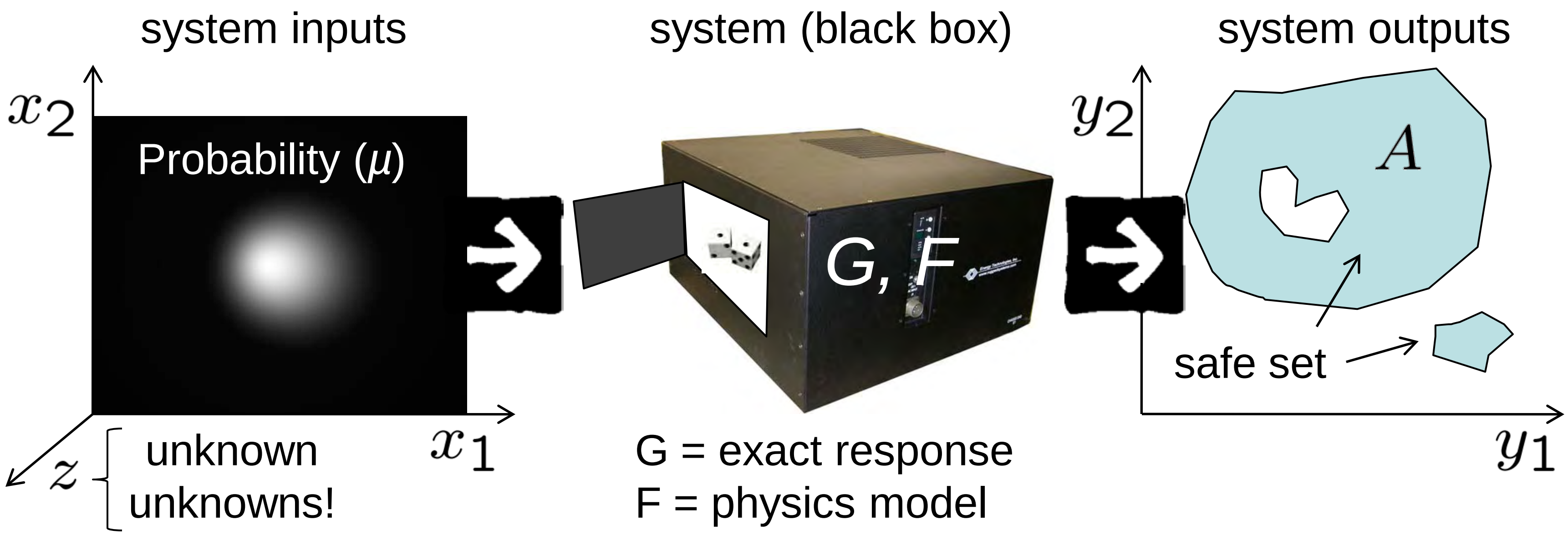
QMU – Essential difficulties



- 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…

QMU – Conservative certification



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

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

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

Example – McDiarmid's inequality

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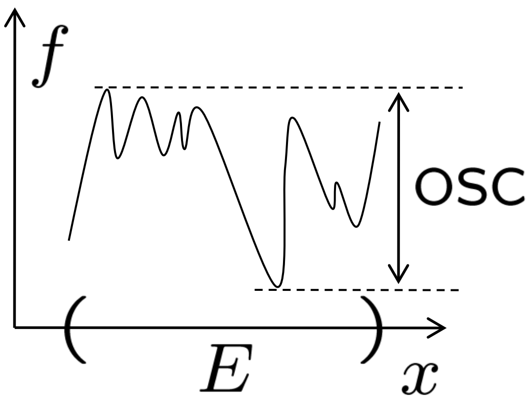
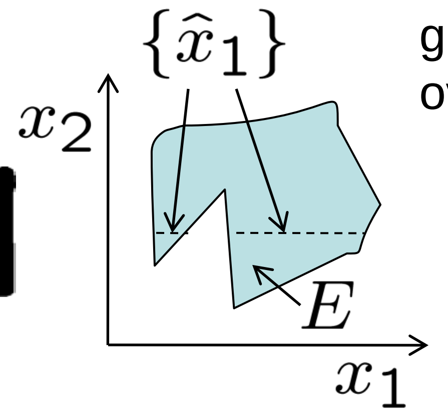
- Function diameters:

computation requires global optimization over parameter space!



One-dimensional diameter



Multidimensional diameter

$\to |f|_D$

- McDiarmid's CoM inequality: $\mathbb{P}[\text{failure}] \leq \text{e}^{-2(M/U)^2}$

$M \equiv \text{margin} = \text{mean output} - \text{threshold} - \text{margin hit}$

$U \equiv \text{uncertainty} = \underbrace{\text{predicted}}_{|F|_D} + \underbrace{\text{modeling}}_{|F-G|_D} + \underbrace{\text{scatter}}_{\sim 2\sigma}$

$|F|_D$ model diameter

$|F-G|_D$ modeling error diameter

$\sim 2\sigma$

Lucas, Owhadi & MO
CMAME (2008)

Example: Certifying threat lethality

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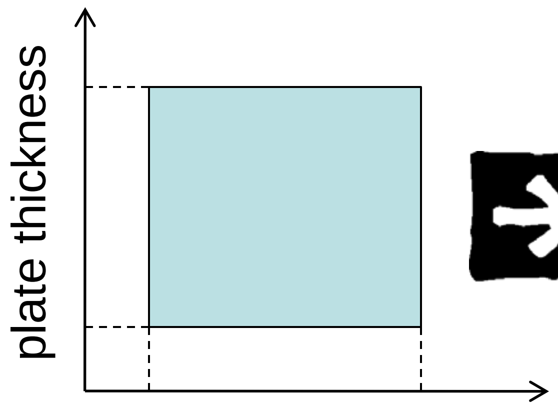
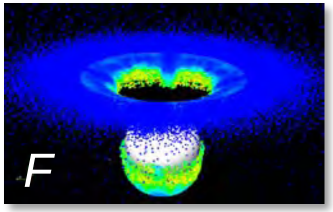
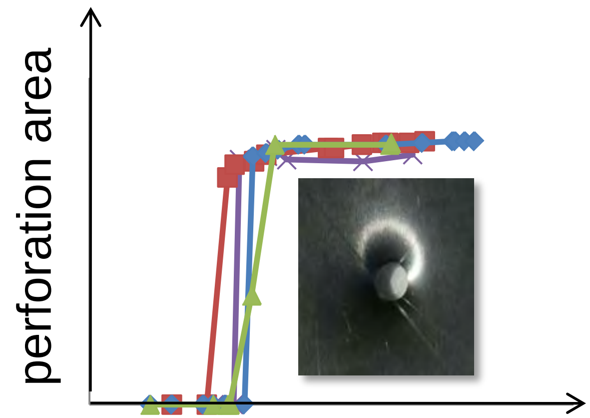
system inputs



system (gas gun)



system outputs



Model diameter $\|F\|_D$	6.24 mm^2
Modeling error $\|F-G\|_D$	5.41 mm^2
Experimental scatter 2σ	0.50 mm^2
Uncertainty $\|F\|_D+\|F-G\|_D+2\sigma$	11.65 mm^2
Empirical mean $<G>$	47.77 mm^2
Margin hit α ($\varepsilon'=0.1\%$)	4.17 mm^2
Confidence factor M/U	3.59

- System certified with very high confidence (PoF < 0.1%)
- Total number of tests required ~ 50
- Total number of calculations ~ 2000

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QMU – Conservative certification

- 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
- Question: Is it possible to compute optimal PoF bounds? (for given information about the system)
- **Optimal Uncertainty Quantification**! (OUQ)

Optimal Uncertainty Quantification

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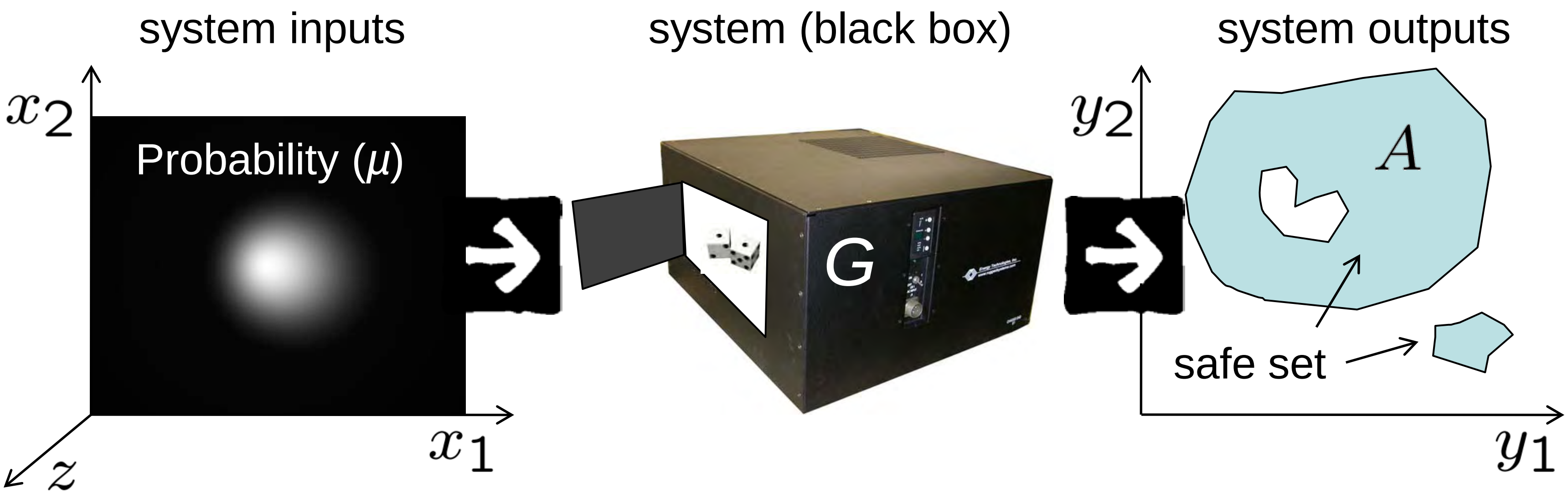

- Wanted: $\mathbb{P}[\text{failure}] = \mathbb{E}_\mu[\{G \in A\}]$
- Assume information about (μ, G): Data, models...
- Admissible set: $\mathcal{A} = \{(\mu, G) \text{ compatible with info}\}$
- Optimal PoF bounds given $\mathcal{A}$:

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

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OUQ – The Reduction Theorem

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

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

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

Then:

$$\inf_{(\mu,G)\in\mathcal{A}} \mathbb{E}_\mu(\{G \in A\}) = \inf_{(\mu,G)\in\mathcal{A}_{\text{red}}} \mathbb{E}_\mu(\{G \in A\})$$

$$\sup_{(\mu,G)\in\mathcal{A}} \mathbb{E}_\mu(\{G \in A\}) = \sup_{(\mu,G)\in\mathcal{A}_{\text{red}}} \mathbb{E}_\mu(\{G \in A\})$$

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

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Example – Seismic risk assessment

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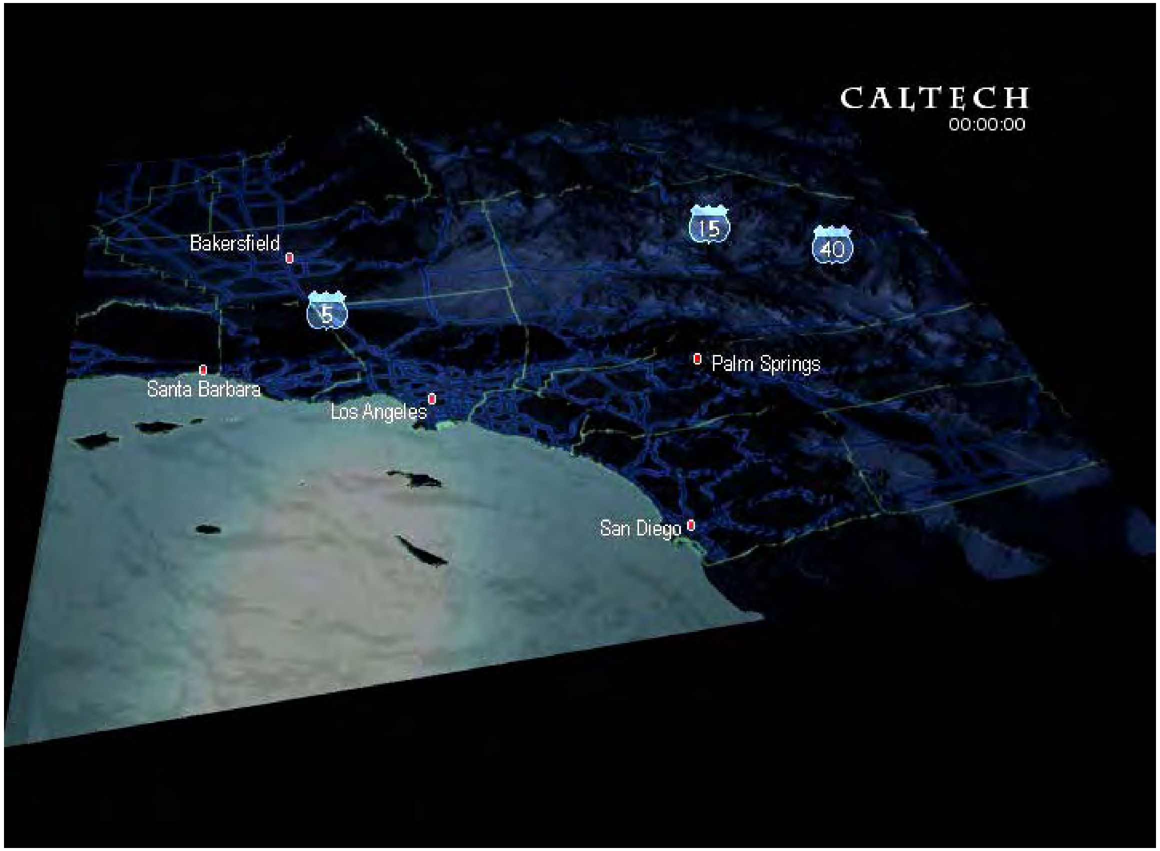
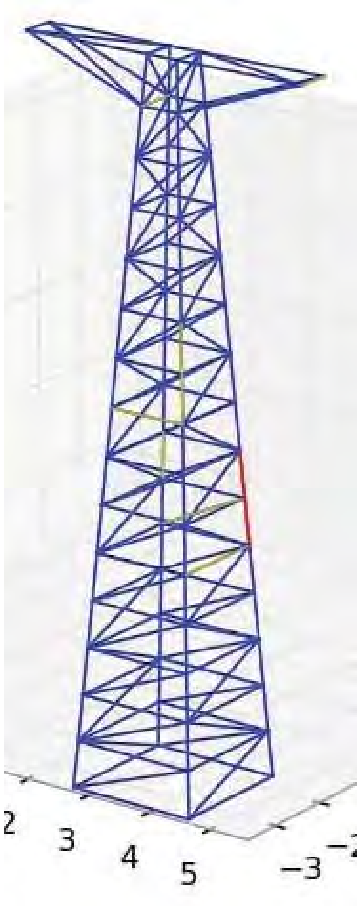


Simulation of seismic waves from rupture initiating at Parkfield, central California, and propagating over Los Angeles basin (http://krishnan.caltech.edu/krishnan/res.html)



3D truss structure of power-line tower

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Example – Seismic risk assessment

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- Ground motion acceleration:

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

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

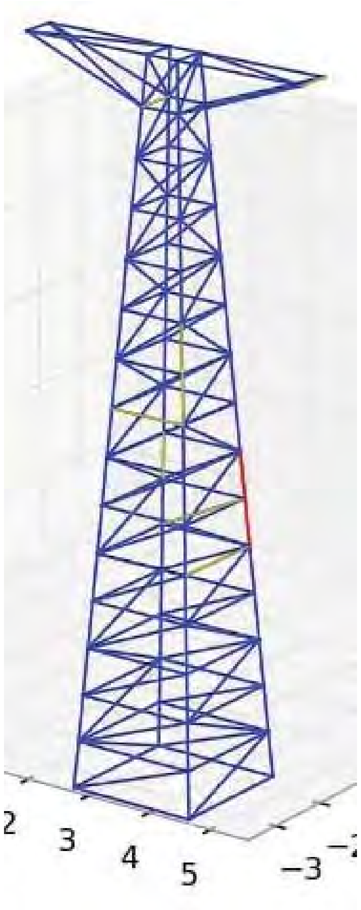
$\psi(t) \equiv$ Transfer function

- Structural response:

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

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

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



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Example – Seismic risk assessment

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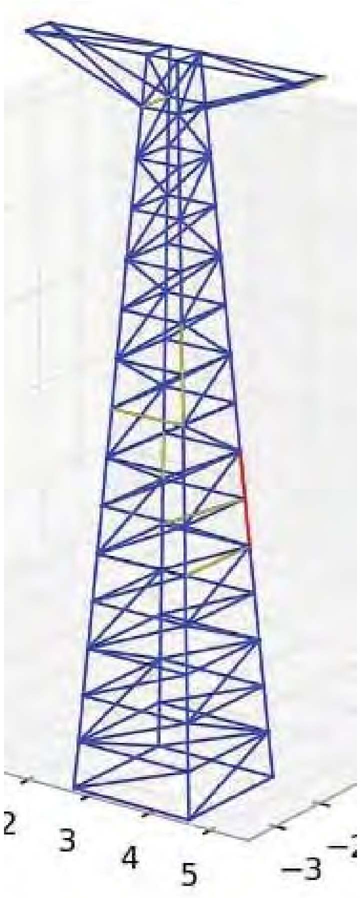
- Assumptions on source term *s(t)*:
  - Piecewise constant in time
  - Random amplitudes in [$-a_{max}$,a_{max}] (given by Richter magnitude M) with zero mean
  - Random time interval durations with bounded mean
- Assumptions on transfer function *ψ(t)*:
  - Piecewise linear in time
  - Random amplitudes with zero mean, bounded L^2 norm
- Reduced OUQ problem: Global optimization in 179 dimensions
- One PoF calculation takes O(24 hours) on O(1000) AMD opteron cluster



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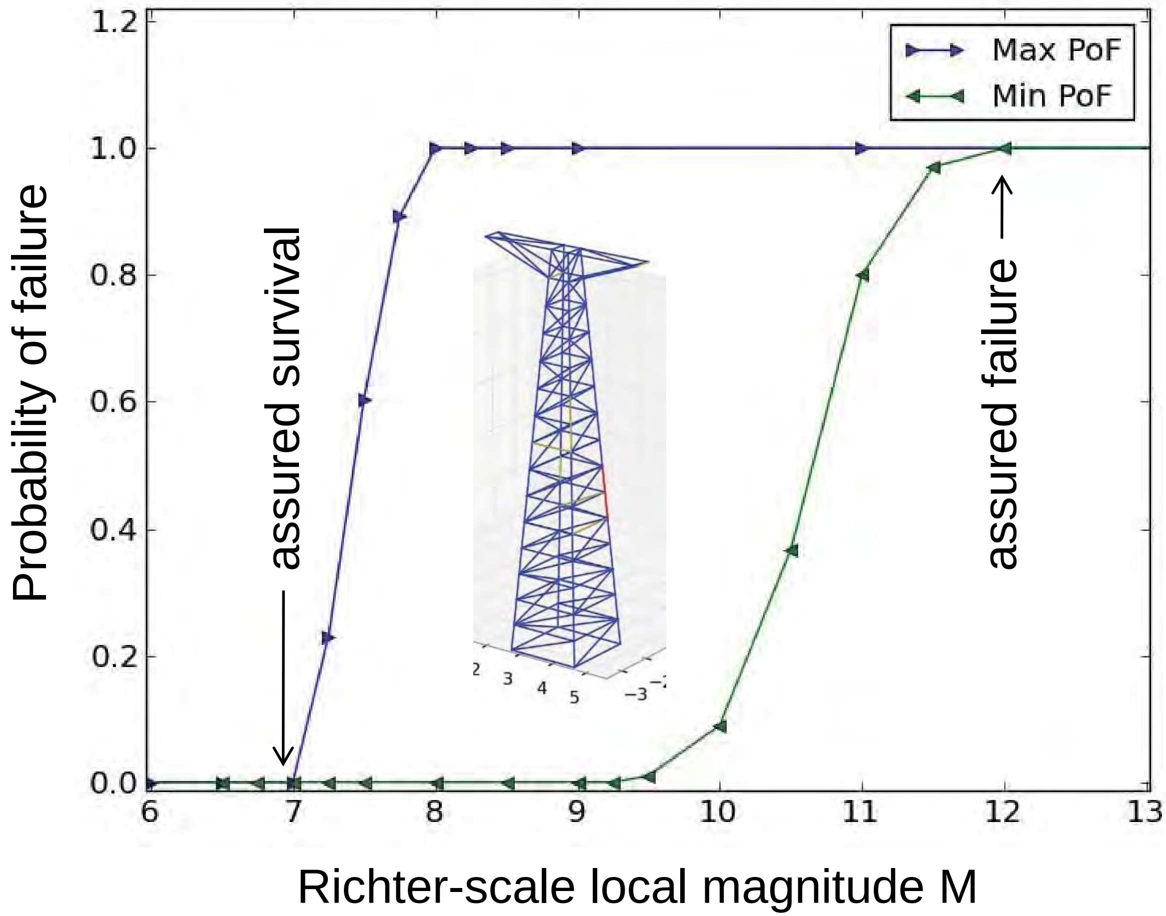

Optimal PoF upper and lower bounds vs. Richter scale magnitude M at hypocentral distance R=25 km, with a_{max} given by Esteva's semi-empirical expression as a function of M

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Concluding remarks – Systems view of Computational Mechanics…

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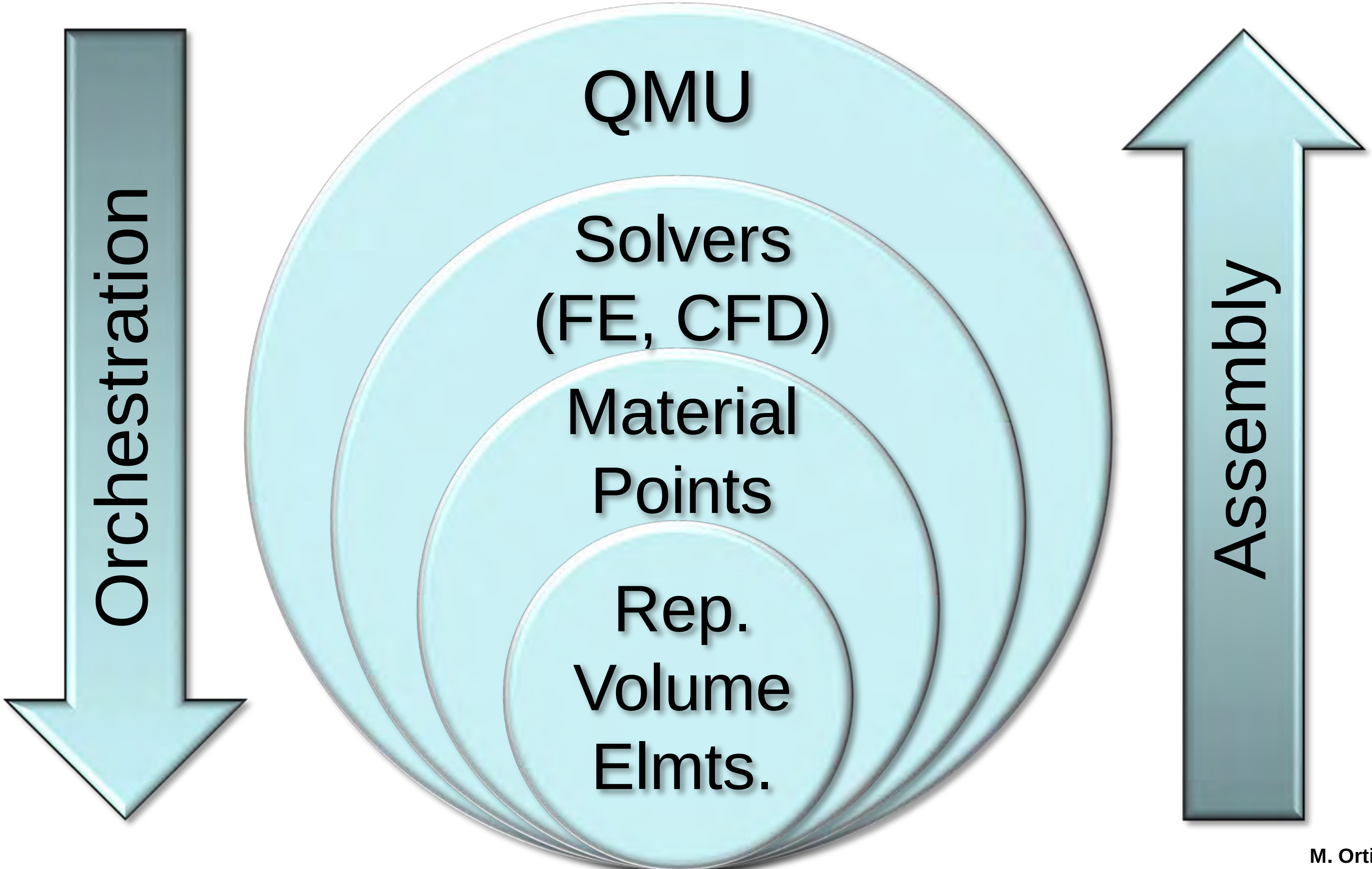

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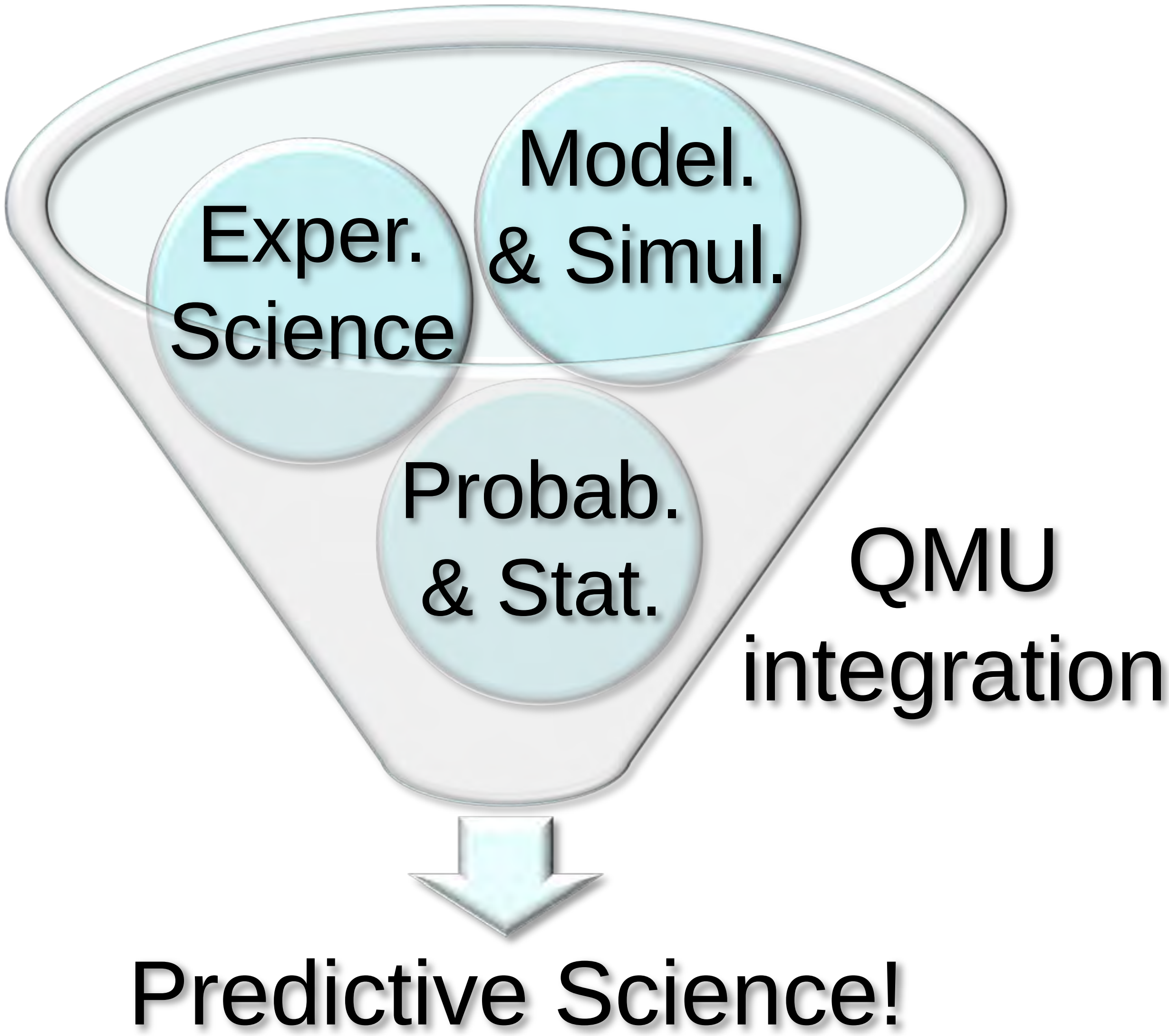
Concluding remarks – Disciplinary view of QMU and Predictive Science



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Concluding remarks…

Thank you!