Model-Based Rigorous Uncertainty Quantification in Complex Systems

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Quantification of margins and uncertainties (QMU)

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- Aim: *Predict mean performance and uncertainty in the behavior of complex physical/engineered systems*
- Example: Short-term weather prediction,
  - Old: Prediction that tomorrow will rain in Warwick…
  - New: *Guarantee* same with 99% confidence…
- *QMU* is important for achieving confidence in high-consequence decisions, designs
- *Paradigm shift* in experimental science, modeling and simulation, scientific computing (*predictive science*):
  - Deterministic → Non-deterministic systems
  - Mean performance → Mean performance + uncertainties
  - Tight integration of experiments, theory and simulation
  - Robust design: Design systems to minimize uncertainty
  - Resource allocation: Eliminate main uncertainty sources

Certification view of QMU

system inputs — response function — performance measures

$$\overbrace{(X_1, \ldots, X_M)}^{\text{system inputs}} \xrightarrow[]{\underbrace{}_{\text{response function}} G} \overbrace{(Y_1, \ldots, Y_N)}^{\text{performance measures}}$$

- Random variables
- Known or unknown pdfs
- Controllable, uncontrollable, unknown-unknowns

System as black box

- Observables
- Subject to performance specs
- Random due to randomness of inputs or of system

Hypervelocity impact as an example of a complex system

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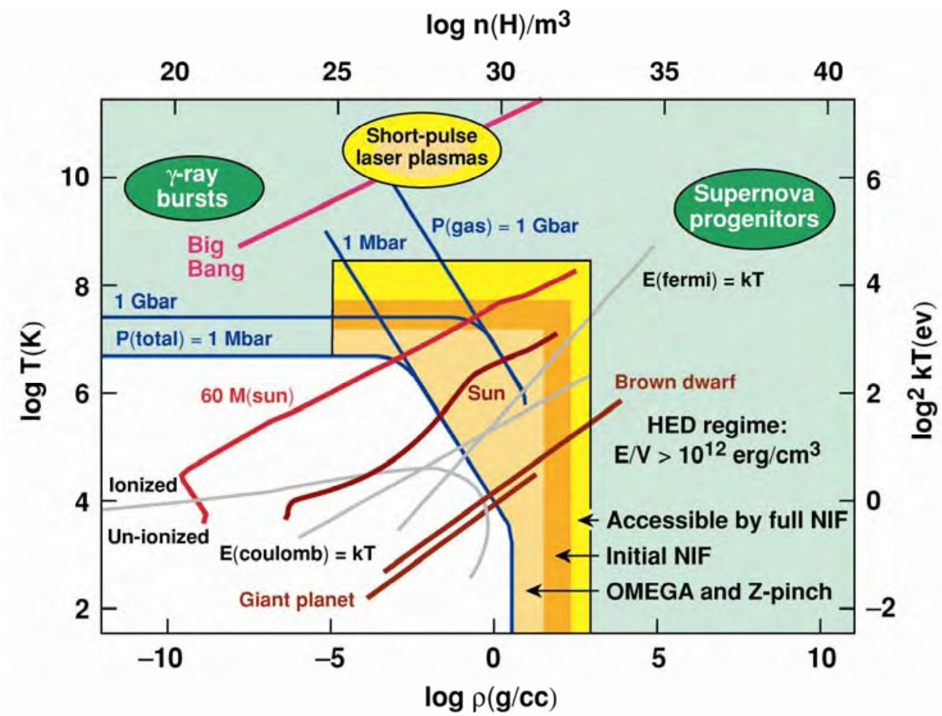
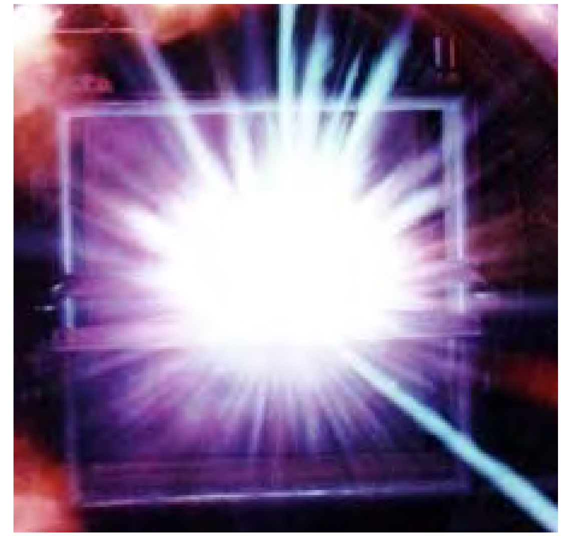
Challenge: Predict *hypervelocity impact* phenomena (10Km/s) with *quantified margins and uncertainties*





NASA Ames Research Center Energy flash from hypervelocity test at 7.9 Km/s

Hypervelocity impact test bumper shield (Ernst-Mach Institut, Freiburg Germany)

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Hypervelocity impact as an example of a complex system

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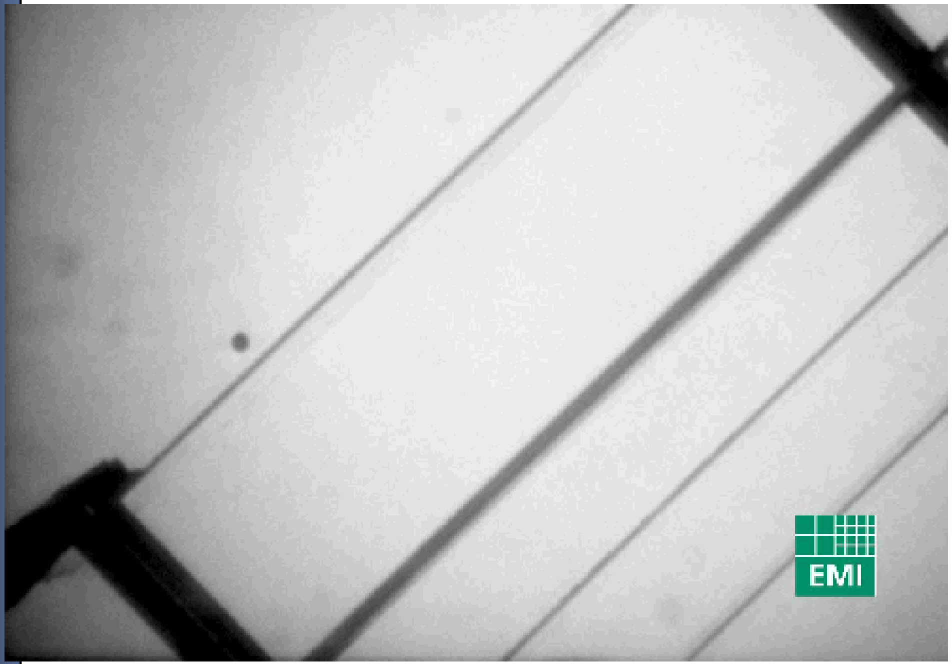
- Hypervelocity impact is of interest to a broad scientific community: Micrometeorite shields, geological impact cratering…



Hypervelocity impact test of multi-layer micrometeorite shield

The International Space Station uses 200 different types of shield to protect it from impacts

Hypervelocity impact at Caltech

Caltech's Small Particle Hypervelocity Impact Range facility
(A.J. Rosakis, Director)

Hypervelocity impact at Caltech

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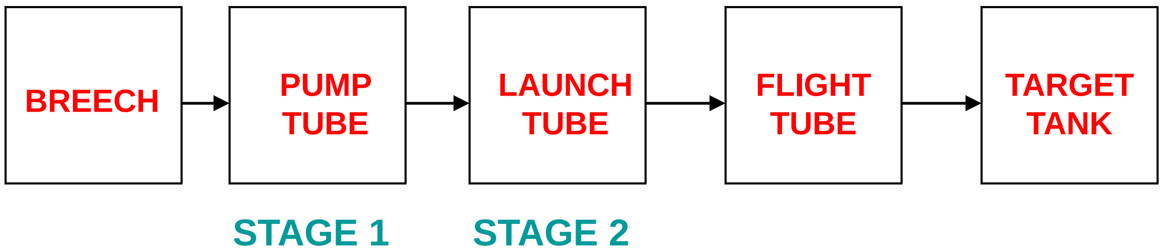
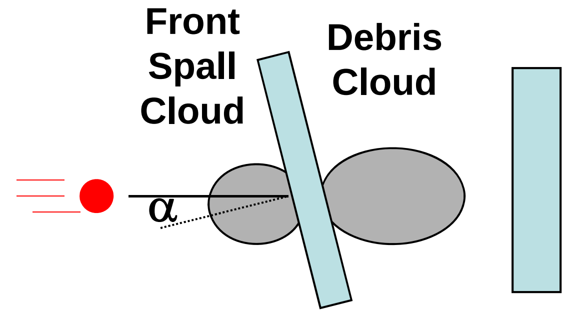
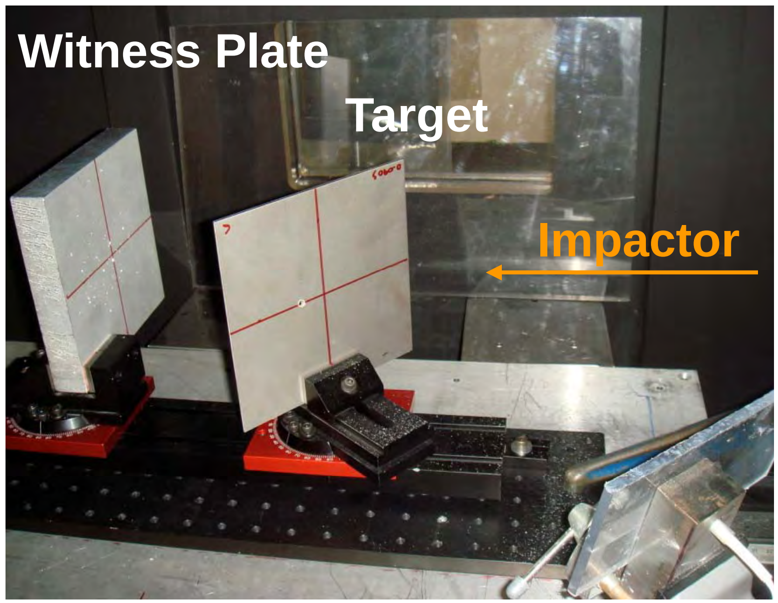




aluminum witness plates replaced by capture media

<u>Target Materials</u>
•Steel
•Aluminum
•*Tantalum*



Ø 71 mil (1×10^{-3} in) launch tube bore

- Impact Speeds: 2 to 10 km/s
- Impact Obliquities: 0 to 80 degrees
- Impactor Mass: 1 to 50 mg

<u>Impactor Materials</u>
•Steel
•Nylon

Hypervelocity impact as system

System inputs (X)	System Outputs (Y)	
	Diagnostics	Metrics
Projectile velocity	Conoscope	Profilometry Perforation area
Projectile mass	CGS	Real-time, full-field back-surface deformation
Number of target plates	VISAR	Real-time back-surface velocimetry
Plate thicknesses	Spectro-photometer	Impact flash, debris and spall clouds, spectra over IR to UV range
Plate obliquities	Capture media	Debris & spall clouds, Particle consistency, size & velocity vector
Projectile/plate materials		

Certification view of QMU

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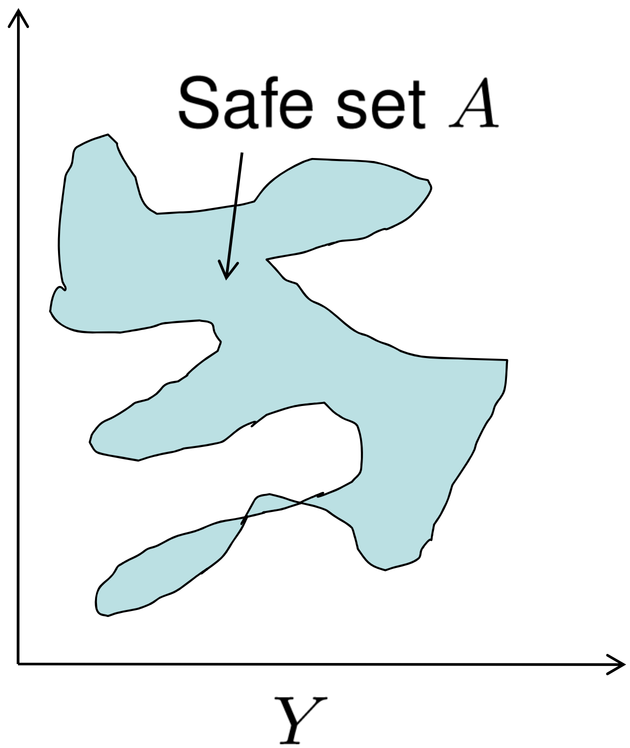
- Certification = Rigorous guarantee that complex system will perform safely and according to specifications



- Certification criterion: Probability of failure must be below tolerance,

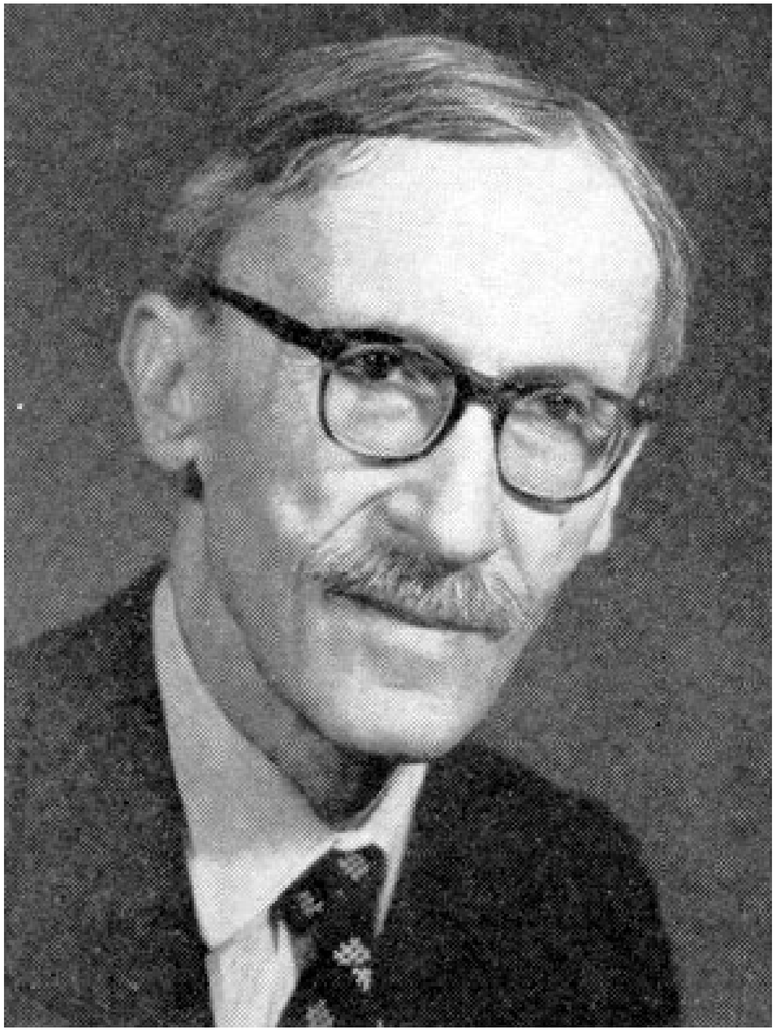
$$\boxed{\mathbb{P}[Y \in A^c] \leq \epsilon}$$

- Alternative (conservative) certification criterion: Rigorous *upper bound* of probability of failure must be below tolerance,

$$\mathbb{P}[Y \in A^c] \leq \boxed{\text{upper bound} \leq \epsilon}$$

- Challenge: Rigorous, measurable/computable upper bounds on the probability of failure of systems

Concentration of measure (CoM)



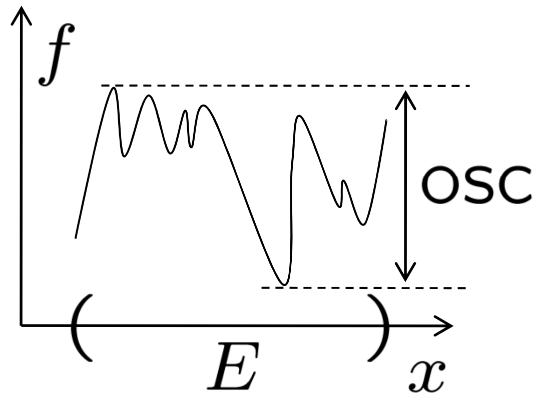
Paul Pierre Levy (1886-1971)

- CoM phenomenon (Levy, 1951): Functions over high-dimensional spaces with small local oscillations in each variable are almost constant
- CoM gives rise to a class of probability-of-failure inequalities that can be used for rigorous certification of complex systems

The *diameter* of a function

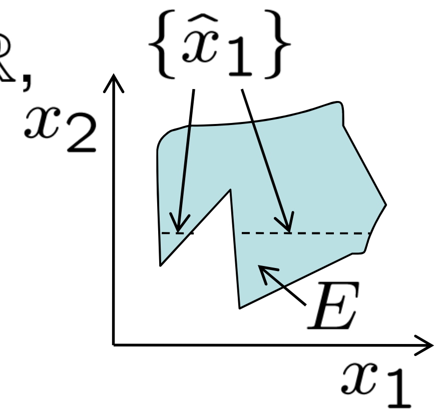
- Oscillation of a function of one variable:

$$\operatorname{osc}(f,E) = \sup_{x\in E} f(x) - \inf_{x\in E} f(x)$$
$$= \sup_{x,x'\in E} |f(x) - f(x')|$$



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

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



- Function diameter:

$$D(f,E) = \sqrt{\sum_{i=1}^{N} D_i^2(f,E)}$$

evaluation requires global optimization!

McDiarmid's inequality

ON THE METHOD OF BOUNDED DIFFERENCES

Colin McDiarmid

(1.2) Lemma: Let $X_1,\dots,X_n$ be independent random variables, with X_k taking values in a set A_k for each k. Suppose that the (measurable) function $f\colon \Pi A_k \to \mathbb{R}$ satisfies

(1.3) $$|f(\underline{x}) - f(\underline{x}')| \le c_k$$

whenever the vectors $\underline{x}$ and $\underline{x}'$ differ only in the kth co–ordinate. Let Y be the random variable $f[X_1,\dots,X_n]$. Then for any $t > 0$,

$$P(|Y - E(Y)| \ge t) \le 2\exp\left[-2t^2/\Sigma c_k^2\right].$$

McDiarmid, C. (1989) "On the method of bounded differences". In J. Simmons (ed.), Surveys in Combinatorics*: London Math. Soc. Lecture Note Series* **141**. Cambridge University Press.

McDiarmid's inequality

Theorem [McDiarmid] *Suppose that:*

i) $\{x_1, \dots, x_N\}$ *are independent random variables,*

ii) $f : E \subset \mathbb{R}^N \to \mathbb{R}$ *is integrable.*

Then, for every $r \geq 0$

$$\mathbb{P}[|\, f - \mathbb{E}[f]\,| \geq r] \leq \exp\left(-2\frac{r^2}{D^2(f,E)}\right),$$

where $D(f,E)$ *is the diameter of* f *over* E*.*

- Bound does not require distribution of inputs
- Bound depends on two numbers: Function *mean* and function *diameter!*

McDiarmid's inequality and QMU

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Corollary *A conservative certification criterion is:*

$$\underbrace{\mathbb{P}[G \leq a]}_{\text{Probability of failure}} \leq \underbrace{\exp\left(-2\frac{(\mathbb{E}[G]-a)_+^2}{D_G^2}\right)}_{\text{Upper bound}} \leq \underbrace{\epsilon}_{\text{Failure tolerance}},$$

- Equivalent statement (confidence factor CF):

$$\text{CF} \equiv \frac{M}{U} \equiv \frac{(\mathbb{E}[G]-a)_+}{D_G} \geq \sqrt{\log\sqrt{\frac{1}{\epsilon}}} \Rightarrow \text{certification!}$$

- Rigorous definition of margin (*M*)
- Rigorous definition of uncertainty (*U*)

Extension to empirical mean

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Theorem [Lucas, Owhadi, MO] *With probability* $1-\epsilon'$,

$$\mathbb{P}[G \leq a] \leq \exp\left(-2\frac{(\langle Y\rangle - a - \alpha)_+^2}{D_G^2}\right),$$

where $\langle Y\rangle = \frac{1}{m}\sum_{i=1}^m Y^i$ *and* $\alpha = D_G m^{-\frac{1}{2}}(-\log\epsilon')^{\frac{1}{2}}$.

- Equivalent statement (confidence factor CF):

$$\text{CF} \equiv \frac{M}{U} \equiv \frac{(\langle Y\rangle - a - \alpha)_+}{D_G} \geq \sqrt{\log\sqrt{\frac{1}{\epsilon}}} \Rightarrow \text{certification!}$$

- Rigorous definition of margin (margin hit!)
- Rigorous definition of uncertainty ($U = D_G$)

Extension to multiple performance measures

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Theorem [Lucas, Owhadi, MO] *A conservative certification criterion is*

$$\mathbb{P}[G_i \notin \prod_{i=1}^{N} [a_i, \infty)] \leq \sum_{i=1}^{N} \exp\left(-2\frac{(\mathbb{E}[G_i] - a_i)_+^2}{D_{G_i}^2}\right) \leq \epsilon.$$

- Equivalent statement (confidence factor CF):

$$\mathrm{CF} = \sqrt{-\log\sqrt{\sum_{i=1}^{N} \exp\left(-2(\mathrm{CF}_i)^2\right)}} \geq \sqrt{\log\sqrt{\frac{1}{\epsilon}}}$$

where: $\mathrm{CF}_i = \dfrac{M_i}{U_i} = \dfrac{\mathbb{E}[G_i] - a_i}{D_{G_i}}$

Multiple performance measures and unknown mean performance

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Theorem [Lucas, Owhadi, MO] *With probability* $1-\epsilon'$,

$$\mathbb{P}[G_i \notin \prod_{i=1}^{N} [a_i, \infty)] \leq \sum_{i=1}^{N} \exp\left(-2\frac{(\langle Y_i\rangle - a_i - \alpha_i)_+^2}{D_{G_i}^2}\right),$$

where $\alpha_i = D_{G_i}\sqrt{\log(N/\epsilon')}/\sqrt{2m}$.

- Equivalent statement (confidence factor CF):

$$\text{CF} = \sqrt{-\log\sqrt{\sum_{i=1}^{N} \exp\left(-2(\text{CF}_i)^2\right)}} \geq \sqrt{\log\sqrt{\frac{1}{\epsilon}}}$$

$$\text{where: } \text{CF}_i = \frac{M_i}{U_i} = \frac{\mathbb{E}[G_i] - a_i - \alpha_i}{D_{G_i}}, \quad \text{margin hit!}$$

McDiarmid's inequality and QMU

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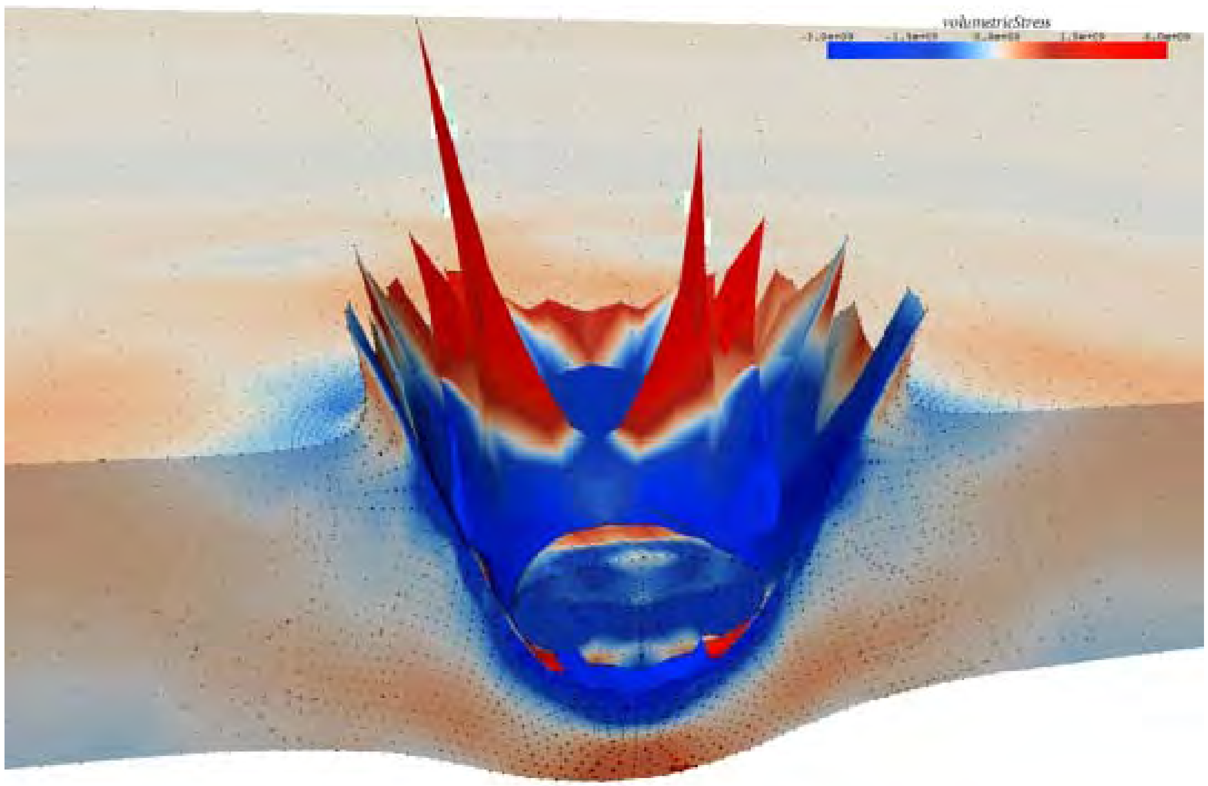
- Direct evaluation of McDiarmid's upper bound requires:
  - Determination of mean performance (e.g., by sampling)
  - Determination of system diameter by solving a sequence of global optimization problems
- Viable approach for systems that can be tested cheaply
- Prohibitively expensive or unfeasible in many cases!
  - Tests too costly, time-consuming
  - Operating conditions are not observable
  - Political/environmental constraints…
- Alternative: Model-based certification!
- Challenge: How can we use physics-based models to achieve rigorous certification with a minimum of testing?

Model-based QMU – The model

$$\overbrace{(X_1,\ldots,X_M)}^{\text{System inputs}} \xrightarrow{\underbrace{\text{Model}}_{F}} \overbrace{(Y_1,\ldots,Y_N)}^{\text{performance measures}}$$



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Model-based QMU – McDiarmid

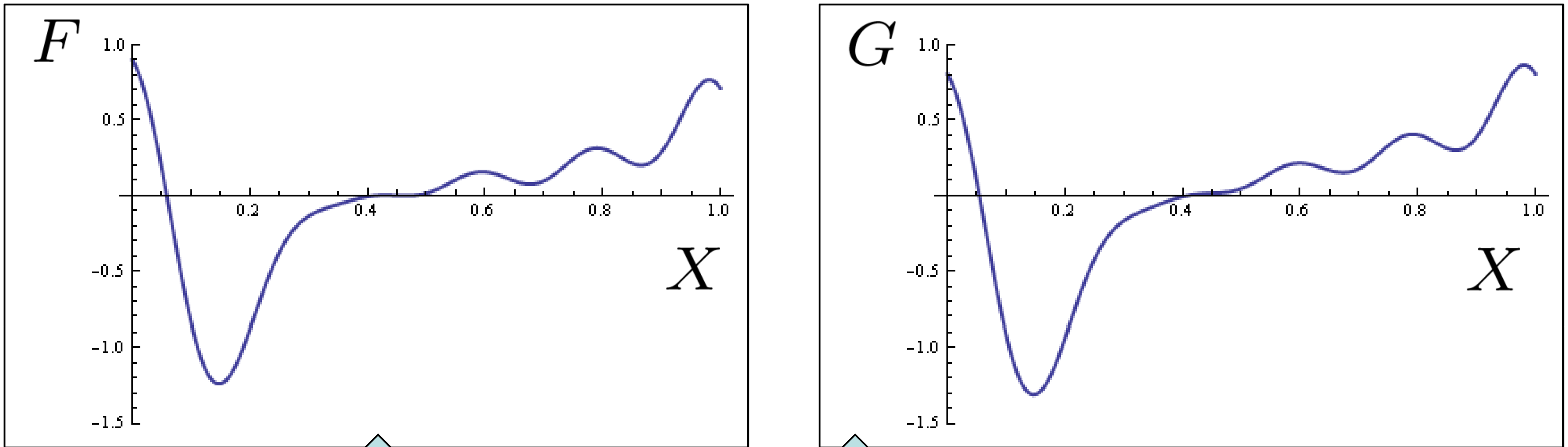
- Two functions that describe the system:
  - Experiment: *G(X)*
  - Model: *F(X)*

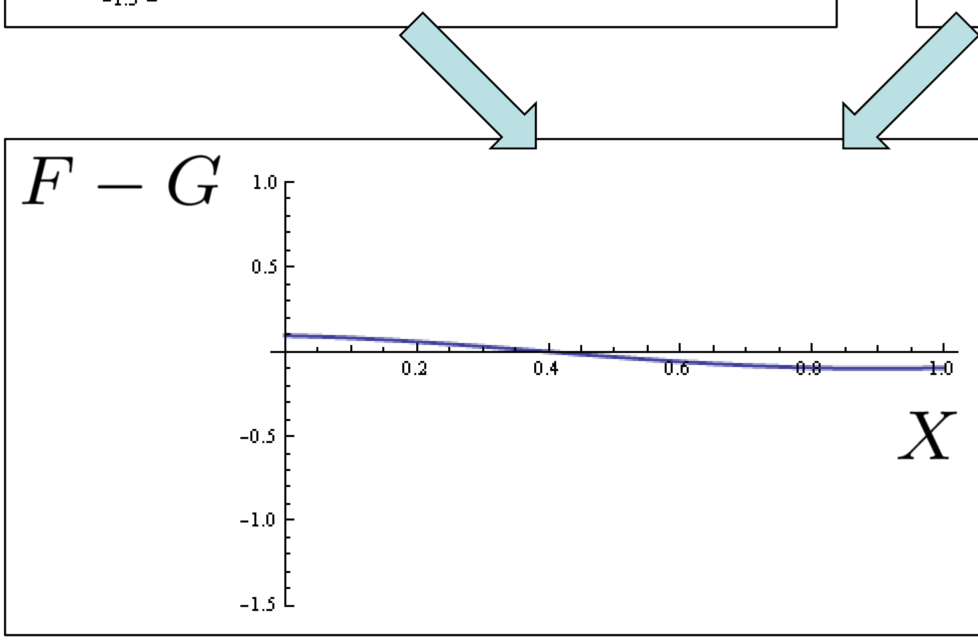
  F(X)-G(X) ≡ Modeling-error function
- Linearity: $\mathbb{E}[G] = \mathbb{E}[F] - \mathbb{E}[F-G]$
- Triangular inequality: $D_G \leq D_F + D_{F-G}$
- Corollary: A conservative certification criterion is:

$$\mathbb{P}[G \leq a] \leq \exp\left(-2\frac{(\mathbb{E}[F] - \mathbb{E}[F-G] - a)_+^2}{(D_F + D_{F-G})^2}\right) \leq \epsilon,$$

- E[*F*]: Model mean; E[*F-G*]: Model mean error
- D_F: ***Model diameter*** (*variability* of model)
- $D_{F\text{-}G}$: ***Modeling error*** (*badness* of model)

Model-based QMU – McDiarmid





- Working assumptions:
  - *F-G* far more regular than *F* or *G* alone
  - Global optimization for $D_{F\text{-}G}$ converges fast
  - Evaluation of $D_{F\text{-}G}$ 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 $D_{F\text{-}G}$ requires (few) experiments
- Rigorous certification not achievable by modeling and simulation alone!

Model-based QMU – Implementation

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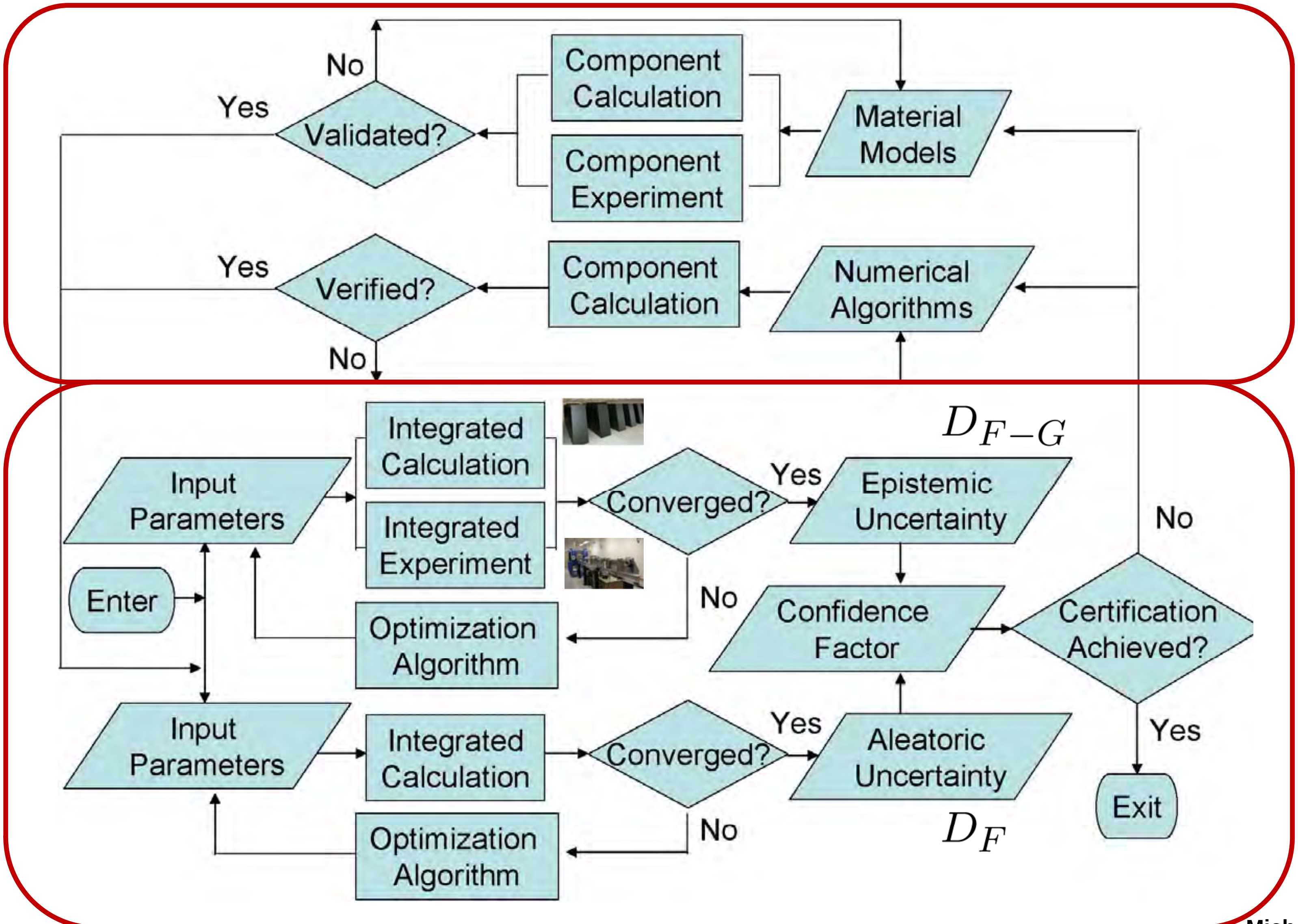
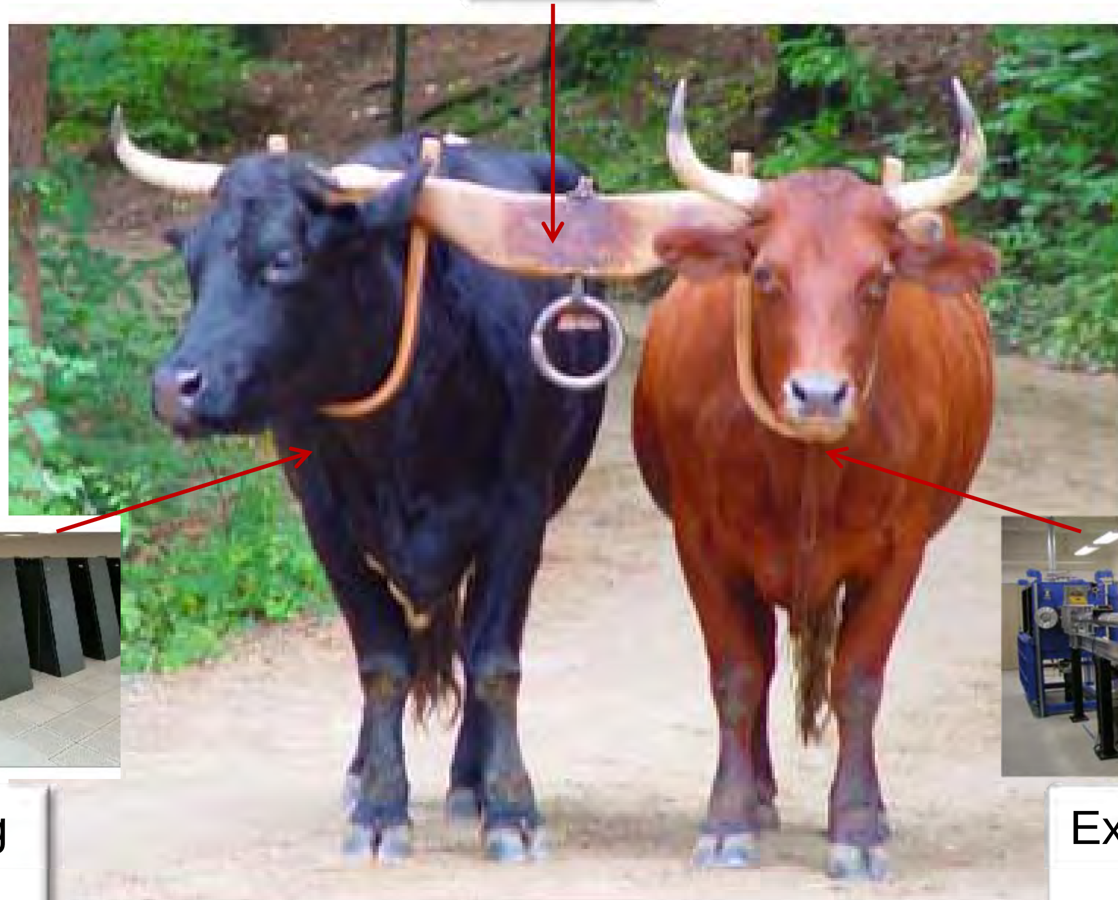


Model-based QMU – Implementation

UQ

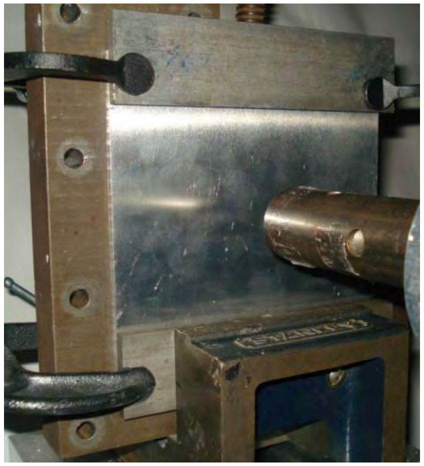


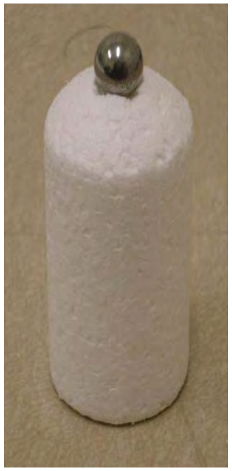
Modeling and Simulation

Experimental Science

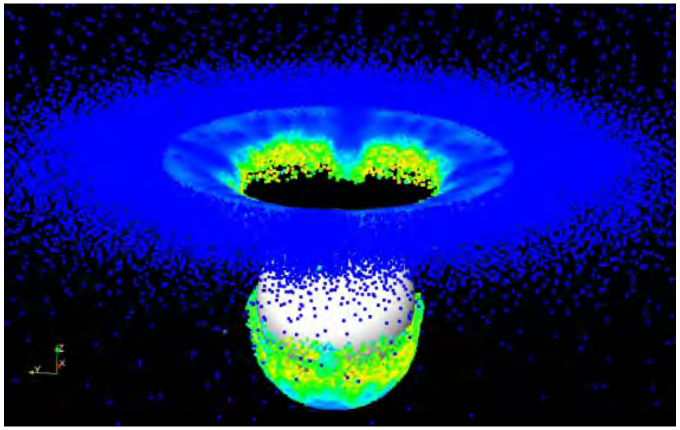
Sample UQ Analysis – Ballistic range

- Target/projectile materials:
  - Target: Al 6061-T6 plates (6"x 6")
  - Projectile: S2 Tool steel balls (5/16")
- Performance measure (output): Perforation area
- Admissible operation range: Perforation area > 0!
- Model parameters (inputs):
  - Plate thickness (0.032''-0.063'')
  - Impact velocity (100-400 m/s)
- Optimal Transportation Meshfree (OTM) solver (sequential)
- Modifier adaption, BFGS; in-house UQ pipeline (Mystic)



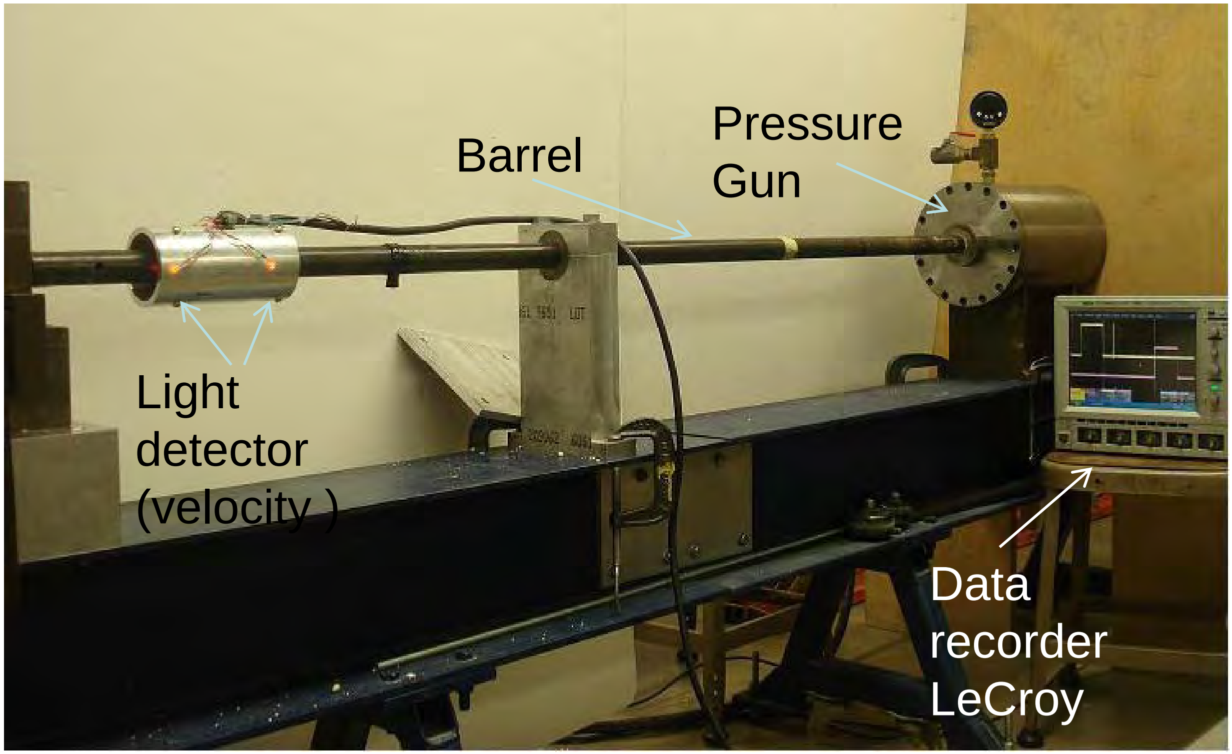


Target and projectile

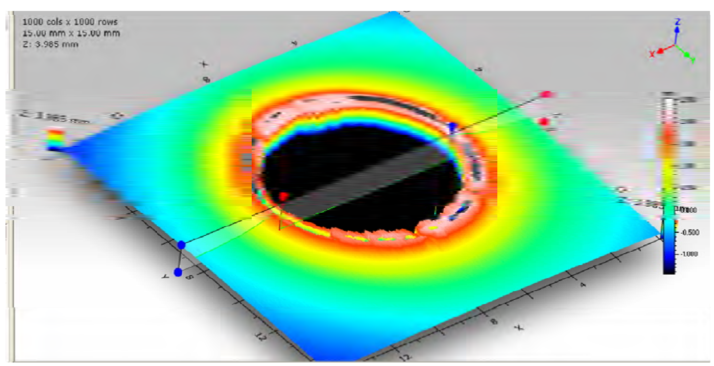


OTM simulation

Sample UQ Analysis – Ballistic range



Optimet MiniConoscan 3000



Sample UQ Analysis – Ballistic range

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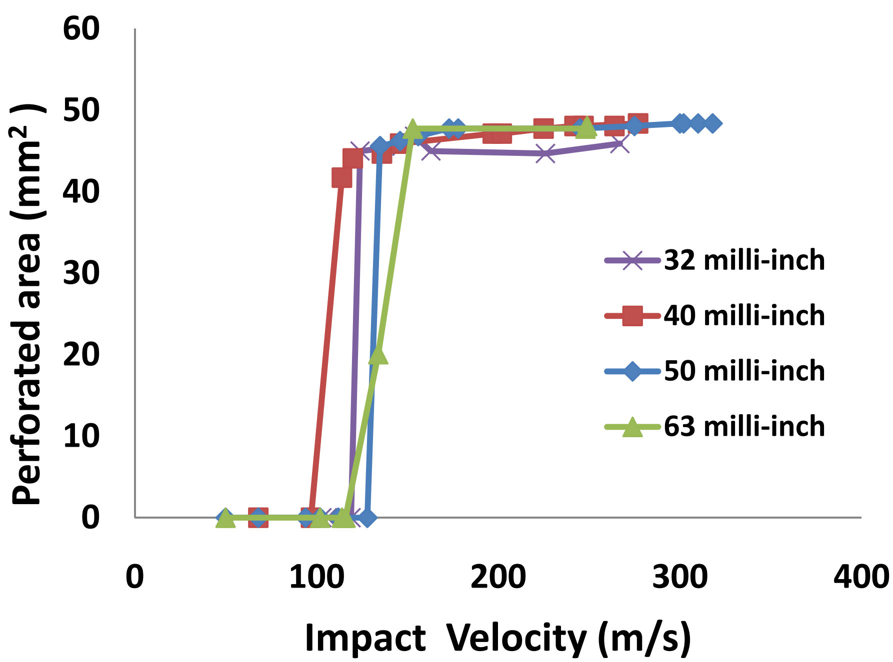

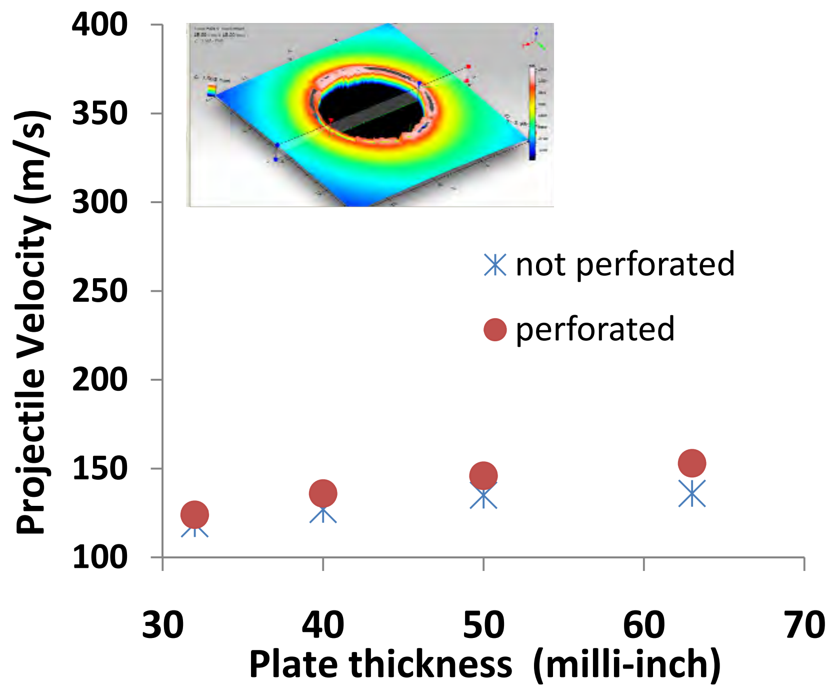

Perforation area *vs*. impact velocity (note small data scatter!)

Perforation/non-perforation boundary

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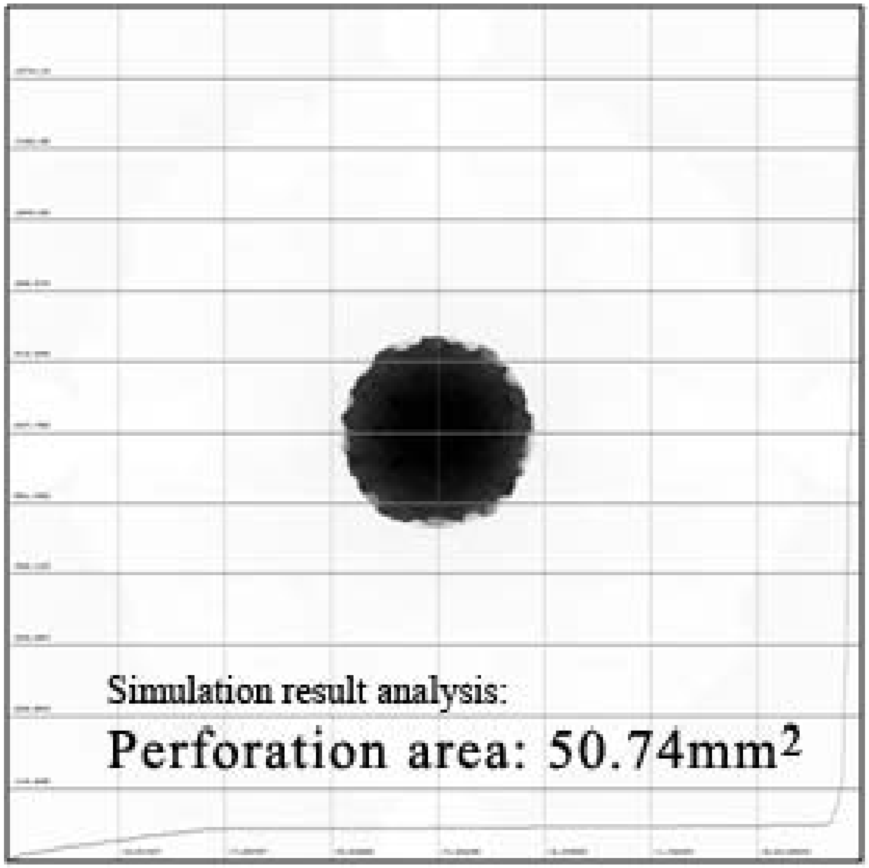
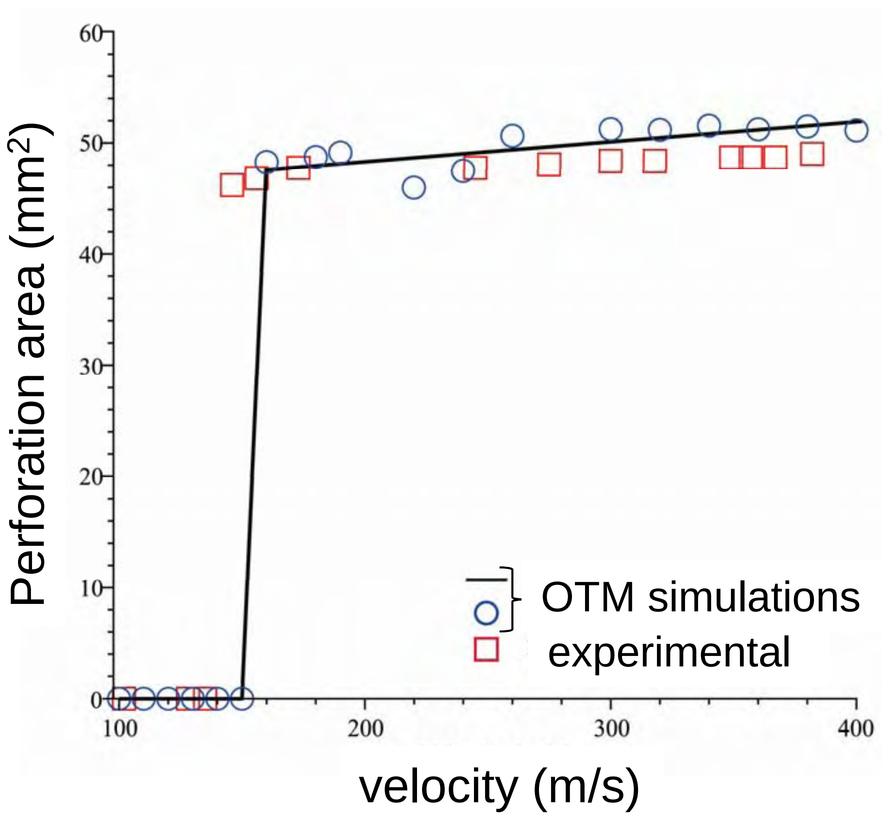
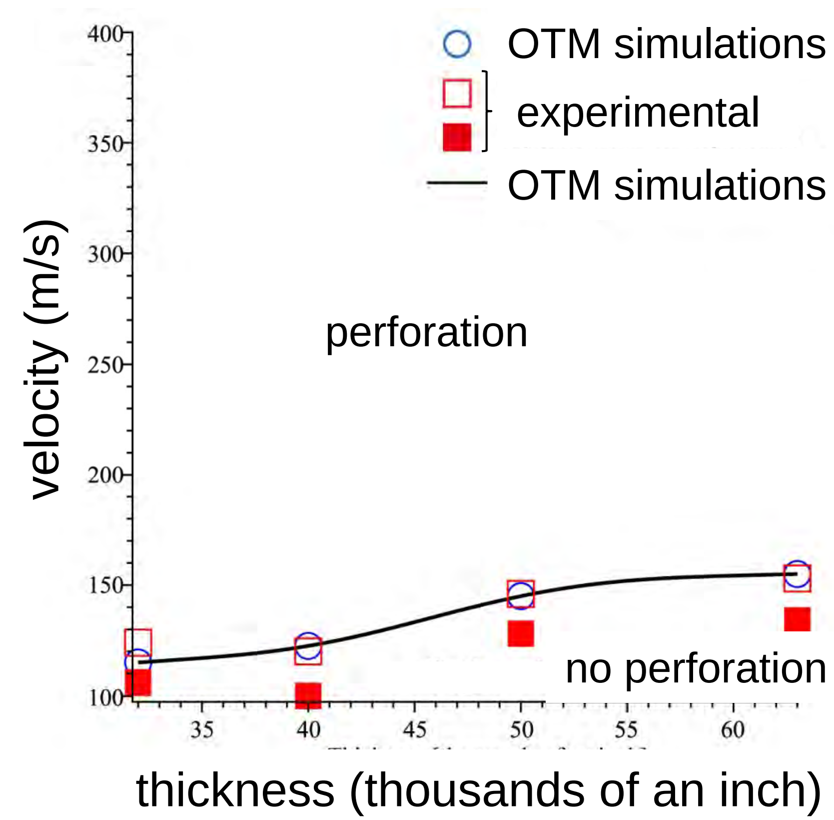
Sample UQ Analysis – Ballistic range



Computed *vs*. measured perforation area

Sample UQ Analysis – Ballistic range





Measured *vs*. computed perforation area

Sample UQ Analysis – Ballistic range

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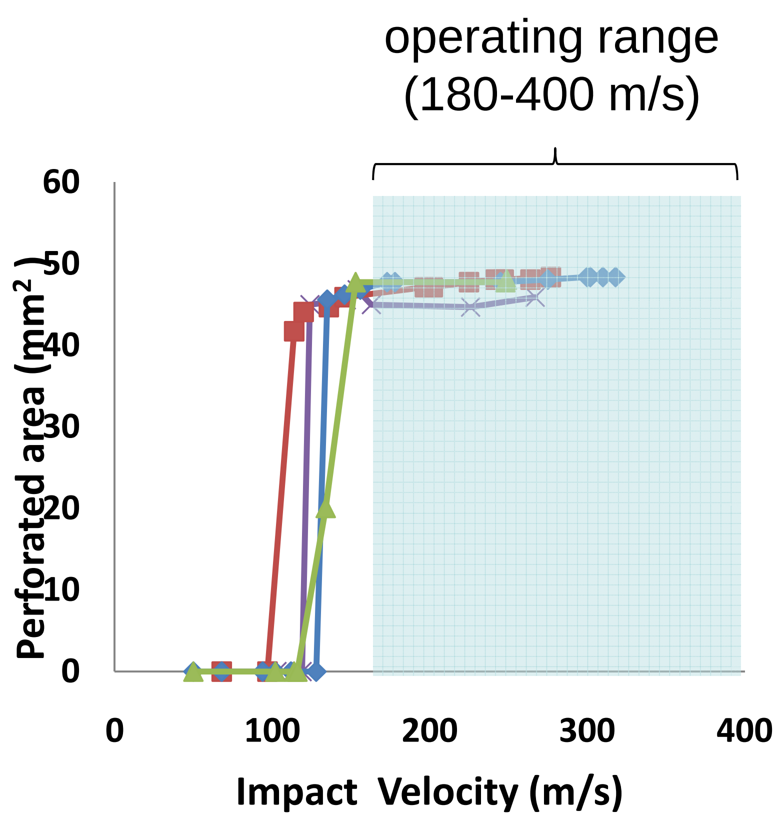
Model diameter D_F	thickness	4.33 mm^2
	velocity	4.49 mm^2
	total	6.24 mm^2
Modeling error $D_{F\text{-}G}$	thickness	4.96 mm^2
	velocity	2.16 mm^2
	total	5.41 mm^2
Uncertainty $D_F + D_{F\text{-}G}$		11.65 mm^2
Empirical mean <*G*>		47.77 mm^2
Margin hit α ($\varepsilon'=0.1\%$)		4.17 mm^2
Confidence factor *M/U*		3.74

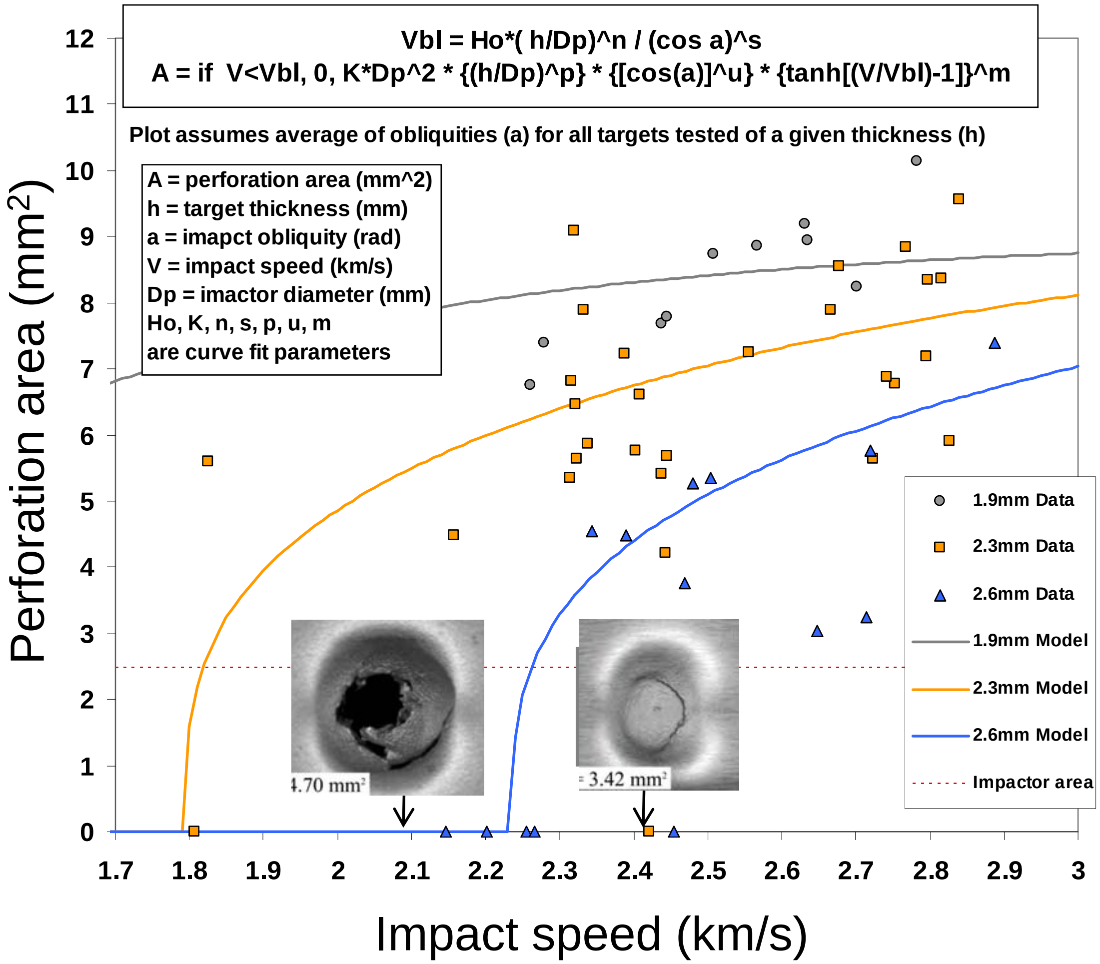


- Perforation can be certified with ~ 1-10^{-12} confidence!
- Total number of tests ~ 50 → Approach feasible!

Beyond McDiarmid - Extensions

- A number of extensions of McDiarmid may be required in practice:
  - Some input parameters cannot be controlled
  - There are unknown input parameters (unknown unknowns)
  - There is experimental scatter (*G* defined in probability)
  - McDiarmid may not be tight enough (convergence?)
  - Model itself may be uncertain (epistemic uncertainty)
  - Data may not be available ‘on demand’ (legacy data)
- Extensions of McDiarmid that address these challenges include:
  - Martingale inequalities (unknown unknowns, scatter…)
  - Partitioned McDiarmid inequality (convergent upper bounds)
  - Optimal Uncertainty Quantification (OUQ)
  - Optimal models (least epistemic uncertainty

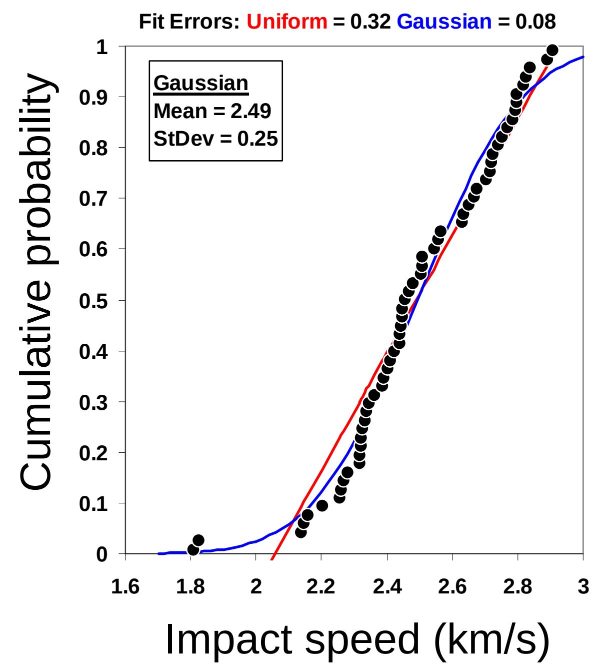
Beyond McDiarmid – Scatter



Experimental ballistic curves (SPHIR)
440 C Steel spherical projectiles
304 Stainless Steel plate targets

- Added challenges:
  - Experimental scatter!
  - Impact velocity uncontrollable!

Measured speed distribution



Beyond McDiarmid – Scatter

known controllable inputs

$$(X_1, \ldots, X_M)$$

$$(Z_1, \ldots, Z_L)$$

uncontrollable inputs & unknown unknowns

Response function

$$G$$

performance measures

$$(Y_1, \ldots, Y_N)$$

Beyond McDiarmid – Scatter

- Let $\langle f \rangle$ denote averaging with respect to uncontrollable variables and unknown unknowns
- Let $f' = f - \langle f \rangle$ be the fluctuation
- **Theorem** [Lashgari, Owhadi, MO] A conservative certification criterion is:

$$\mathbb{P}[G \leq a] \leq \exp\left(-2\frac{(\mathbb{E}[\langle F \rangle] - \mathbb{E}[\langle F - G \rangle] - a)_+^2}{(D_{\langle F \rangle} + D_{\langle F-G \rangle} + \underbrace{D_{G'}})^2}\right) \leq \epsilon$$

measure of experimental scatter!

- Simulations and experiments must be averaged wrt uncontrolled variables and unknown unknowns
- Data scatter contributes to uncertainty!

Beyond McDiarmid – Scatter

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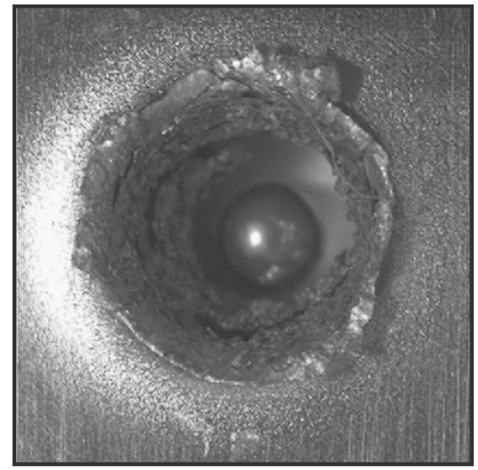
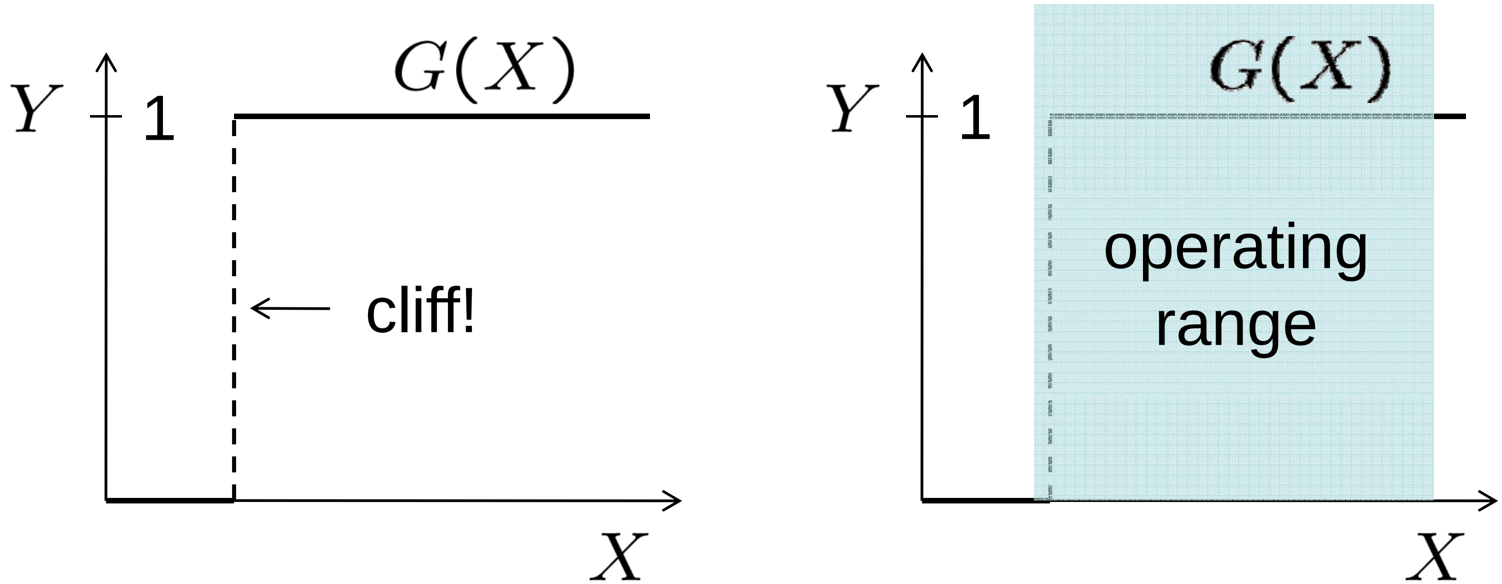
Diameters	Model $D_{\langle F \rangle}$	thickness	1.82 mm^2
		obliquity	2.41 mm^2
		total	3.02 mm^2
	Modeling error $D_{\langle F-G \rangle}$	thickness	1.80 mm^2
		obliquity	4.50 mm^2
		total	4.85 mm^2
	Experimental scatter $D_{G'}$	total	7.78 mm^2
Mean values	Model E[F]	total	3.30 mm^2
	Modeling error E[F-G]	total	0.32 mm^2



Steel-on-steel, 2.6 km/s
Perforation and impactor

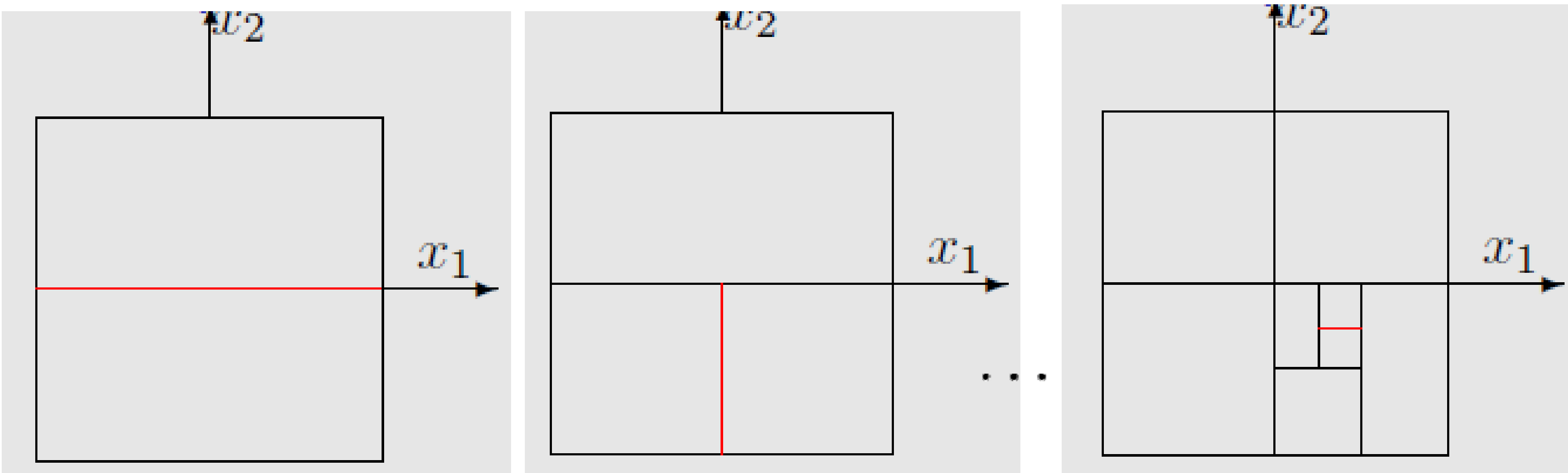
- Perforation cannot be certified with any reasonable confidence!

Beyond McDiarmid - Partitioning



- Mean performance: $\mathbb{E}[G] = 1$
- Function diameter: $D_G = 1$
- McDiarmid probability upper bound for no-perforation:
  $= e^{-2} \approx 0.135335$
- McDiarmid inequality too coarse for cliff behavior!

Beyond McDiarmid - Partitioning



Theorem [Sullivan *et al.*] If F continuous, the sequence

$$\sum_{i=1}^{N} \mathrm{Prob}\left[A_i\right] \exp\left(-2\frac{(a-\mathbb{E}\left[F|A_i\right])_+^2}{D_{F|A_i}^2}\right)$$

converges to $\mathrm{Prob}[F \geq a]$.

Beyond McDiarmid – Optimal UQ

CALTECH PSAAP

- What is the least probability of failure upper bound given what is known about the system?
- Best probability of failure upper bound given that probability μ of inputs and response function G are in a set A*:*

$$\sup_{(\mu,G)\in\mathcal{A}} \mu[G(X) \leq a]$$

- Can be reduced, to finite-dimensional optimization (Choquet theory, representation of linear functionals by measures on extreme points, moment problems…)
- Example: Mean performance and diameter known
- Explicit solutions for finite-dimensional inputs (Owhadi *et al*.), optimal McDiarmid-type inequalities!

Concluding remarks…

- QMU represents a paradigm shift in predictive science:
  - Emphasis on predictions with *quantified uncertainties*
  - Unprecedented integration between simulation and experiment
- QMU supplies a powerful organizational principle in predictive science: *Theorems run entire centers*!
- QMU raises theoretical and practical challenges:
  - Tight and measureable/computable probability-of-failure upper bounds (need theorems!)
  - Efficient global optimization methods for highly non-convex, high-dimensionality, noisy functions
  - Effective use of massively parallel computational platforms, heterogeneous and exascale computing
  - High-fidelity models (multiscale, effective behavior…)
  - Experimental science for UQ (diagnostics, rapid-fire testing…)…