Model-Based Rigorous Uncertainty Quantification in Complex Systems

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ASC/PSAAP Centers

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PSAAP: Predictive Science Academic Alliance Program

Hypervelocity impact as an example of a complex system

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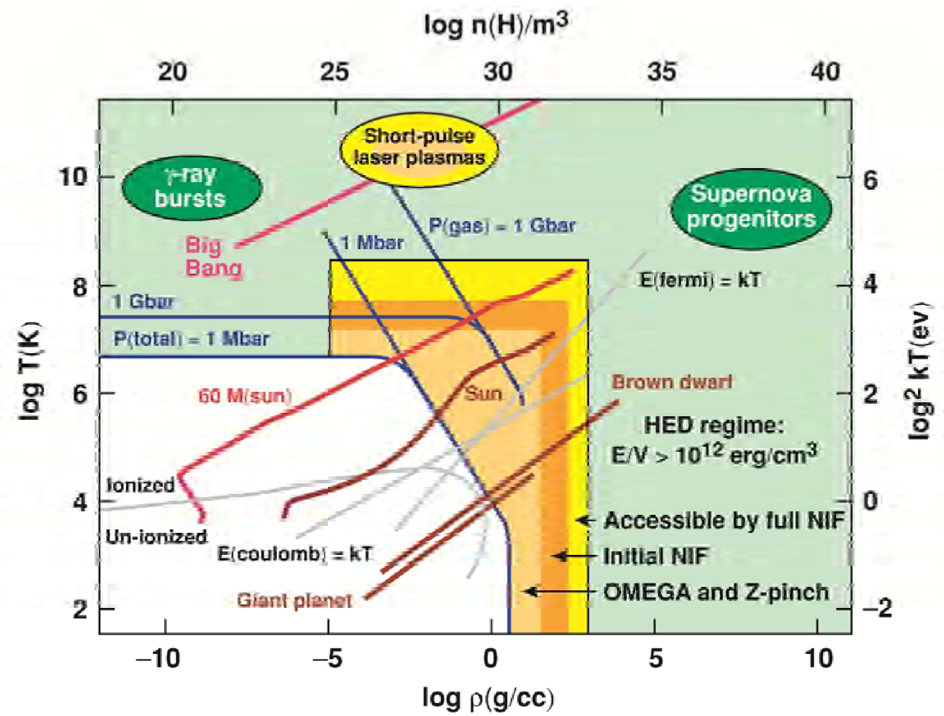
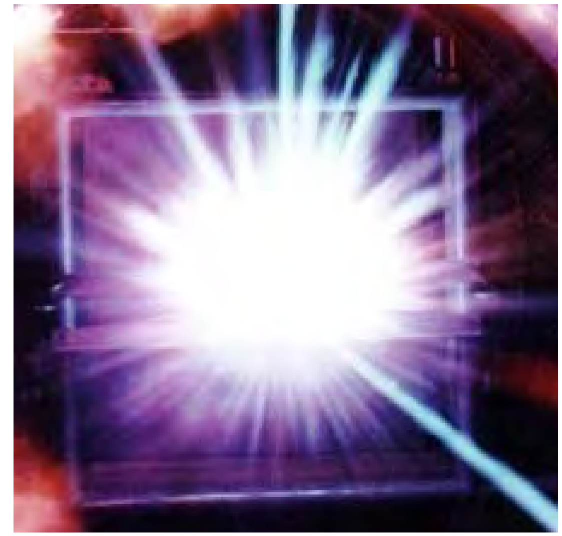
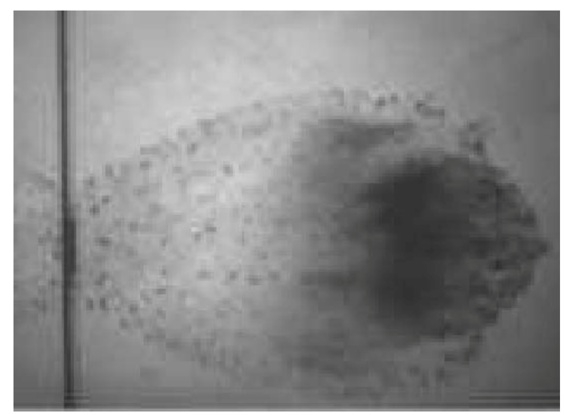
Challenge: Predict *hypervelocity impact* phenomena (10Km/s) with ***quantified margins and uncertainties***





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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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 Buenos Aires…
  - 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

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

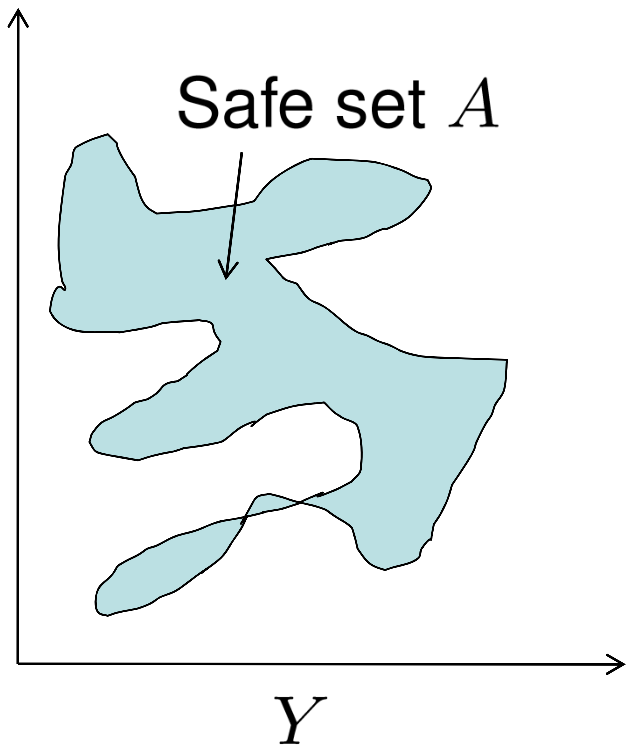
- Random variables
- Known or unknown pdfs
- Controllable, uncontrollable, unknown-unknowns

System as black box

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

Certification view of QMU

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



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

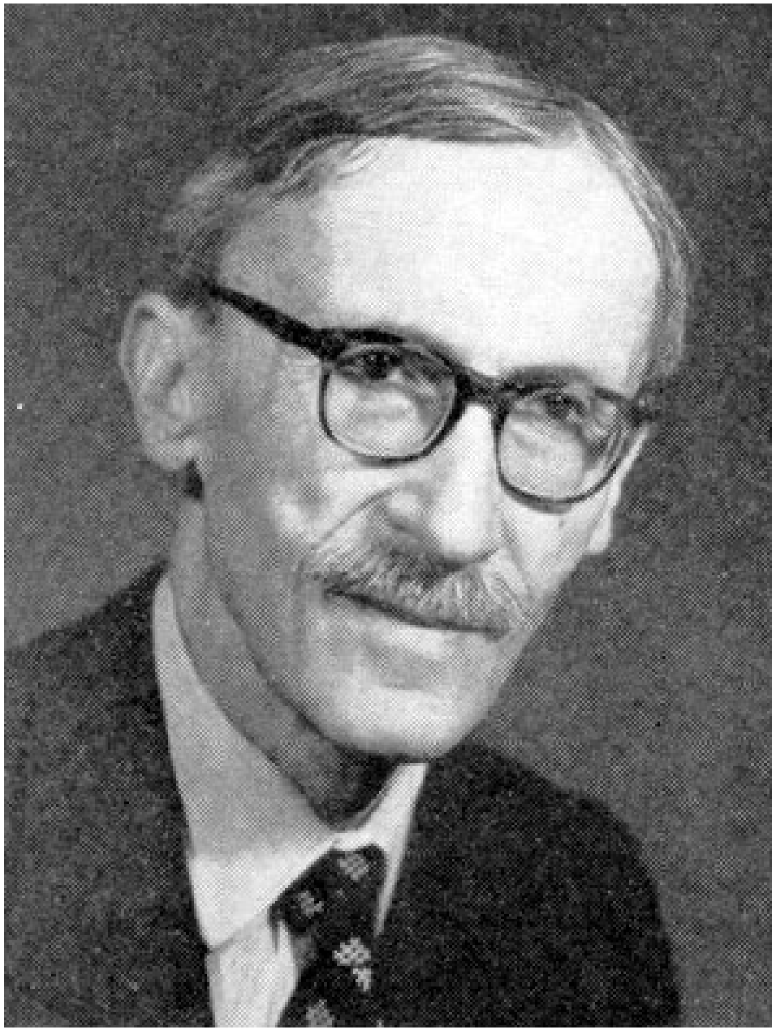
$$\mathbb{P}[Y \in A^c] \le \epsilon$$

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

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

- 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

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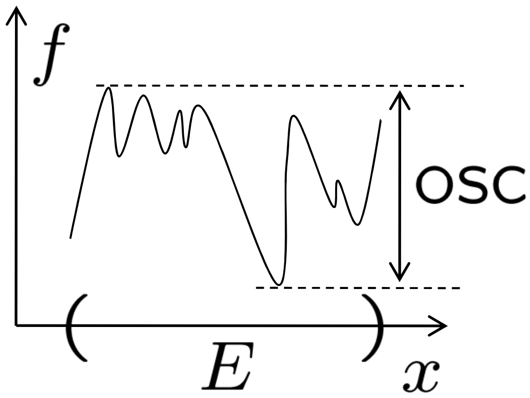
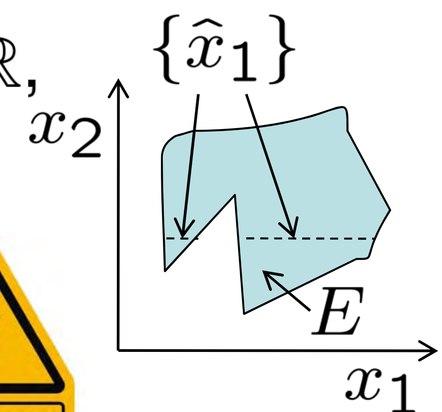
- Oscillation of a function of one variable:

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



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

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



- Function diameter:

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

evaluation requires global optimization!

McDiarmid's inequality

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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 $f\left[X_1,\dots,X_n\right]$. 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 only: Function ***mean*** and function ***diameter****!*

McDiarmid's inequality and QMU

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*)

McDiarmid's inequality and QMU

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- CoM Uncertainty Quantification (UQ) 'does the job':
  - Rigorous upper bounds on PoFs for complex systems
  - Rigorous definitions of 'uncertainty' and 'margin'
  - Does not require knowledge of input parameters pdfs
  - Reduces UQ to determination of:
    - Mean performance $E[G]$
    - System diameter D_G
- But determination of response diameter is a global optimization problem over parameter space: Solution requires exceedingly many function evaluations
- Strictly experimental implementation is often impractical
- Alternative: ***Model-Based Uncertainty Quantification!***

Model-Based QMU

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$$\overbrace{(X_1,\ldots,X_M)}^{\text{system inputs}} \xrightarrow{\overbrace{\quad F \quad}^{\text{response function}}} \overbrace{(Y_1,\ldots,Y_N)}^{\text{performance measures}}$$

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

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

System model

Model-based QMU – Perfect model

System model

- Assume ***deterministic system*** (no scatter)
- Assume ***model is perfect*** (F=G)
- Assume that *mean performance* and *system diameter* can be ***computed exactly***
- Then UQ can be carried out entirely in cyber-space, ***no experiments are required!***

Case Study – Steel/Al ballistics

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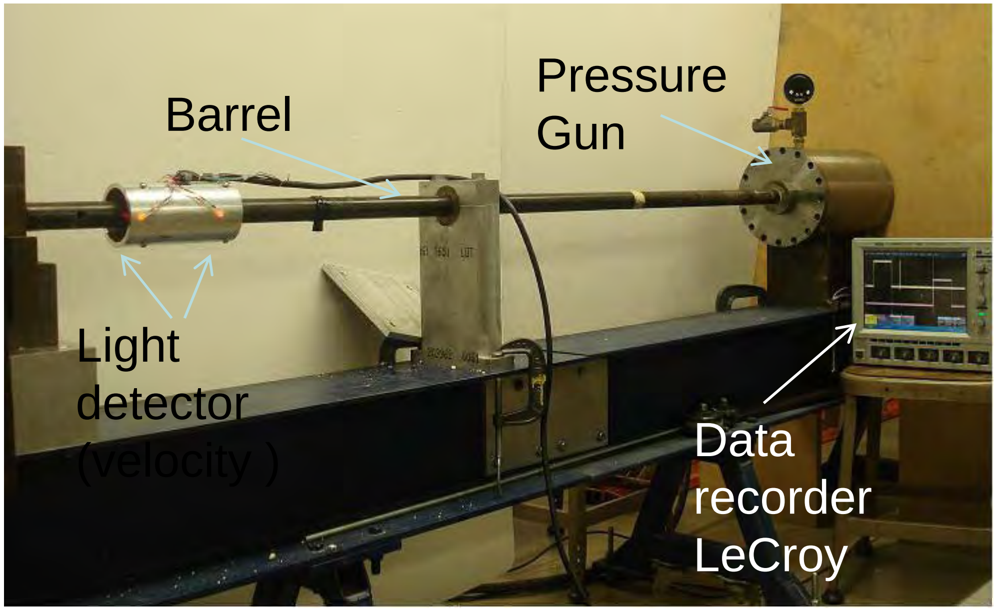
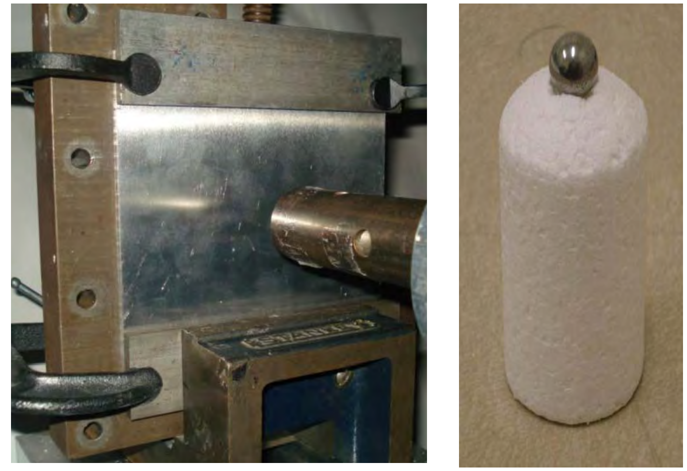
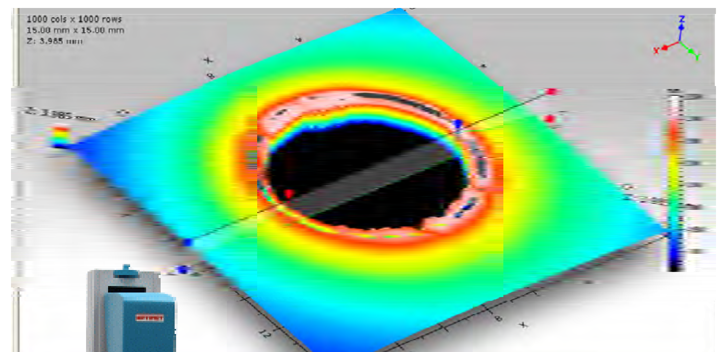




Target and projectile



Optimet MiniConoscan 3000

- 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

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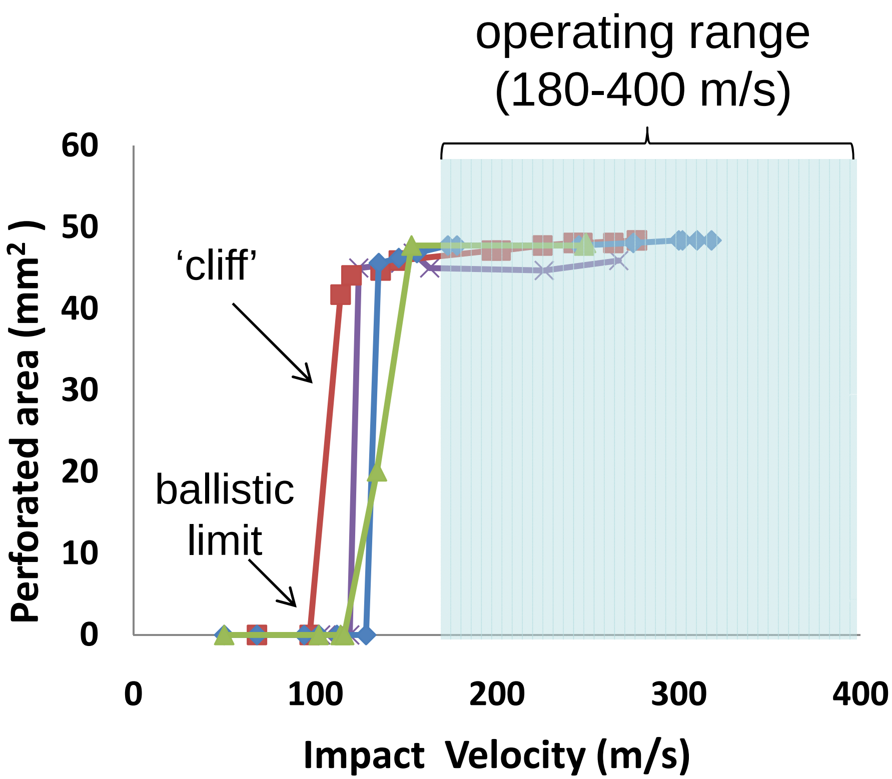
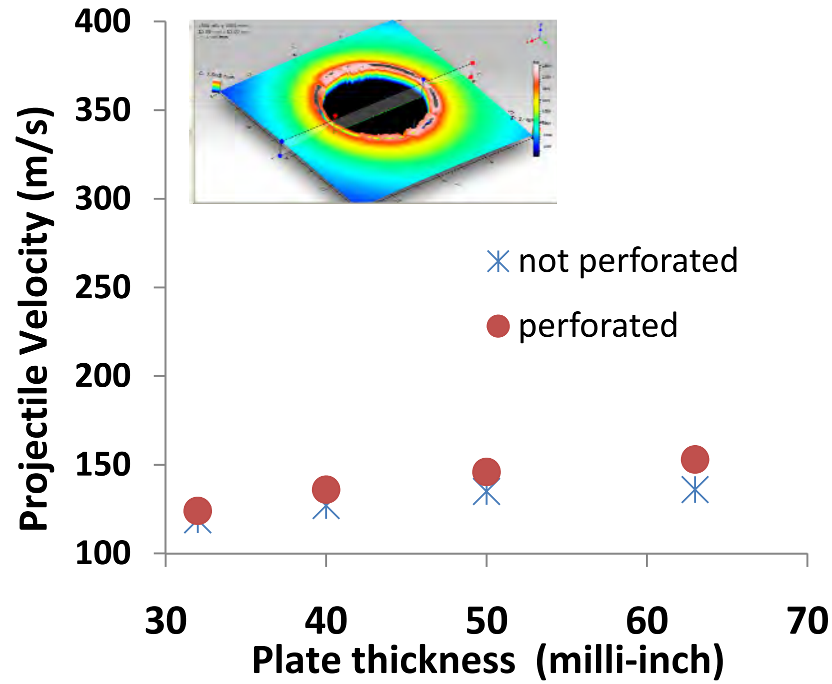


Perforation area *vs*. impact velocity (note small data scatter!)



Perforation/non-perforation boundary

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

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Optimal-Transportation Meshfree (OTM) model of terminal ballistics

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- Optimal transportation theory is a useful tool for generating geometrically-exact discrete Lagrangians for flow problems
- Inertial part of discrete Lagrangian measures distance between consecutive mass densities (in sense of Wasserstein)
- Discrete Hamilton principle of stationary action: Variational time integration scheme:
  - Symplectic, time reversible, exact conservation
  - Variational convergence (Γ-convergence, B. Schmidt)
- Extension to inelasticity: Variational constitutive updates

Li, B., Habbal, F. and Ortiz, M., *IJNME*, **83** (2010) 1541-1579

OTM – Spatial discretization

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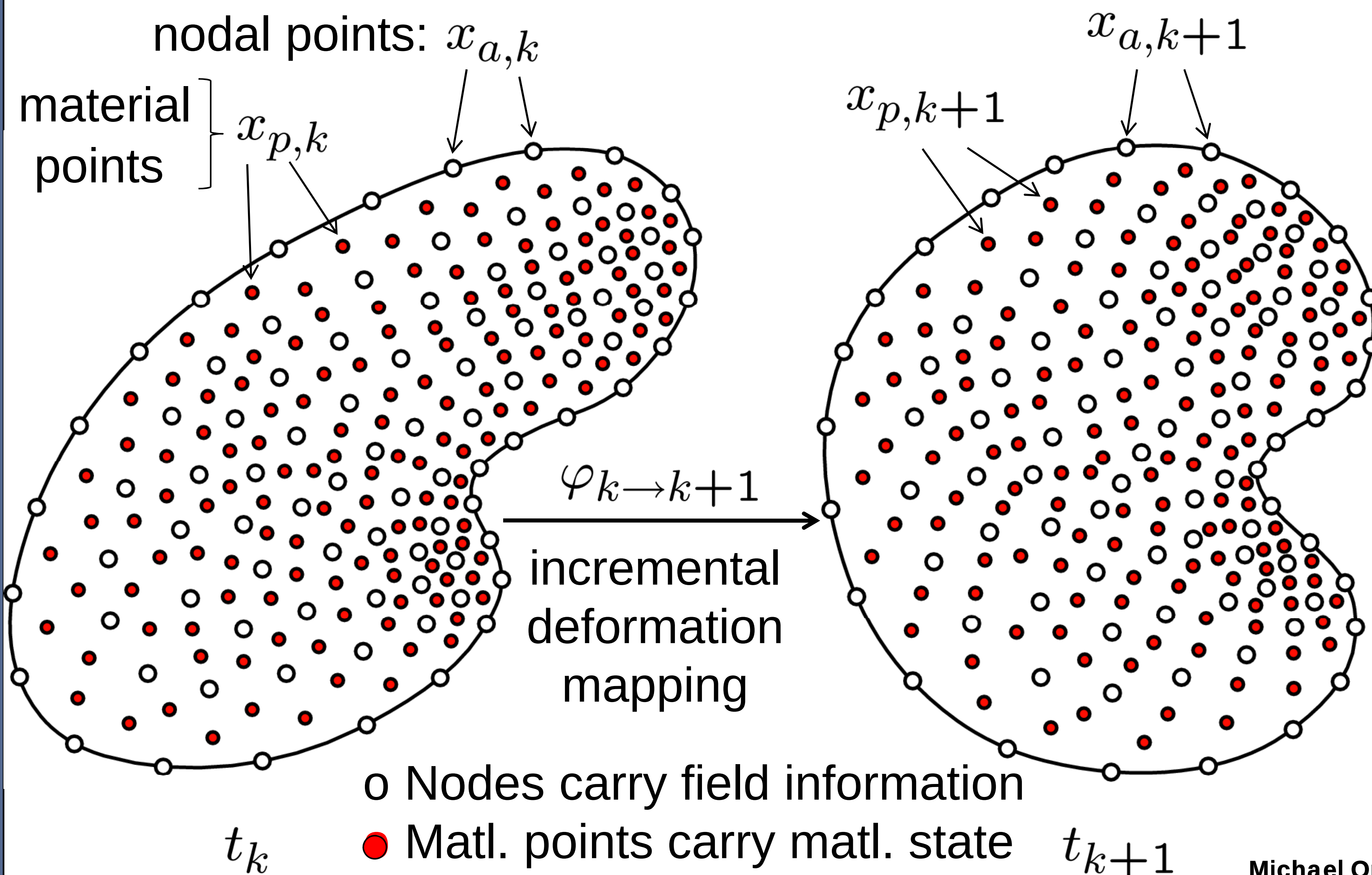
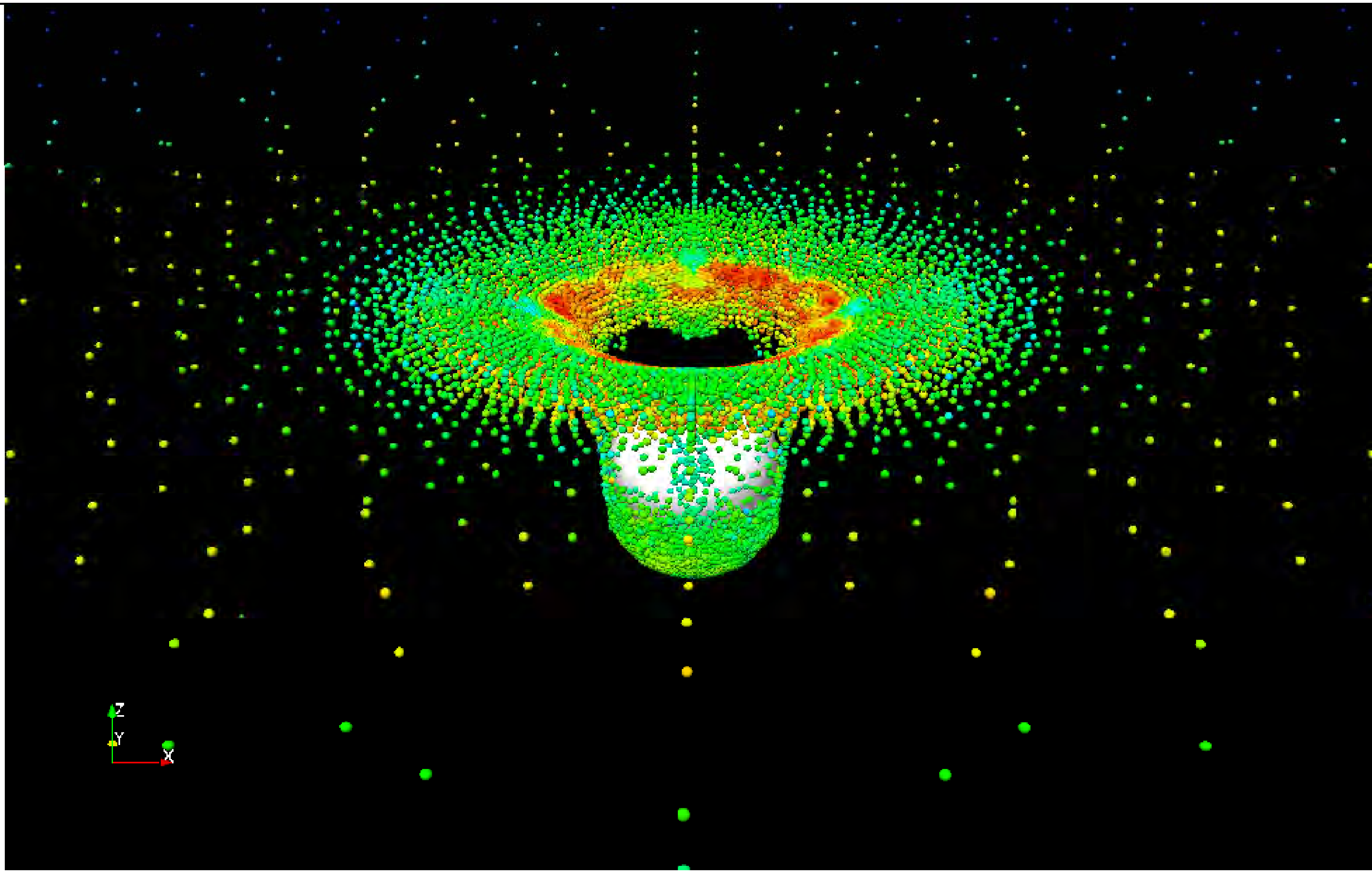


o Nodes carry field information

● Matl. points carry matl. state

OTM – Nodal point set



Steel projectile/aluminum plate: Nodal set

OTM – Material point set

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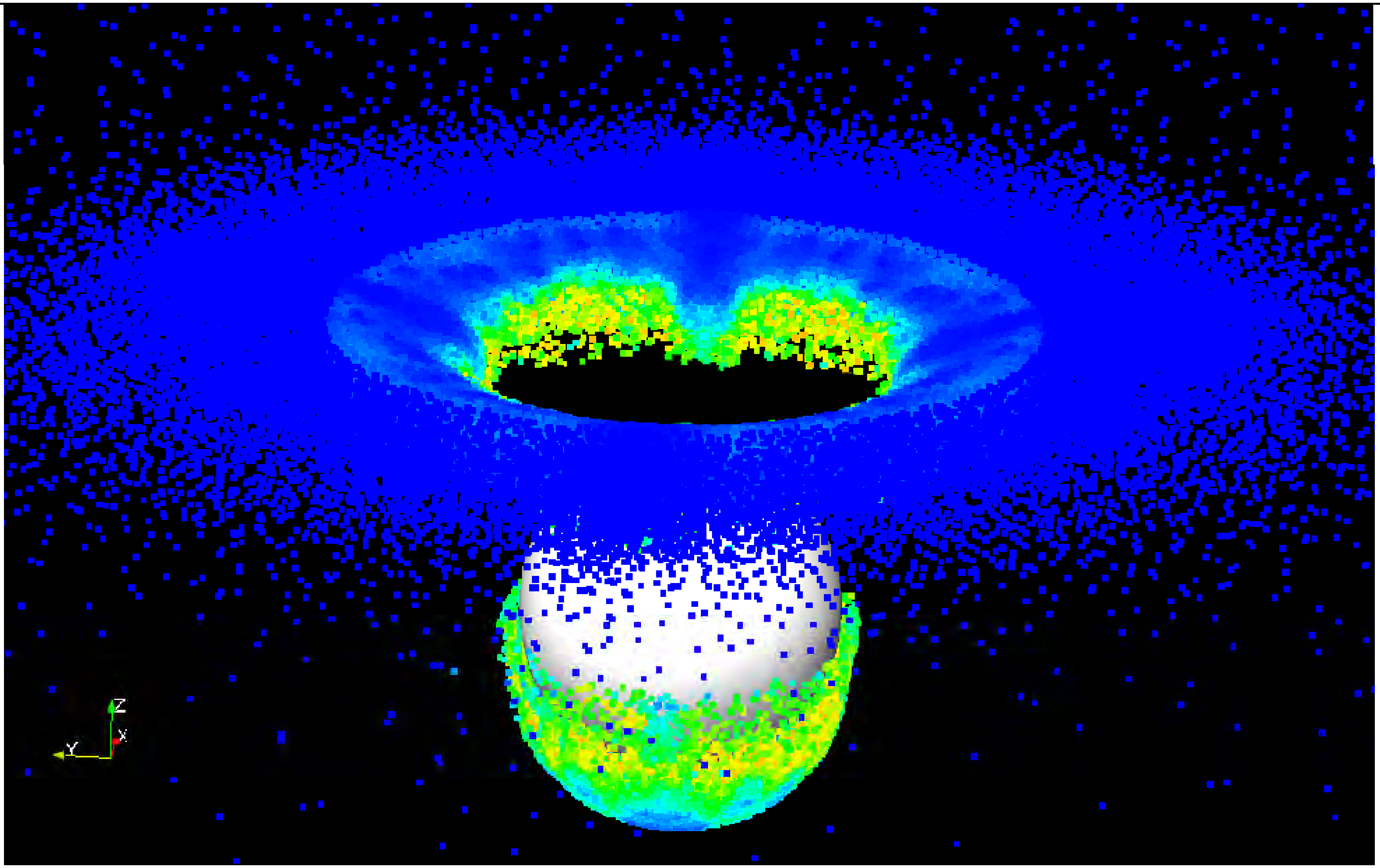
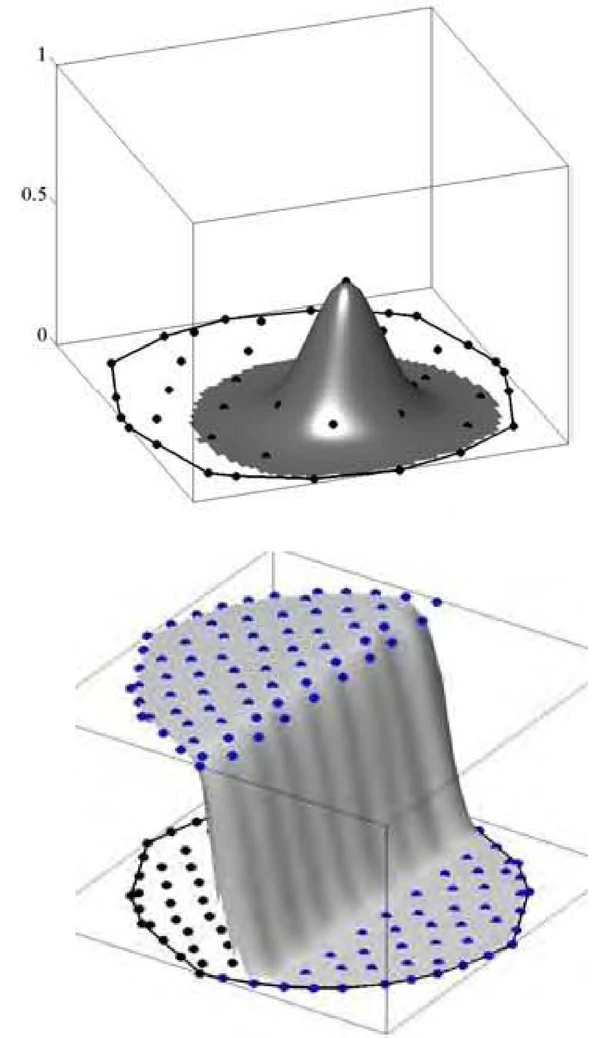


Steel projectile/aluminum plate: Material point set

OTM — Max-ent interpolation

- Max-ent interpolation is smooth, meshfree
- Finite-element interpolation is recovered as a limit
- Rapid decay, short range
- Monotonicity, maximum principle
- Good mass lumping properties
- Kronecker-delta property at the boundary:
  - Displacement boundary conditions
  - Compatibility with finite elements



Arroyo, M. and Ortiz, M., *IJNME*, **65** (2006) 2167-2202

OTM — Spatial discretization

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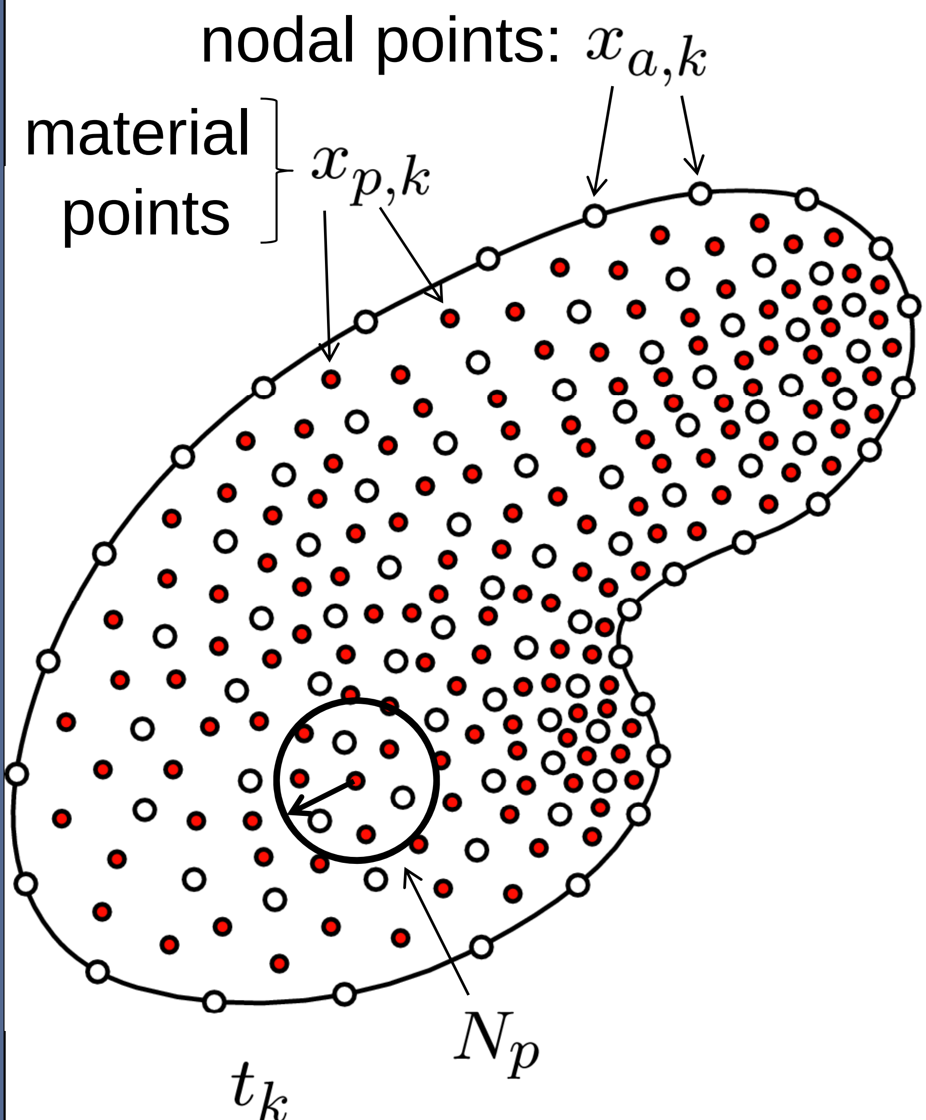

- Max-ent interpolation at material point *p* determined by nodes in its local environment *Np*
- Local environments determined 'on-the-fly' by range searches
- Local environments evolve continuously during flow (dynamic reconnection)
- Dynamic reconnection requires no remapping of history variables!

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OTM – Flow chart

(i) Explicit nodal coordinate update:

$$x_{k+1} = x_k + (t_{k+1} - t_k)(v_k + \frac{t_{k+1} - t_{k-1}}{2} M_k^{-1} f_k)$$

(ii) Material point update:

position: $x_{p,k+1} = \varphi_{k\to k+1}(x_{p,k})$

deformation: $F_{p,k+1} = \nabla\varphi_{k\to k+1}(x_{p,k}) F_{p,k}$

volume: $V_{p,k+1} = \det \nabla\varphi_{k\to k+1}(x_{p,k}) V_{p,k}$

density: $\rho_{p,k+1} = m_p / V_{p,k+1}$

(iii) Constitutive update at material points

(iv) Reconnect nodal and material points (range searches), recompute max-ent shape functions

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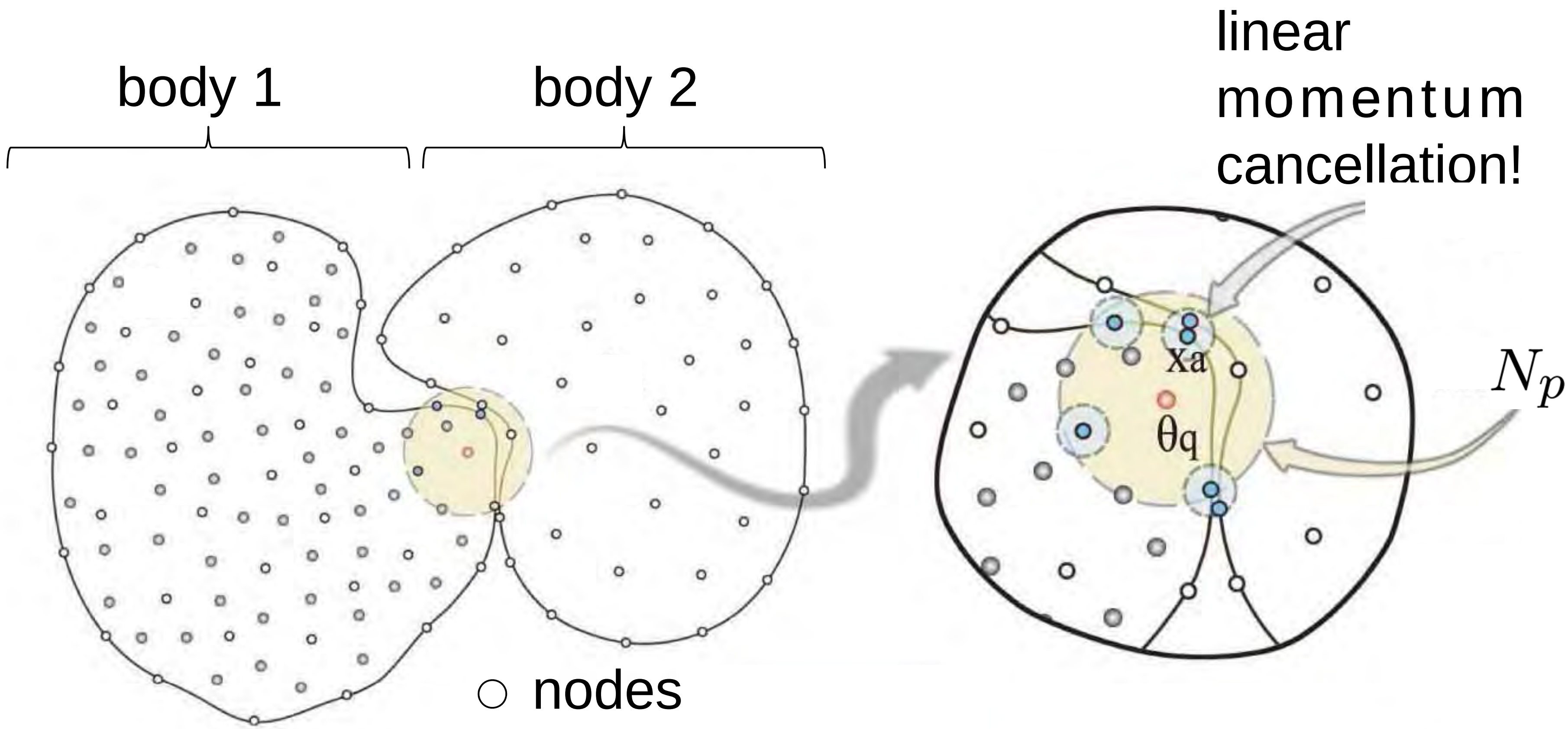
OTM – Seizing contact

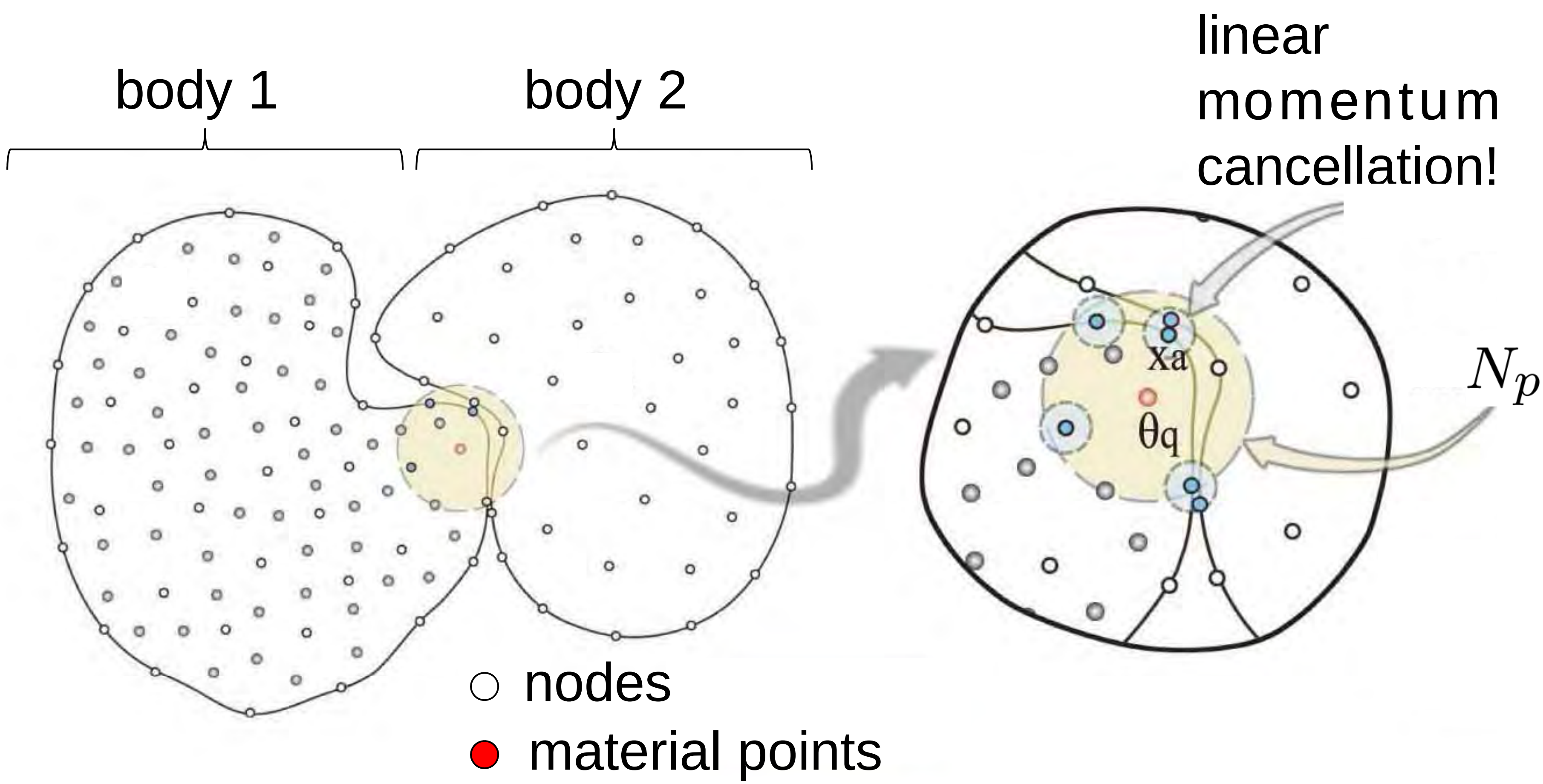


○ nodes

● material points

Seizing contact (infinite friction) is obtained for free in OTM! (as in other material point methods)

OTM — Seizing contact



Seizing contact (infinite friction) is obtained for free in OTM! (as in other material point methods)

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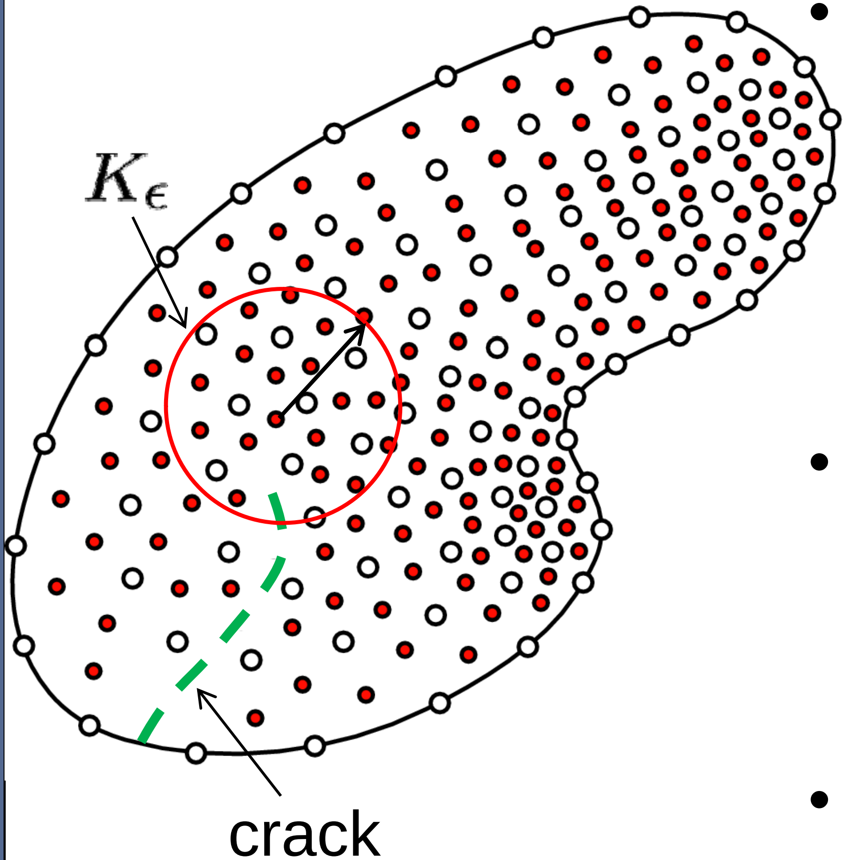
OTM - Fracture & fragmentation



$$G_\epsilon \sim \frac{h^2}{|K_\epsilon|} \int_{K_\epsilon} W(\nabla u)\, dx$$

- Proof of convergence of variational element erosion to Griffith fracture:
  - Schmidt, B., Fraternali, F. and Ortiz, M., SIAM J. Multiscale Model. Simul., **7**(3) (2009) 1237-1366.
- OTM implentation: Variational erosion of material points (by ε-neighborhood construction),

$$G_\epsilon \geq G_c$$

- Alternatively: Material point failure + comminution:
  - Pandolfi, A., Conti, S. and Ortiz, M., JMPS, **54** (2006) 1972-2003

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OTM – Terminal ballistics

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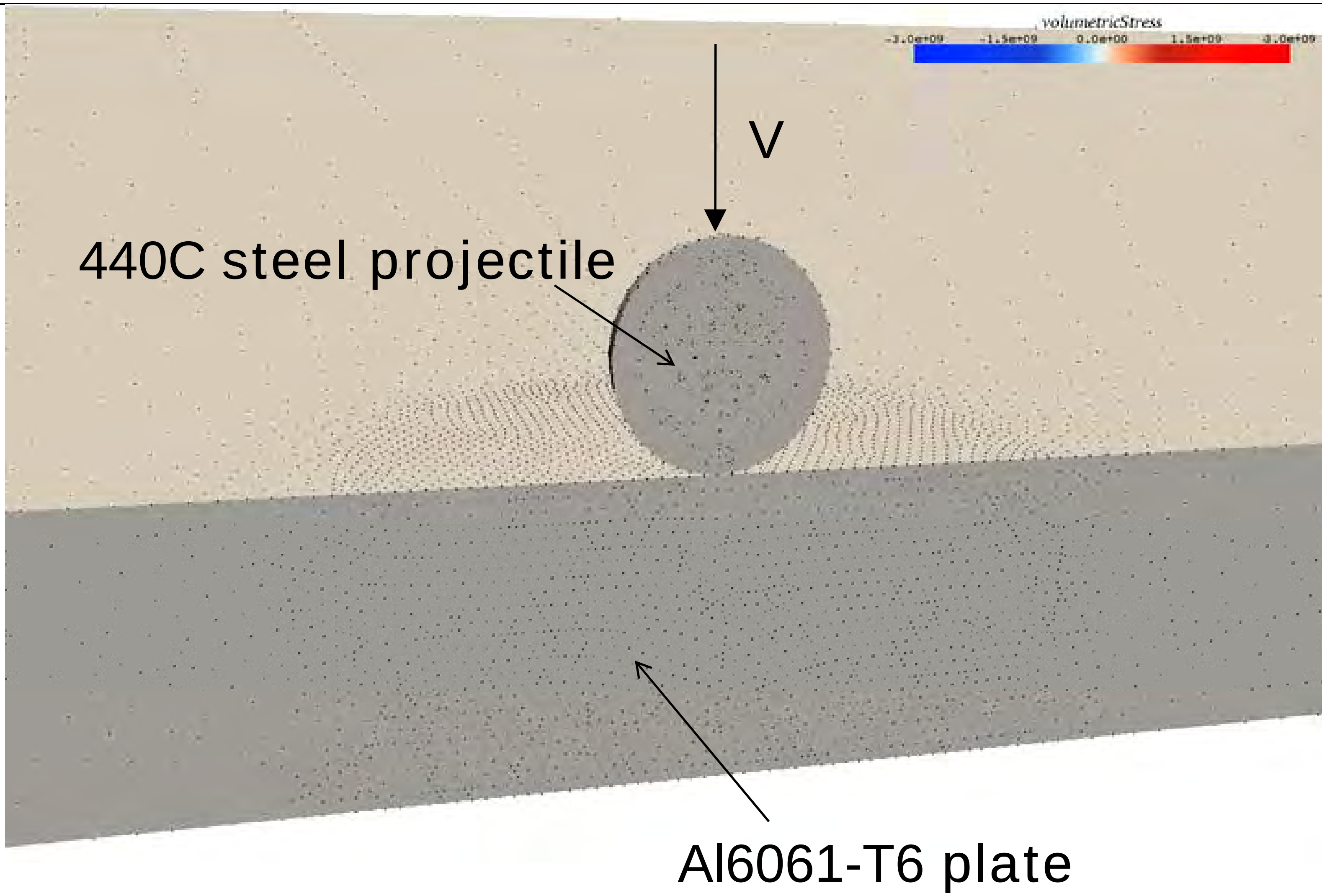

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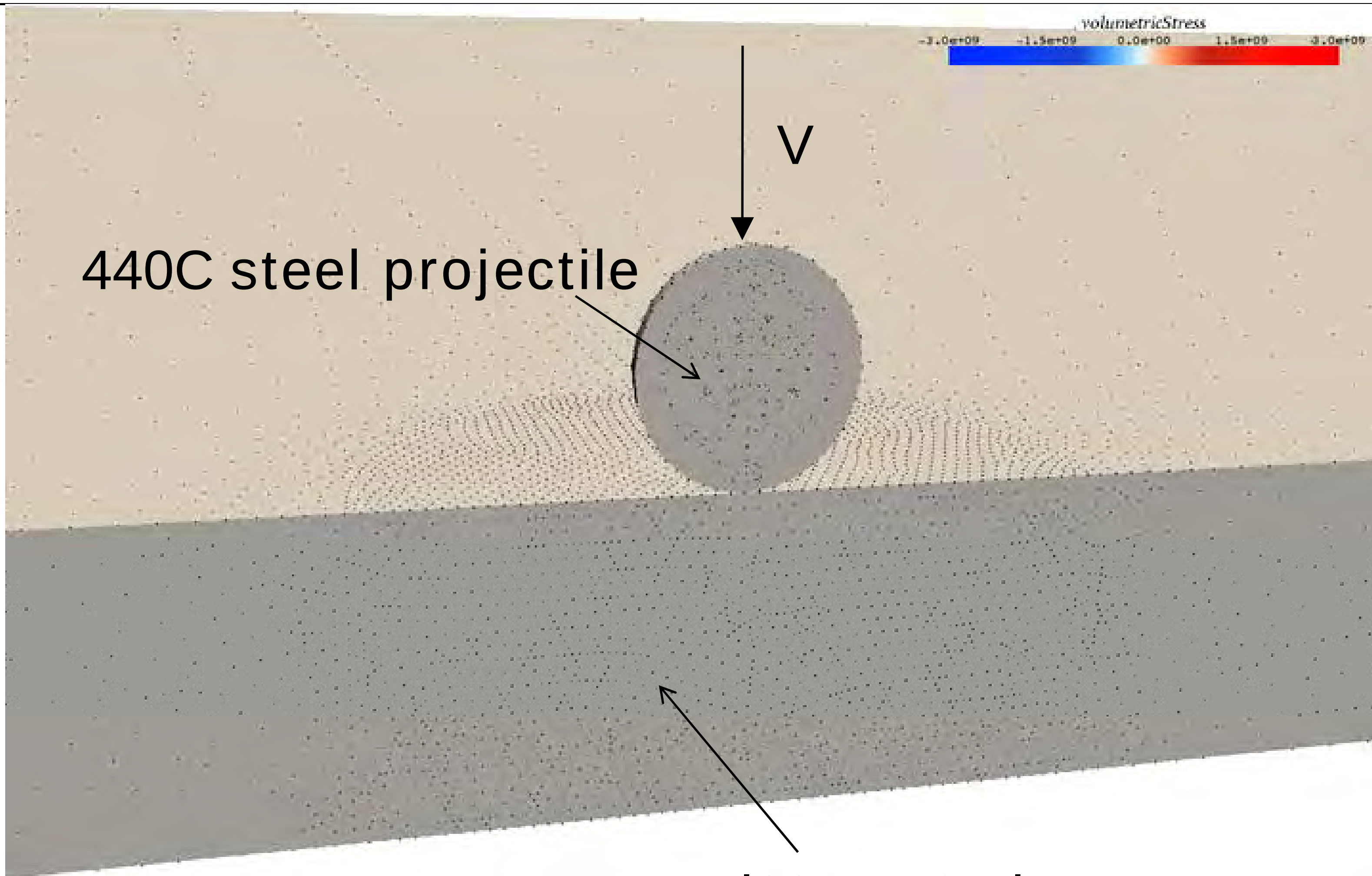
OTM – Terminal ballistics



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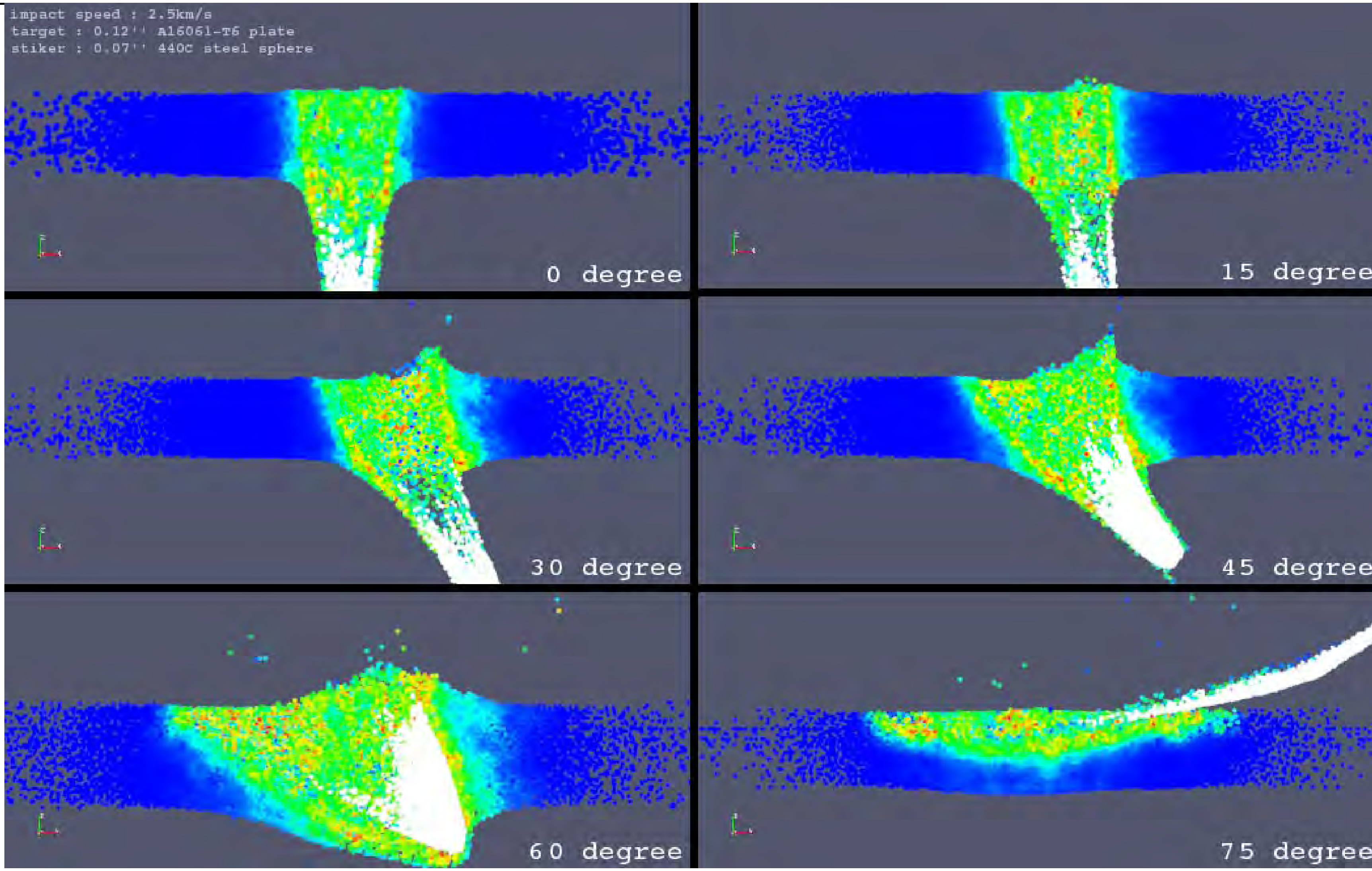
OTM – Terminal ballistics



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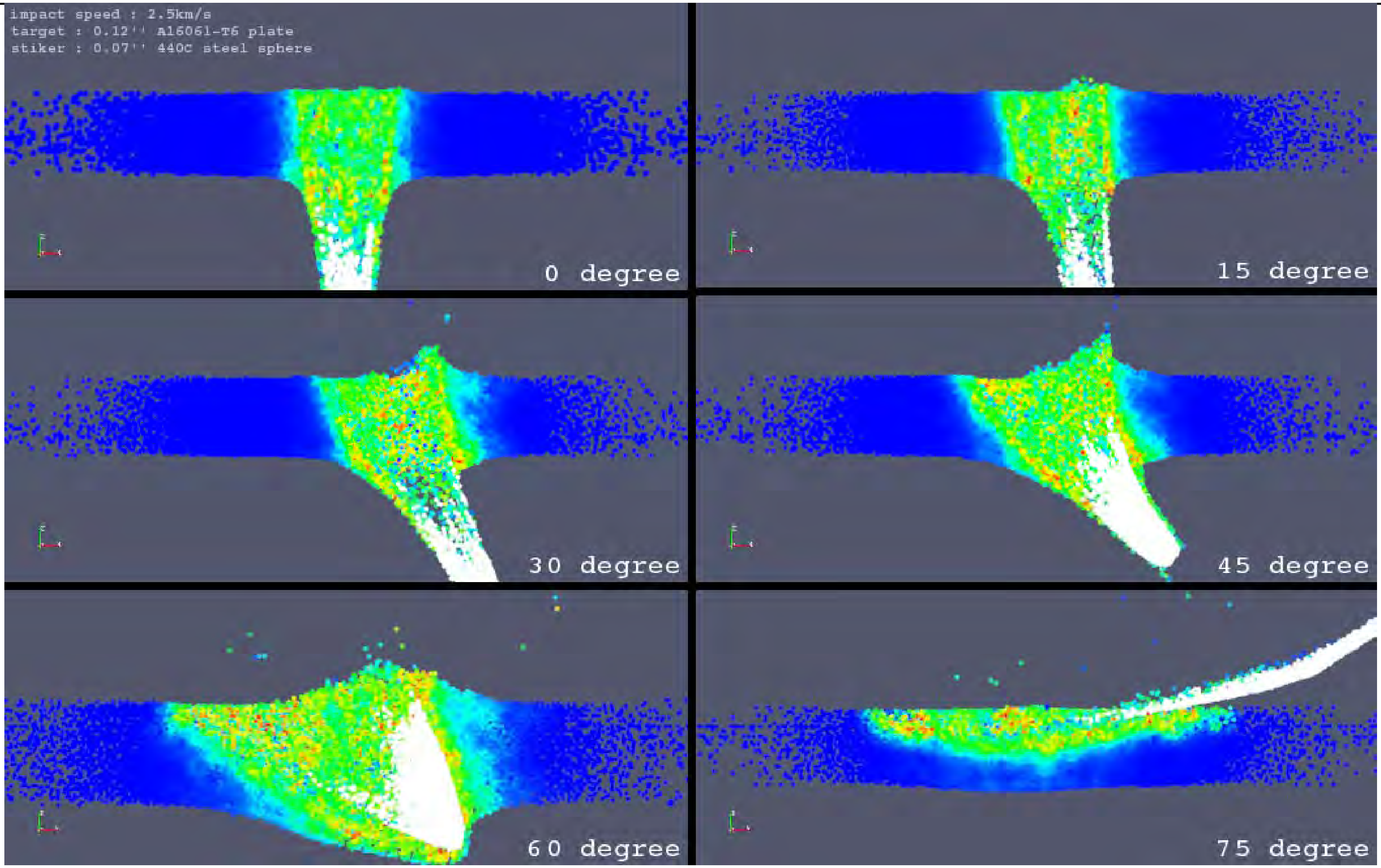
OTM – Terminal ballistics



Case Study I – Steel/Al ballistics

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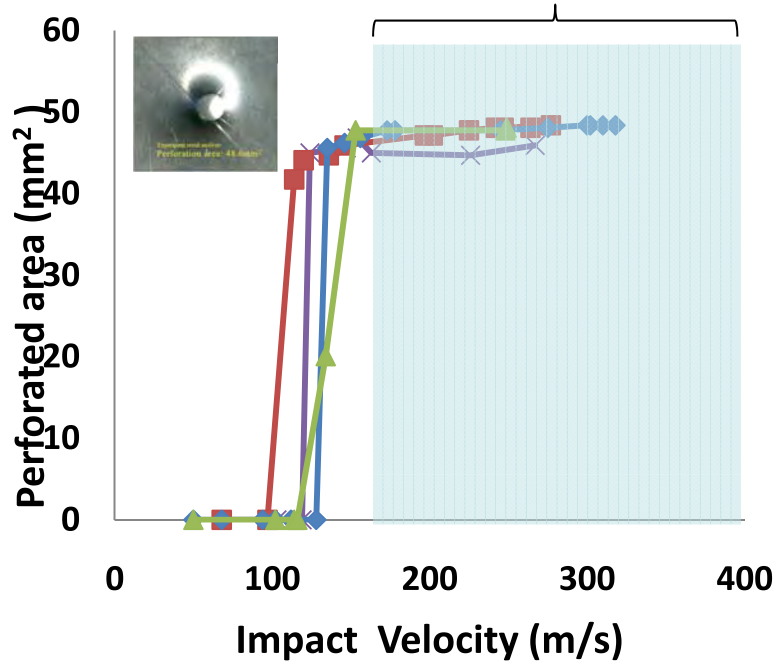
- McDiarmid inequality:

$$\mathrm{PoF} = \mathbb{P}[F \le a] \le \mathrm{e}^{-2\mathrm{CF}^2}$$

$$CF = \frac{M}{U} = \frac{(\mathbb{E}[F]-a)_+}{D_F}$$

Model diameter D_F	thickness	4.33 mm^2
	velocity	4.49 mm^2
	total	6.24 mm^2
Model mean *E[F]*		47.77 mm^2
Confidence factor *M/U*		7.66

operating range (180-400 m/s)



Steel/Al ballistics response function

- Lethality can be certified with ~ 10^{-51} confidence!
- Number of response function evaluations ~ 2,000

Uncertainty quantification ‘crimes’

- Models are inexact in general!
- How does lack of model fidelity contribute to uncertainty?
- Is rigorous model-based certification possible in the face of modeling error?
- Mean performance *E[F]* cannot be computed exactly for complex systems
- Instead, mean performance *E[F]* is approximated by empirical mean:

$$\mathbb{E}[G] \approx \frac{1}{m}\sum_{i=1}^{m} Y^i \equiv \langle Y \rangle$$

- What is the effect of the empirical mean approximation on uncertainty quantification?

UQ crime and punishment

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

  F(X)-G(X) ≡ Modeling-error function
- McDiarmid bound monotonic in diameter
- Triangular inequality: $D_G \leq D_F + D_{F-G}$
- Conservative certification criterion:

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

- $\alpha = U m^{-\frac{1}{2}}(-\log \epsilon')^{\frac{1}{2}}$ *: **Margin hit** (emp. mean)*
- D_F: ***Model diameter*** (*variability* of model)
- D_{F-G}: ***Modeling error*** (*badness* of model)

Model-based QMU – McDiarmid

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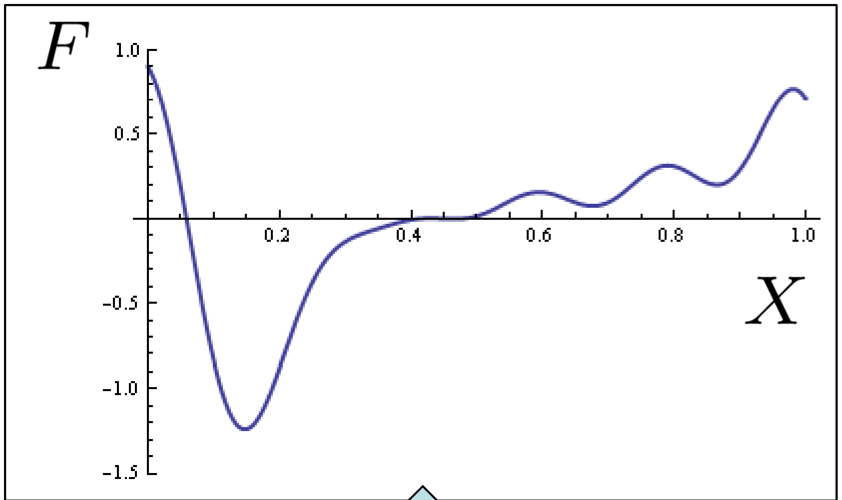
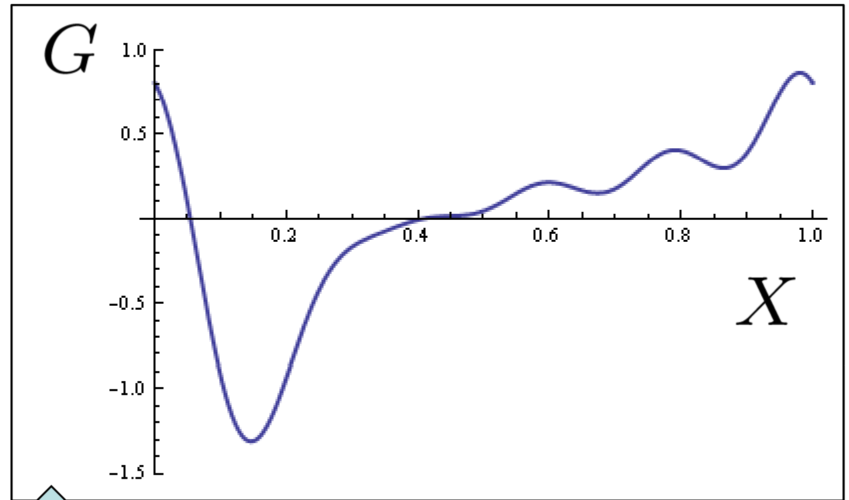
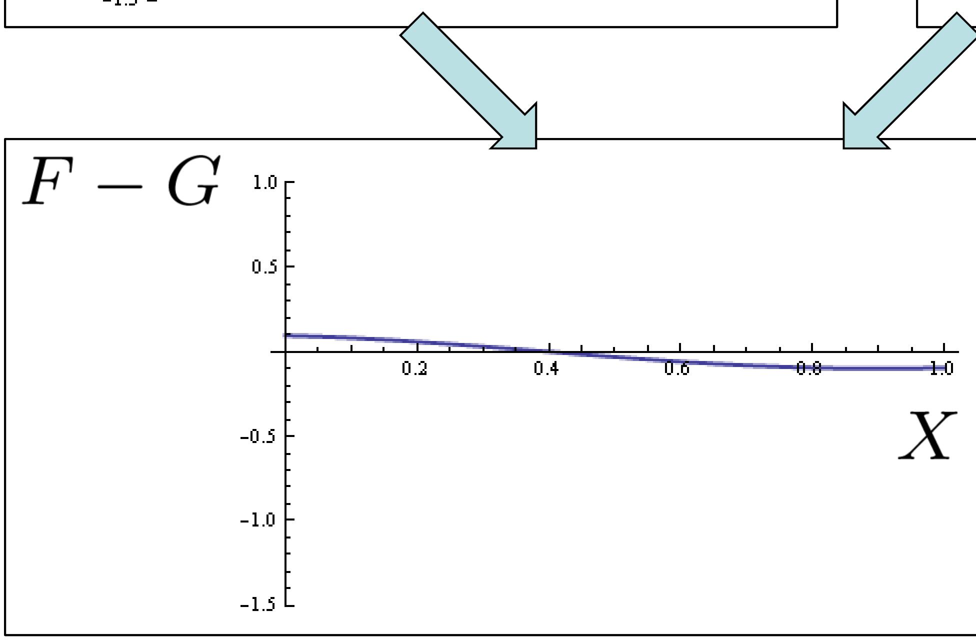






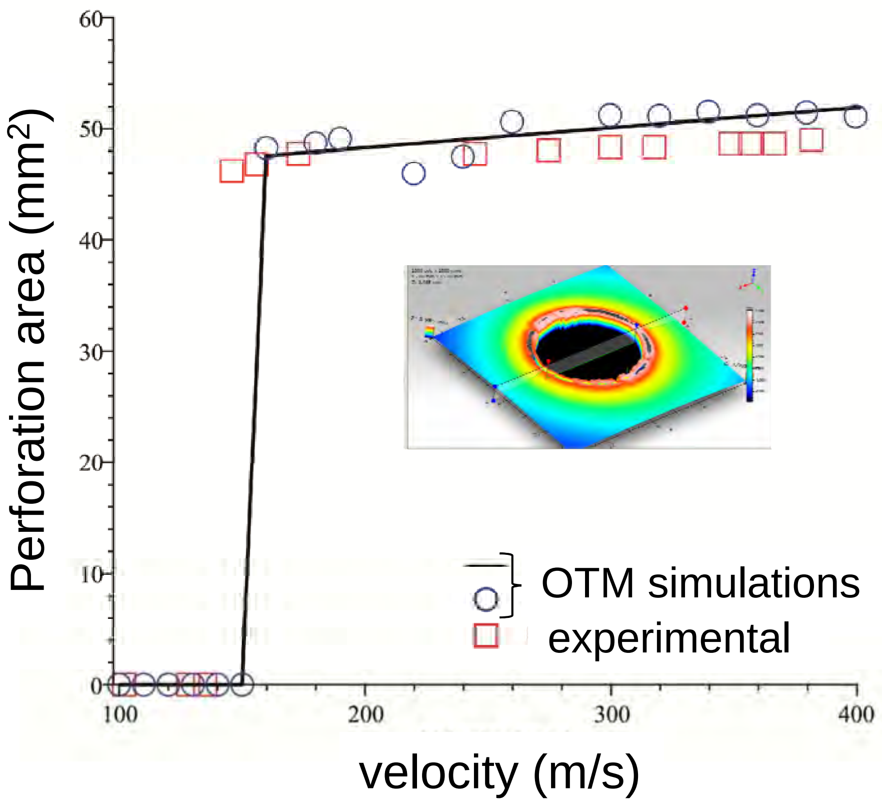
- Working assumptions:
  - *F-G* far more regular than *F* or *G* alone
  - Global optimization for $D_{F\text{-}G}$ converges fast (e.g. BFGS)
  - Evaluation of $D_{F\text{-}G}$ requires few experiments

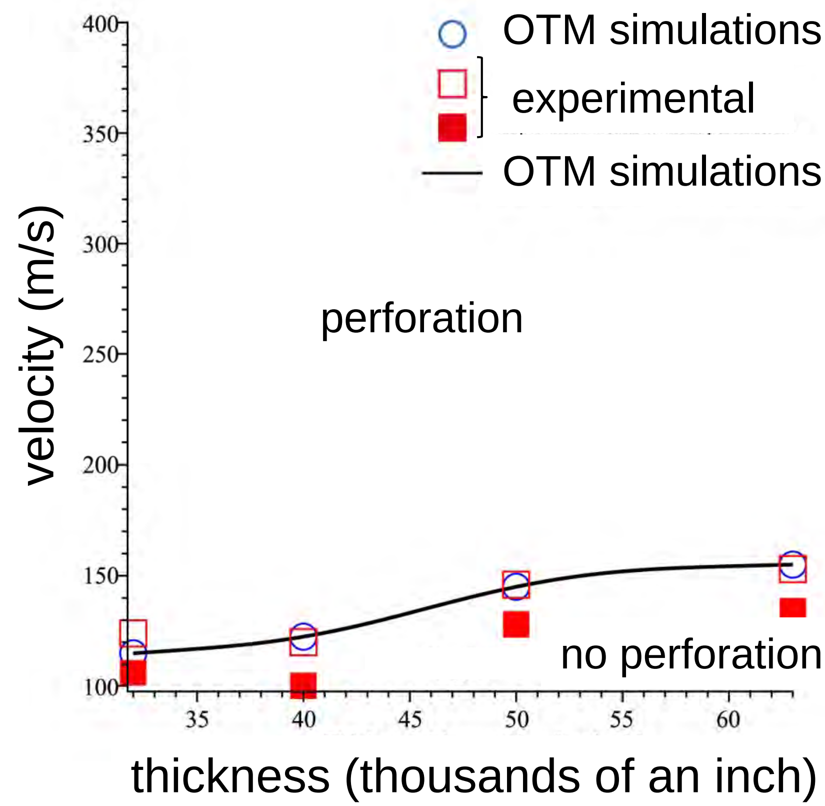
Model-based QMU – McDiarmid

- 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!

Case Study – OTM modeling error





Measured *vs*. computed perforation area

Sample UQ Analysis – Ballistic range

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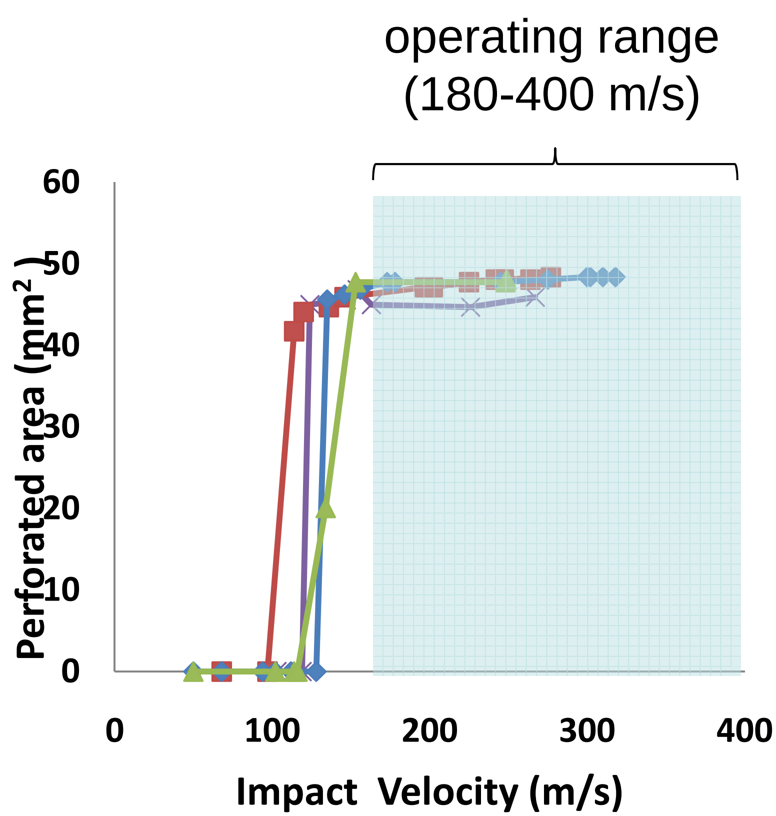
Model diameter D_F	thickness	4.33 mm^2
	velocity	4.49 mm^2
	total	6.24 mm^2
Modeling error $D_{F\text{-}G}$	thickness	4.96 mm^2
	velocity	2.16 mm^2
	total	5.41 mm^2
Uncertainty $D_F + D_{F\text{-}G}$		11.65 mm^2
Empirical mean $\langle Y \rangle$		47.77 mm^2
Margin hit α (ε'=0.1%)		4.17 mm^2
Confidence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



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

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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)

Concluding remarks…

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- 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…)…

Concluding remarks…