'Full Physics' and Uncertainty Quantification as Drivers for Exascale Computing

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California Institute of Technology

SimTech Colloquium
Universität Stuttgart, December 18, 2012

DoE/ASC/PSAAP Centers

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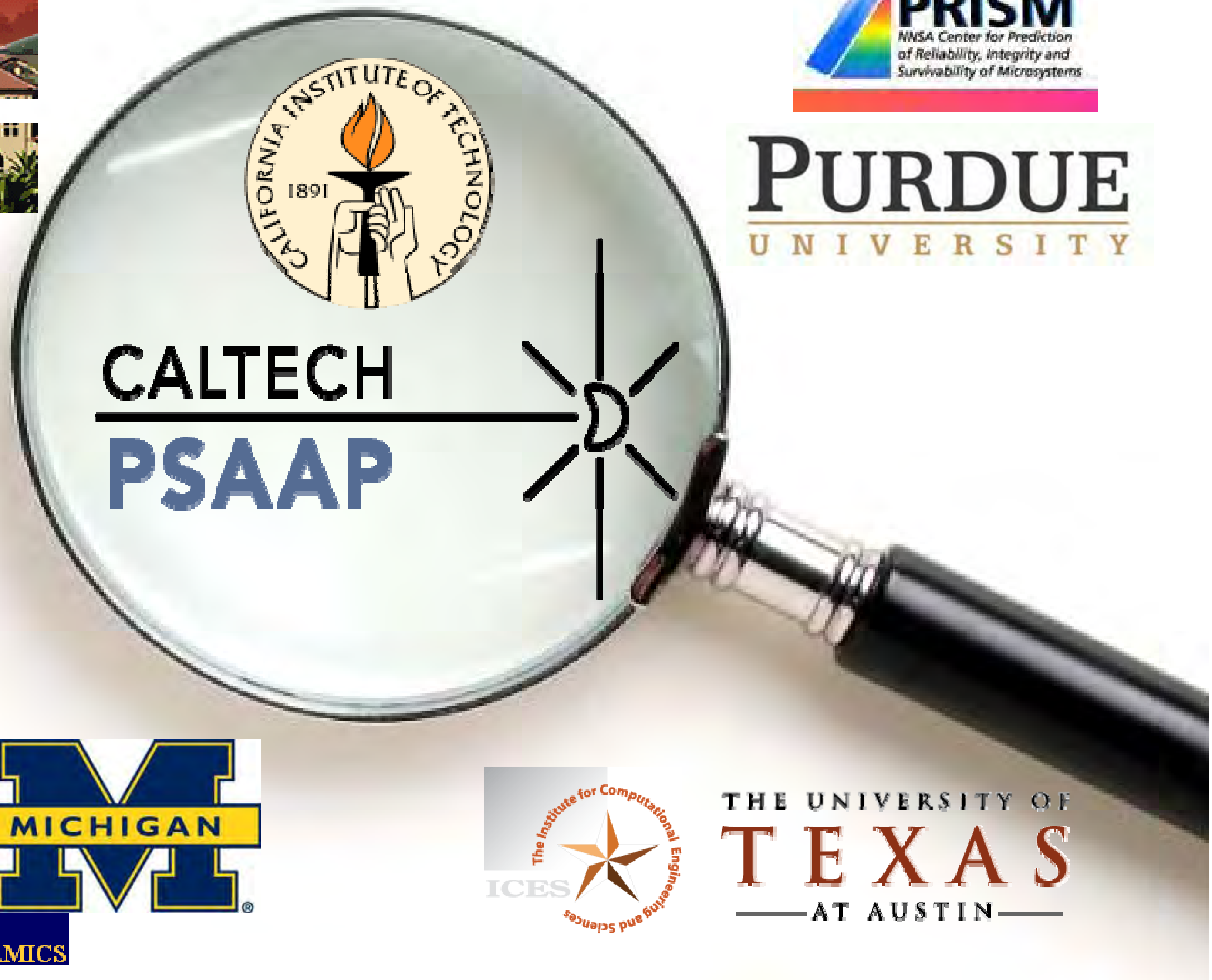
STANFORD UNIVERSITY

PSAAP

PRISM

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

PURDUE UNIVERSITY



CENTER FOR RADIATIVE SHOCK HYDRODYNAMICS

MICHIGAN

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The Institute for Computational Engineering and Sciences

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The Predictive Science challenge

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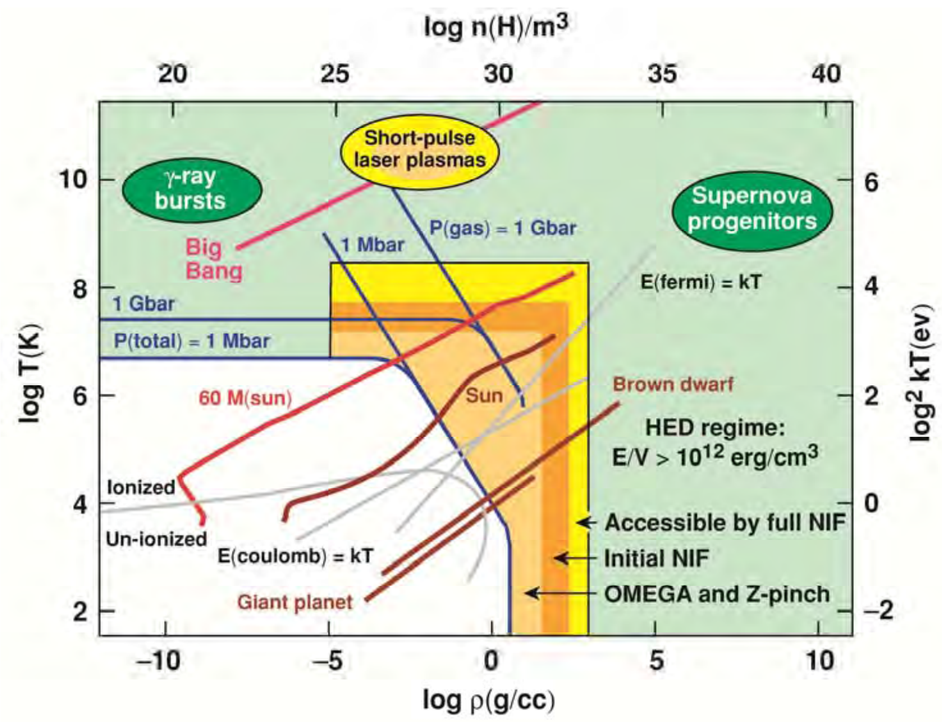
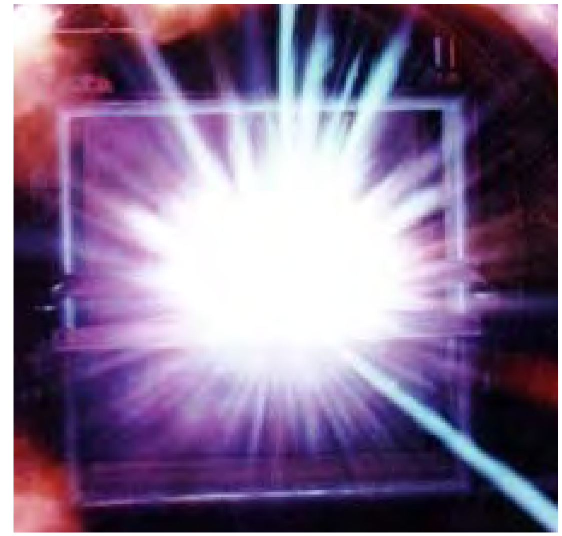
Aim: Demonstrate Predictive Science
in the field of hypervelocity impact
(impact velocities up to 10Km/s)





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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The Predictive Science Paradigm

- **Aim:** *Predict the behavior of complex physical/engineered systems* ***with quantified uncertainties***
- **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

The Predictive Science Paradigm

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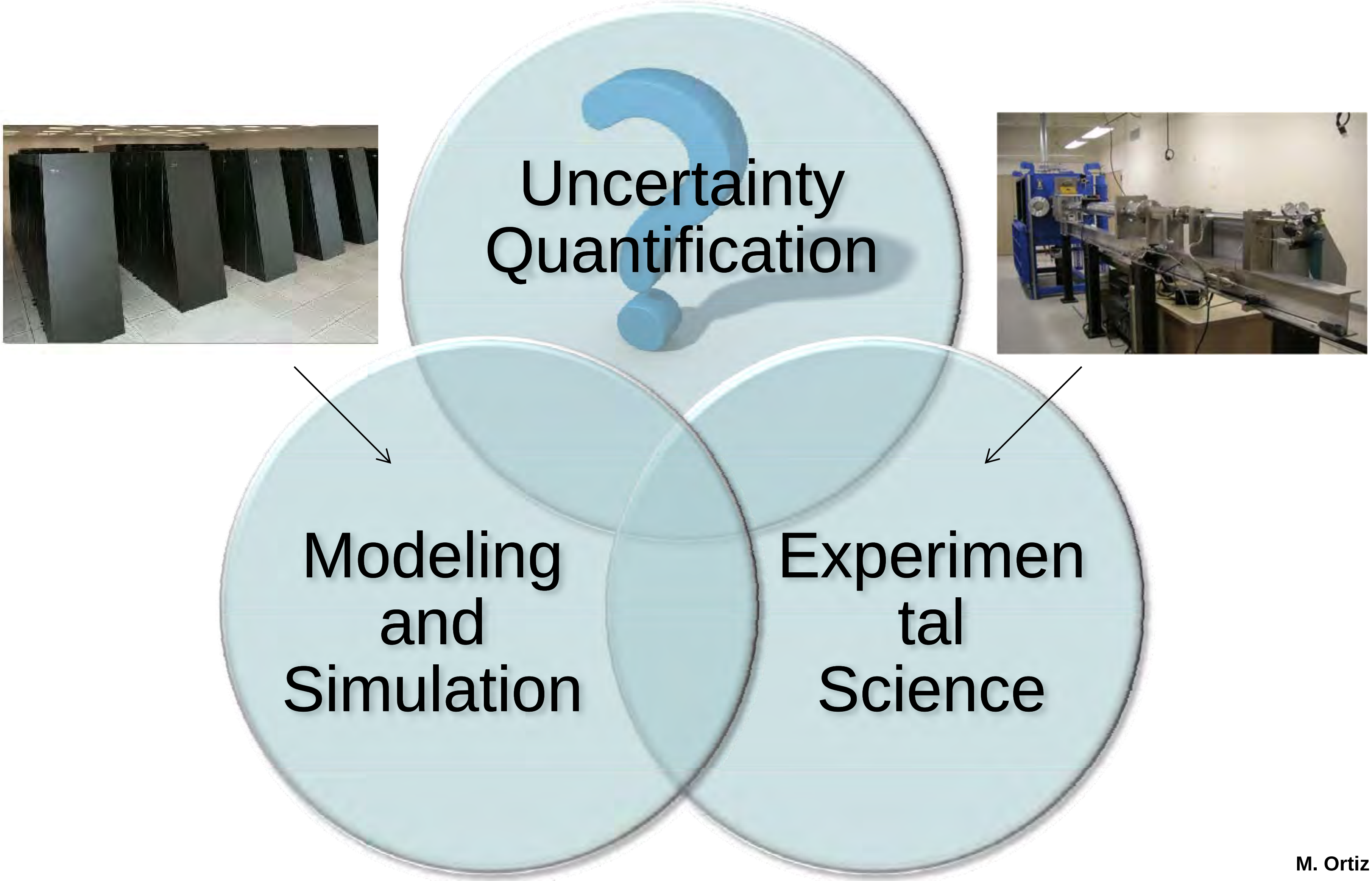

The Predictive Science Paradigm

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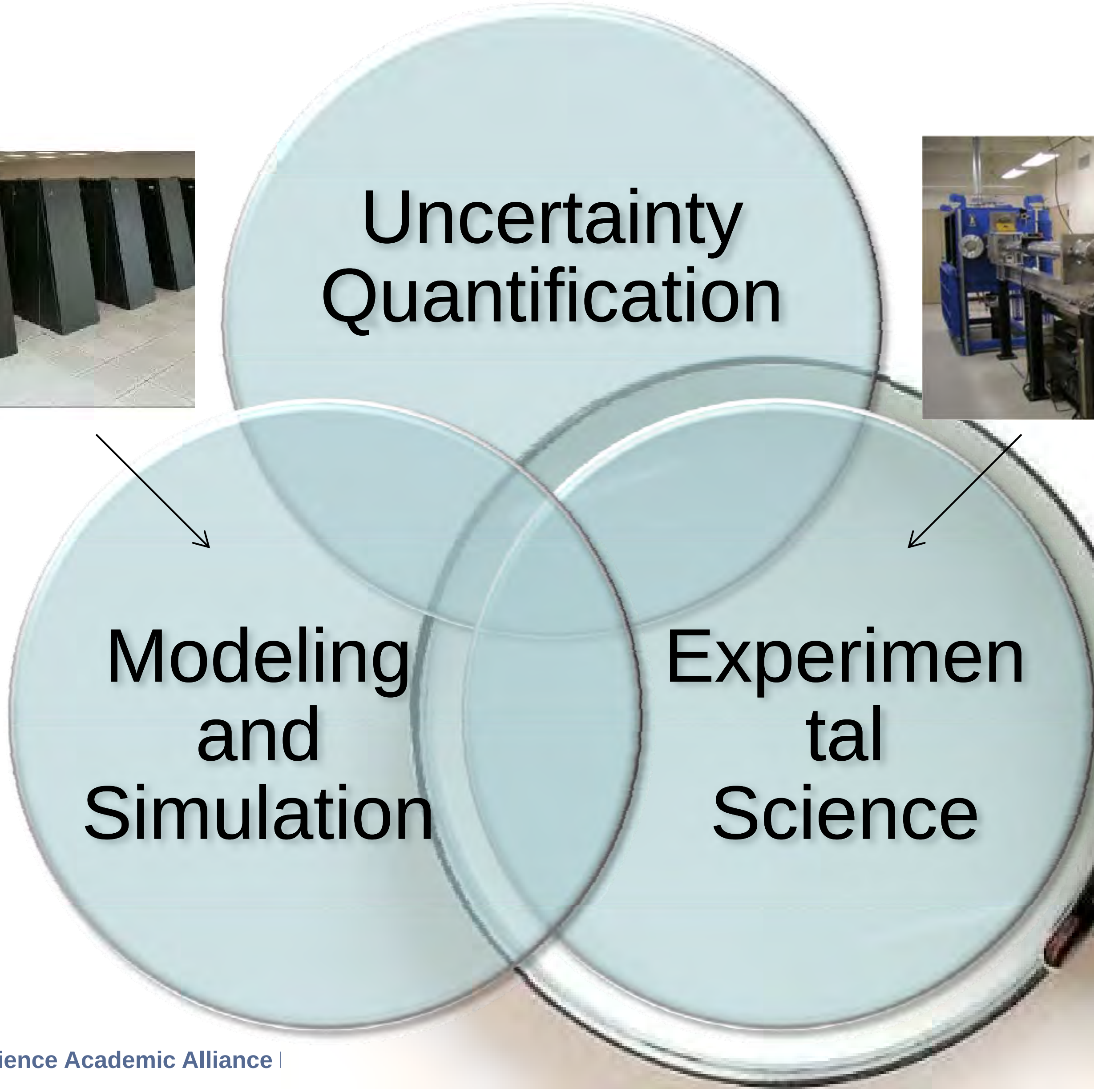

Hypervelocity Impact Testing

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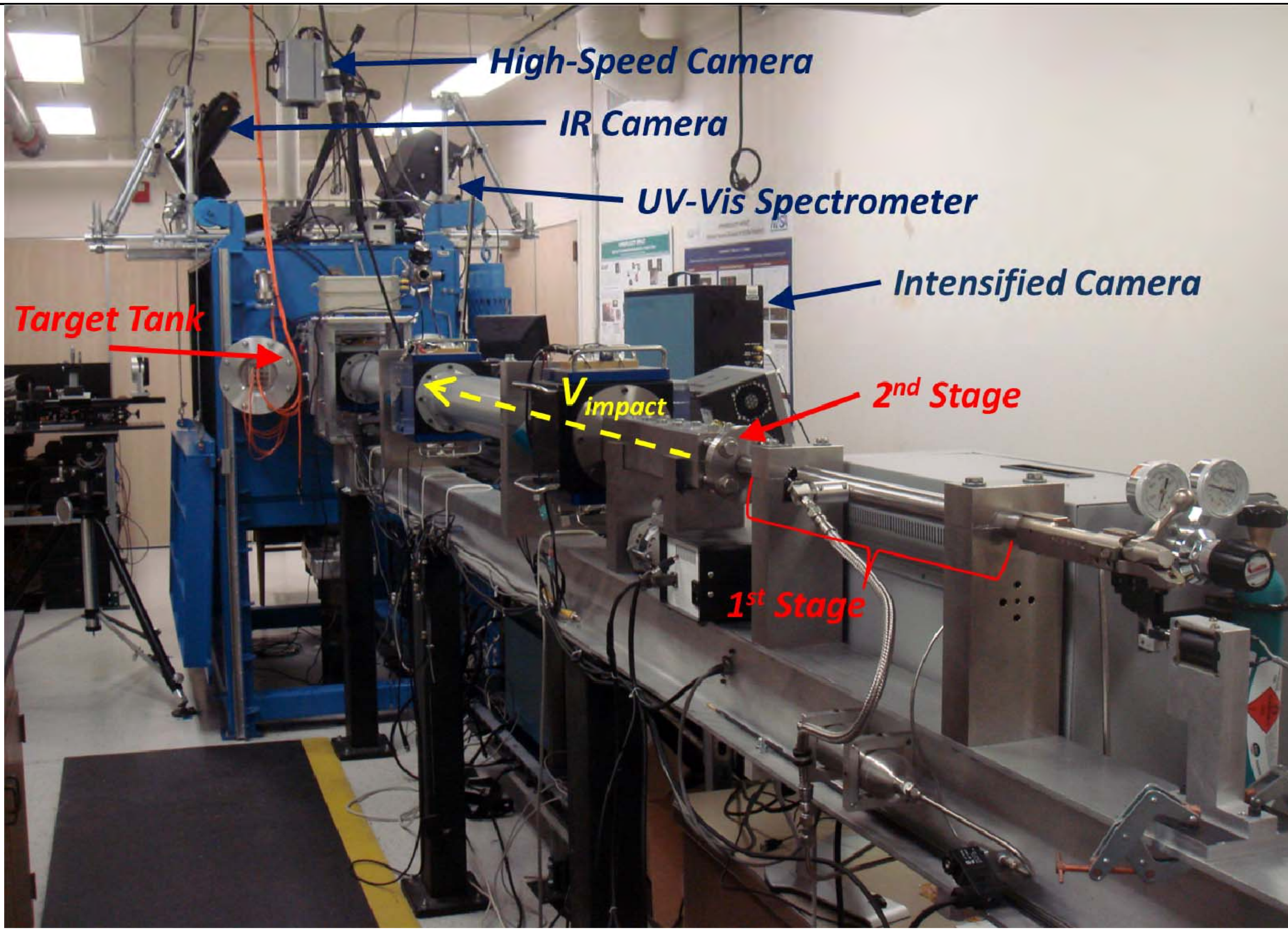

Catech's Small Particle Hypervelocity Impact Range (SPHIR)

Hypervelocity Impact Testing

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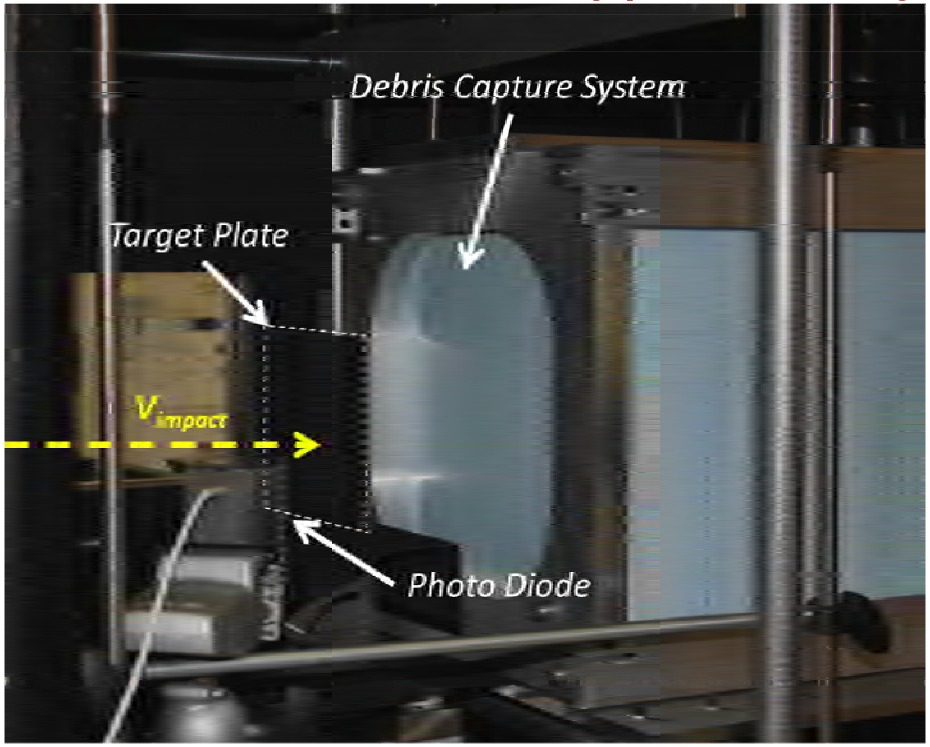
Small Particle Hypervelocity Impact Range (SPHIR)



- Two-Stage Light-Gas Gun
- 1.8 mm bore diameter

Target Materials
•Steel
•Aluminum
•*Tantalum*

Test configuration parameters:
- Impact Speeds: 2 to 10 km/s
- Impact Obliquities: 0 to 80 degrees
- Impactor Mass: 1 to 50 mg
- Target plate thickness: 0.5-3 mm

Impactor Materials
•440 C Steel
•6/6 Nylon

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Hypervelocity Impact Diagnostics

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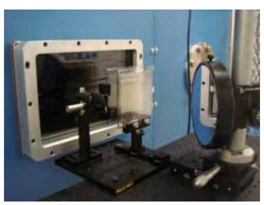
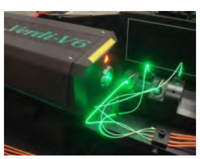
Diagnostic Technique | **Performance Measures**

Post Mortem Profilometry → **Routine**
- Perforation Area
- Target back-surface slope
- …

In Situ Side-Lighting Shadowgraphs → **Operational**
- Bulge formation
- Ejecta/debris cloud formation
- Ejecta/debris cloud distribution



In Situ CGS by Transmission → **Operational**
- Index of refraction gradient of Ejecta and Debris cloud



In Situ VISAR → **Operational**
- Back-surface normal velocity

In Situ Spectrometry → **Operational**
- Emission spectra
- Thermal distribution of target/debris cloud

SPHIR – Post Mortem Profilometry

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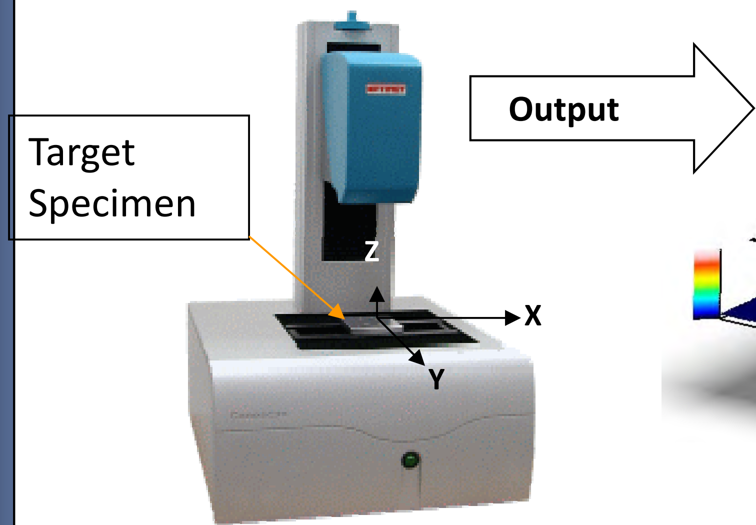
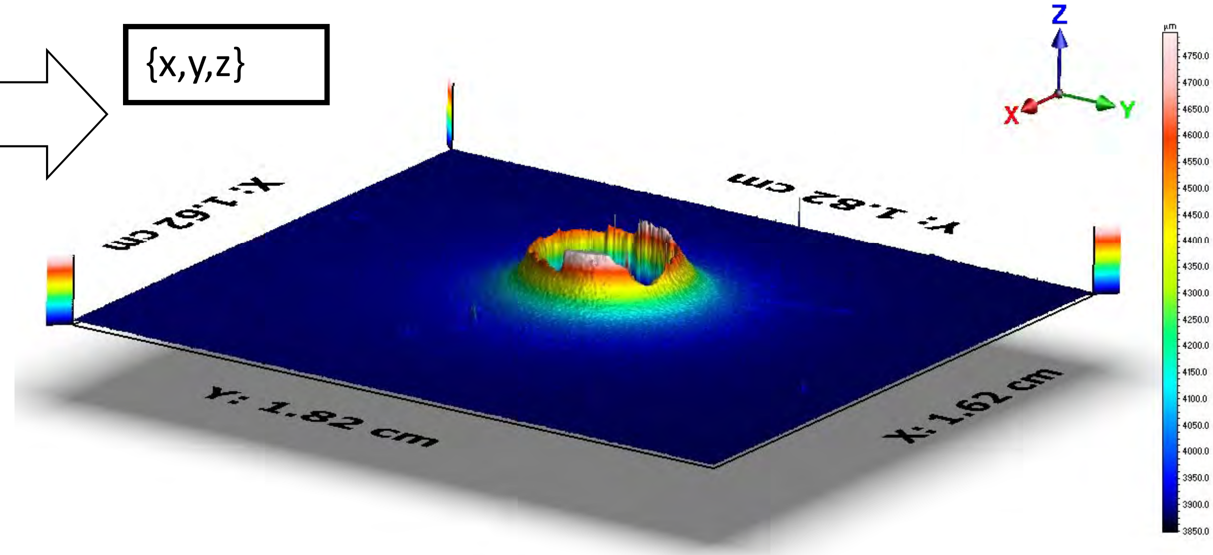
Optimet MiniConoscan 3000



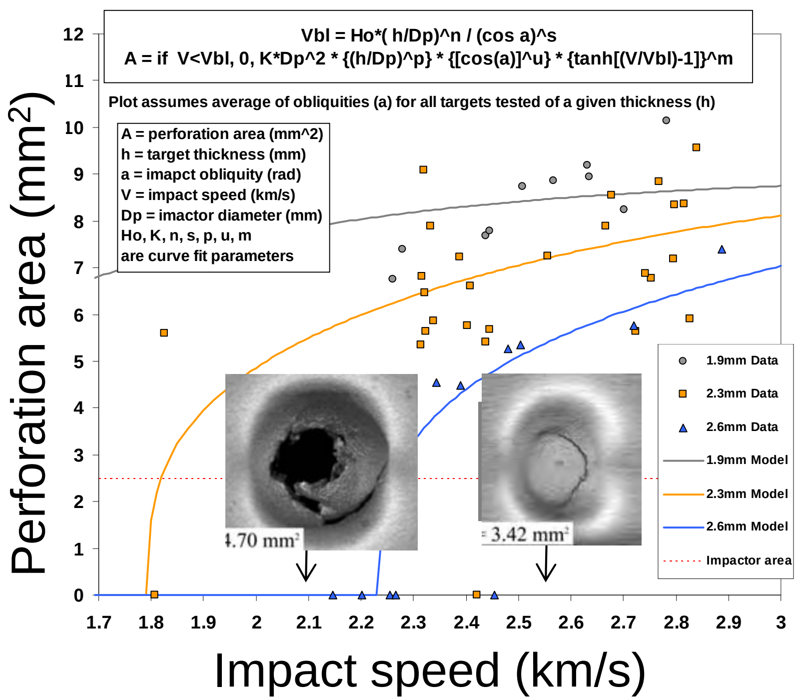


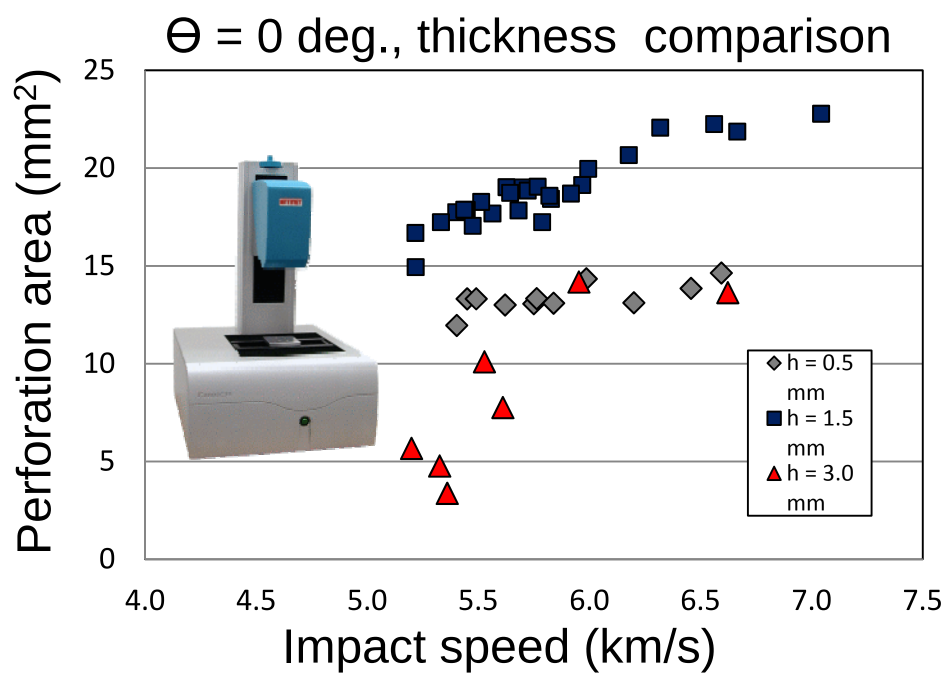
- Produces surface map as {x,y,z} coordinate table
- Scans 101 mm x 101 mm area
- 25 micron resolution in x, y, z

Accurately measures post-test target deformation features for comparison with numerical simulation

- ***Target Perforation area***
- ***Back-surface slope map***

SPHIR – Perforation area data





440 C Steel spherical projectiles
304 Stainless Steel plate targets

6/6 nylon cylindrical projectiles
6061-T6 aluminum plate targets

SPHIR – Laser Side Lighting System

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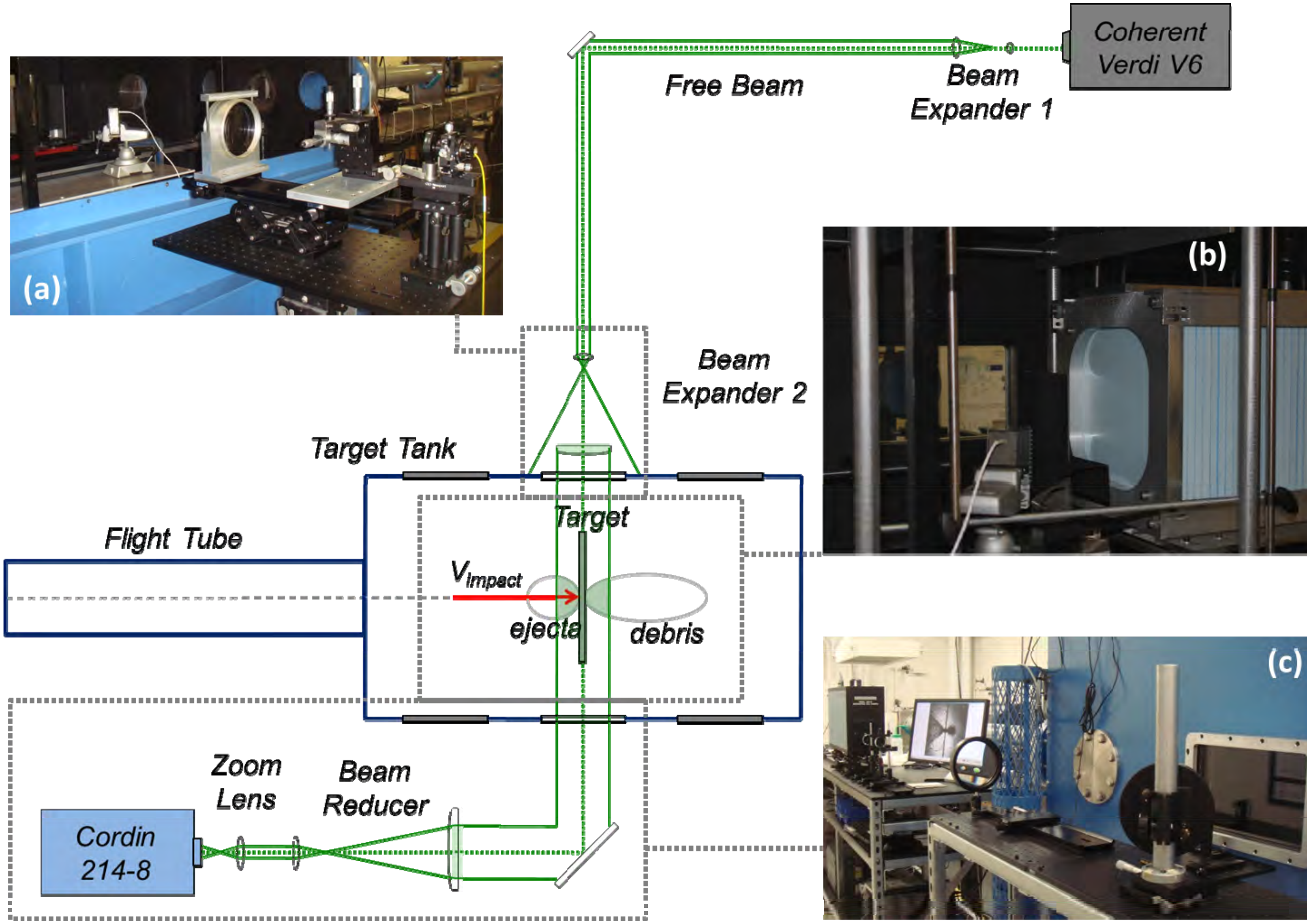

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SPHIR – Shadowgraph Data

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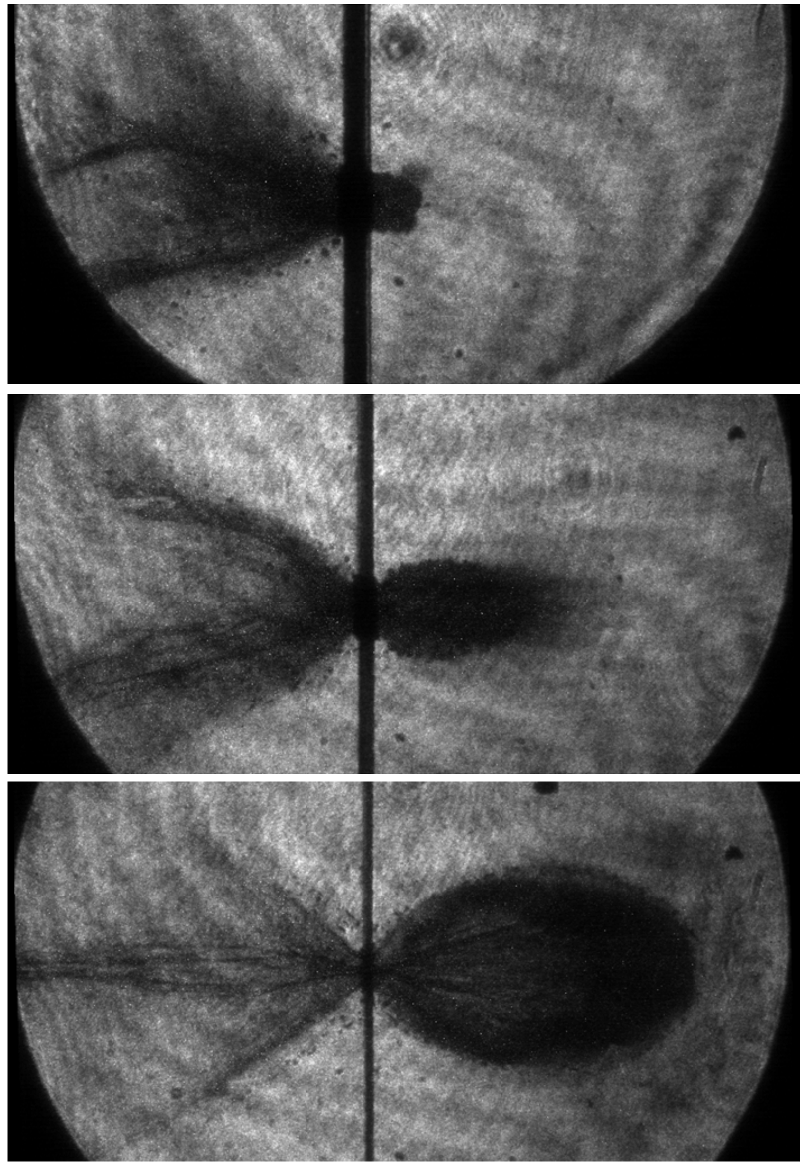
h = 3.0 mm
v_{impact} = 5.95 km/s

h = 1.5 mm
v_{impact} = 6.00 km/s

h = 0.5 mm
v_{impact} = 6.31 km/s



Nylon 6/6 Impactor
L/D=1 Cylinder

6061-T6 Al. Target

P_{atm}= 1.0 Torr

t = 10.3 μs

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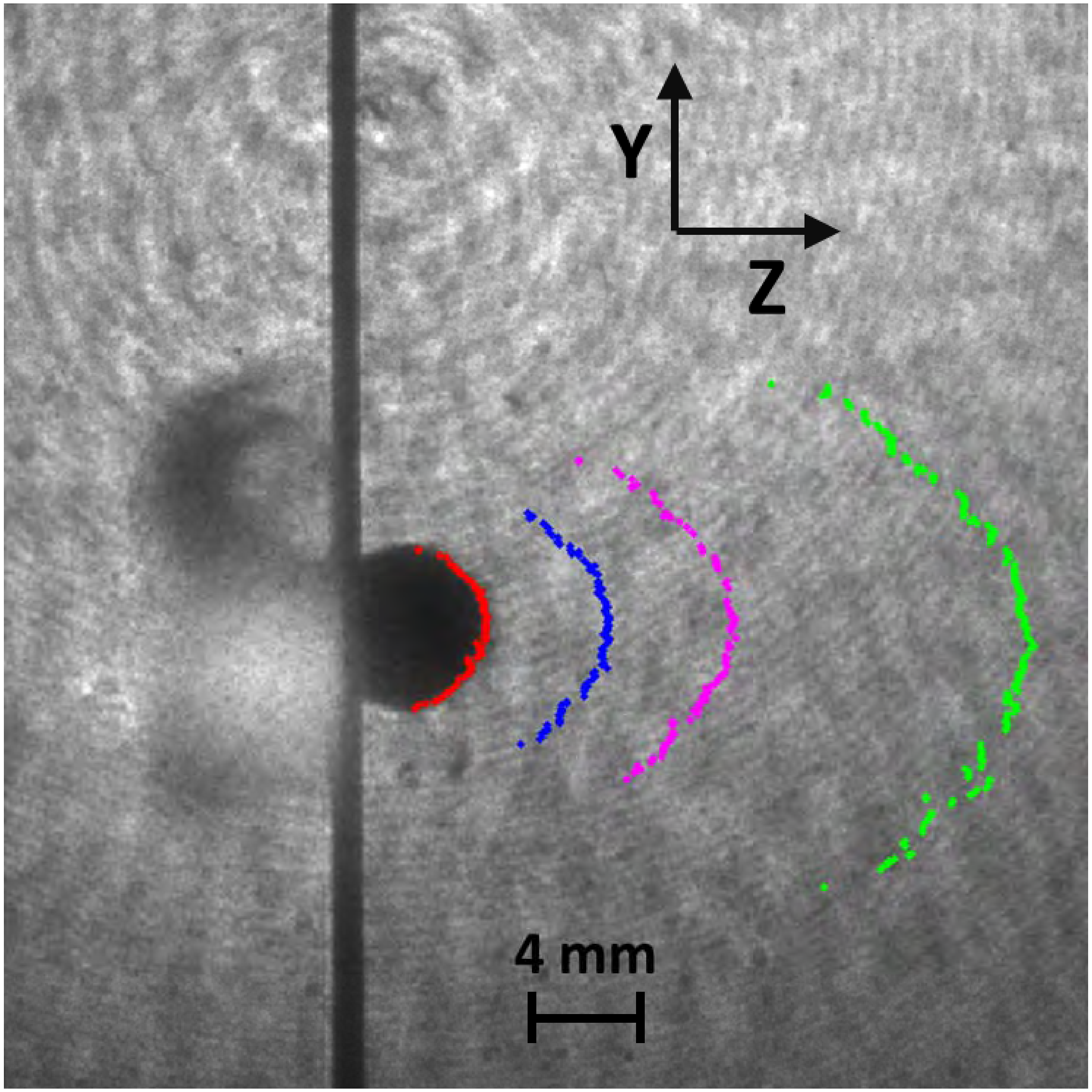
SPHIR – Debris Front Data



SPHIR – Debris Capture Data

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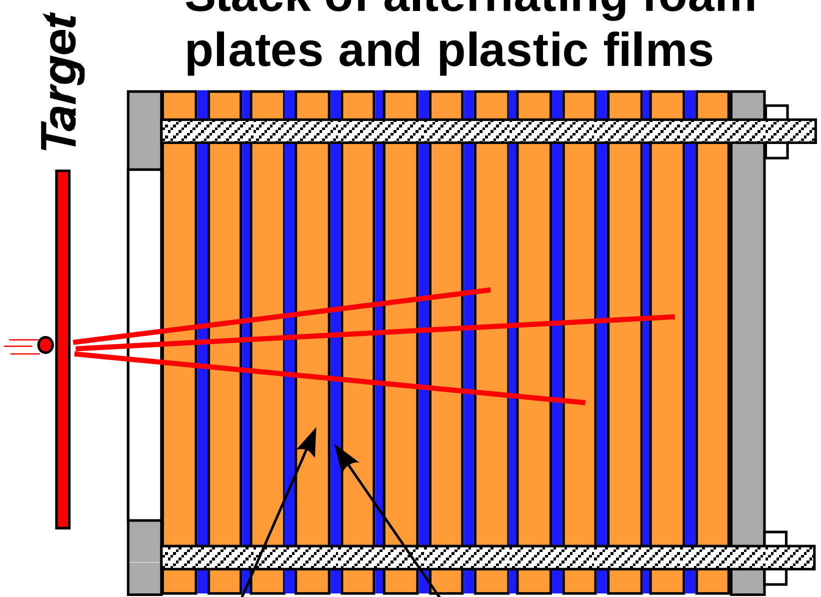
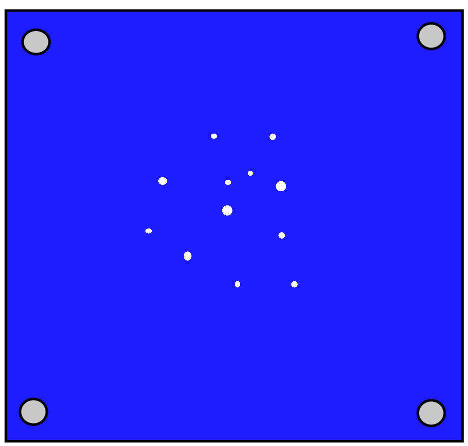
Stack of alternating foam plates and plastic films



- Architectural Foam
- **1 lb/ft3**
- **inexpensive**
- **highly engineered (controlled ptys)**

Opaque plastic film



Film sheet after test

Measurements

(1) X-Y position of debris particle perforations on each film [dispersion of debris]
(2) Size of debris particle perforations [debris particle size]
(3) #1 combined with film distance from target perforation site gives debris particle direction and penetration path length in foam [related to mass & velocity of debris particle]
(4) Recovery of debris material from selected tests

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High Strain-Rate Testing (HSRT)

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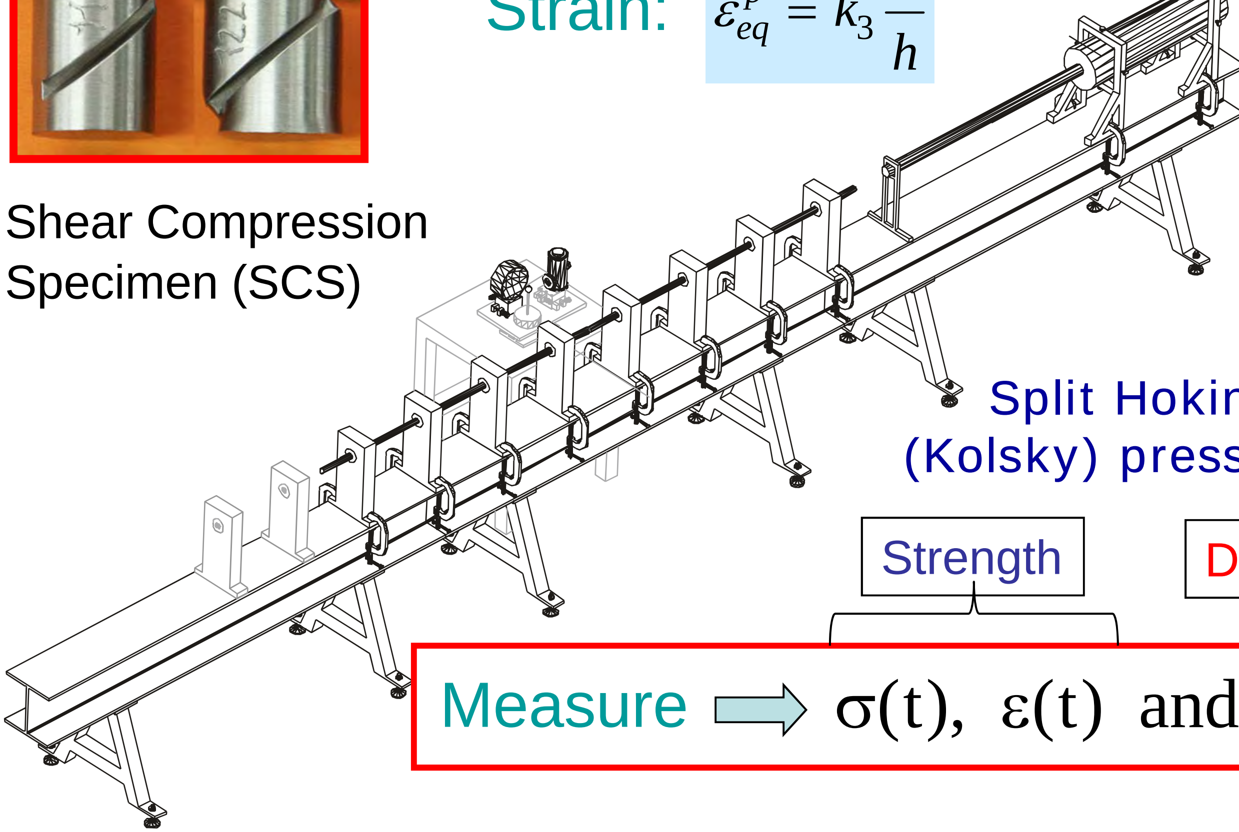
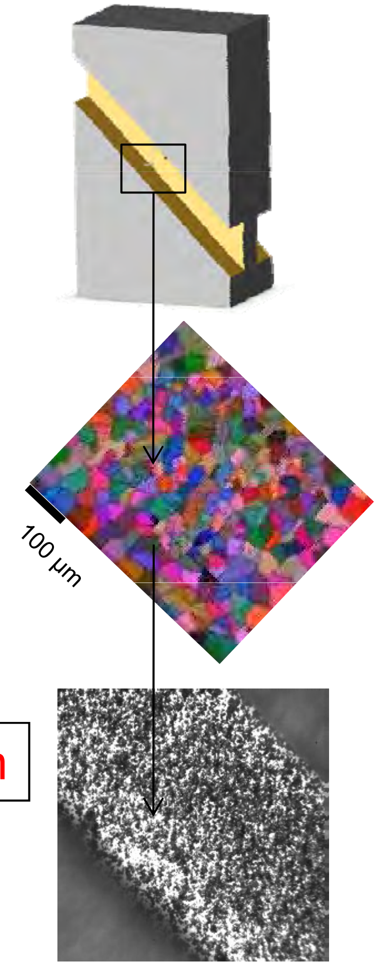
Shear Compression Specimen (SCS)

Stress: $\sigma_{eq} = k_1 (1 - k_2 \varepsilon^p_{eq}) \frac{P}{Dt}$

Strain: $\varepsilon^p_{eq} = k_3 \frac{d}{h}$



Split Hokinson (Kolsky) pressure bar



Strength | Dissipation

Measure ⇨ $\sigma(t)$, $\varepsilon(t)$ and $\theta(t)$

Full-field imaging, Sub-grain resolution

Caltech's High Strain-Rate Testing (HSRT) facility
(Prof. G. Ravichandran, Director)

High Strain-Rate Testing (HSRT)

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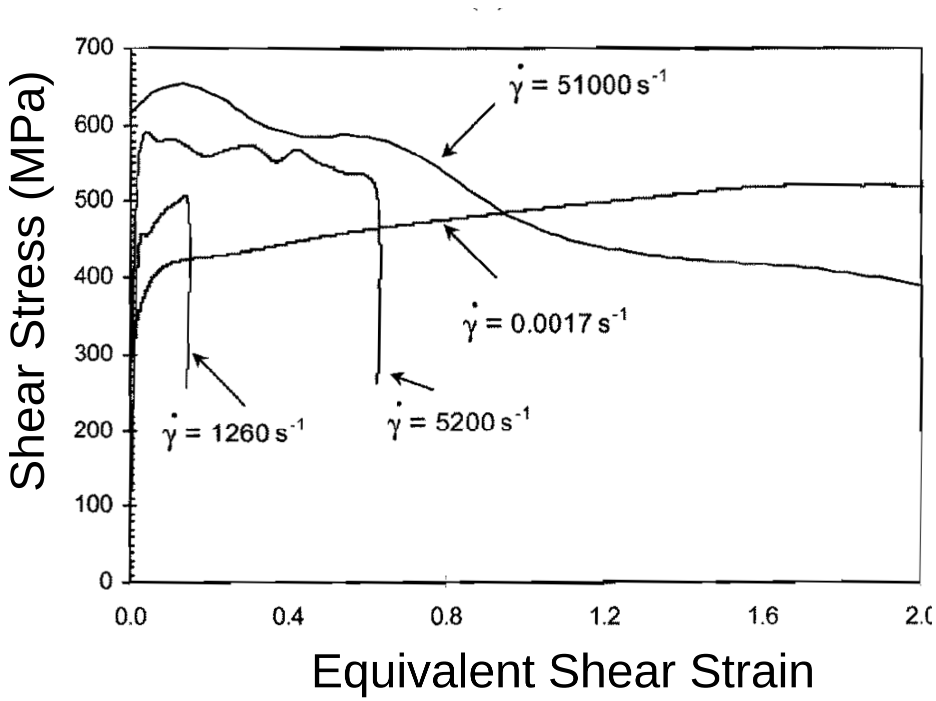
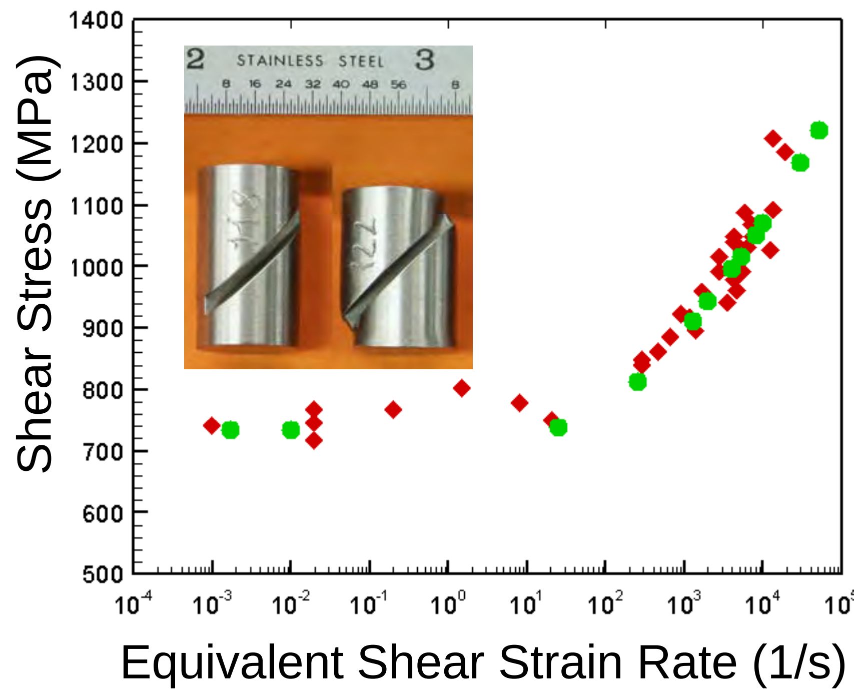
Shear-compression specimen test





M. Vural, D. Rittel and G. Ravichandran, "Large strain mechanical behavior of 1018 cold-rolled steel over a wide range of strain rates," *Metallurgical and Materials Transactions A*, Vol. 34A (2003) p. 2873.

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High Strain-Rate Testing (HSRT)

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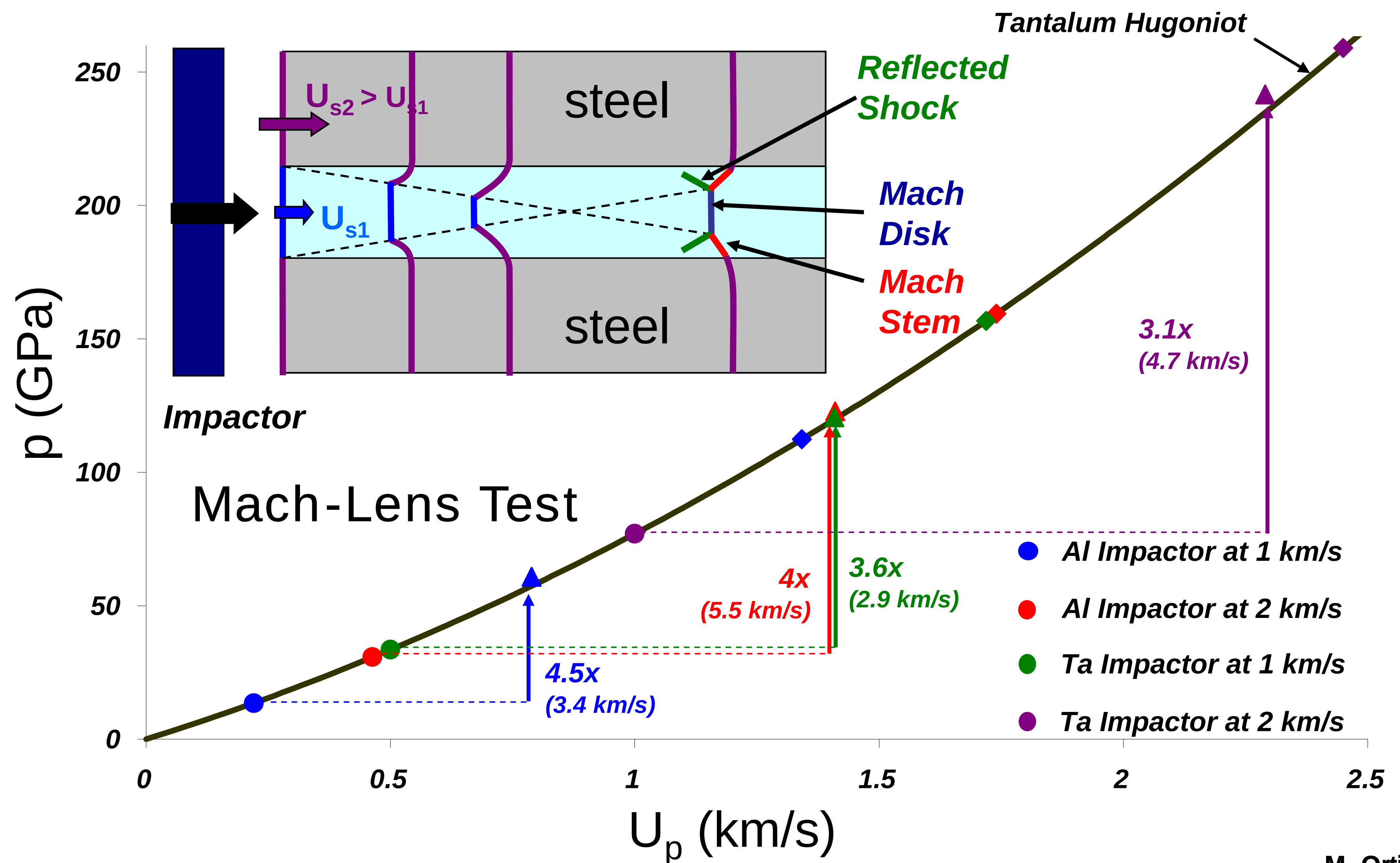

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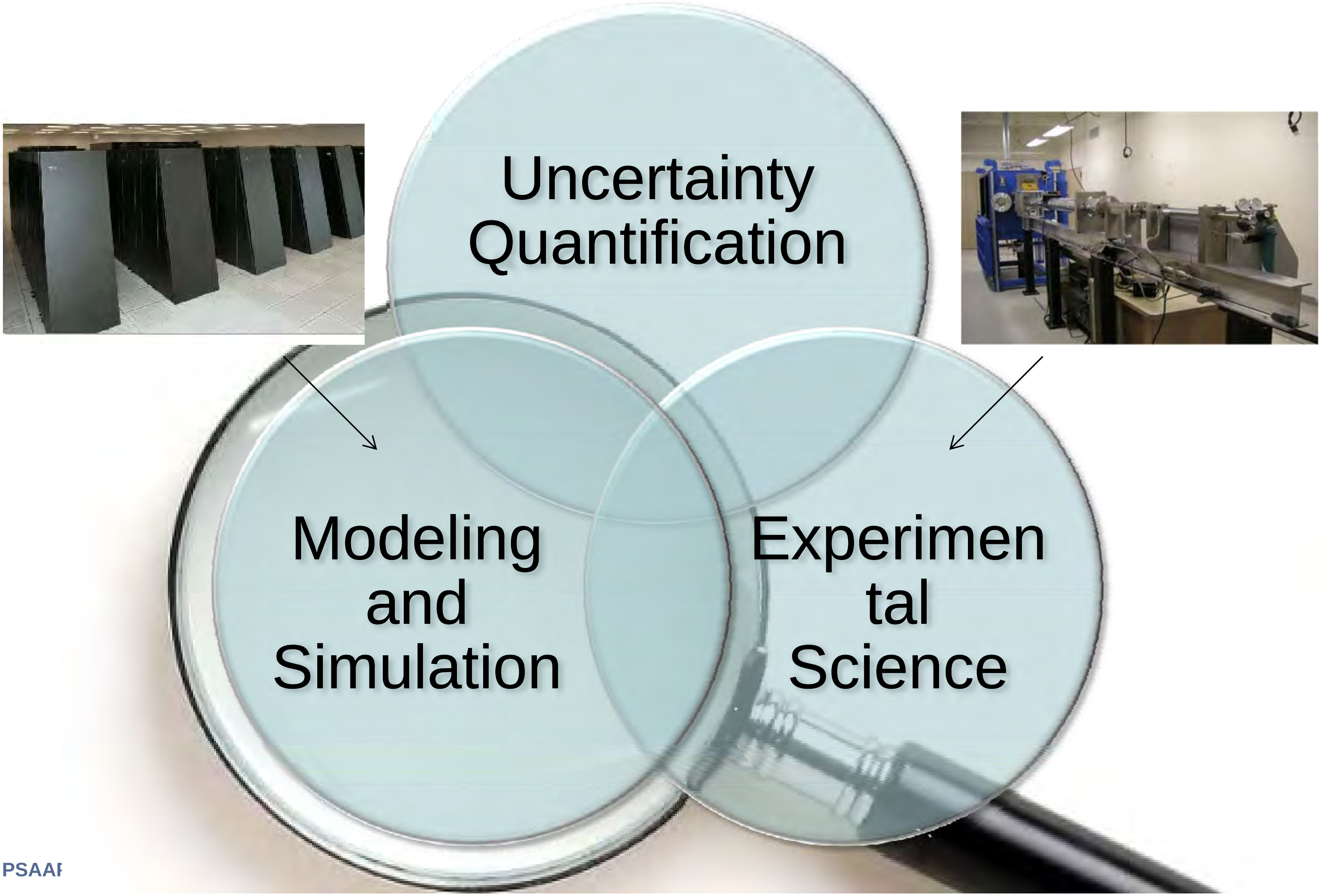
Experimental data at Caltech

- Experimental Science, full-device testing, component and materials testing, essential to Predictive Science: ***No data, no prediction!***
- The Caltech center houses experimental facilities:
  - **Small Particle Hypervelocity Impact Range**
  - High-Strain Rate Facility (constitutive characterization)
- The material characterization facilities supply material data for ***model calibration and validation***
- Hypervelocity impact facility defines performance measures to be predicted and supplies quantitative data for ***Uncertainty Quantification***

The Predictive Science Paradigm



Hypervelocity Modeling & Simulation

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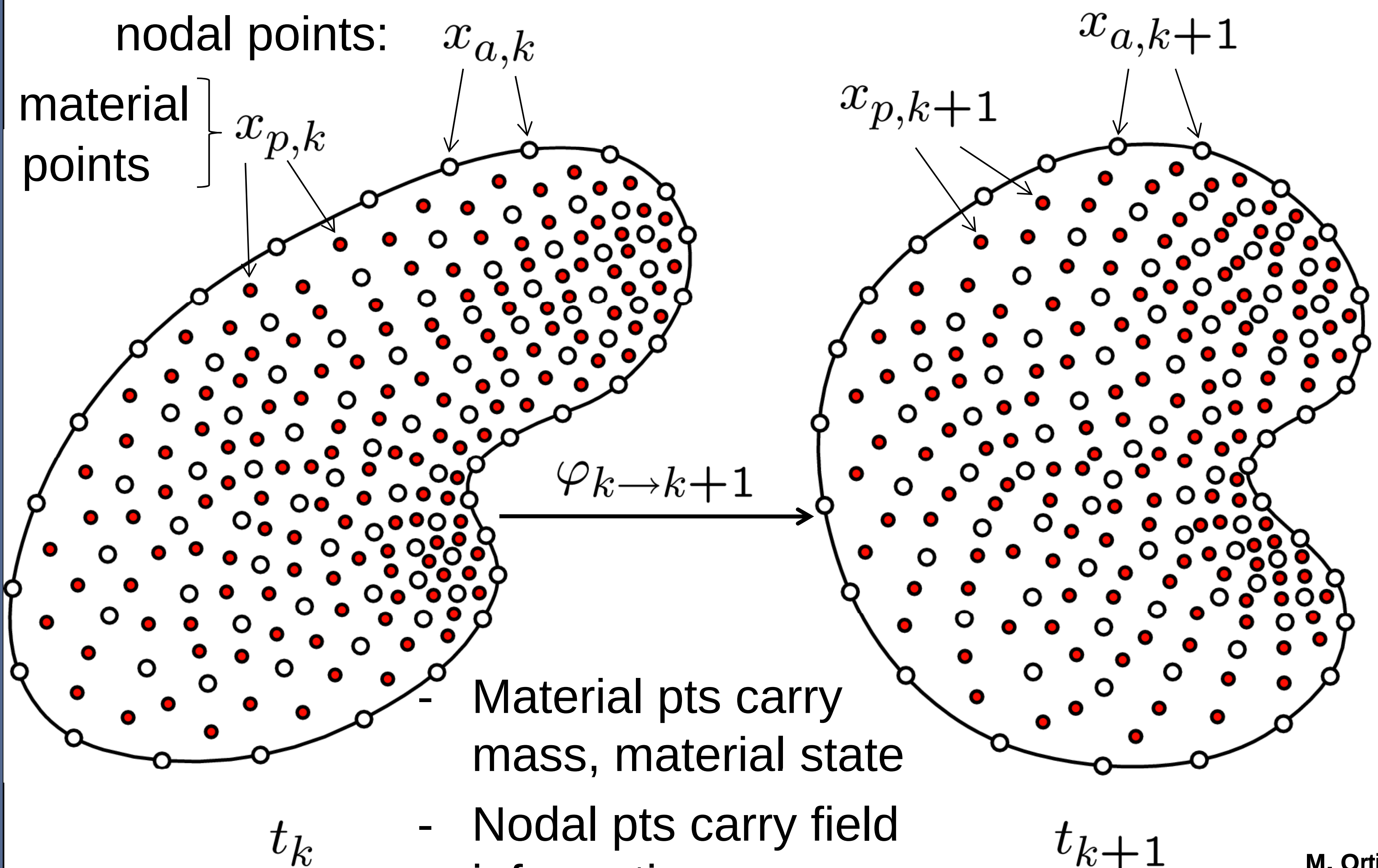
- Phenomena that ***challenge modeling and simulation***:
  - Plasma magneto-hydrodynamics
  - Coupled multiphase large-deformation thermo-plasticity
  - Fracture, fragmentation, collisions/contact
- Physics that ***challenge modeling and simulation***:
  - Pressure ~ 1-2 Mbar, strain rates ~ 10^{11} 1/s, temp ~ 10^4 K
  - melting and vaporization, dissociation, ionization, plasma
  - luminescence and radiative transport
  - hydrodynamic instabilities, mixed-phase flows, mixing
  - solid-solid phase transitions, high-strain-rate deformation, thermo-mechanical coupling
  - fracture, fragmentation, spall and ejecta, deformation instabilities such as shear banding

Optimal-Transportation Meshfree



- Material pts carry mass, material state
- Nodal pts carry field information

OTM meshfree spatial discretization

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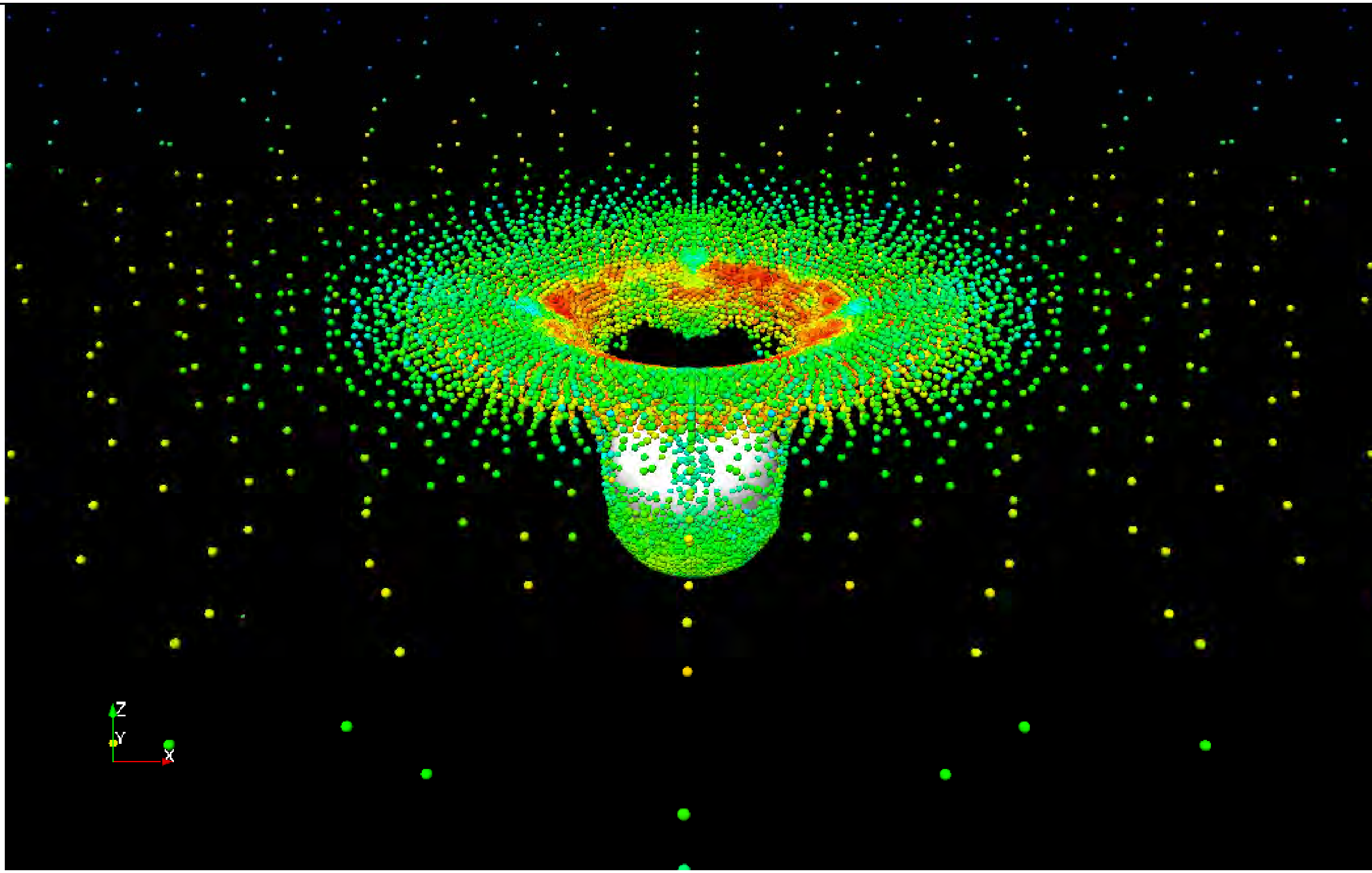

Steel projectile/aluminum plate: Nodal set

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OTM meshfree spatial discretization

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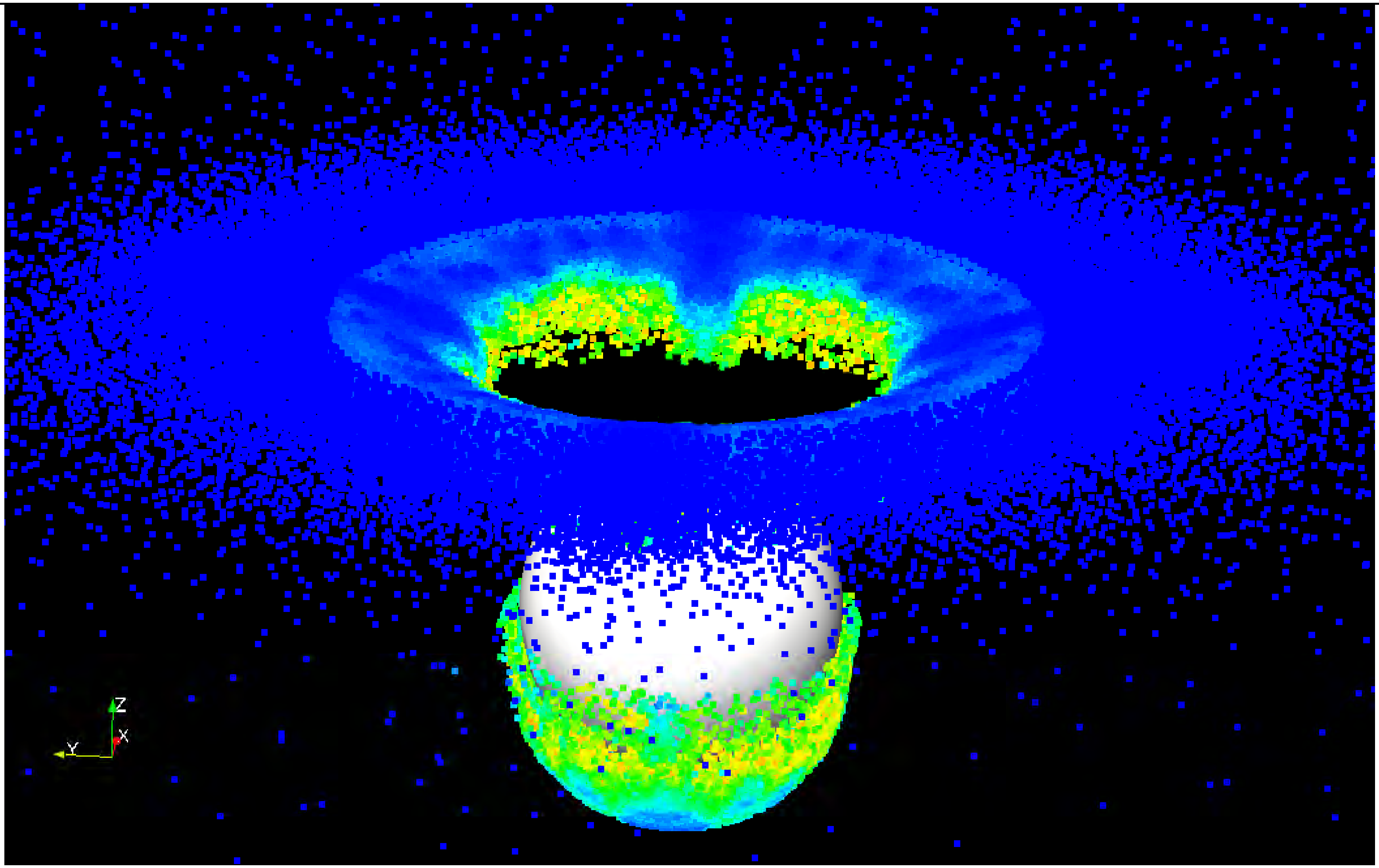

Steel projectile/aluminum plate: Material point set

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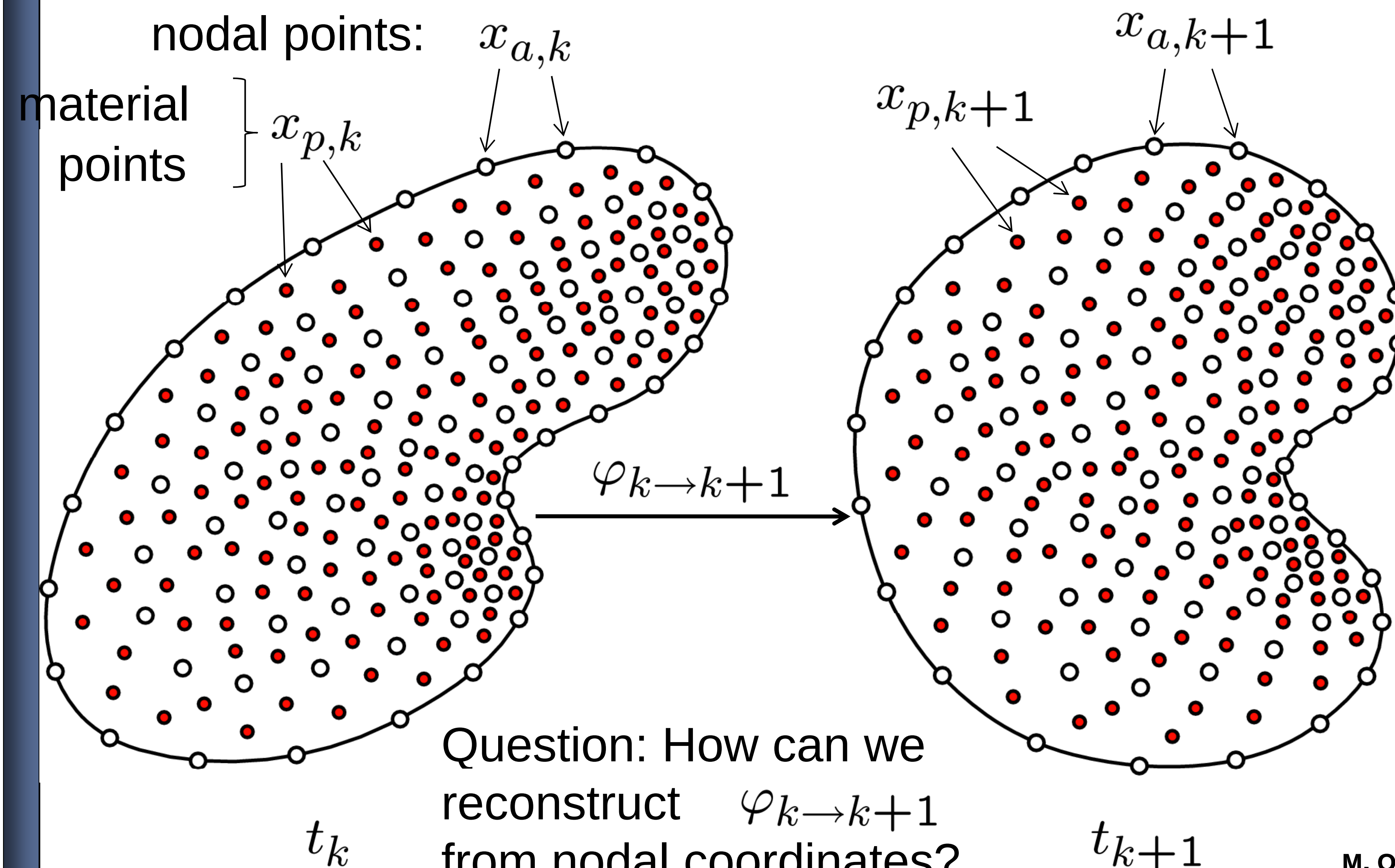
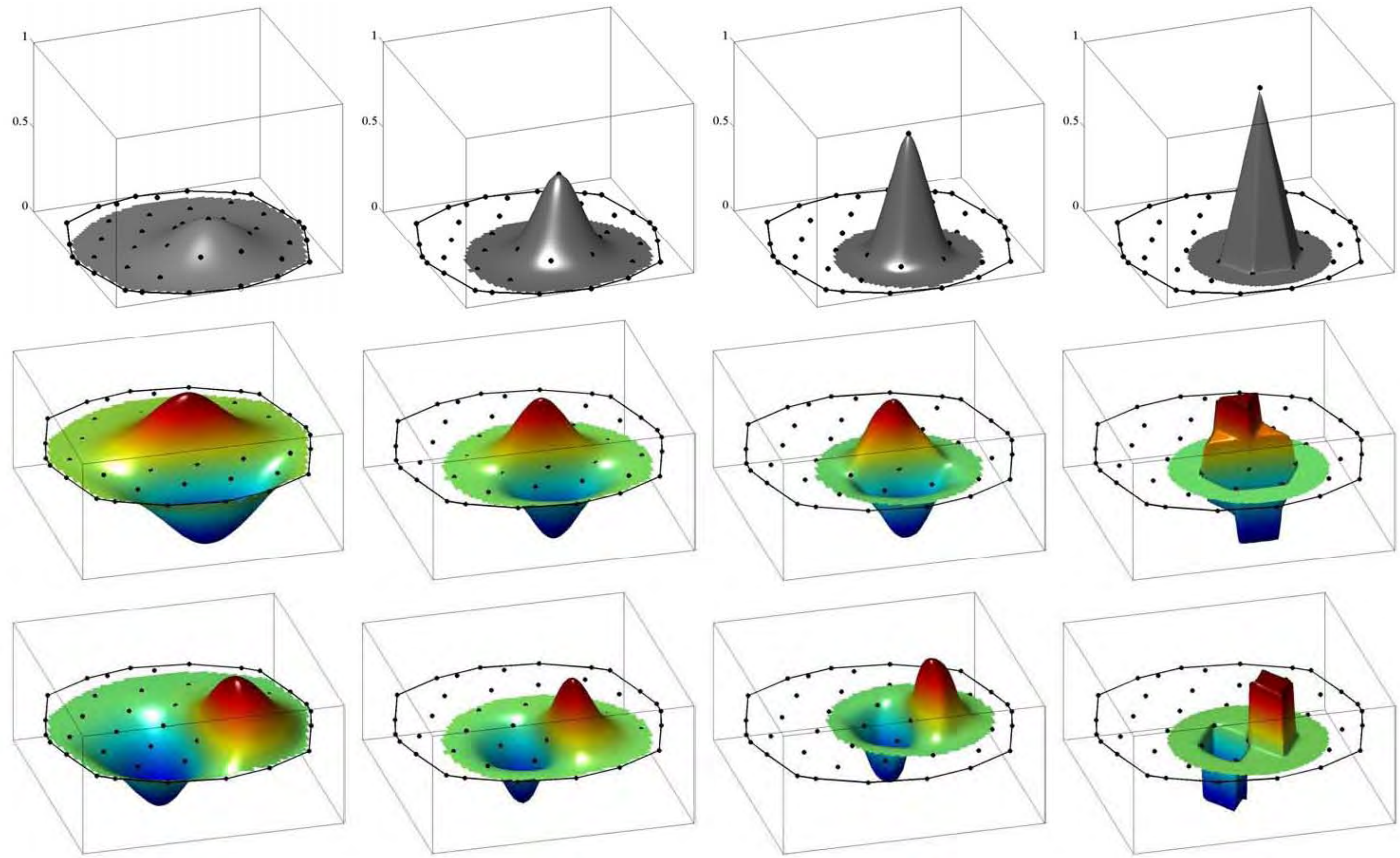
Meshfree spatial discretization



Question: How can we reconstruct $\varphi_{k\to k+1}$ from nodal coordinates?

Max-ent spatial interpolation



$\gamma = 0.8$ $\gamma = 1.8$ $\gamma = 2.8$ $\gamma = 6.8$

Max-ent shape functions of decreasing entropy

Arroyo, M. & MO*, Int. J. Numer. Meth. Engr.*, **65**:2167-2202, 2006

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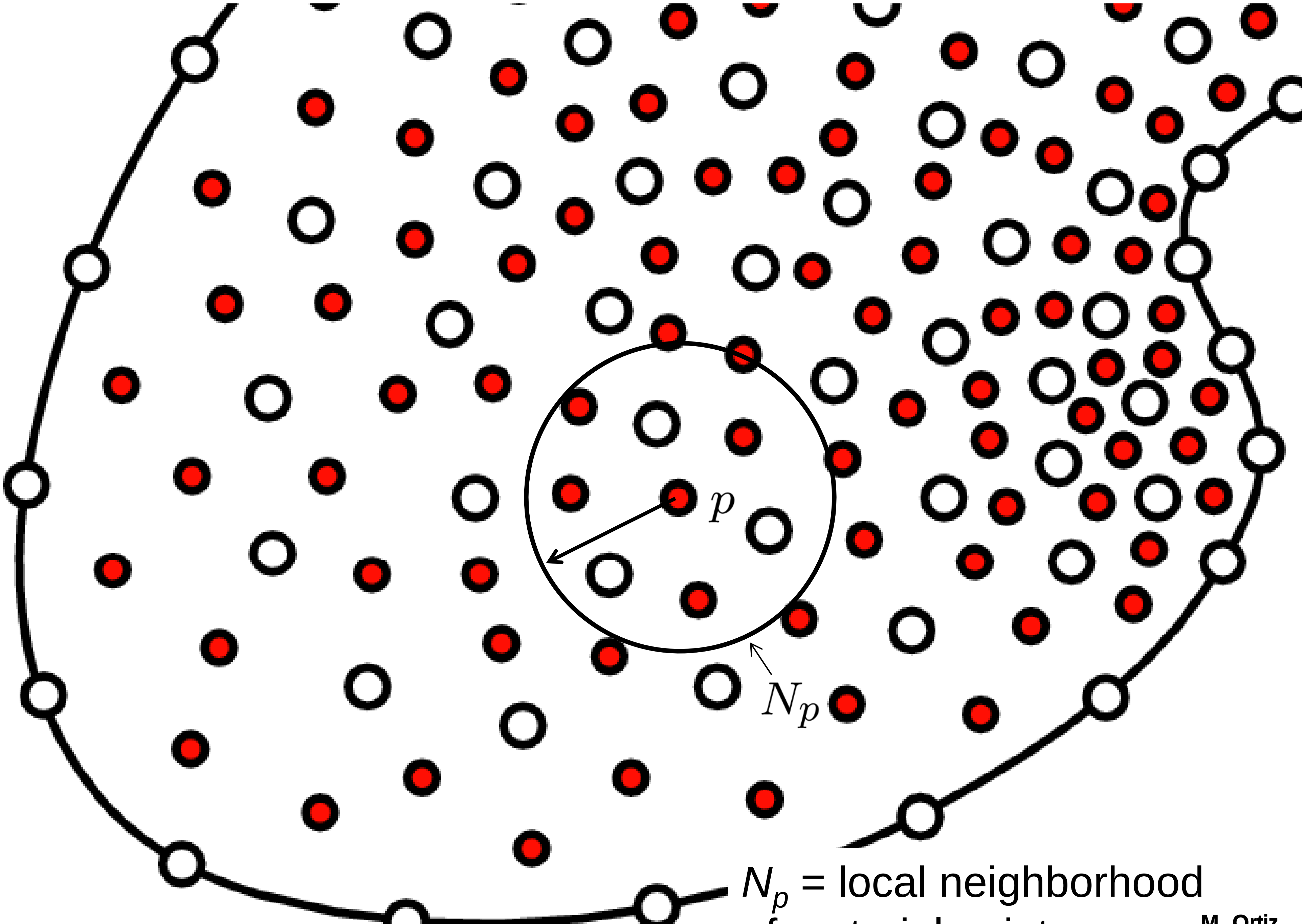
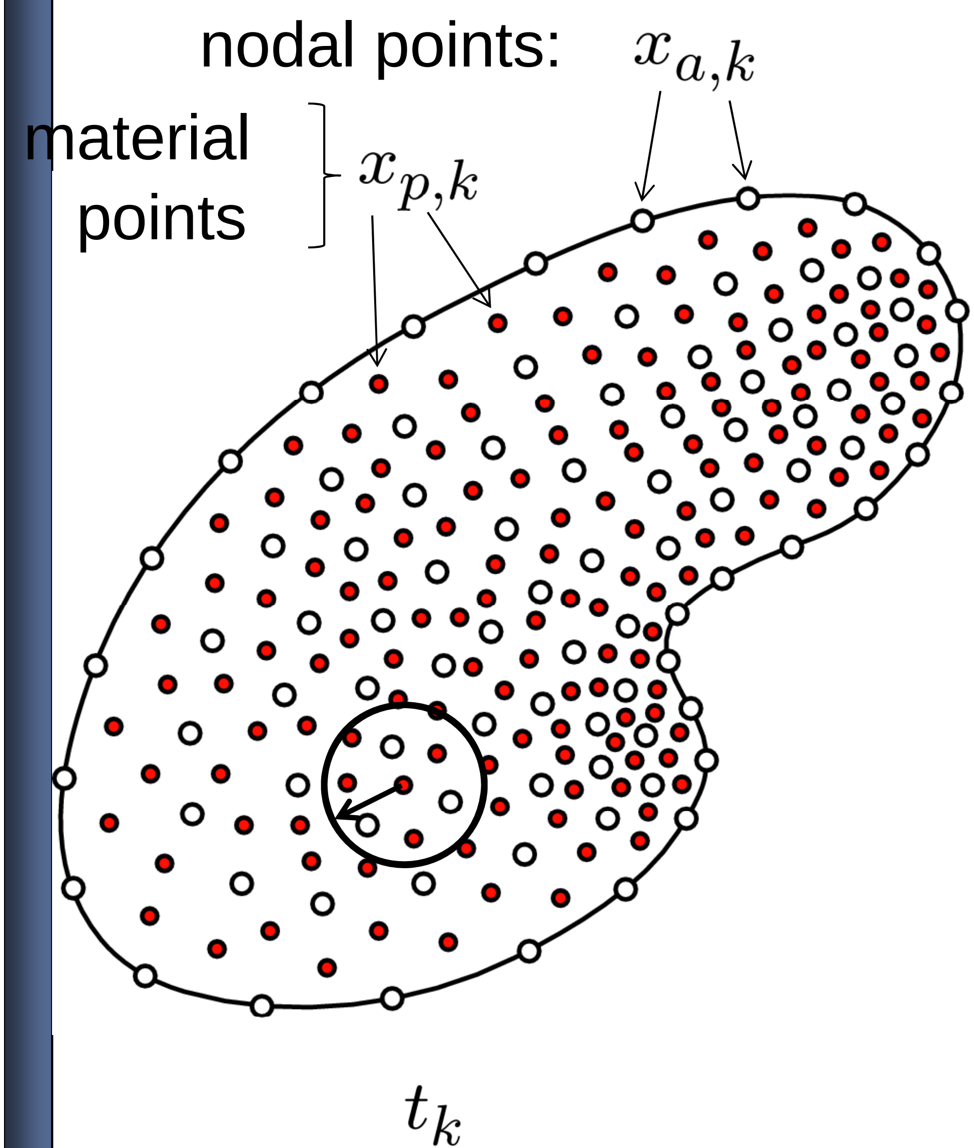


N_p = local neighborhood of material point p

Max-ent spatial discretization



- Max-ent interpolation at material point *p* determined by nodes in its local environment N_p *only*
- 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 – Seizing contact

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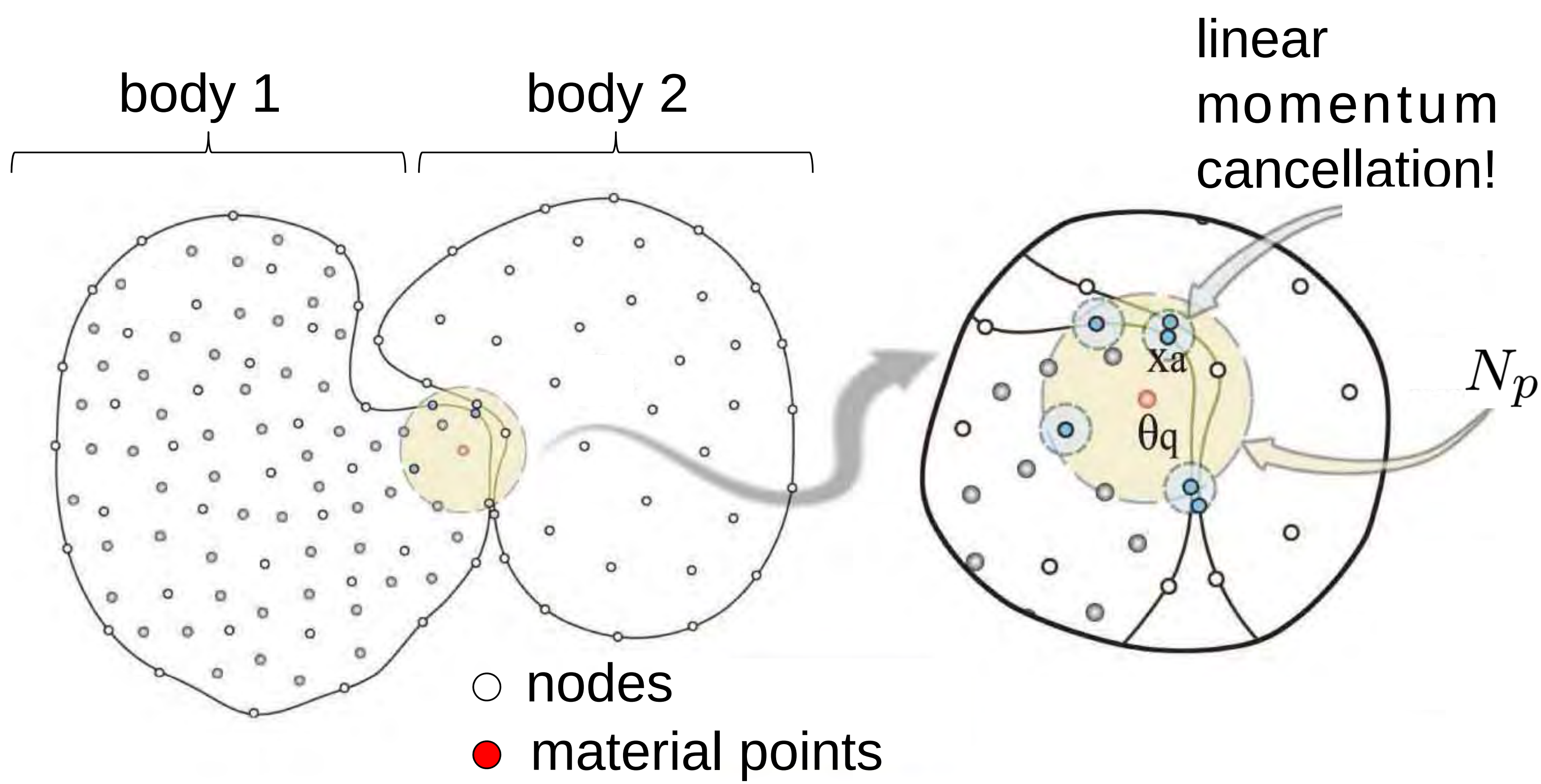
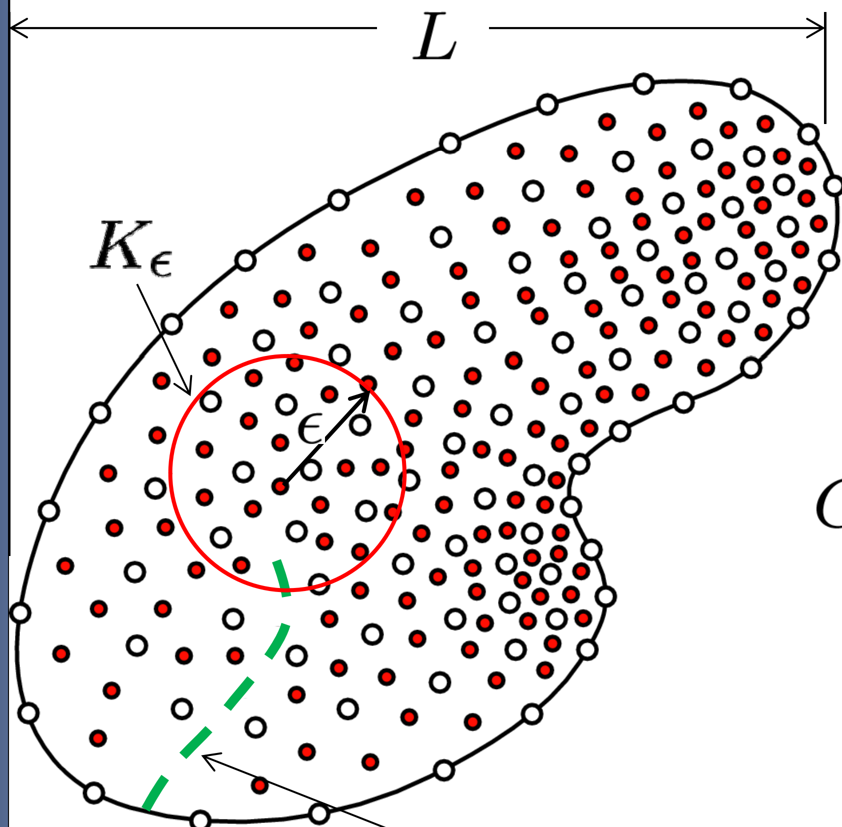


Seizing contact (infinite friction) is obtained for free in OTM!

OTM – Material-point erosion



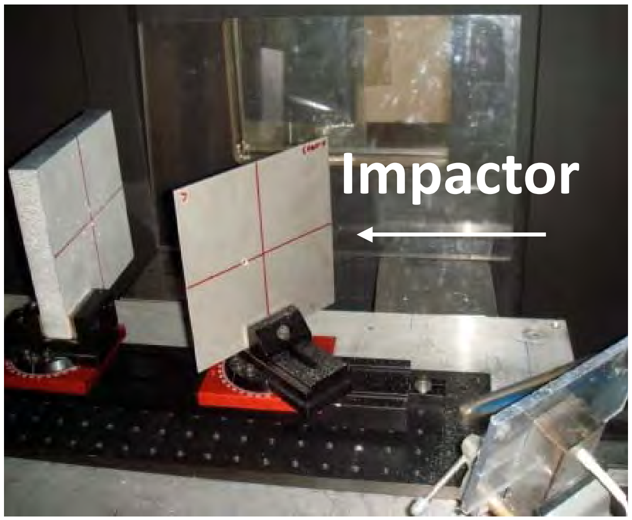
Schematic of ε-neighborhood construction

- ε-neighborhood construction: Choose h << ε << L
- Erode material point if

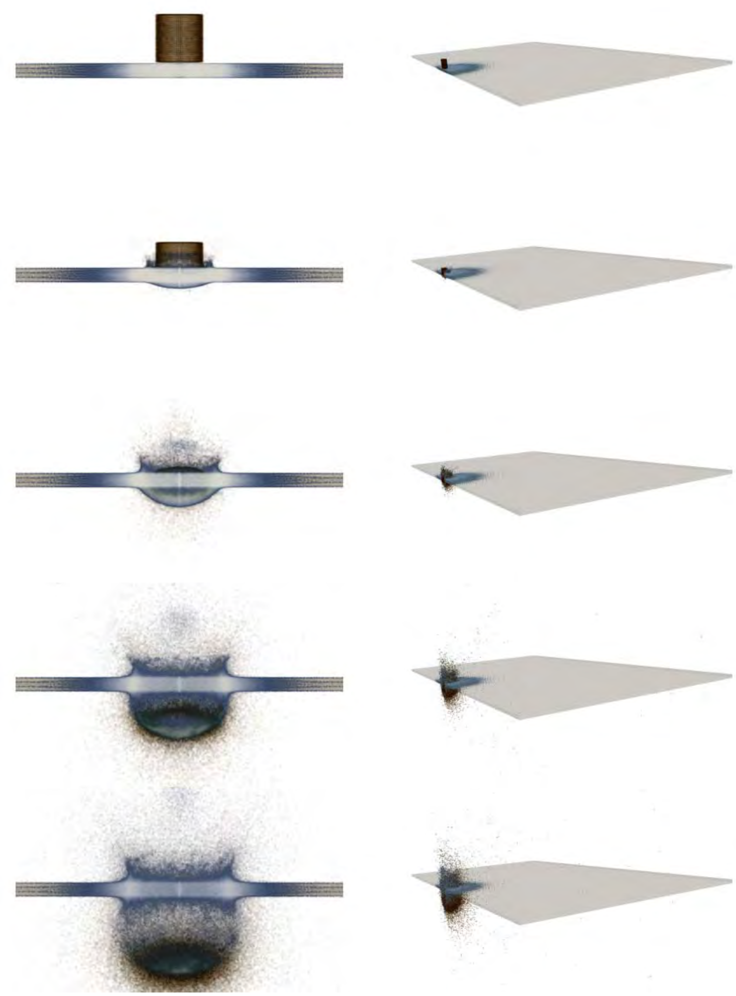
$$G_\epsilon \sim \frac{h^2}{|K_\epsilon|} \int_{K_\epsilon} W(\nabla u)\, dx \geq G_c$$

- Proof of convergence to Griffith fracture:
  – *Schmidt, B., Fraternali, F. & MO, SIAM J. Multiscale Model. Simul.*, **7**(3):1237-1366, 2009.

Hypervelocity impact - Simulation

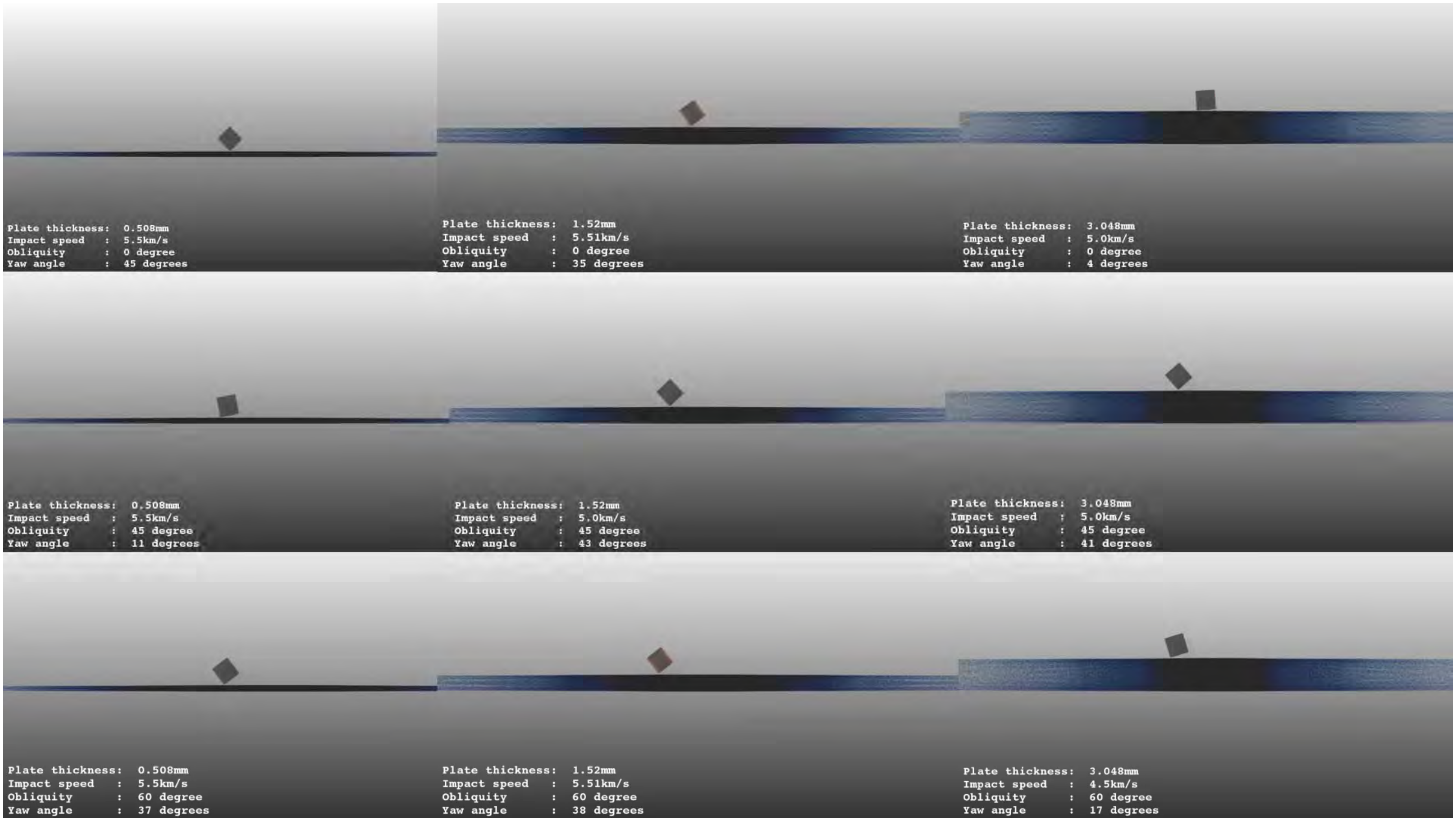


Caltech's hypervelocity Impact facility

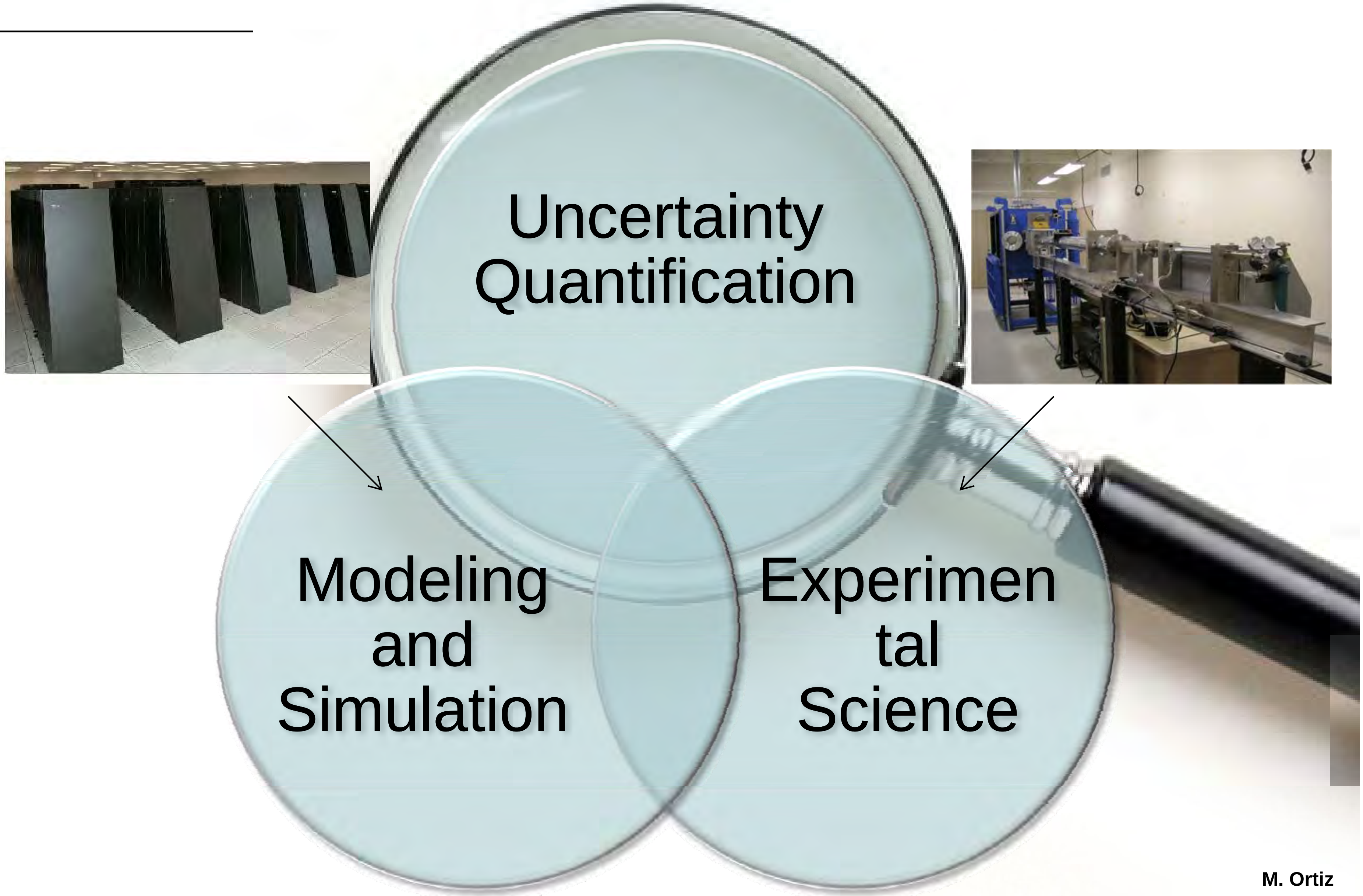


OTM simulation, 5.2 Km/s, Nylon/Al6061-T6, 20 million points

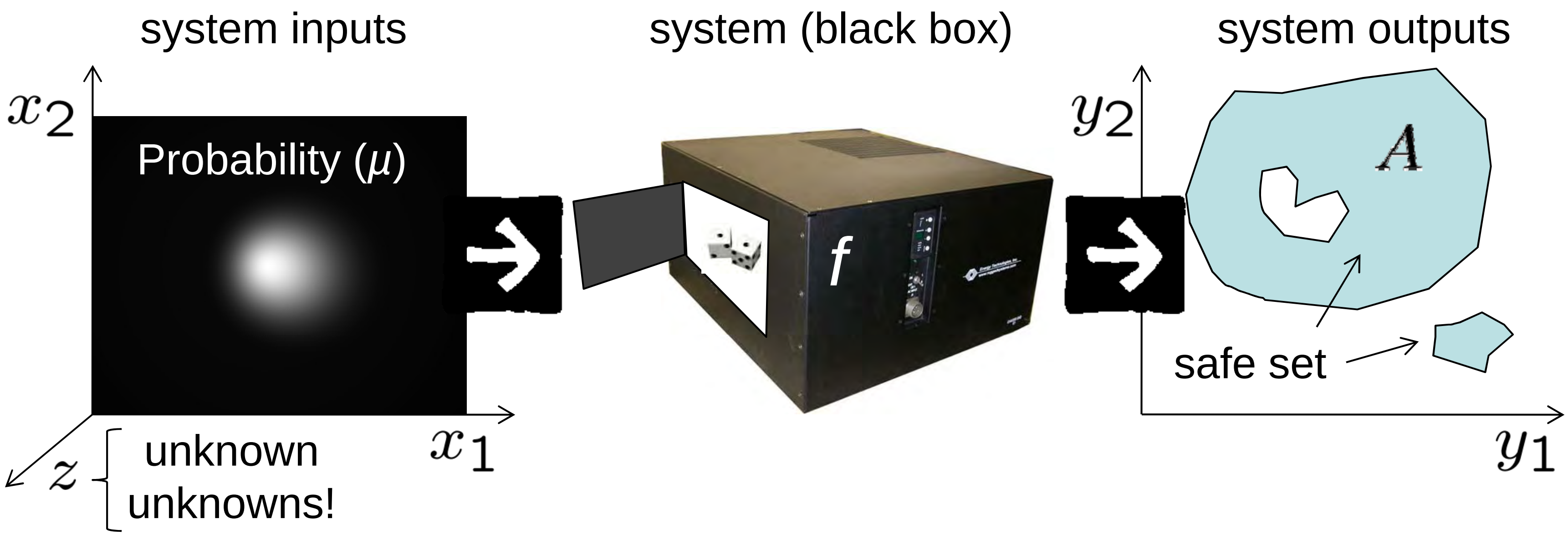
Solvers — Massively Parallel OTM



The Predictive Science Paradigm



Uncertainty Quantification (UQ)



- Black box: $x \equiv$ inputs, $y \equiv$ outputs
- Response function: $y = f(x)$
- Exact probability of outcomes:

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

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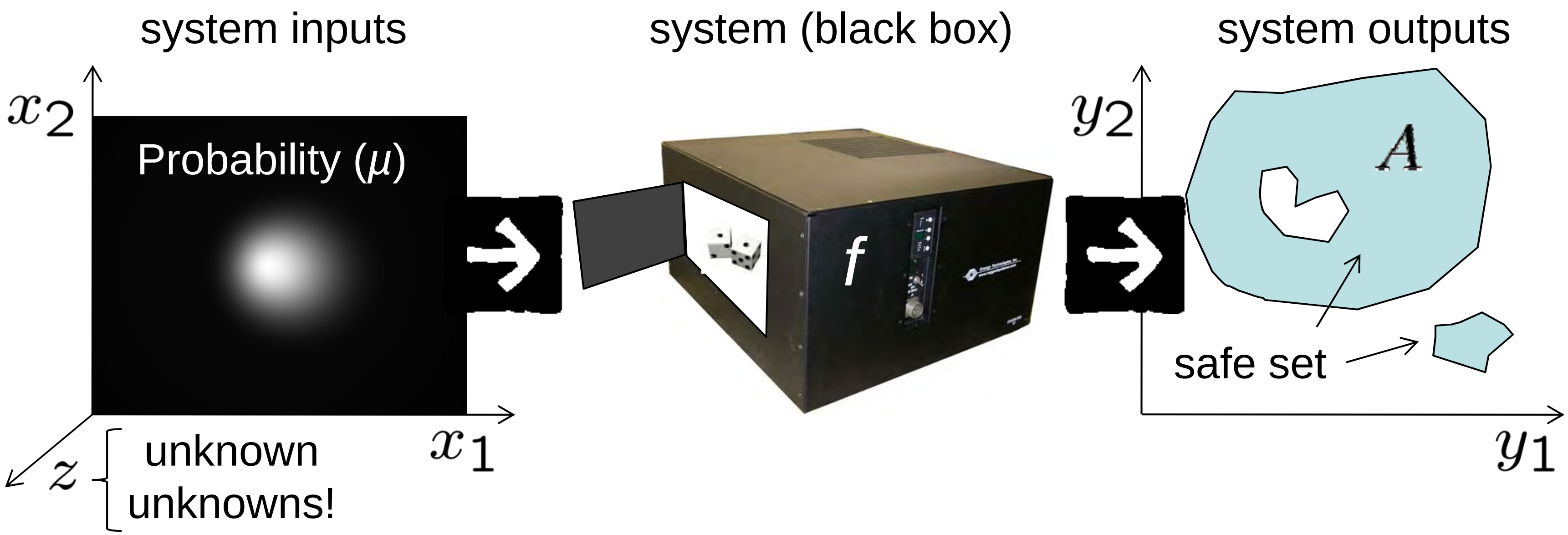
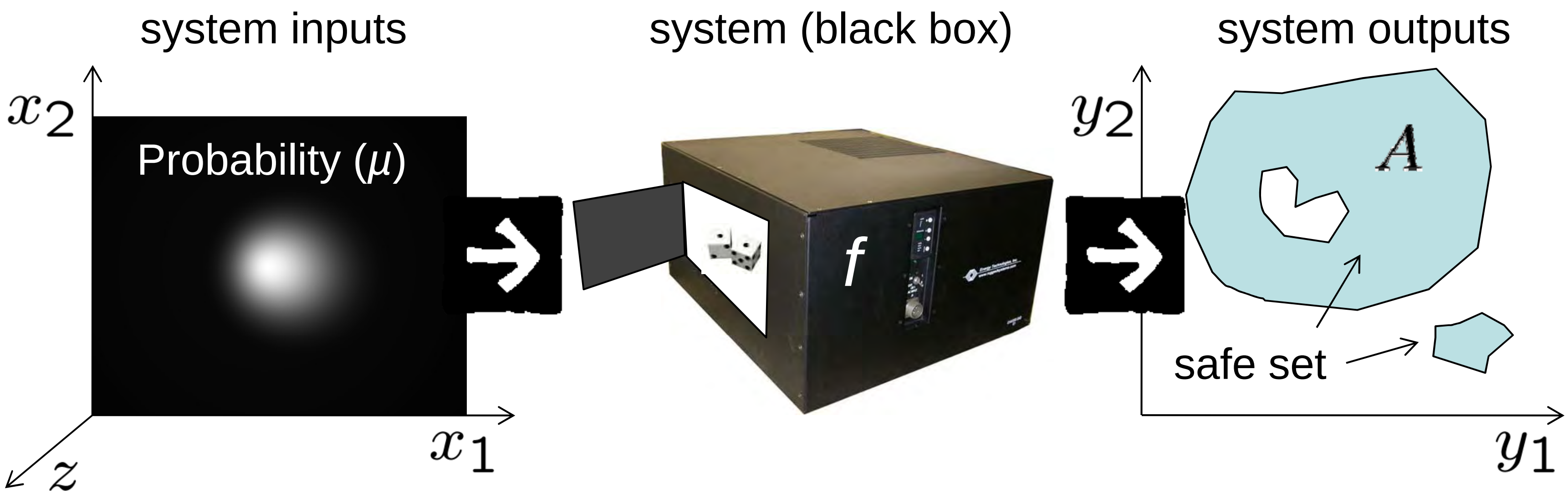
UQ – Essential difficulties



- 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…

Optimal Uncertainty Quantification



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

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

OUQ – The Reduction Theorem

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

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

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

Then:

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

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

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

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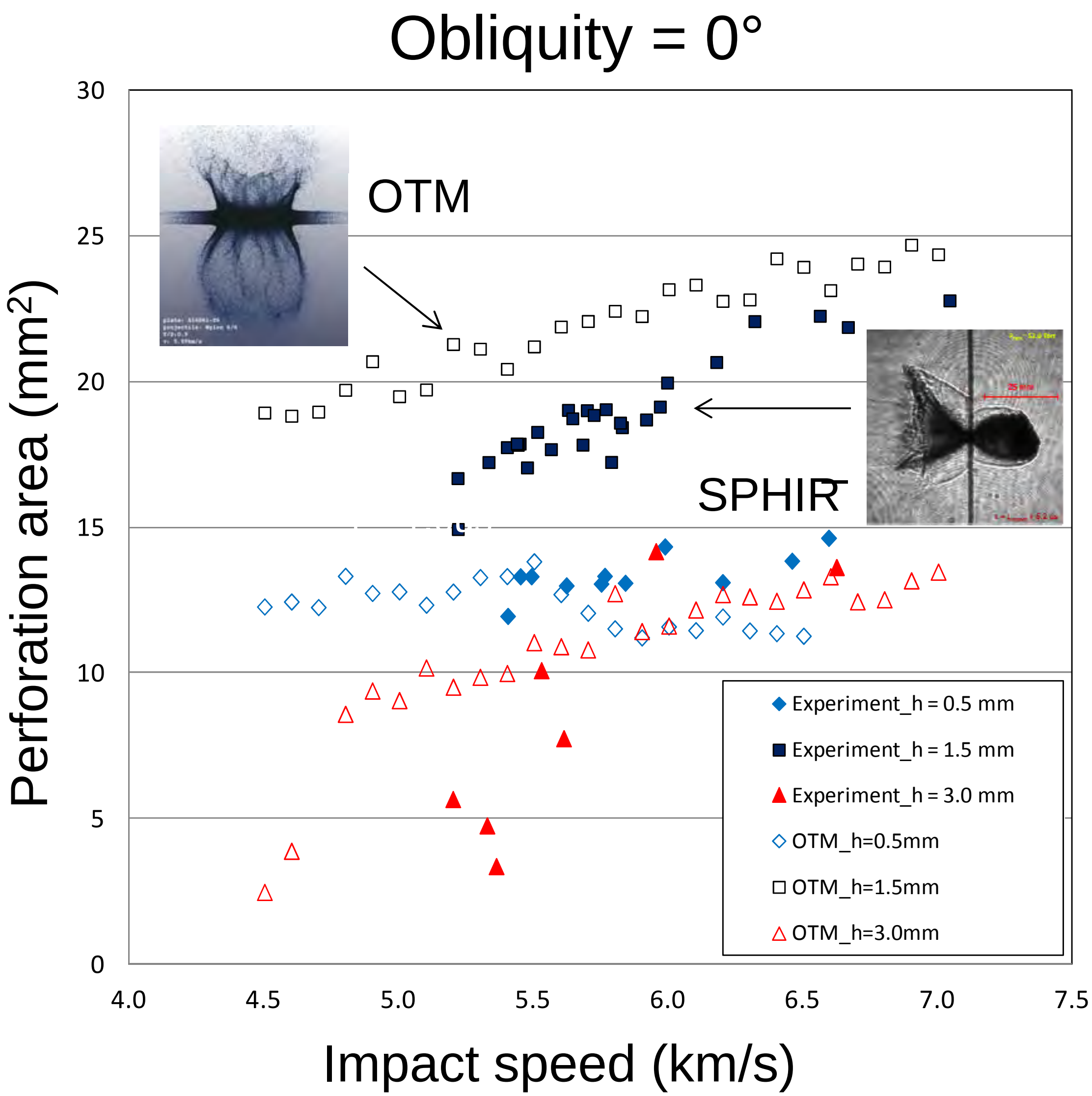
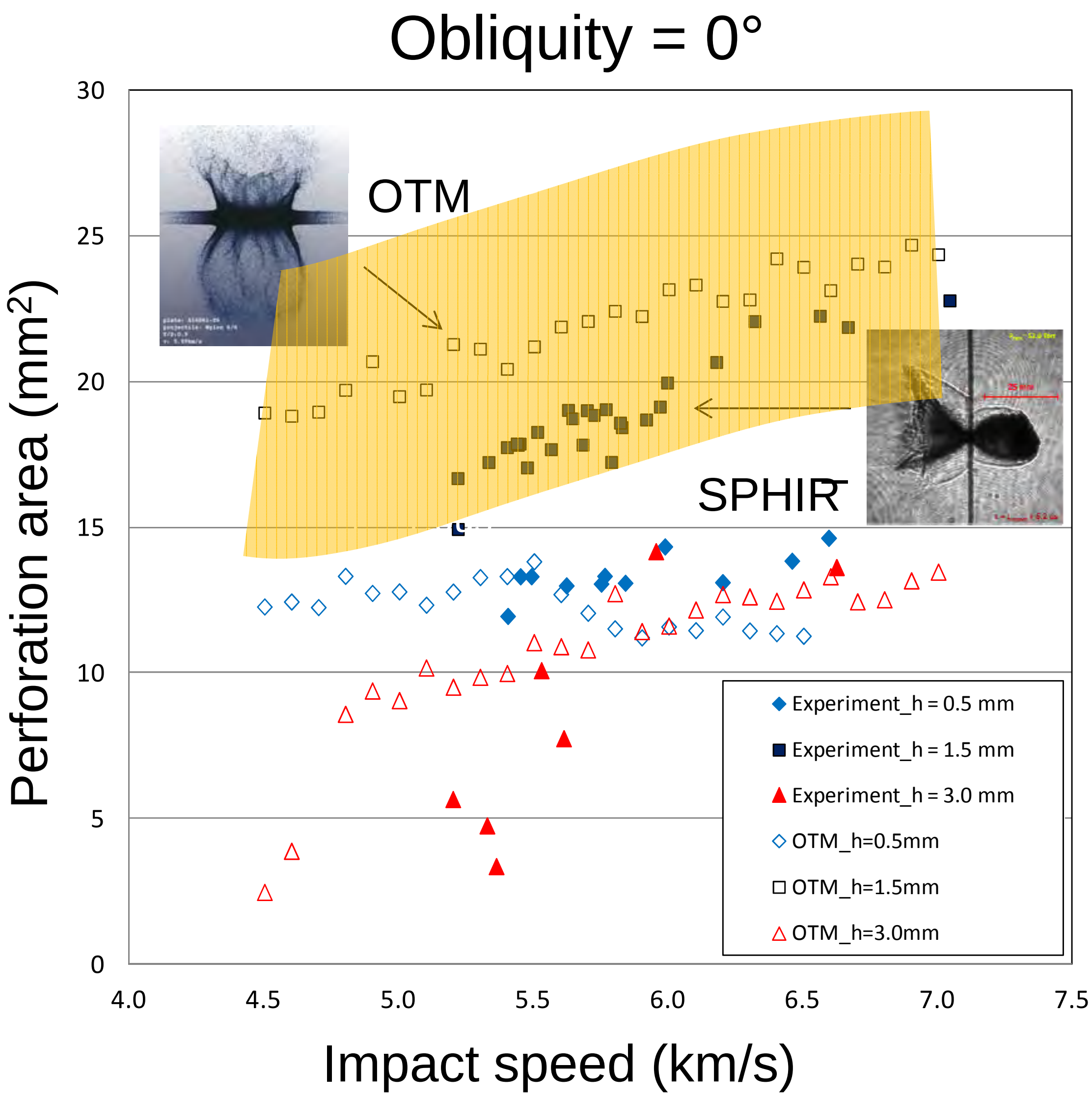
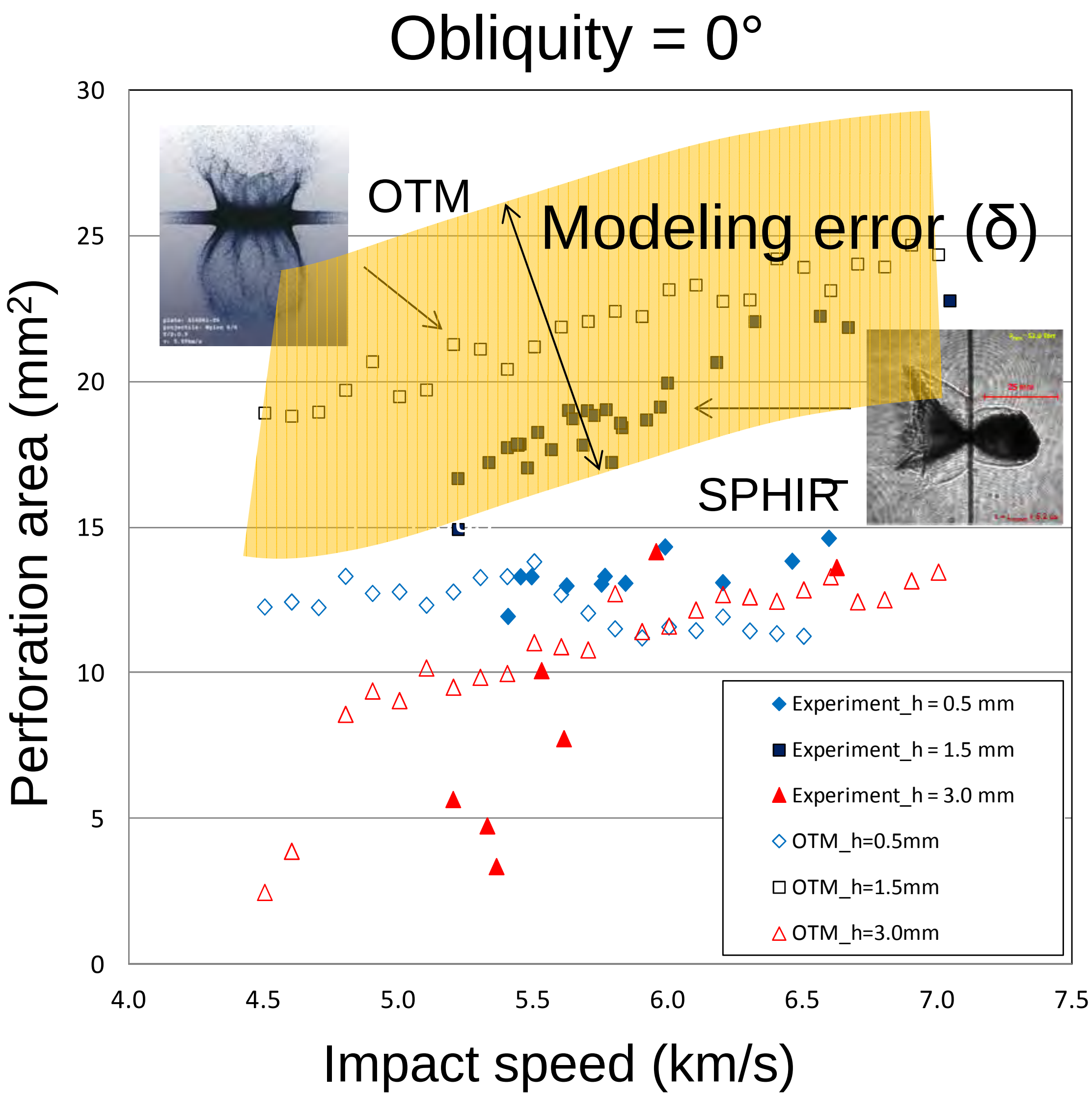
OUQ – Model based protocol



OUQ – Model based protocol



OUQ – Model based protocol



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Hypervelocity — Model-based OUQ

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Caltech's SPHIR facility

- Inputs: $x \equiv \begin{cases} h \in [1.524, 2.667]\,\text{mm} \\ \theta \in [0, \frac{\pi}{6}] \\ v \in [2.1, 2.8]\,\text{km}\,\text{s}^{-1} \end{cases}$
- Output: $y \equiv$ perforation area

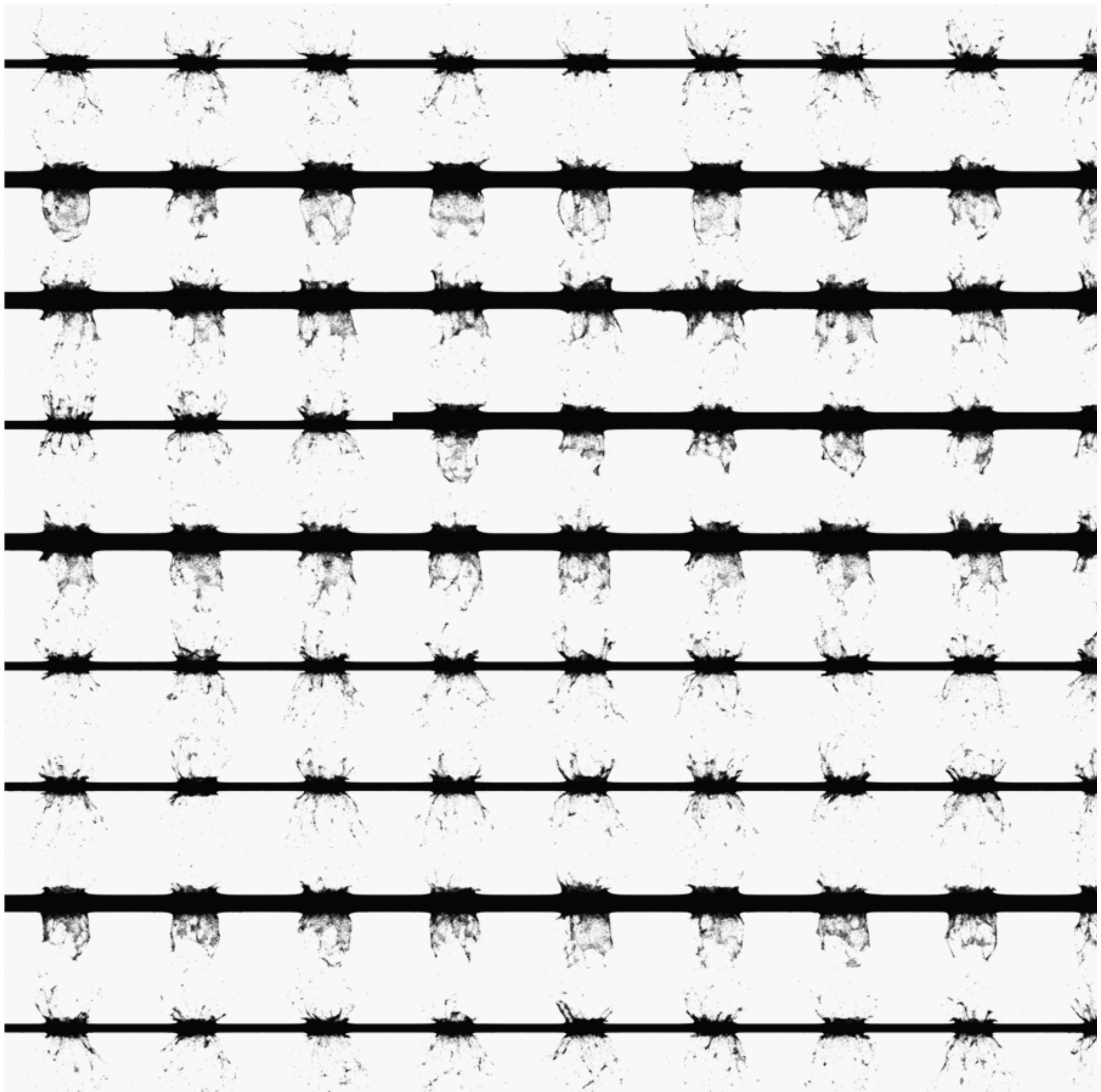
- Admissible set:

$$\mathcal{A} \equiv \left\{ (f, \mu) \,\middle|\, \begin{array}{c} d(f, f_{\text{OTM}}) \leq \delta \\ \mu = \mu_1 \otimes \mu_2 \otimes \mu_3 \end{array} \right\}$$

- Reduced admissible set:

$$\mathcal{A}_{\text{red}} \equiv \left\{ (f, \mu) \,\middle|\, \begin{array}{c} d(f, f_{\text{OTM}}) \leq \delta, \\ \mu = \mu_1 \otimes \mu_2 \otimes \mu_3, \\ \mu_i = \alpha_i \delta_{a_i} + (1 - \alpha_i)\delta_{b_i},\ i = 1, 2, 3 \end{array} \right\}$$

Hypervelocity – OUQ/OTM calcs.

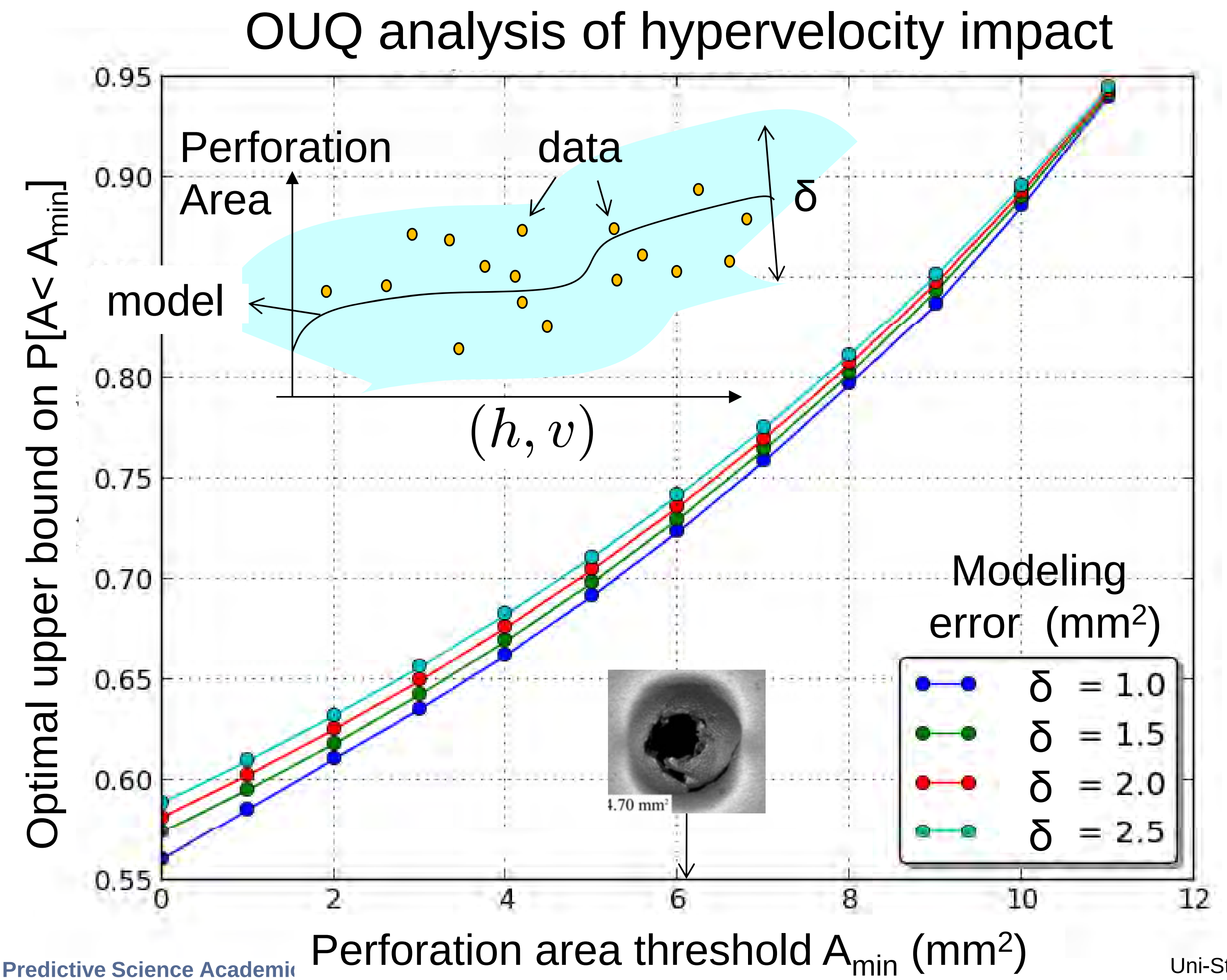


OTM calculations based On engineering material models with first principles input (EoS, elastic moduli, viscosity, melting, cohesive energy…)

- Each point averages 4 runs with different yaw angles (uncontrollable)
- Each run uses ~1million material points to model plate and projectile
- Each run is performed using 512 mpi tasks in 10 hours on: hera, glory, mapache, moonlight, cab, chama and others

M. Ortiz

Hypervelocity — Model-based OUQ



OUQ – Critique and outlook

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- The optimal bounds on probabilities of outcomes tend to be loose, i.e., the ***levels of uncertainty*** regarding the behavior of complex systems are often ***unacceptably high***. Path forward?
- In order to ***reduce uncertainty*** we need:
  - More data (but this may not be possible of too expensive)
  - Better statistics: Larger samples, larger parametric dimension…
  - Higher fidelity models, 'full physics': Quantum mechanical? Atomistic? Coarse-grained atomistic? Multiscale?
- These drivers (***'full-physics, uncertainty quantification***) place increasing demands on computing power: ***Exascale Computing!***

Outlook for Exascale Computing

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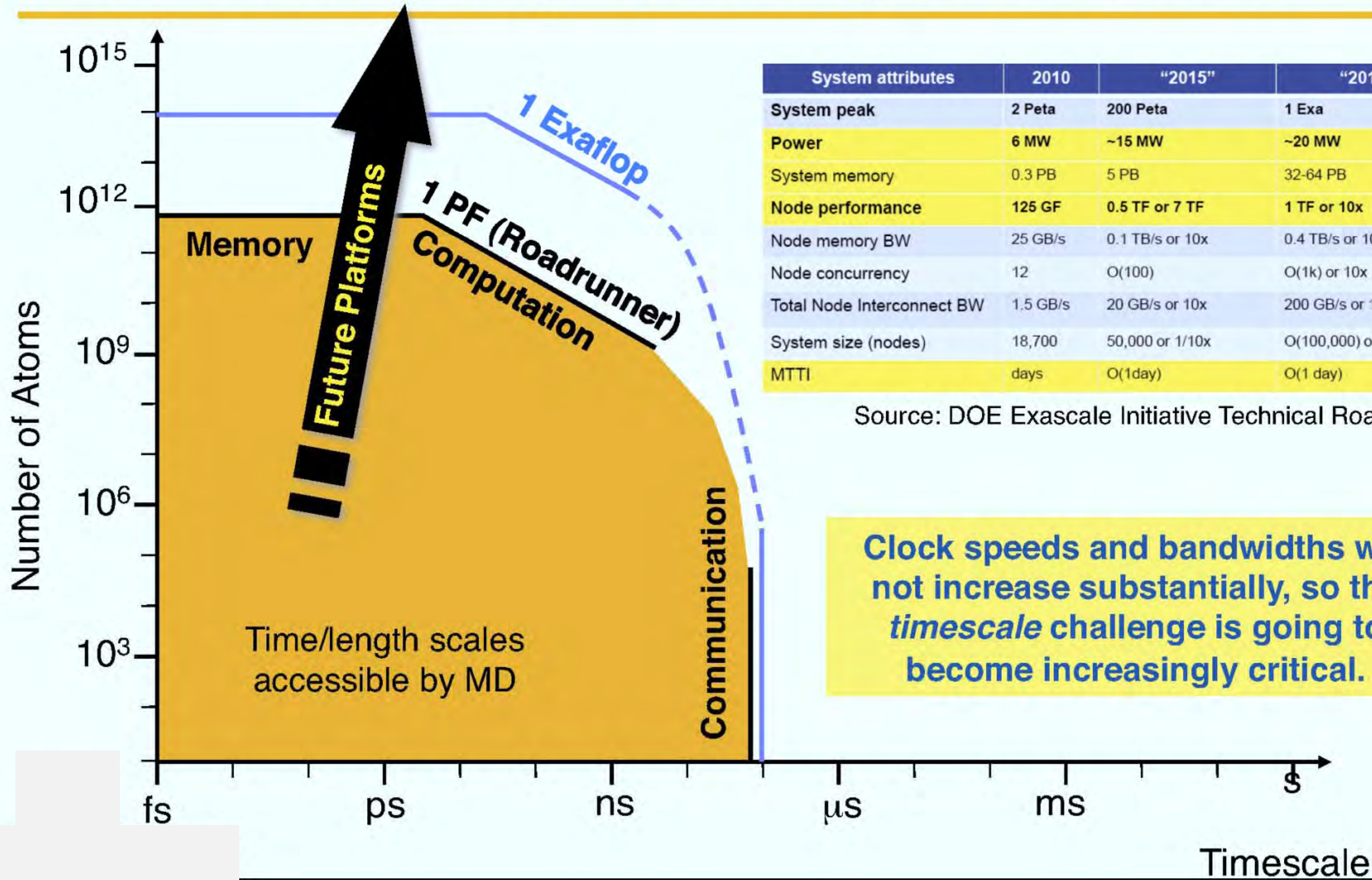
Current trends will increase the *length*, but not *time*, scales accessible by molecular dynamics simulation



System attributes	2010	"2015"	"2018"
System peak	2 Peta	200 Peta	1 Exa
Power	6 MW	~15 MW	~20 MW
System memory	0.3 PB	5 PB	32-64 PB
Node performance	125 GF	0.5 TF or 7 TF	1 TF or 10x
Node memory BW	25 GB/s	0.1 TB/s or 10x	0.4 TB/s or 10x
Node concurrency	12	O(100)	O(1k) or 10x
Total Node Interconnect BW	1.5 GB/s	20 GB/s or 10x	200 GB/s or 10x
System size (nodes)	18,700	50,000 or 1/10x	O(100,000) or 1/10 x
MTTI	days	O(1day)	O(1 day)

Source: DOE Exascale Initiative Technical Roadmap

Clock speeds and bandwidths will not increase substantially, so the *timescale* challenge is going to become increasingly critical.

(From: Timothy C. Germann, LANL, April 25-28, 2011)

Outlook for Exascale Computing

- Computer architectures are becoming increasingly heterogeneous and hierarchical, with greatly increased flop/byte ratios, architectural design uncertain…
- The algorithms, programming models, and tools that will thrive in this environment must mirror these characteristics, codes will need to be rewritten…
- SPMD bulk synchronous parallelism (message passing, MPI…) will no longer be viable…
- Power, energy, and heat dissipation are increasingly important, presently unsolved technological bottleneck
- Traditional global checkpoint/restart is becoming impractical (fault tolerance and resilience!)
- Analysis and visualization…

Evolution of Predictive Science…

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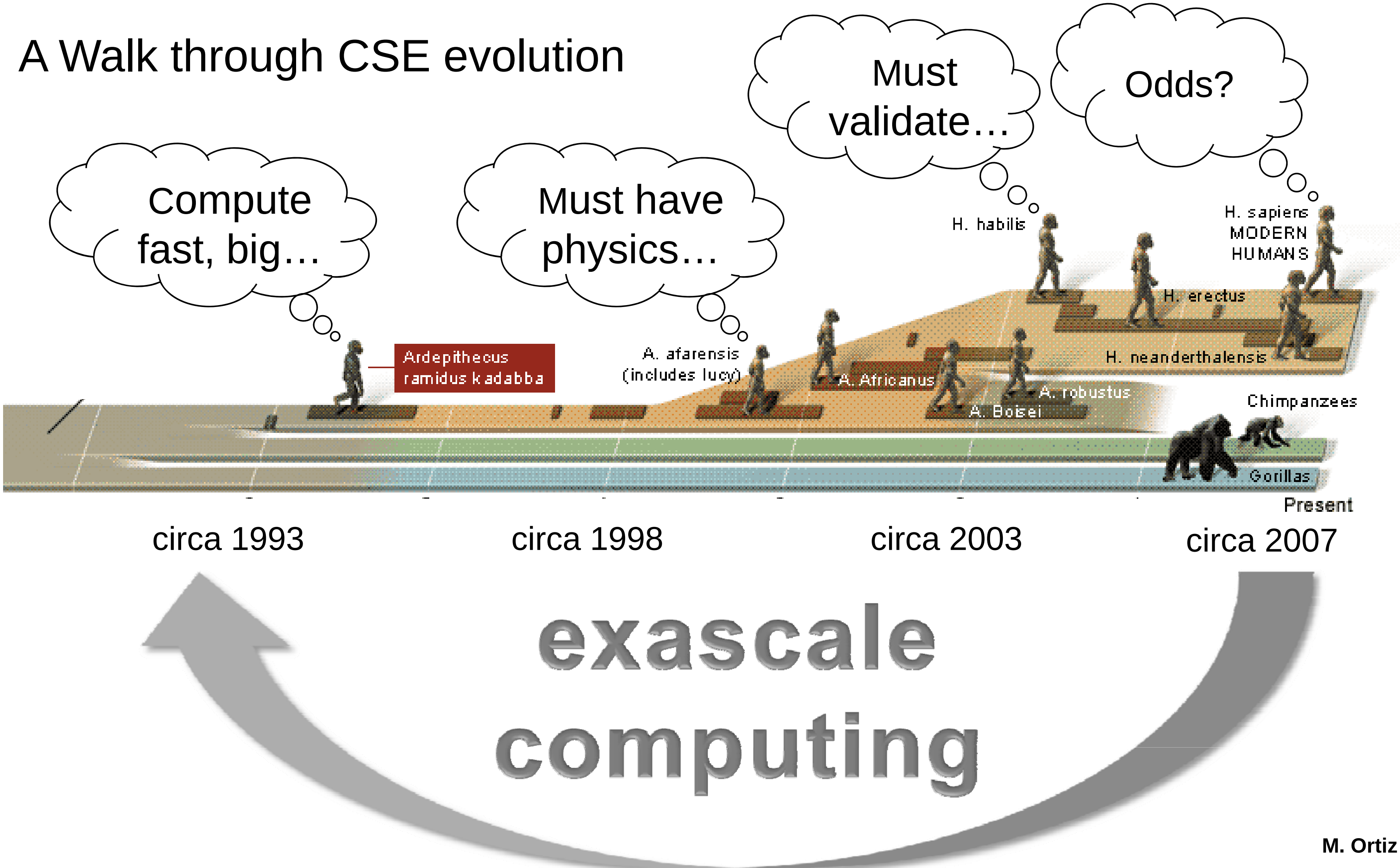
A Walk through CSE evolution



M. Ortiz

Concluding remarks…

Thank you!