‘Full Physics’ and Uncertainty Quantification as Drivers for Exascale Computing

M. Ortiz
California Institute of Technology

SimTech Colloquium
Universität Stuttgart, December 18, 2012
DoE/ASC/PSAAP Centers

STANFORD UNIVERSITY

PSAAP

CALTECH

PSAAP

PURDUE UNIVERSITY

CENTER FOR RADIATIVE SHOCK HYDRODYNAMICS

THE UNIVERSITY OF TEXAS AT AUSTIN
The Predictive Science challenge

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

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

NASA Ames Research Center Energy flash from hypervelocity test at 7.9 Km/s
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 $\rightarrow$ Non-deterministic systems
  - Mean performance $\rightarrow$ Mean performance + Uncertainty

Old single-calculation paradigm  New ensemble-of-calculations paradigm
The Predictive Science Paradigm

- Uncertainty Quantification
- Modeling and Simulation
- Experimental Science

PSAAP: Predictive Science Academic Alliance Program

M. Ortiz
Uni-Stuttgart 12/12-5
The Predictive Science Paradigm

Uncertainty Quantification

Modeling and Simulation

Experimental Science
Catech’s Small Particle Hypervelocity Impact Range (SPHIR)

M. Ortiz

Uni-Stuttgart 12/12-7
Hypervelocity Impact Testing

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

PSAAP: Predictive Science Academic Alliance Program

M. Ortiz
Uni-Stuttgart 12/12-8
Hypervelocity Impact Diagnostics

**Diagnostic Technique**

- **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

**Performance Measures**

PSAAP: Predictive Science Academic Alliance Program

M. Ortiz

Uni-Stuttgart 12/12-9
SPHIR — Post Mortem Profilometry

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

\[ V_{bl} = \frac{H_0 (\frac{h}{D_p})^n}{(\cos a)^s} \]

\[ A = \begin{cases} 0, & \text{if } V < V_{bl} \\ K \cdot D_p^2 \cdot \left( \frac{h}{D_p} \right)^p \cdot (\cos a)^u \cdot \tanh \left( \frac{V}{V_{bl}} - 1 \right)^m \end{cases} \]

- \( A = \) perforation area (mm²)
- \( h = \) target thickness (mm)
- \( a = \) impact obliquity (rad)
- \( V = \) impact speed (km/s)
- \( D_p = \) imactor diameter (mm)
- \( H_0, K, n, s, p, u, m \) are curve fit parameters

\[ \Theta = 0 \text{ deg., thickness comparison} \]

440 C Steel spherical projectiles
304 Stainless Steel plate targets
6/6 nylon cylindrical projectiles
6061-T6 aluminum plate targets

M. Ortiz
Uni-Stuttgart 12/12-11
SPHIR – Shadowgraph Data

Nylon 6/6 Impactor
L/D=1 Cylinder

6061-T6 Al. Target

$P_{atm} = 1.0$ Torr

$t = 10.3 \, \mu s$

$h = 3.0 \, \text{mm}$
$v_{\text{impact}} = 5.95 \, \text{km/s}$

$h = 1.5 \, \text{mm}$
$v_{\text{impact}} = 6.00 \, \text{km/s}$

$h = 0.5 \, \text{mm}$
$v_{\text{impact}} = 6.31 \, \text{km/s}$
SPHIR – Debris Front Data

M. Ortiz
Uni-Stuttgart 12/12- 14
SPHIR – Debris Capture Data

**Stack of alternating foam plates and plastic films**

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

**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

M. Ortiz
Uni-Stuttgart 12/12- 15
High Strain-Rate Testing (HSRT)

Stress: \[ \sigma_{eq} = k_1 (1 - k_2 \varepsilon_{eq}^p) \frac{P}{D t} \]

Strain: \[ \varepsilon_{eq}^p = k_3 \frac{d}{h} \]

Shear Compression Specimen (SCS)

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

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

Split Hokinson (Kolsky) pressure bar

Strength Dissipation

Full-field imaging, Sub-grain resolution

M. Ortiz
Uni-Stuttgart 12/12-16
High Strain-Rate Testing (HSRT)

Shear-compression specimen test


M. Ortiz

Uni-Stuttgart 12/12- 17
High Strain-Rate Testing (HSRT)

Impactor at 1 km/s

$t_{\text{up}} > t_{\text{down}}$

steel

Reflected Shock

Mach Disk

Mach Stem

Tantalum Hugoniot

$p$ (GPa)

$U_p$ (km/s)

Al Impactor at 1 km/s

Al Impactor at 2 km/s

Ta Impactor at 1 km/s

Ta Impactor at 2 km/s

M. Ortiz

Uni-Stuttgart 12/12-18

PSAAP: Predictive Science Academic Alliance Program
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

Uncertainty Quantification

Modeling and Simulation

Experimental Science

PSAAP: Predictive Science Academic Alliance Program
Hypervelocity Modeling & Simulation

- 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

M. Ortiz
Uni-Stuttgart 12/12- 21
Optimal-Transportation Meshfree

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

Nodal points: $x_{a,k}$, $x_{p,k}$, $x_{p,k+1}$, $x_{a,k+1}$

PSAAP: Predictive Science Academic Alliance Program

M. Ortiz
Uni-Stuttgart 12/12-22
OTM meshfree spatial discretization

Steel projectile/aluminum plate: Nodal set

M. Ortiz
Uni-Stuttgart 12/12-23
Stein projectile/aluminum plate: Material point set

M. Ortiz

Uni-Stuttgart 12/12-24
Meshfree spatial discretization

nodal points: $x_{a,k}$

material points $x_{p,k}$

$\mathcal{X}_{k \rightarrow k+1}$

Question: How can we reconstruct from nodal coordinates?
Max-ent spatial interpolation

Max-ent shape functions of decreasing entropy

$N_p = \text{local neighborhood of material point } p$
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!
OTM — Seizing contact

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

M. Ortiz
Uni-Stuttgart 12/12-29
OTM – Material-point erosion

• ε-neighborhood construction: Choose \( h << \varepsilon << L \)

• Erode material point if

\[
G_\varepsilon \sim \frac{h^2}{|K_\varepsilon|} \int_{K_\varepsilon} W(\nabla u) \, dx \geq G_C
\]

• Proof of convergence to Griffith fracture:

Schematic of ε-neighborhood construction
Hypervelocity impact - Simulation

Caltech’s hypervelocity Impact facility

Impactor

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

PSAAP: Predictive Science Academic Alliance Program
### Solvers — Massively Parallel OTM

<table>
<thead>
<tr>
<th>Plate thickness</th>
<th>Impact speed</th>
<th>Obliquity</th>
<th>Yaw angle</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.50mm</td>
<td>5.5km/s</td>
<td>0 degree</td>
<td>10 degrees</td>
</tr>
<tr>
<td>1.52mm</td>
<td>5.5km/s</td>
<td>0 degree</td>
<td>15 degrees</td>
</tr>
<tr>
<td>3.04mm</td>
<td>5.5km/s</td>
<td>0 degree</td>
<td>15 degrees</td>
</tr>
</tbody>
</table>

---

PSAAP: Predictive Science Academic Alliance Program

M. Ortiz
Uni-Stuttgart 12/12- 35
The Predictive Science Paradigm

Uncertainty Quantification

Modeling and Simulation

Experimen tal Science

PSAAP: Predictive Science Academic Alliance Program

M. Ortiz

Uni-Stuttgart 12/12-36
Uncertainty Quantification (UQ)

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

$$E_{\mu}[\{f \in A\}] = \int \left\{ \begin{array}{ll} 1, & \text{if } f(x) \in A \\ 0, & \text{if } f(x) \notin A \end{array} \right\} d\mu(x)$$
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 $(\mu, f)$: Data, models...
- Admissible set: $A = \{(\mu, f) \text{ compatible with info}\}$
- Wanted: Optimal probability bounds,

$$\inf_{(\mu, f) \in A} \mathbb{E}_\mu[\{f \in A\}] \leq \sup_{(\mu, f) \in A} \mathbb{E}_\mu[\{f \in A\}]$$
Theorem [Owhadi et al. (2011)] Suppose that

\[ \mathcal{A} = \left\{ (\mu, f) \mid \mathbb{E}_\mu[\varphi_1] \leq 0, \ldots, \mathbb{E}_\mu[\varphi_n] \leq 0 \right\} \]

Let:

\[ \mathcal{A}_{\text{red}} = \left\{ (\mu, f) \in \mathcal{A} \mid \mu = \sum_{i=1}^{n} \alpha_i \delta_{x_i}, \alpha_i \geq 0, \sum_{i=1}^{n} \alpha_i = 1 \right\} \]

Then:

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

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

• OUQ problem is reduced to optimization over finite-dimensional space of measures: Program feasible!
Obliquity = 0°

- **OTM**
- **SPHIR**

![Graph showing perforation area vs. impact speed for different OTM and SPHIR experiments.]

- **Perforation area (mm²)**
- **Impact speed (km/s)**

- **Symbols and Legends**:
  - Circle: Experiment_h = 0.5 mm
  - Square: Experiment_h = 1.5 mm
  - Triangle: Experiment_h = 3.0 mm
  - Open Circle: OTM_h = 0.5 mm
  - Open Square: OTM_h = 1.5 mm
  - Open Triangle: OTM_h = 3.0 mm

---

PSAAP: Predictive Science Academic Alliance Program

M. Ortiz

Uni-Stuttgart 12/12- 41
Obliquity = 0°

Impact speed (km/s) vs Perforation area (mm²)

- Experiment_h = 0.5 mm
- Experiment_h = 1.5 mm
- Experiment_h = 3.0 mm
- OTM_h = 0.5 mm
- OTM_h = 1.5 mm
- OTM_h = 3.0 mm

M. Ortiz
Uni-Stuttgart 12/12- 42
OUQ – Model based protocol

Obliquity = 0°

Impact speed (km/s)

Perforation area (mm²)

Modeling error (δ)

OTM

SPHIR

Experiment_h = 0.5 mm
Experiment_h = 1.5 mm
Experiment_h = 3.0 mm
OTM_h = 0.5 mm
OTM_h = 1.5 mm
OTM_h = 3.0 mm
Hypervelocity — Model-based OUQ

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

- Output: \( y \equiv \text{perforation area} \)

- Admissible set:
  \[
  A \equiv \left\{ (f, \mu) : \frac{d(f, f_{\text{OTM}})}{\mu} \leq \delta \right\}
  \quad \mu = \mu_1 \otimes \mu_2 \otimes \mu_3
  \]

- Reduced admissible set:
  \[
  A_{\text{red}} \equiv \left\{ (f, \mu) : \frac{d(f, f_{\text{OTM}})}{\mu} \leq \delta, \quad \mu = \mu_1 \otimes \mu_2 \otimes \mu_3, \quad \mu_i = \alpha_i \delta_{a_i} + (1 - \alpha_i) \delta_{b_i}, \quad i = 1, 2, 3 \right\}
  \]

Caltech's SPHIR facility

M. Ortiz
Uni-Stuttgart 12/12- 44
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 ~1 million 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
Uni-Stuttgart 12/12- 45
Hypervelocity — Model-based OUQ

OUQ analysis of hypervelocity impact

Optimal upper bound on $P[A < A_{\min}]$

Perforation Area

Data

Model

$(h, v)$

Modeling error (mm²)

$\delta = 1.0$

$\delta = 1.5$

$\delta = 2.0$

$\delta = 2.5$

Perforation area threshold $A_{\min}$ (mm²)
• 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…
• These drivers (‘fullphysics, uncertainty quantification) place increasing demands on computing power: Exascale Computing!
Outlook for Exascale Computing

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

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

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…

A Walk through CSE evolution

Compute fast, big...
Must have physics...
Must validate...
Odds?

Exascale computing

circa 1993
circa 1998
circa 2003
circa 2007
Concluding remarks...

Thank you!

PSAAP: Predictive Science Academic Alliance Program

M. Ortiz
Uni-Stuttgart 12/12- 51