Research and Future Directions for Simulating Extreme Events
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Justine Johannes
Engineering Sciences Center, Director
Sandia National Laboratories
jejohan@sandia.gov
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Sandia’s unique core mission has shaped the institution and it’s capabilities

Always / Never

“Always” refers to the reliability that we require for effective nuclear deterrence. Deterrence works because we know that if the President were to call on our nuclear arsenal, those weapons would function as designed. And our adversaries know it. “

“Never” refers to the dire consequences of failure. Think about the incredible power of nuclear weapons, and you realize that you absolutely cannot accept potential nuclear yield in an accident or terrorist event.
“Always / Never” construct has enabled tools relevant to extreme event studies

Sierra Mechanics – SNL core engineering mechanics code family

Computational Simulation Capabilities

CTH Shock Physics Code

Diagnostic and physics model development

Impact Velocity = 0.315 km/s

Large scale model validation and event simulation

Workflow supporting analysis

CAD Model

Mesh

Time

Distance

Computational Simulation Capabilities

Sierra Mechanics – SNL core engineering mechanics code family
Sandia has been called upon to support investigations of national importance

- **USS Iowa Investigation** (April 19, 1989)
- TWA Flight 800 Accident Investigation (July 1997)
- Post 9/11 Vulnerability Studies (Nov 11, 2001)
- **Columbia Space Shuttle Accident** (February 4, 2003)
- **I-35W bridge collapse in Minneapolis** (August 1, 2007)
- BP Deepwater Horizon Oil Spill Accident (Sept 8, 2010)
- Aircraft Vulnerability (Jan 11, 2013)
- **Traumatic Brain Injury** (on-going)
USS Iowa accident investigation

- Training accident occurred in 2nd turret, 47 sailors were killed.

- The Navy concluded that Clayton Hartwig intentionally placed an incendiary device between two propellant bags to kill himself.

- Sandia was chosen by Congress to conduct independent investigation.
Sandia pulled from a broad set of capabilities (thermal, fluid, chemical, and structural) for investigation

- Forensic evidence combined with the Sandia analyses led to the conclusion that the explosion was an accident
- Sandia presented their results to the Navy Sea System command:
  - The next day the Chief of Naval Operations retired
  - The Navy formally apologized to the family of Clayton Hartwig and the families of the deceased sailors

Computational and experimental results caused initial naval results to be reconsidered
Columbia accident investigation

SNL created database of expected sensor output as a function of impact severity, used by NASA on subsequent flights

SwRI test demonstrated foam impact was probable cause of Columbia accident

Use smooth particle hydrodynamic model of foam, hex model in Pronto 3D of RCC wing leading edge panels

Sandia Simulation

Experimental Validation, SwRI
I-35 Minneapolis bridge collapse

As the capacity was exceeded, a plastic hinge formed in the gusset plate and subsequent tearing from rivet line resulted in bridge failure.
Traumatic brain injury (TBI) studies

Differentiating Capability - Digital Head-Neck Models

Motivation
- Understand blast exposure leading to TBI
- Injury investigation
- Helmet design & assessment

POCs: Paul A. Taylor, PI (pataylo@sandia.gov), Douglas A. Dederman, PM (dadeder@sandia.gov)
Research activities and future directions

Increasing the physics understanding
- Material model development
- Experimental diagnostics and test

Improving computational methods
- Multi scale materials modeling
- Coupled multi-physics approaches
- Marker methods and multi-field techniques

Creative problem solving
- Automated geometry “as-built”
- Automated ensemble calculations

Next generation computing platforms
Developing and utilizing improved physics models

Developing and utilizing physics models for non-ideal explosives offers challenges.

- Advanced scientific computing
  - Mesoscale analysis (movie)
  - Molecular Dynamics
- Novel diagnostics needed
- Advanced reactive models development

CTH simulation

Time = 0.000 μs
Advancing diagnostics and experimental methods

Kolsky bar activities for high-rate compression, tension, and torsion experiments on materials at room and high temperatures

ORVIS diagnostic to gain statistics of material shock behavior in space and time

Explosive Powder Bed (Potassium Chlorate and Powdered Sugar)

POC: Dr. Marcia A. Cooper (macoope@sandia.gov)

POC: Dr. Bo Song
Homogenization may filter physics necessary to predict failure. To predict reliability with true Uncertainty Quantification, we must locally enrich physics by incorporating the microstructure. The stress field resulting from homogenization theory can miss potential fracture initiation locations.

To predict reliability with true Uncertainty Quantification, we must locally enrich physics by incorporating the microstructure.

POC: Joe Bishop
Computational techniques for coupled, multi-physics

- Air and Fluid Shock
- Reacting Flow-Thermal-Structure
- Pervasive material and structural failure
- High Mach Fluid-structure-interaction

- Underwater blast on Structure
- Fire-Structural Collapse
- Captive Carry Fluid Structure Interaction
- Blast-on-Structures
- Rocket Motor propellant-structure Interaction
- Reacting flows-structural response
Computational methods advancement

Material Point Method with Multi-Field

- Lagrangian material points are moved through a Eulerian background mesh
- Being investigated as a way to better simulate impact and penetration
- Improved handling of history-dependent constitutive models versus Eulerian methods
- Does not require re-meshing as in standard Lagrangian FEM
- Separate field velocities for different materials being implemented into CTH
- Implicit Continuous-fluid Eulerian method to address time scale issues

Fun Fact: As a result of a joint effort between UCLA’s mathematics department and Walt Disney Animation Studios, MPM was successfully used to simulate snow in the film Frozen

(SNL-LANL and Joint SNL and DoD collaborations contribute to capability)
Work flow coupled with high performance computing - unprecedented exploration of design space

Challenges and Opportunities

• Ensemble analysis requires new toolsets designed for an unprecedented scale of parallel data analysis
• A novel approach using web servers is allowing users to access metadata and graphics with unprecedented speed
• Feature recognition, data mining, and user feedback are essential for understanding ensembles of runs

Approach

Describe Designs of Interest

Sampling the Design Space

Measure Quantities of Interest (QOIs)

Fix limits of design space

Noisy Sampling?

Yes

No

Determine “Good” Runs (Expert feedback)

Determine local optima

QOI 1

Tip Velocity
7.1  2.7  2.8
2.1  4.7  4.2
3.5  2.2  5.0

QOI 2

Target Penetration
2.3  0.2  6.0
3.4  2.5  1.6
5.6  1.7  0.5

Impact

Base Line Design

Final Design
• 2X Performance
• 50% Less Mass
• Less Collateral Damage

POC: Steve Attaway, John Korbin
Integration with computed tomography for rapid as-built analysis – creative problem solving

Opportunity

- Tomography has been advancing rapidly
- Emerging high performance computing capabilities allow precise geometric detail when required.
- Parallel processing along with novel sensor technologies are driving a revolution in x-ray scanning
- Incorporation of new technologies into our numerical analysis capabilities

POC: Steve Attaway, John Korbin
Next generation computing

Challenges:
- Many-core or Accelerators?
- Memory layout?
- Memory speed?
- I/O for very large data?
- Data movement?
- Resiliency?
- Power?

Opportunities:
- Software needs to change to keep up
- Can we do the same amount of work faster in smaller packages
- Can we do more of the same type of work better, e.g., insert UQ
- Can we enable more predictive simulations with multi-scale and multi-physics

Blast on Structure Simulation
LANL Cielo 32-64k Cores
The challenges and opportunities are abundant!

- Increased knowledge of the driving physics
- Improving the computational approaches and diagnostic capabilities
- Novel problem solving
- Preparing for next generation computing platforms