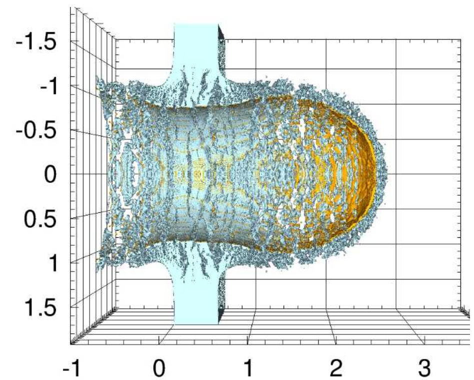
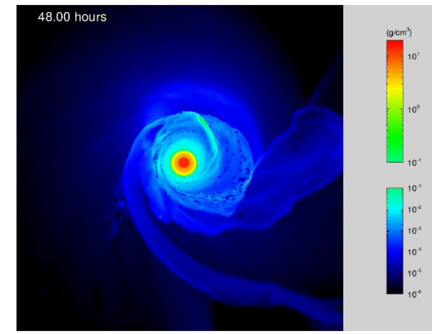
Exceptional service in the national interest

Sandia National Laboratories





Research and Future Directions for Simulating Extreme Events

UCSD Center for Extreme Events Research Kickoff Meeting

February 9, 2015

Justine Johannes

Director of Engineering Sciences Center

Sandia National Laboratories

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Acknowledgements – it takes a village

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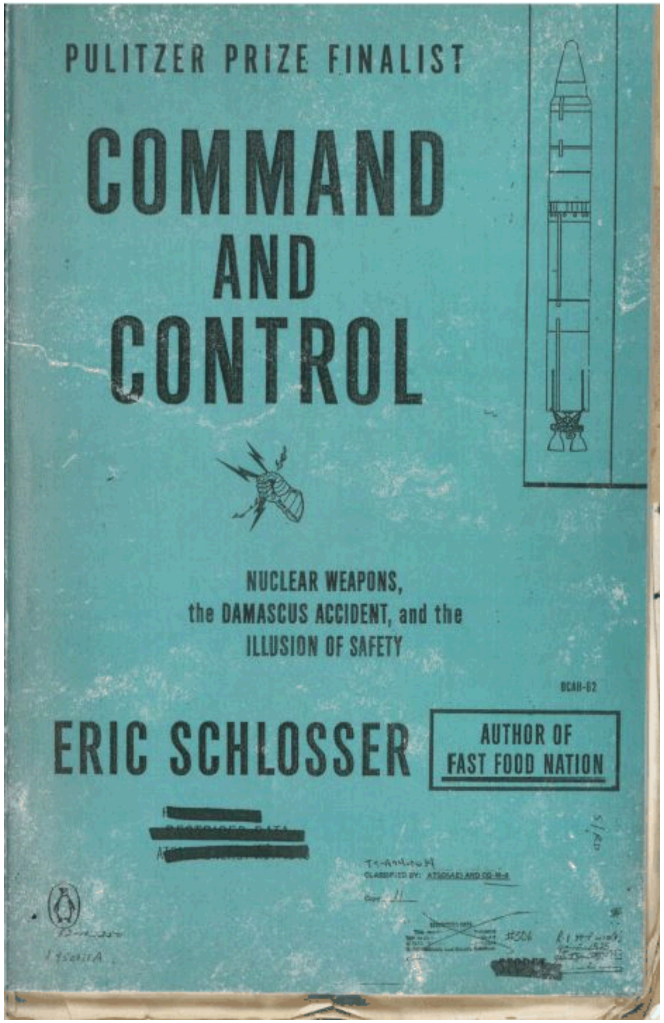
Sandia's mission require expertise in the response to extreme environments

Sandia National Laboratories

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.



Core expertise is called upon to support investigations of National importance

Sandia National Laboratories

- *USS Iowa Investigation (April 19, 1989)*
- Post 9/11 Vulnerability Studies (Nov 11, 2001)
- *Columbia Space Shuttle Accident (Jan. 16, 2003)*
- *I-35W bridge collapse in Minneapolis (August 1, 2007)*
- BP Deepwater Horizon Oil Spill Accident (Sept 8, 2010)
- Aircraft Safety Analyses (Jan 11, 2013)
- *Traumatic Brain Injury (on-going)*

Sandia's mission has created unique capabilities and expertise that allow understanding of extreme events.

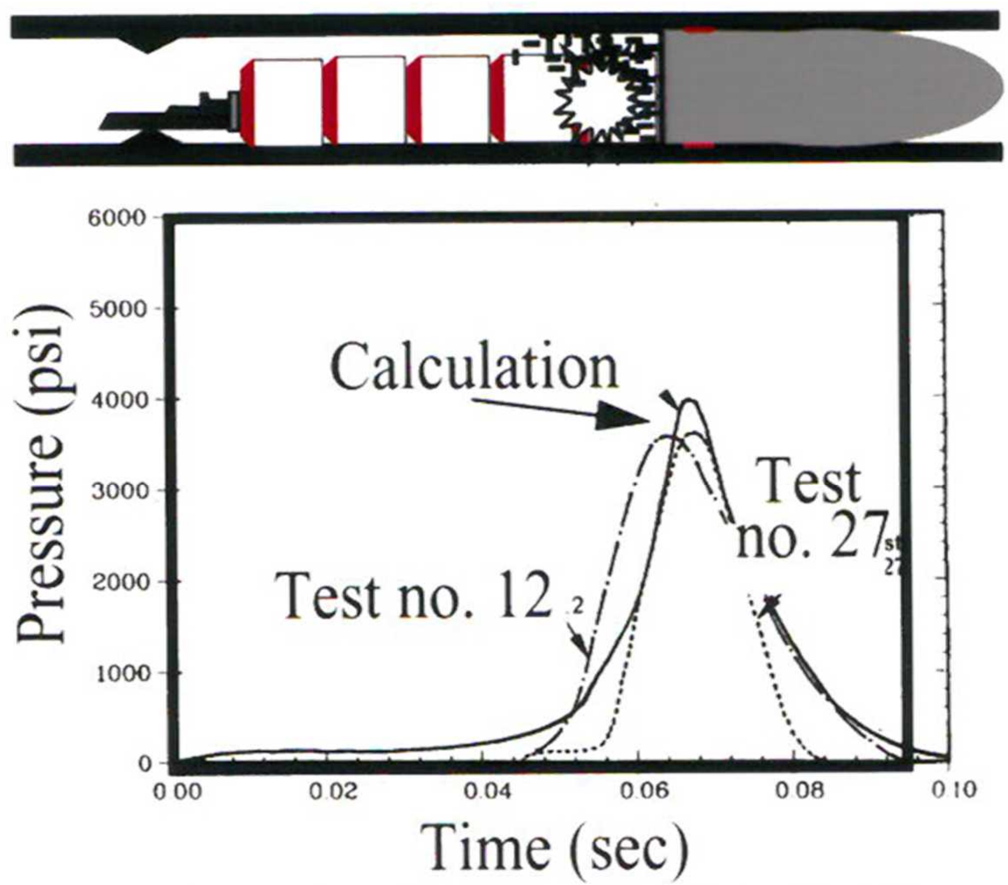
Sandia expertise were requested to support the USS Iowa accident investigation

- Training accident occurred in 2^{nd} turret on April 19, 1989, 47 sailors were killed in the blast and fire.
- The Naval Investigation Service concluded that Clayton Hartwig intentionally placed an incendiary device between two propellant bags to kill himself
- Sandia National Laboratories was chosen by Congress to conduct independent investigation.

Computational and experimental tools were required to adequately resolve the cause of accident

Sandia conducted a variety of analyses: thermal, fluid, structural, combustion, chemical, and structural

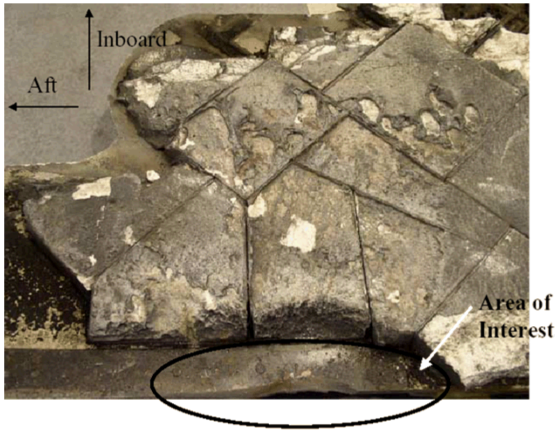
- **Results of forensic evidence combined with the Sandia analyses led to the conclusion that the explosion an accident**
- **Sandia presented their results to the Navy Sea System command:**
  - **The next day the Chief of Naval Operations retired**
  - **The Navy formally apologized to the family of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



Interior Ballistics Analysis

Computational and experimental capabilities provided confidence for a different decision

The Columbia Orbiter broke up at ~9AM CST on Saturday, February 4 at ~230Kft Altitude



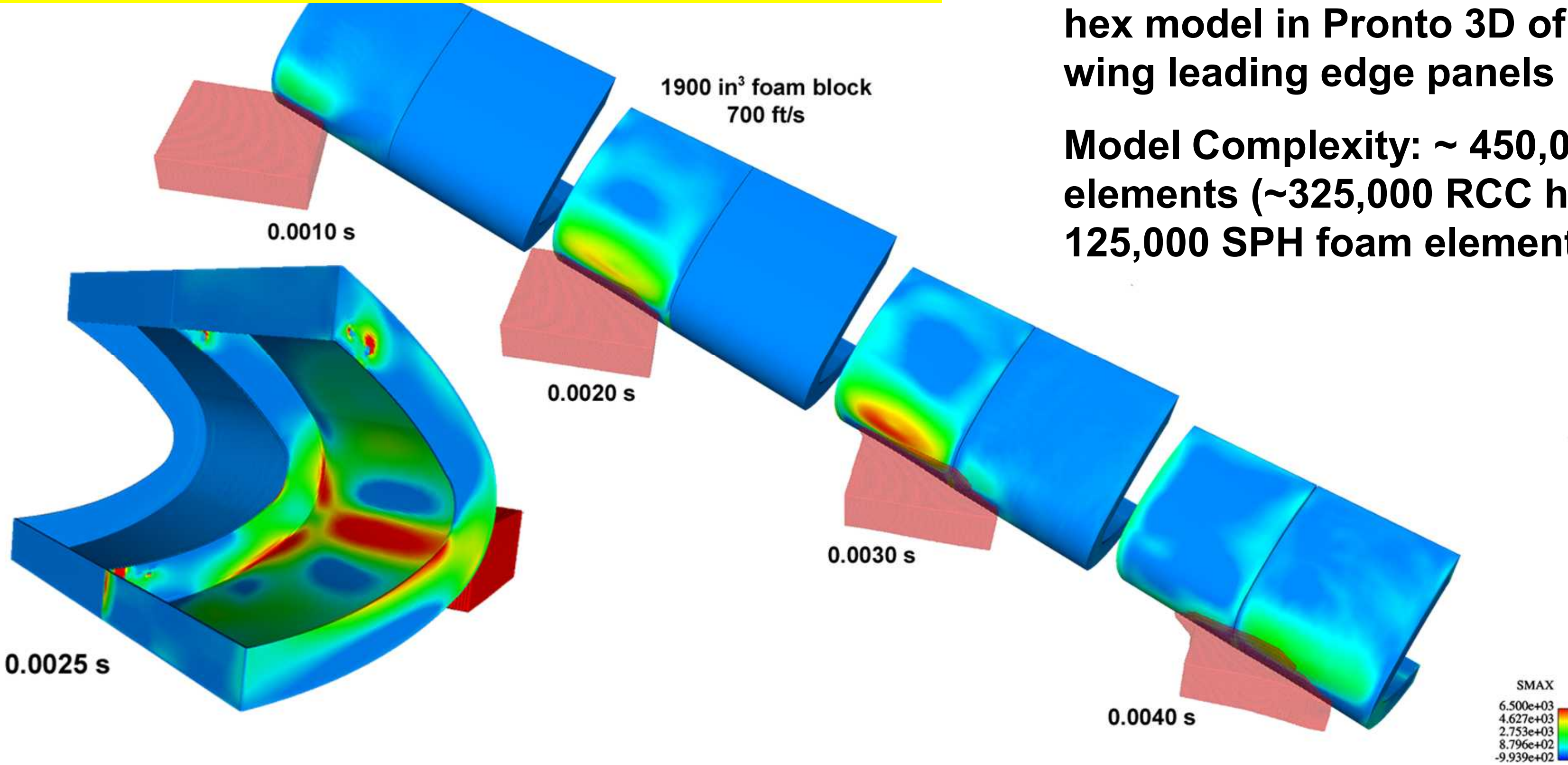
From the gathered debris (shown at KSFC) early scenarios of the cause were being developed by NASA

Sandia analyses concluded that foam impact could cause Reinforced Carbon-Carbon panel damage

SwRI Test of July 11 demonstrated foam impact was the probable cause of the Columbia Accident

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

Model Complexity: ~ 450,000 elements (~325,000 RCC hex, 125,000 SPH foam elements);

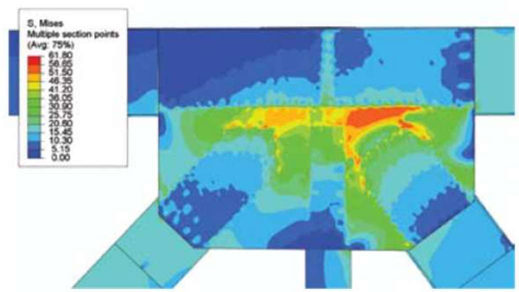


SNL created database of expected sensor output as a function of impact severity , used by NASA on subsequent flights

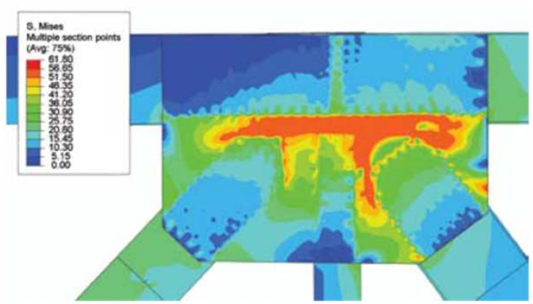
I-35 Minneapolis bridge collapse Accident Details, August 1, 2007

- During rush hour the 8-lane westbound portion of I-35 bridge over the Mississippi collapsed in Minneapolis.
- 13 people died, 34 seriously injured, and 111 minor injuries – construction on the bridge limited the traffic, ironically triggering and controlling fatalities.

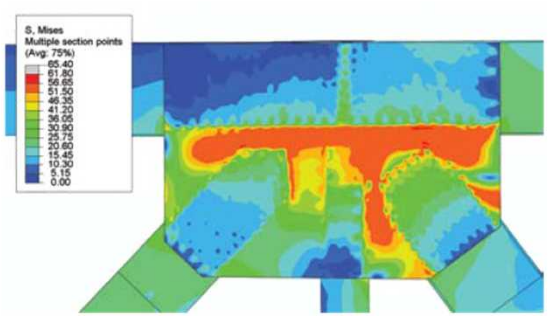
Sandia analysts provided the insight to explain the analysis and forensic evidence



Stress at bridge opening, 1967



Stress in joint after 1977 and 1998 renovations



Stress in joint Aug, 2007 at time of collapse

Collapse was a geometrically induced failure: As the capacity was exceeded, a plastic hinge formed in the gusset plate and subsequent tearing from rivet line resulted in bridge failure

Familiarity with large-deformation failure of structures was critical to understanding what had transpired

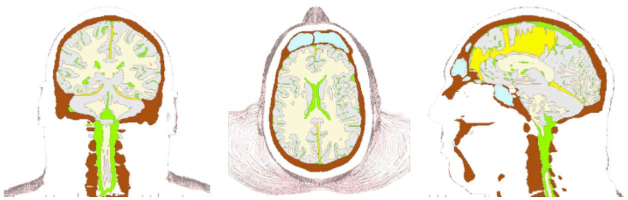
Stress in critical bridge gusset plate

Computer Simulation of Blast Exposure leading to Traumatic Brain Injury (TBI)

Sandia National Laboratories

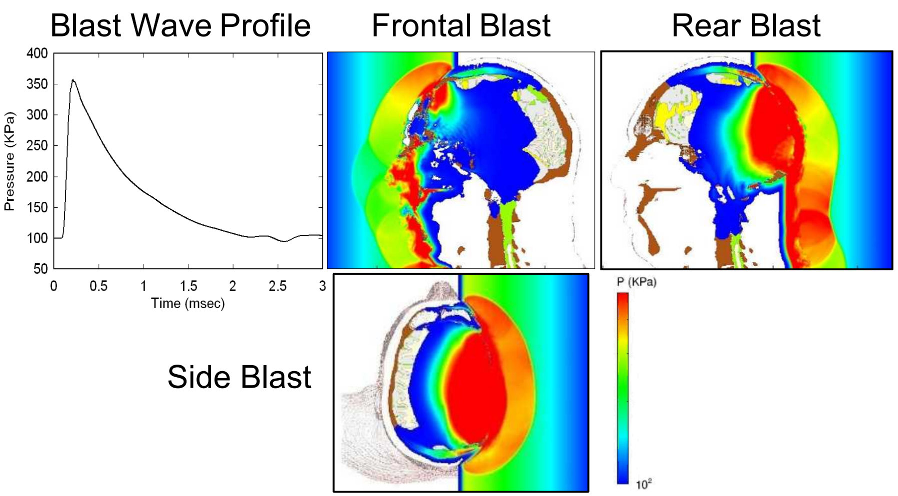
Motivation

- Warfighter Personal Protective Equipment (PPE) development is principally based on laboratory/field testing of prototype designs
- Need high-fidelity computer modeling & simulation tools to:
  - Understand blast exposure leading to TBI
  - Injury investigation
  - Helmet design assessment



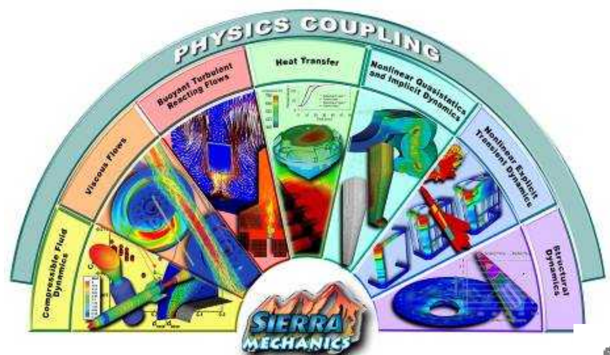
Differentiating Capability - Digital Head-Neck Models

- Anatomically correct distributions of soft tissue & bone at 1mm resolution
- Represented by advanced constitutive models
- Utilization of computational tools



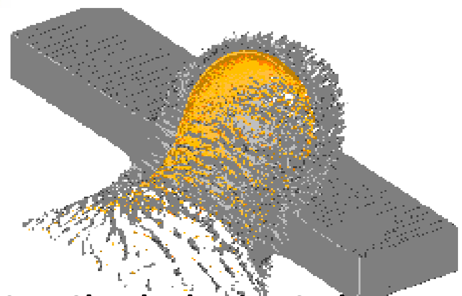
POCs: Paul A. Taylor, PI (pataylo@sandia.gov)
Douglas A. Dederman, PM (dadeder@sandia.gov)

Capability Base for Extreme Event Studies are Derived from Core Mission and Enable Rapid Response

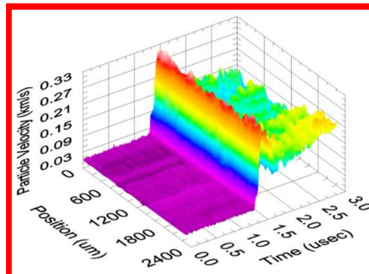


Sierra Mechanics – SNL core engineering mechanics code family

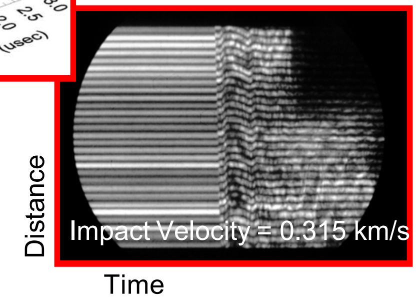
Computational Simulation Capabilities

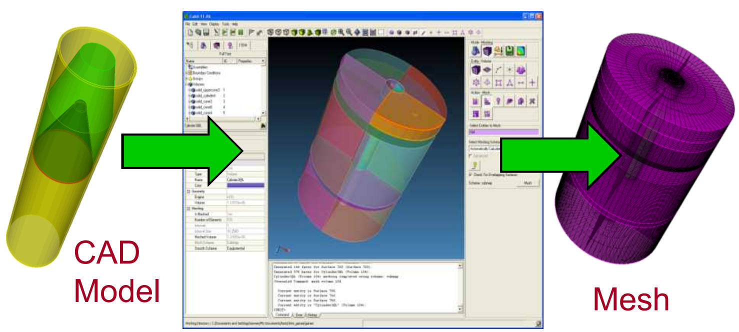


CTH Shock Physics Code



Diagnostic and material model development





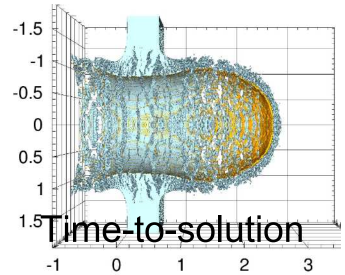
Workflow supporting analysis

Large scale model validation and event simulation

Research Activities and Future Directions
Some places where Sandia is investing

Increasing the Physics Understanding - Predictivity

- Material Model Development - Non-Ideal Explosives
- Multi scale materials modeling
- Experimental Diagnostics



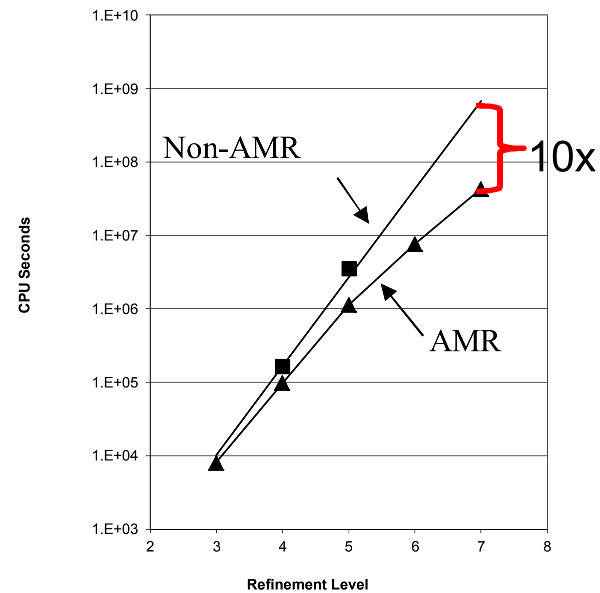
General Structural Failure

Improving Computational Methods

- Coupled multi-physics approaches
- Computational Methods - Marker Methods and Multi-techniques

Creating Solutions – time to solution, depth of solution

- Automated geometry from CT scans of as-built
- Automated ensemble calculations

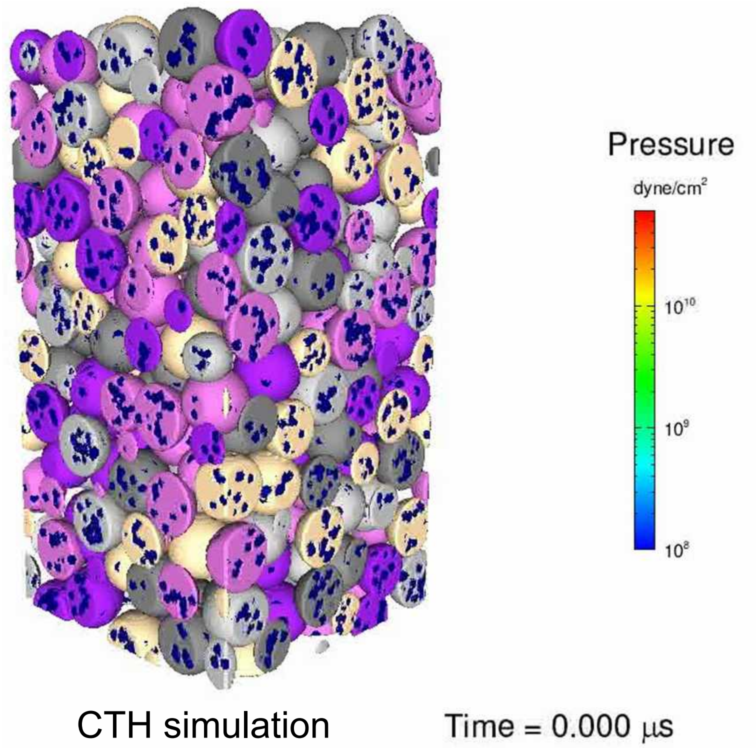


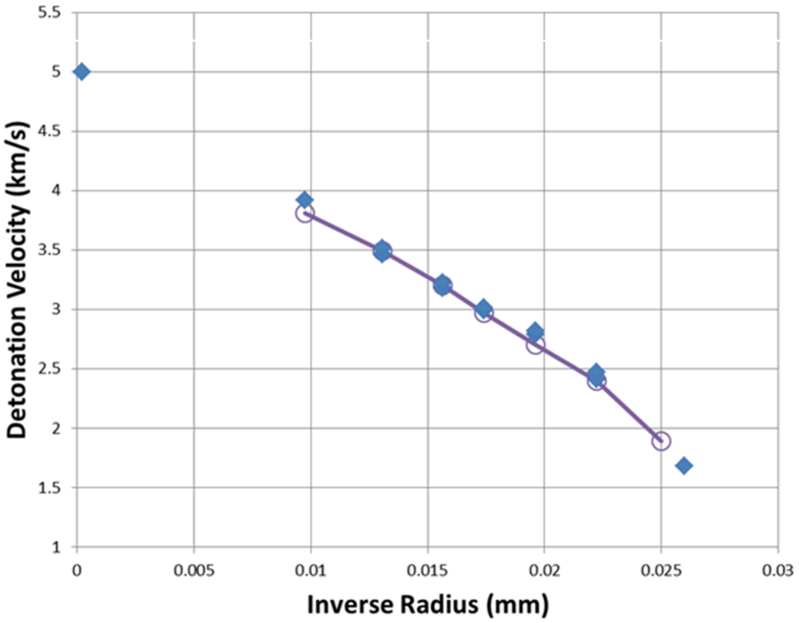
Next Generation computing platforms

Developing and Utilizing Improved Physics models Often an Opportunity for Model Predictivity

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

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

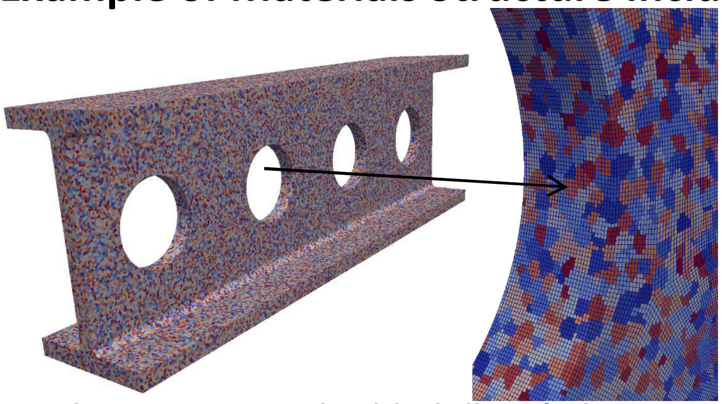




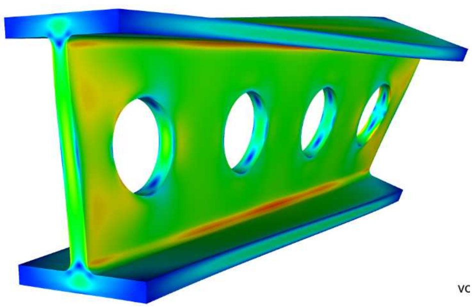
Material-Structural, Multiscale Modeling Approaches

(Material fracture & Structural failure are inherently linked through multi-scale issues)

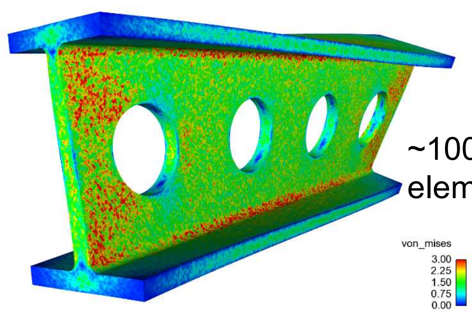
Example of Materials Structure Inclusion



grain structure embedded directly in structure



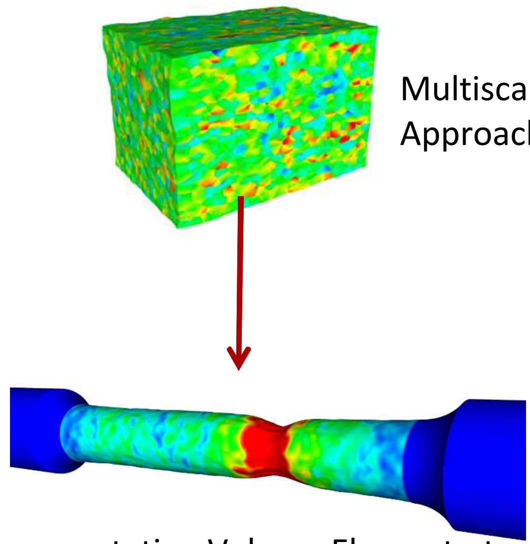
Stress field using homogenized properties.



~100M elements

Grain Scale Direct Numerical Simulations are becoming feasible for research

Multiscale techniques must keep Advancing



Multiscale FE^2 Approach

Structure

Representative Volume Element at Material integration points

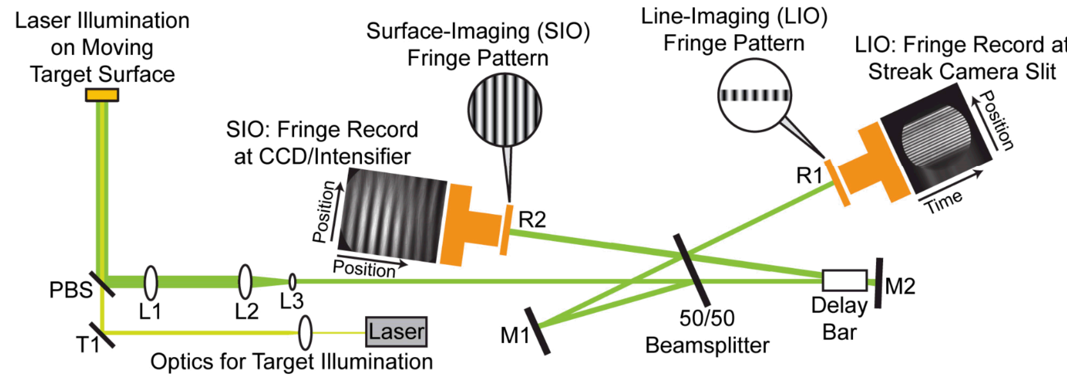
Many Opportunities for Advancement:

- **Concurrent Multiscale models?**
- **Atomistics informed multiscale?**
- **Other approaches….**

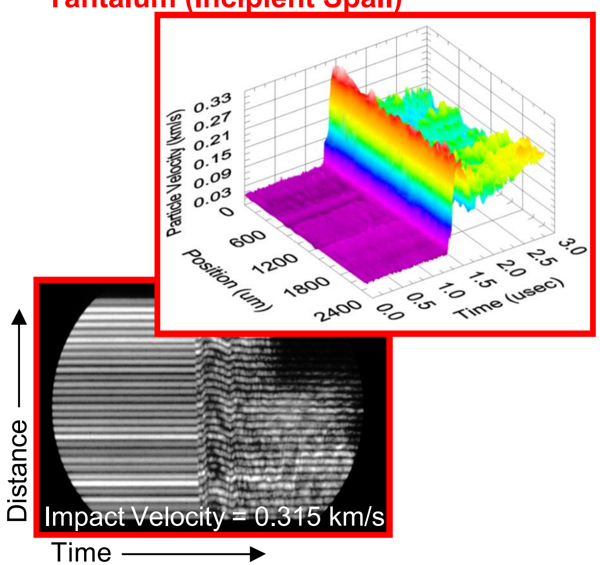
Advancing Diagnostics for Physics Model Development and Model Validation

Sandia has been developing ORVIS diagnostic to gain statistics of material shock behavior quantified in space and time

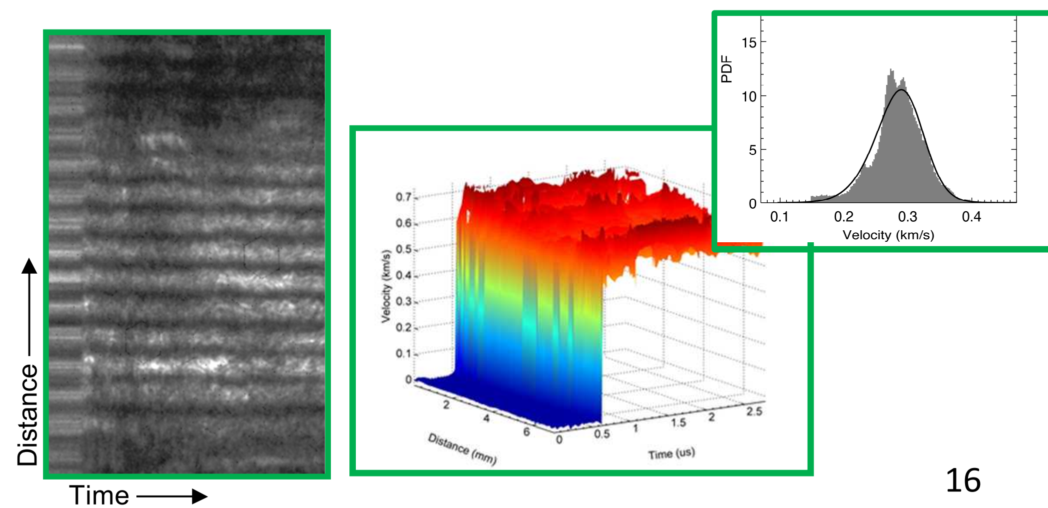
Optically Recording Velocity Interferometer System infers surface velocity from changes in interference fringe phase



Tantalum (Incipient Spall)



Explosive Powder Bed (Potassium Chlorate and Powdered Sugar)



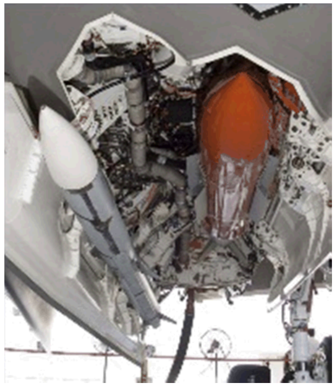
POC: Dr. Marcia A. Cooper (macoope@sandia.gov)

Computational Techniques for Coupled, Multi-Physics

An area of focus for predicting complex Sandia

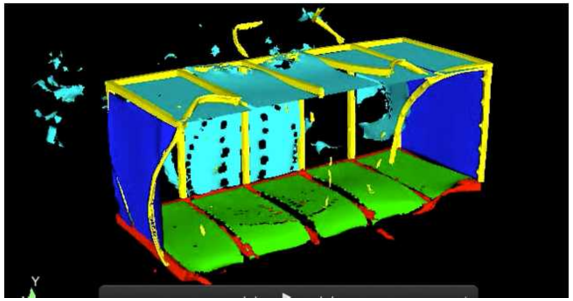
- **Air and Fluid Shock**
- **Reacting Flow-Thermal-Structure**
- **Pervasive material and structural failure**
- **High Mach Fluid-structure-interaction**

Underwater blast on Structure

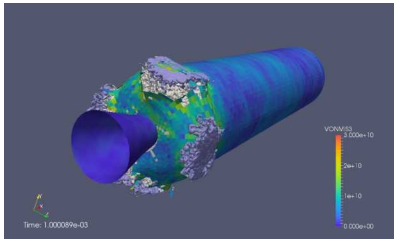


Captive Carry Fluid Structure Interaction

Fire-Structural Collapse



Blast-on-Structures



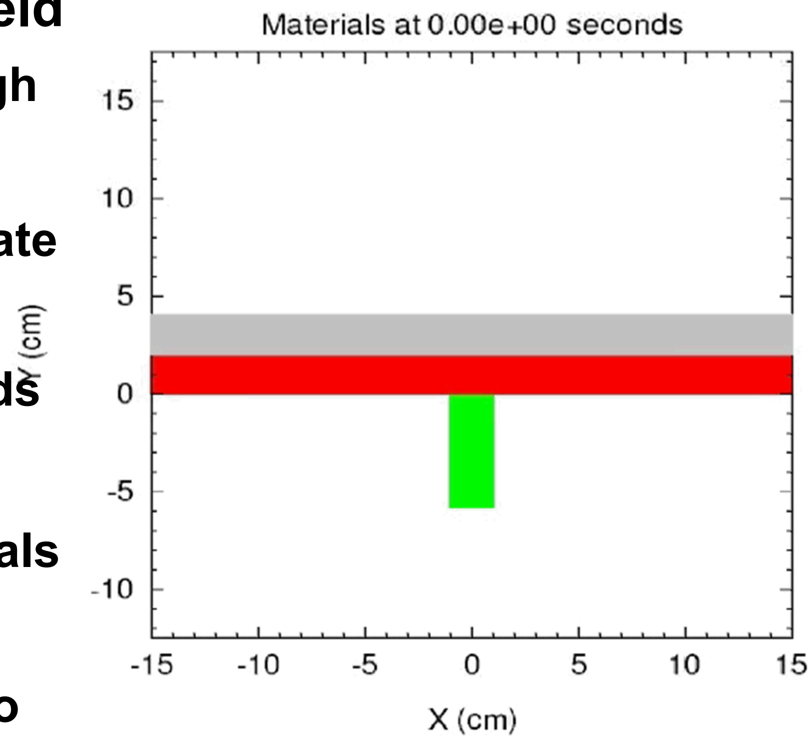
Rocket Motor propellant-structure Interaction

Reacting flows-structural response

Computational Methods Advancement Offers Opportunity for Collaboration

Material Point Method (MPM) with Multi-Field

- Lagragian material points are moved through a Eulerian background mesh
  - CTH is used as the 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
  - Allows for material separation
- Implicit Continuous-fluid Eulerian method to address time scale issues



Projectile passing through steel and aluminum using Multifield and Markers.

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 2013 computer-animated film Frozen

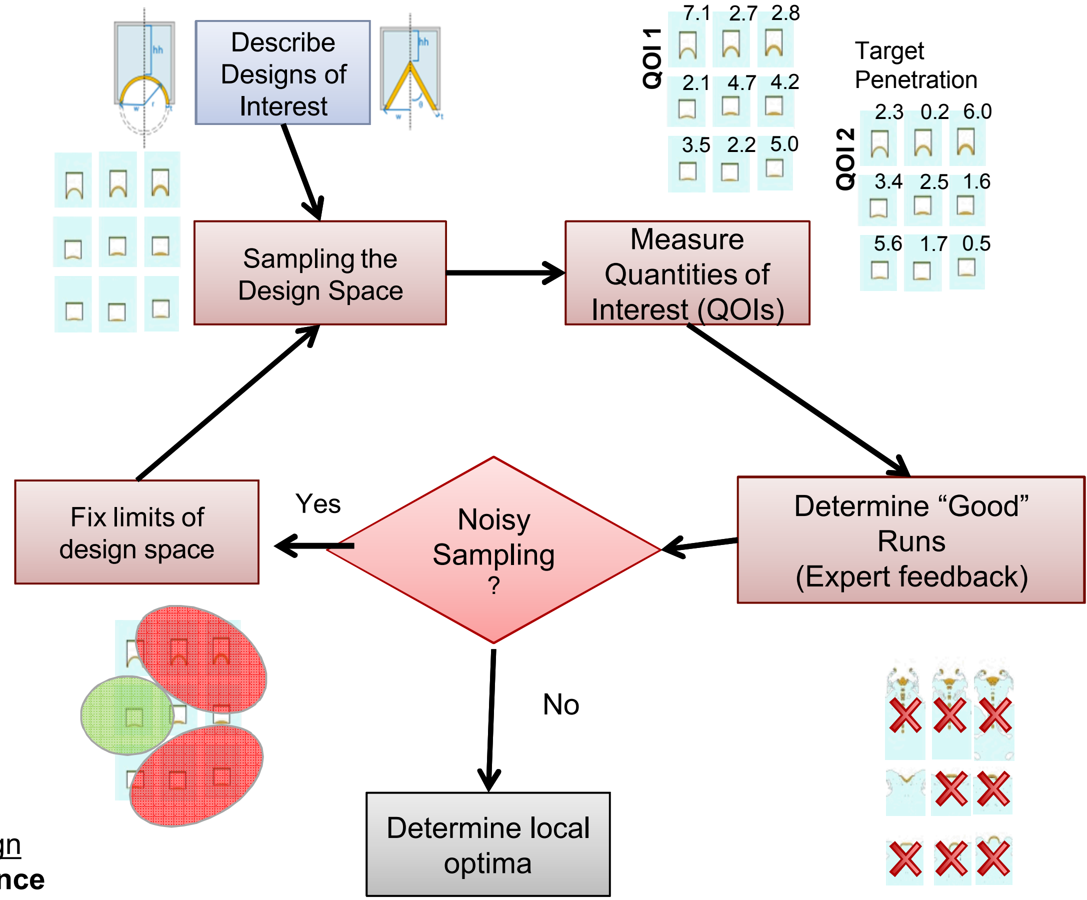
(SNL-LANL and Joint SNL and DoD collaborations contribute to capability)

Work Flow Coupled with High Performance Computing Can Allow Unprecedented Exploration of Design Space

Challenges and Opportunities

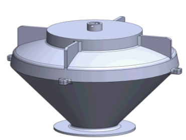
- Ensemble analysis requires new toolsets designed for an unprecedented scale of parallel data analysis
- A novel approach using web servers is allowing users to access metadata and graphics with unprecedented speed
- Feature recognition, data mining, and user feedback are essential for understanding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

Approach



Impact

Base Line Design



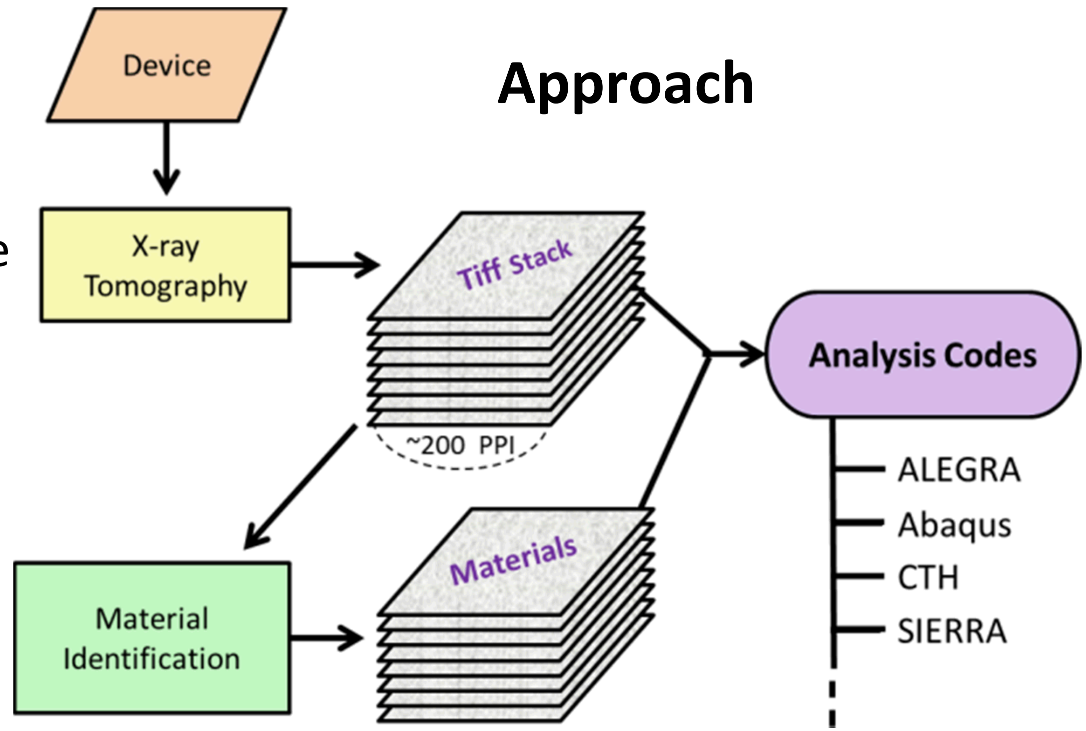
Final Design
- 2X Performance
- 50% Less Mass
- Less Collateral Damage

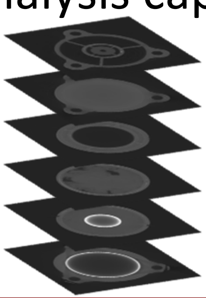
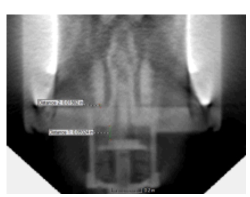
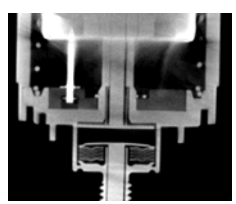
Integration with Computed Tomography for Rapid As-Built Analysis – Creative Problem Solving for the

Opportunity

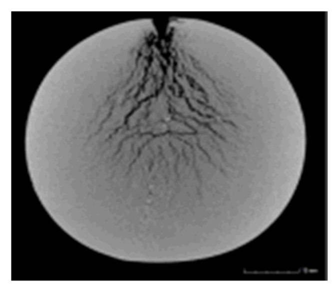
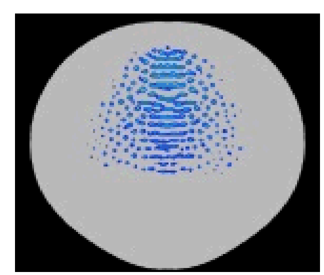
- Tomography has been advancing at an incredible rate
- Emerging high performance computing capabilities allow precise geometric detail when required.
- Parallel processing along with novel sensor technologies are driving a revolution in x-ray scanning
- We have the opportunity to shape the integration of these new technologies into our numerical analysis capabilities

Approach



A Shaped charge
Tiff Stack

Void Nucleation and Growth

High Performance Computing is facing a new disruption in technology - We've been here before

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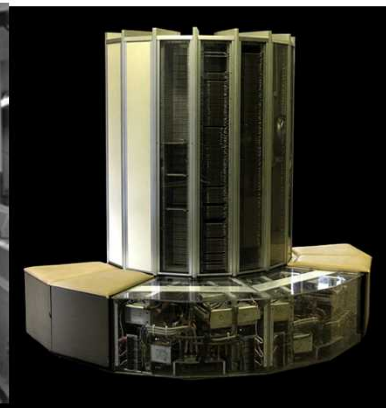
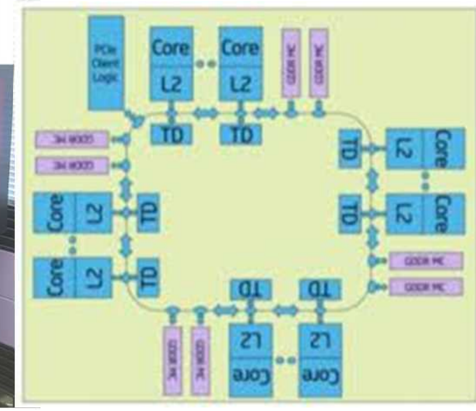




Mainframes
60's to 70's

Vector Supercomputers
70's to early 90's

Massively parallel systems
1990's to 2010

Multilevel, heterogeneous, energy and memory constrained

ROOM → MACHINE → CABINET → CHIP

COMPLEXITY

Technology disruptions require a significant increase in reengineering of our codes

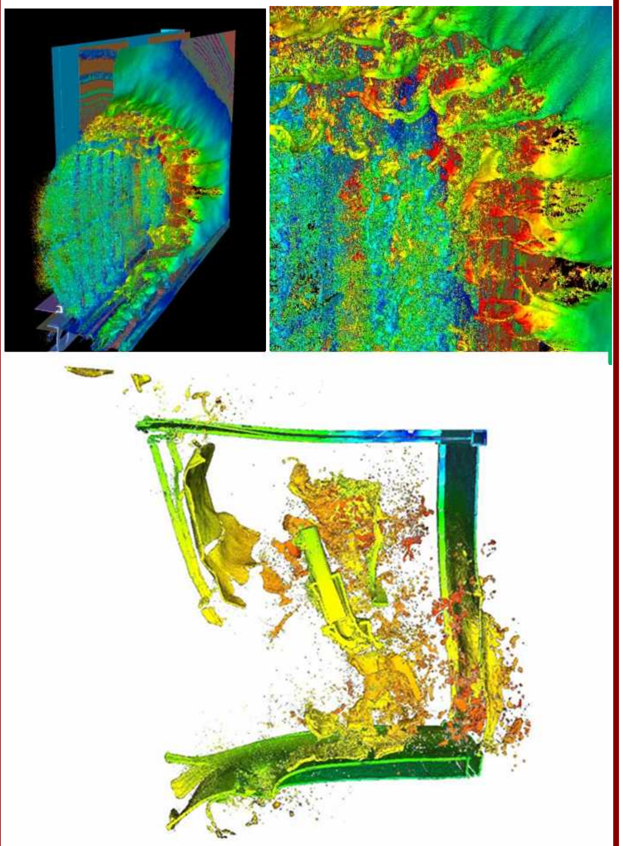
Next Generation Computing Brings good challenges and opportunities

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 techniques**
- **Preparing for next generation computing platforms!**

What does this all mean?

Sandia National Laboratories

Lot's of Questions:

- **Many-core or Accelerators?**
- **Memory layout?**
- **Memory speed?**
- **I/O?**
- **Data movement?**
- **Resiliency?**
- **Power?**

Dramatic Changes even without getting to Exascale

- **GPGPUs (General Purpose Graphics Processors)**
- **Xenon Phi (Intel MIC)**
- **AMD Fusion (Blend of FPU with CPUs)**
- **Low power ARM (Low power processors)**
- **Whatever else is cooking in the labs…**

Implications:

- Continued computing performance increases, but significantly different than in the past
- Software needs to change to keep up
- Can do the same amount of work faster in smaller packages
- Can do more of the same type of work better, e.g, insert UQ
- Can do much more work, e.g, enable more predictive simulations with Multi-scale and Multi-physics

CTH - Time to Solution capabilities allows problems to be solved in a timely manner

Problem Setup

DIATOM – Extensive Geometry Primitives; External Solid Geometries Supported (STLs, Exodus, etc)
Geometry inserted into mesh at run time therefor doesn't require meshed objects (like FE)

Trivial to Refine

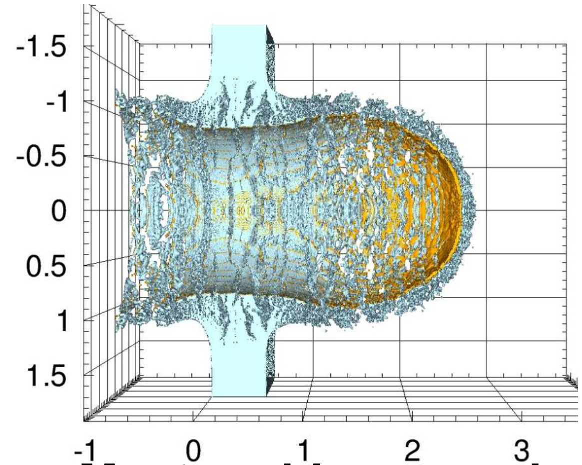
Flat Mesh – 3 line change in input deck
AMR - 1 line change in input deck

Excellent Performance

Massively parallel
Favorable scaling through 1M cores
AMR - Large performance gains

Inline Graphics

Spymaster – on-the-fly graphics allows images to be generated as the calculation runs



Most problems can be set-up in a couple of hours!

Deepwater Horizons Production Platform

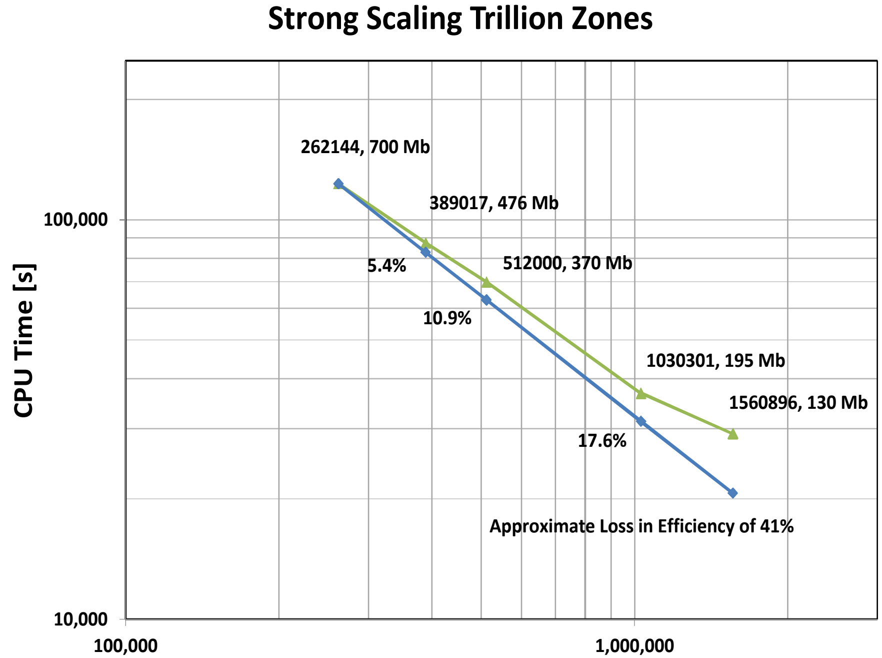
The BP Macondo Well experienced a blow-out, allowing oil and gas to rise uncontrolled up to the platform

- The explosion on the surface rig caused the death of 11 people, with subsequent loss of the control of the floating platform, which sank 36 hours later.
- DOE science team dispatched to help BP with national laboratory expertise
- Sandia was asked to provide and understanding the state of strain in the pipe from these events and figure out how many pipes were inside the riser from the external shape

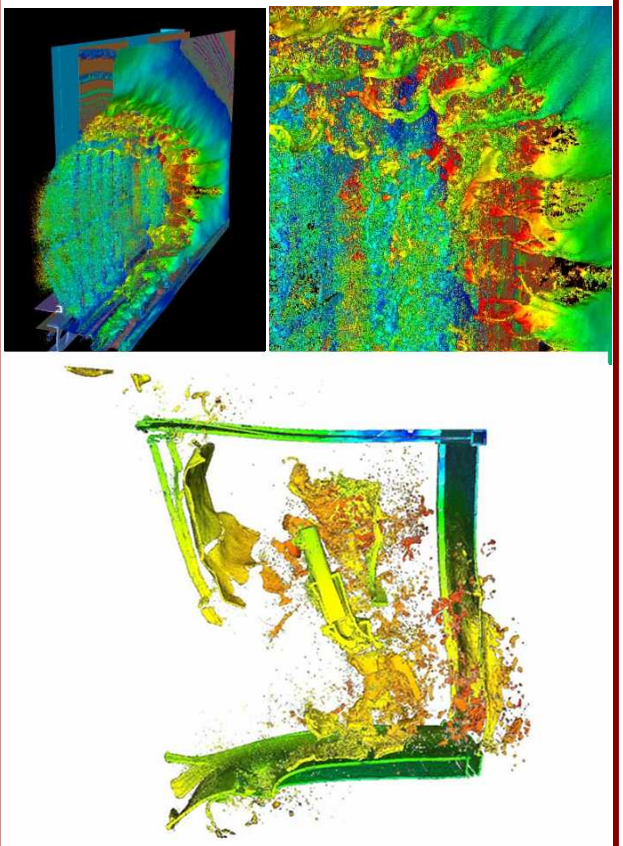
Analysis Conclusions: Internal pressure had to have been present during bend-over of pipe. *The tenuous state of the well head piping proved to be the most important finding* – which hastened attempts to remove the well head and abandon oil 'catching' options. The new well head allowed the flow to be stopped in a controlled manner, and allow subsequent permanent cementing of the well.

CTH is Well Positioned to Adapt to Evolving Architectures and Next Generation Computing Platforms

CTH Scaling on LLNL Sequoia



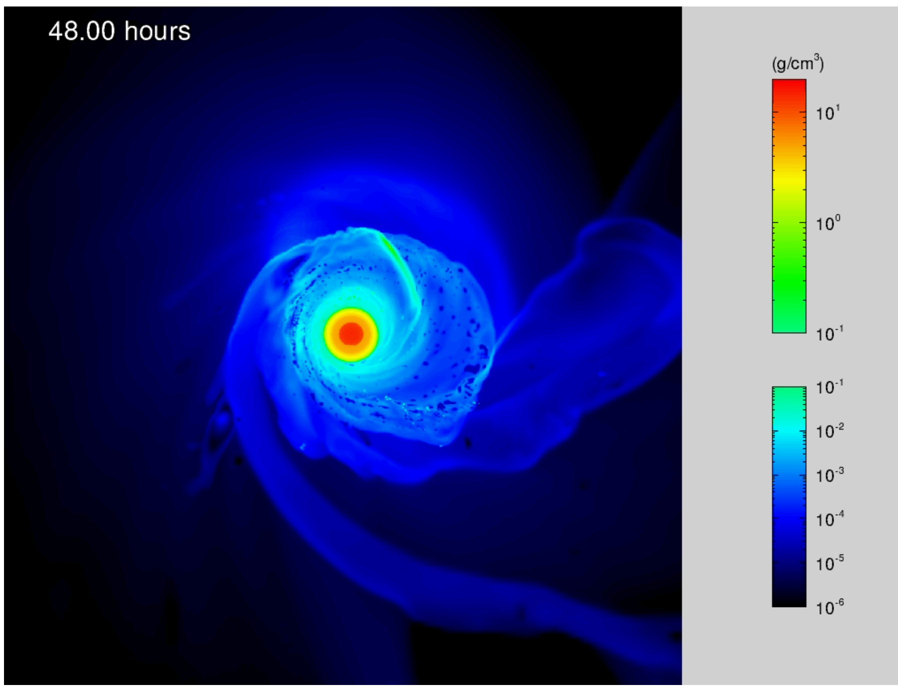
- Core principles: local data, scalable algorithms, vectorizable loops
- Currently addressing: Multi-threading (OpenMP & OpenACC), memory footprint, improved vectorization. Using advanced diagnostic utilities to identify inefficiencies within CTH on specific architectures. Hardware we are focusing on are NGP platforms Trinity and Sierra

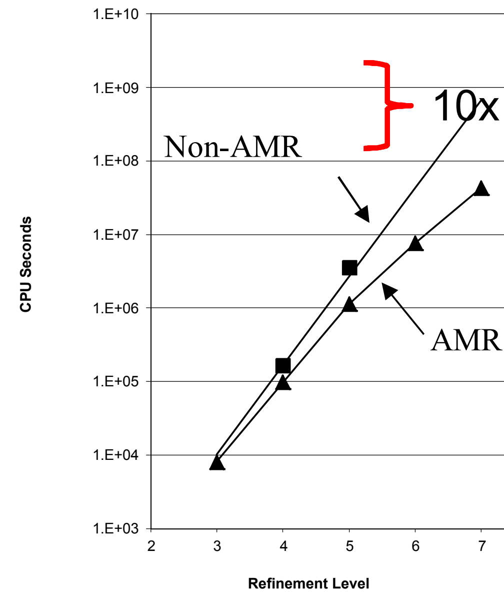


Blast on Structure Simulation LANL Cielo 32-64k Cores

Adaptive Mesh Refinement (AMR) in CTH

- AMR was added to CTH in 1998-2001
  - In 2002 we could see ~10x performance gain (vs. non-AMR) on the largest problems
- Today we routinely see 10x performance gains…
  - and occasionally see 200-300x on the largest problems





Formation of Moon

54-hour, AMR-CTH simulation with self-gravity, 40 million zones, equivalent to 20 billion zones without AMR (2011)

- 500x memory gain, 200-300x performance gain