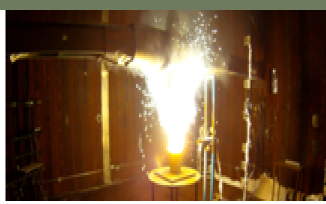
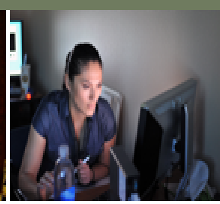
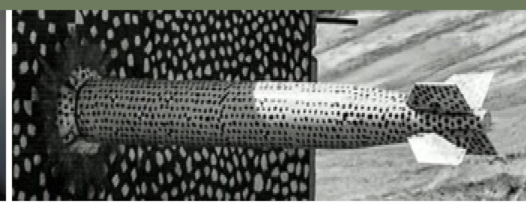
SAND2020-0865PE

SANDIA NATIONAL LABORATORIES AND THE FUTURE OF ENGINEERING AND SIMULATION







Walt Witkowski
Senior Manager, Computational Simulation Group
Engineering Sciences Center

NASA Langley Visit

January 28, 2020

Sandia National Laboratories

Exceptional service in the national interest

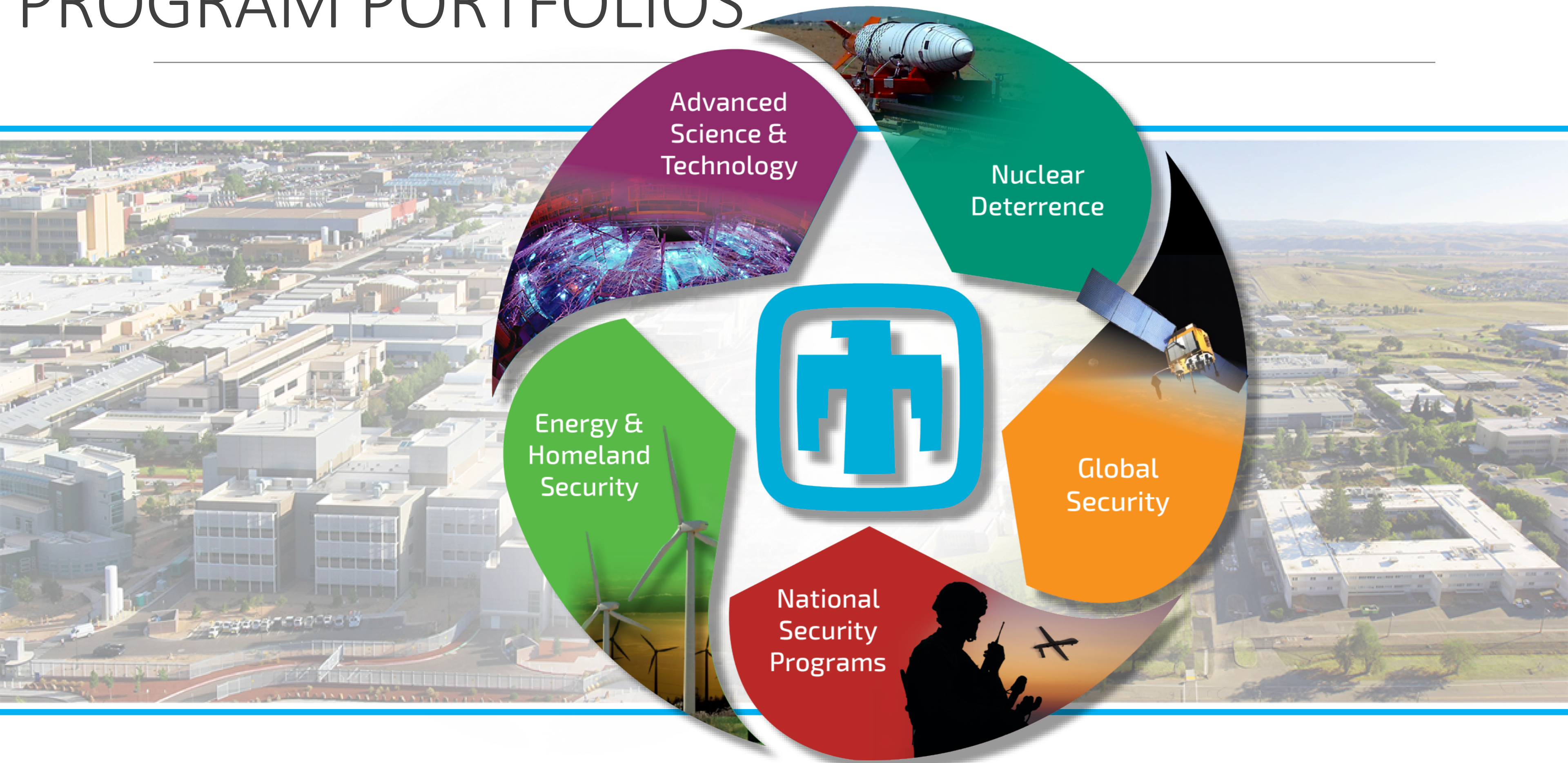
Then….

- July 1945: Los Alamos creates Z Division
- Nonnuclear component engineering
- November 1, 1949: Sandia Laboratory established

Now….

- Core mission in Nuclear Weapons
- Addressing the nation's most challenging National Security problems
  - USS Iowa (1989)
  - TWA Flight 800 Accident (1997)
  - Post 9/11 Vulnerability Studies (2001)
  - Columbia Space Shuttle Accident (2003)
  - I-35W bridge collapse in Minneapolis (2007)
  - BP Deepwater Horizon Oil Spill Accident (2010)
  - Aircraft Vulnerability (2013)
  - Waste Isolation Plant Leak (2014)

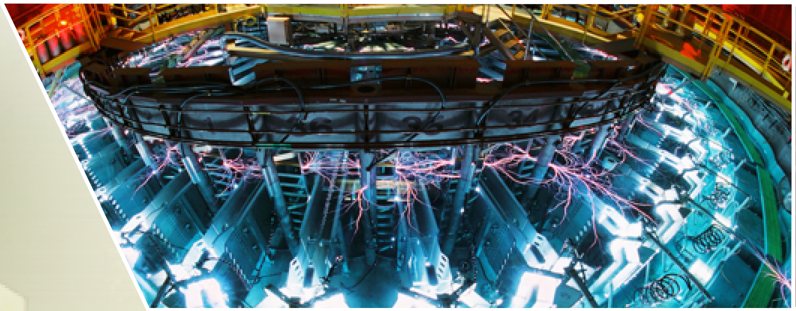
SANDIA HAS FIVE MAJOR PROGRAM PORTFOLIOS



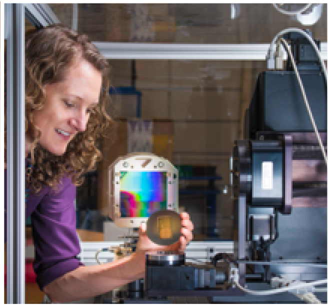
ADVANCED SCIENCE & TECHNOLOGY

Research Foundations play an integral role in stewarding our capabilities

Nanodevices &
Microsystems

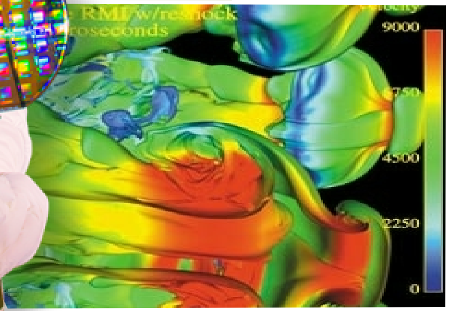


Radiation Effects & High Energy Density Science



Materials Science

Computing & Information Science



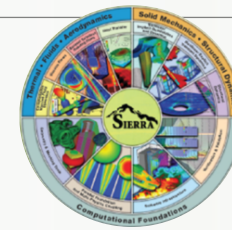
Engineering Science

Geoscience

Bioscienc
e

SCIENCE-BASED ENGINEERING KEY TO MISSION SUCCESS

Integrating multidisciplinary efforts to advance the science of the possible for Sandia's missions



Modeling and Simulation

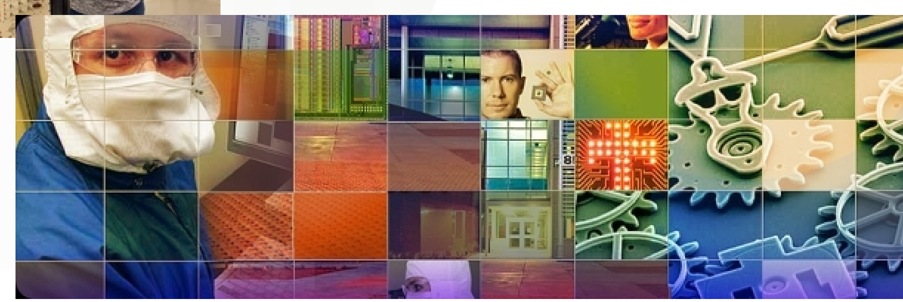
- High Performance Computing
- Software tools
- Uncertainty Quantification (UQ)

Advanced Experimental Capabilities

- Radiation effects
- Engineering environments
- Materials characterization and production

Microelectronics

- Microsystems & Engineering Sciences Applications (MESA) Fab
- Development of advanced semiconductor materials

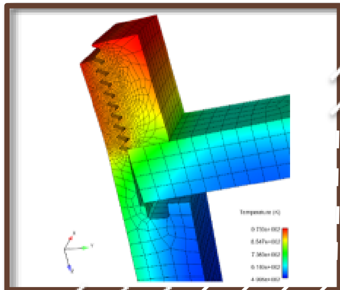


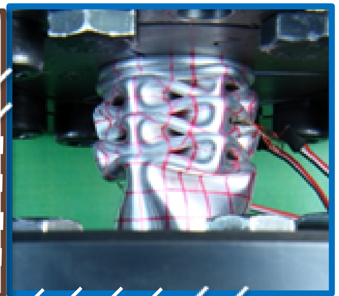
ENGINEERING SCIENCE CENTER PURPOSE

Provide validated, science-based engineering expertise, capabilities and solutions to inform critical engineering decisions.

- We integrate theory, computational simulation and experimental discovery/validation across length and time scales to develop the technical basis for complex systems.
- We steward a breadth of engineering disciplines: Aerosciences, Fire Sciences, Fluid Mechanics, Energetics, Shock Physics, Solid Mechanics, Structural Dynamics, Thermal Sciences, Computational Simulation and Engineering Analysis.

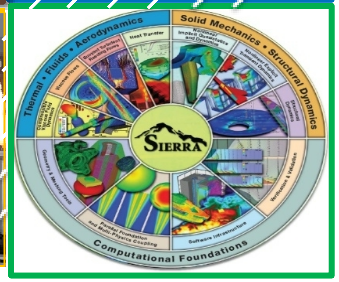
Engineering Analysis





Engineering Science Physical Phenomena

Environmental Simulation & Test



Computational Simulation Technology

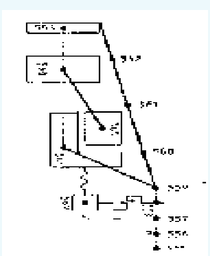
WE HAVE DELIVERED INCREASING *MODEL* FIDELITY

Enabled by platform and software advances

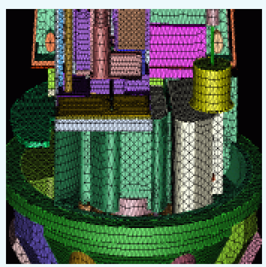
Enormous progress in computational mechanics over the past 3 decades.

- Computer architectures
- Geometric details
- Physics in computational models
- Scalable algorithms
- Multiphysics simulation codes

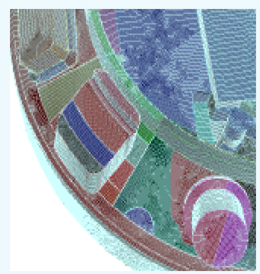
ASC Sequoia Supercomputer at LLNL
98,304 nodes x 16 cores; 20 petaflops



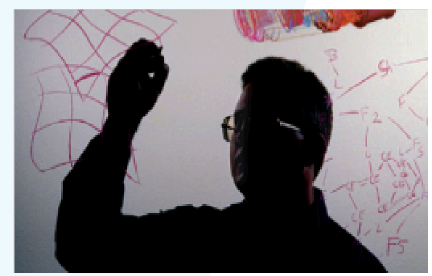
1970s:
200 DOF



ca. 2000
8M DOF



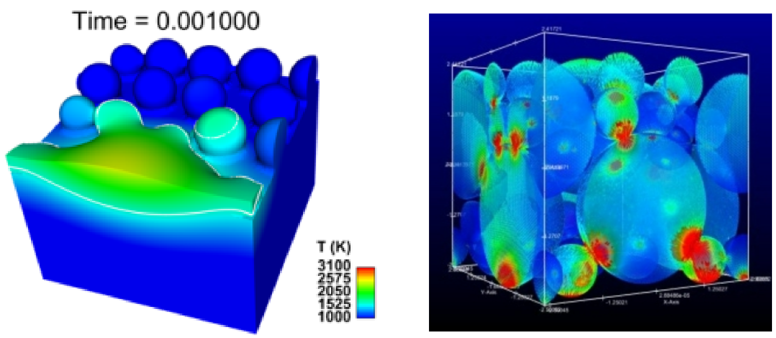
ca. 2008
40M DOF



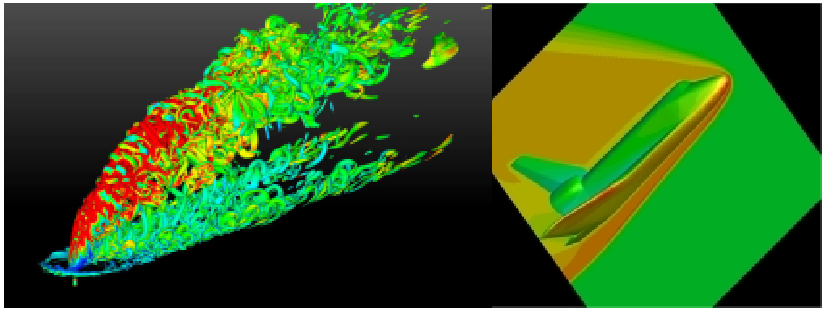
Solving previously intractable problems

ENGINEERING ANALYSIS EXAMPLES

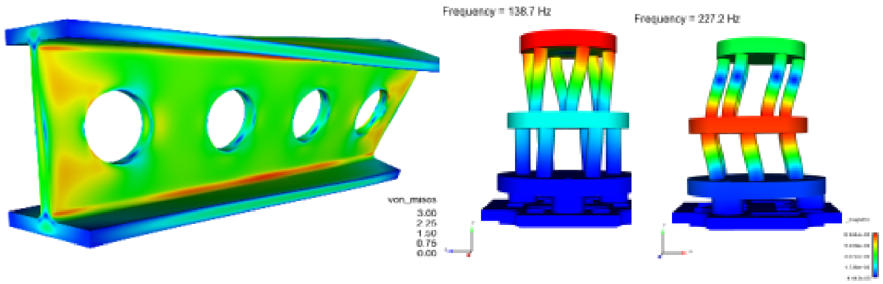
Manufacturing and Fluid Flows



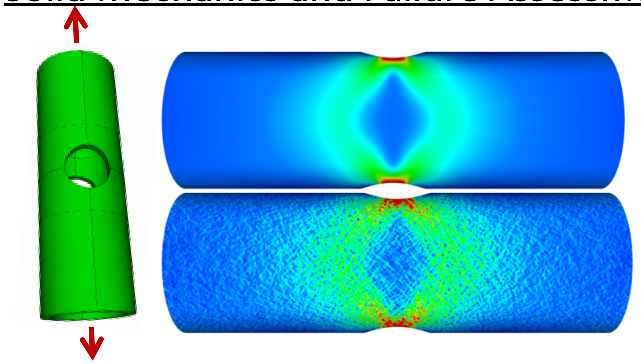
Aeroscience and Flight Phenomena



Structural Dynamics

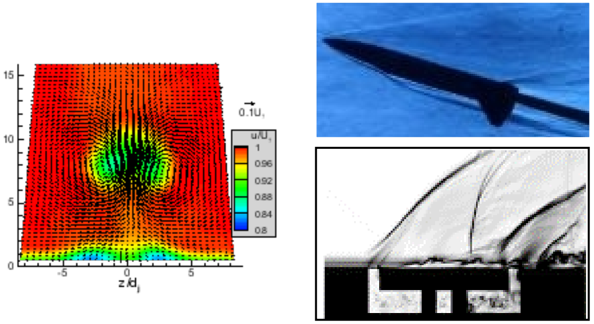


Solid Mechanics and Failure Assessment

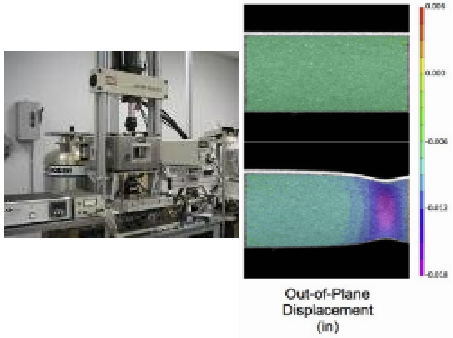


EXPERIMENTAL DIAGNOSTICS AND PHENOMENOLOGY

High Speed Compressible Flows

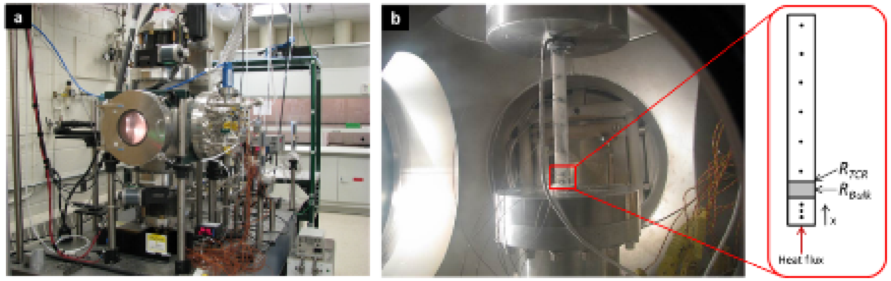


Full Field Mechanical Strain and Motion

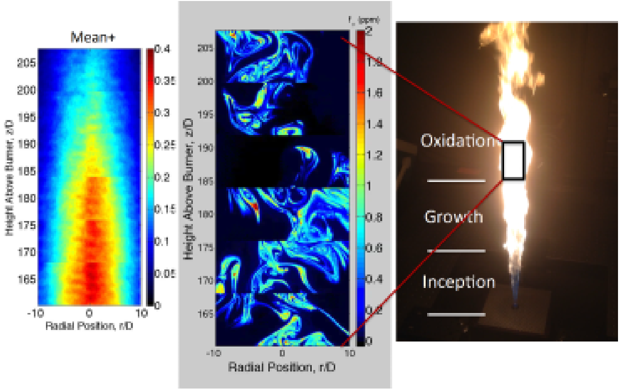


Laser-based Thermal/Flow diagnostics

Thermal Property Measurements



Fire Imaging and Spectroscopy

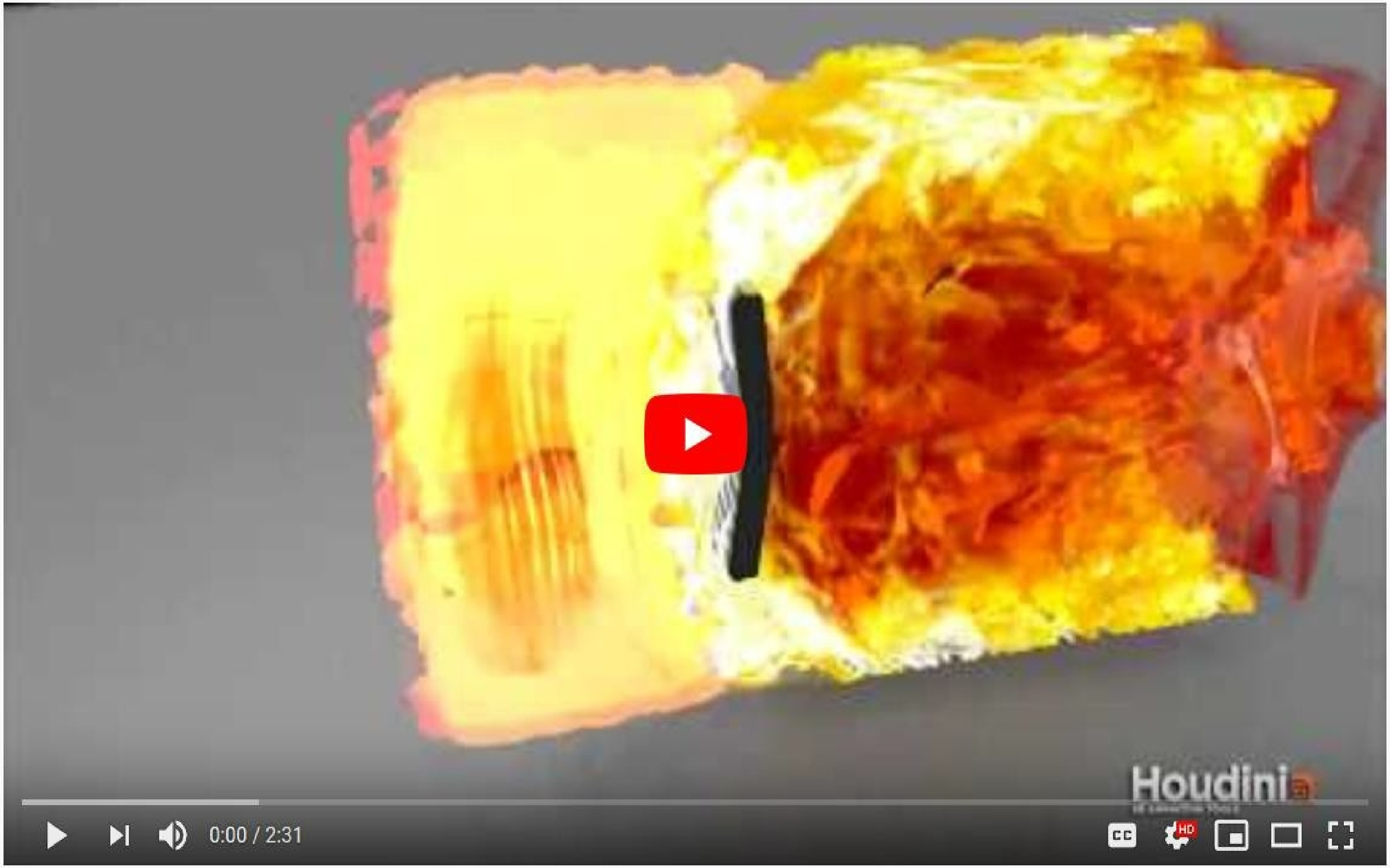


LARGE SCALE ENVIRONMENTAL TESTING

We have to be ready for a challenge!

- If called upon, how do we defend our predictions?
- What evidence is necessary to support our claims?
- It depends on what questions will be answered by the decision maker using the simulation results and testing data AND the associated risk with the decision being wrong

Engineering Sciences Overview



Engineering Sciences at Sandia Labs

- https://www.youtube.com/watch?v=o1qAjLSEv0A

Strategy

Drive understanding and innovation by integrating theory, computational simulation, and experimental discovery and validation to elucidate and credibly predict the behavior of complex physical phenomena and systems.

We seek high risk/payoff leading edge R&D that:

- Advance the scientific and engineering understanding of relevant physical phenomena
- Drive innovation in and broad usage of state-of-the-art, credible computational modeling and simulation tools
- Accelerate the development of diagnostics for data and phenomena discovery, model validation, and enhancement of our test and evaluation capabilities

Engineering Sciences IA Focus Areas

1. Fundamental and Coupled Physics Phenomena

   Discovery and development of predictive models for engineering science phenomena needed to predict the performance of components and systems.

2. Next Generation Engineering Simulation

   Development of efficient and accurate modeling and simulation techniques are required in the design, development, qualification and sustainment stages of complex systems, across a wide variety of length and time scales.

3. Diagnostics and Experimental Capabilities for Engineering Applications

   Development of novel diagnostics and experimental testing capabilities are needed to capture phenomena and responses across multiple time and length scales up to, and including, the system level.

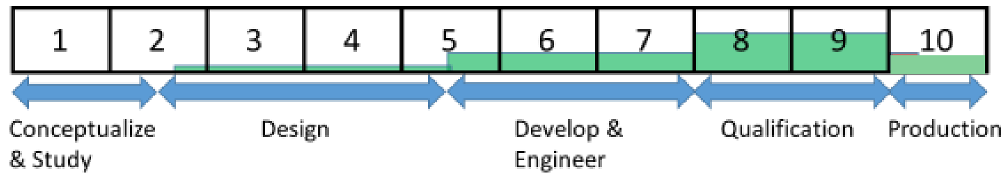
4. Engineering Data Integration and Interrogation

   Formulation and integration of data science techniques to identify and extract buried knowledge/trends in massive engineering data ensembles (either experiments, computational simulation or a combination of the two) or large single data sets exhibiting extreme temporal and spatial resolution.

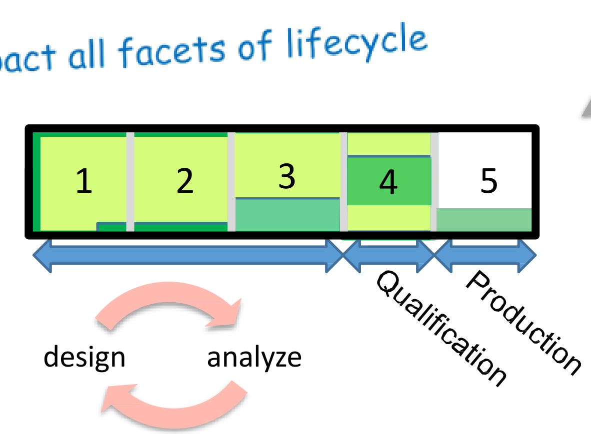
Engineering Agility is….

…a Lab-level/NNSA-level goal

Current Life extension program has a duration of 10 years:



Enable and impact all facets of lifecycle

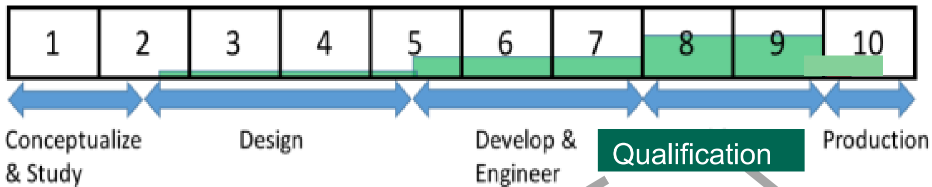


10 → 5 yrs…

…maybe 3 years!!

"Fast cycles of learning" with 100s of Virtual builds

ModSim Impact on Qualification Phase



ModSim footprint across normal, abnormal & hostile environments

- 10s of use cases/scenarios,
- ~10,000 simulations,
- 12 million CPU days

Significant up-front investment

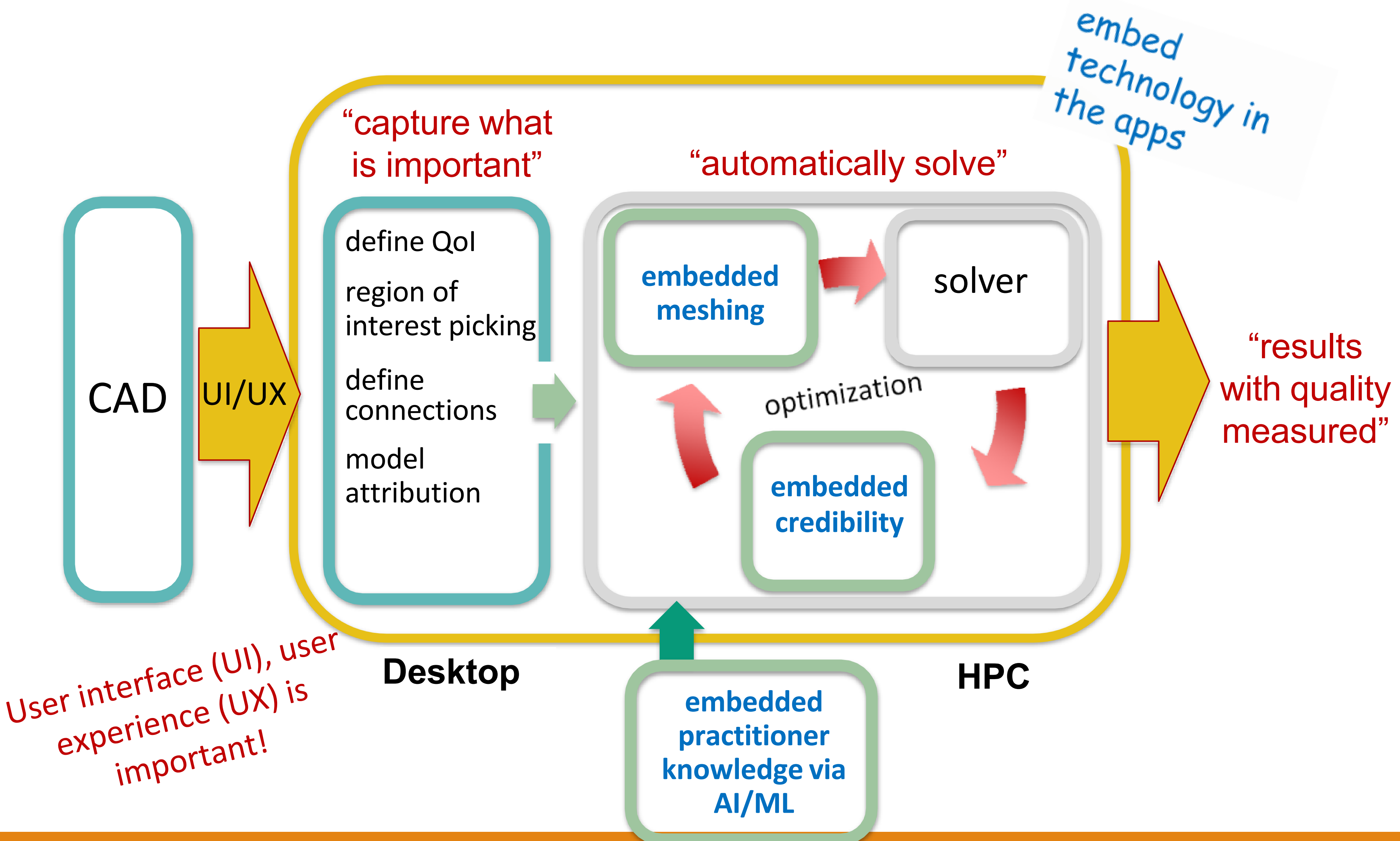
2 year lead-time to generate FE models, and develop ModSim plan, Credibility plan

Normal Thermal | Normal Mechanical | Flight Spin Rocket motor performance | NBSA performance | Abnormal Thermal | Abnormal Mechanical | Hostile Blast | Hostile Radiation | Energy Deposition

Normal Environments | Abnormal Environments | Hostile Environments

Next Generation Simulation (NGS)

enables users to do engineering!

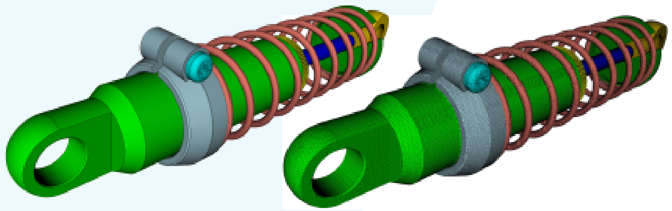


Next Generation Simulation effort is taking us from "months to minutes"

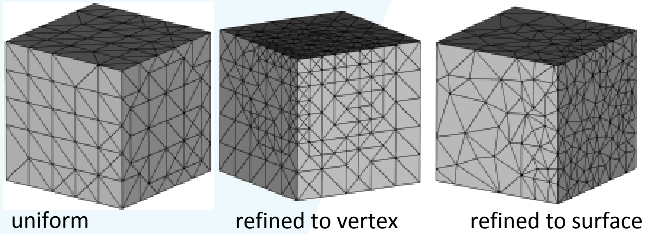
Complex parts and assemblies typically require months of analyst time addressing CAD deficiencies and building acceptable hex meshes

NGS is automated meshing that captures features larger than a specified length-scale and "gracefully ignore" smaller geometric features using tets

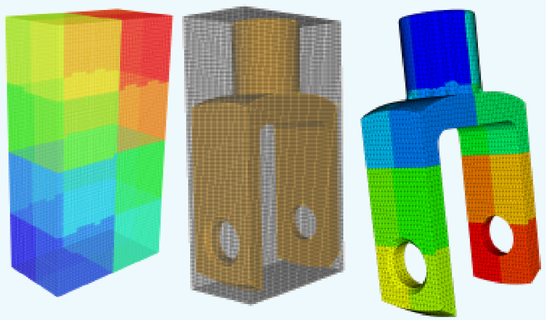
Assemblies
Interfaces, enclosures



Adaptivity
arbitrary overlay grids

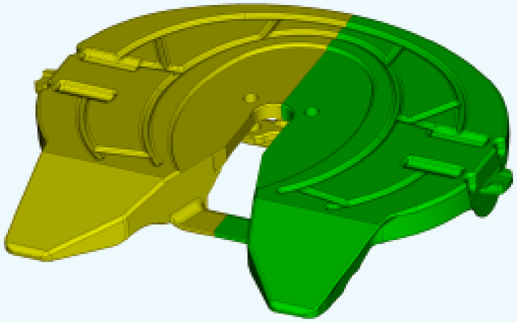


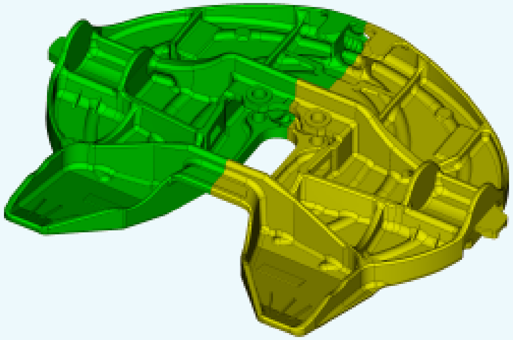
Parallel
performance & scalability

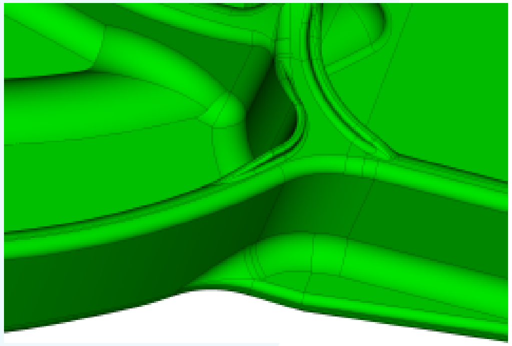


PREVIOUSLY AN ‘IMPOSSIBLE PART TO MESH’

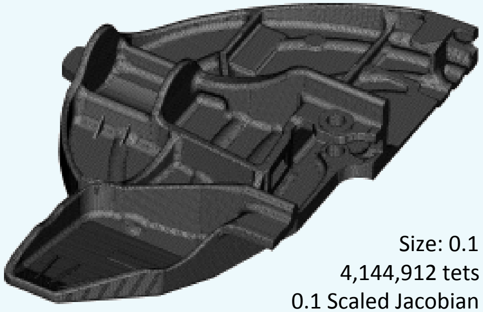
Semi tractor Fifth Wheel CAD model with multiple geometry issues



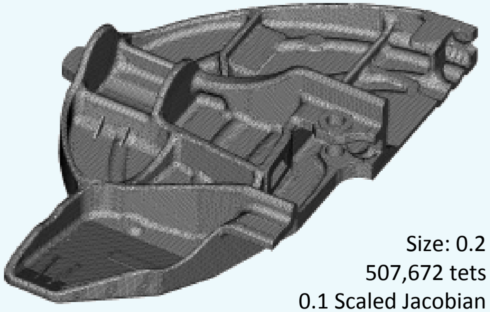




Meshing TAT: 50 minutes

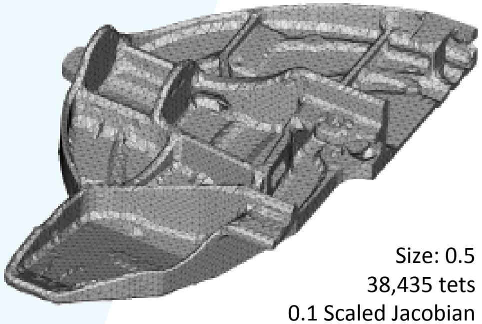


Size: 0.1
4,144,912 tets
0.1 Scaled Jacobian



Size: 0.2
507,672 tets
0.1 Scaled Jacobian

Meshing TAT: 3 minutes



Size: 0.5
38,435 tets
0.1 Scaled Jacobian

Topology optimization using PLATO

Impact on Design:

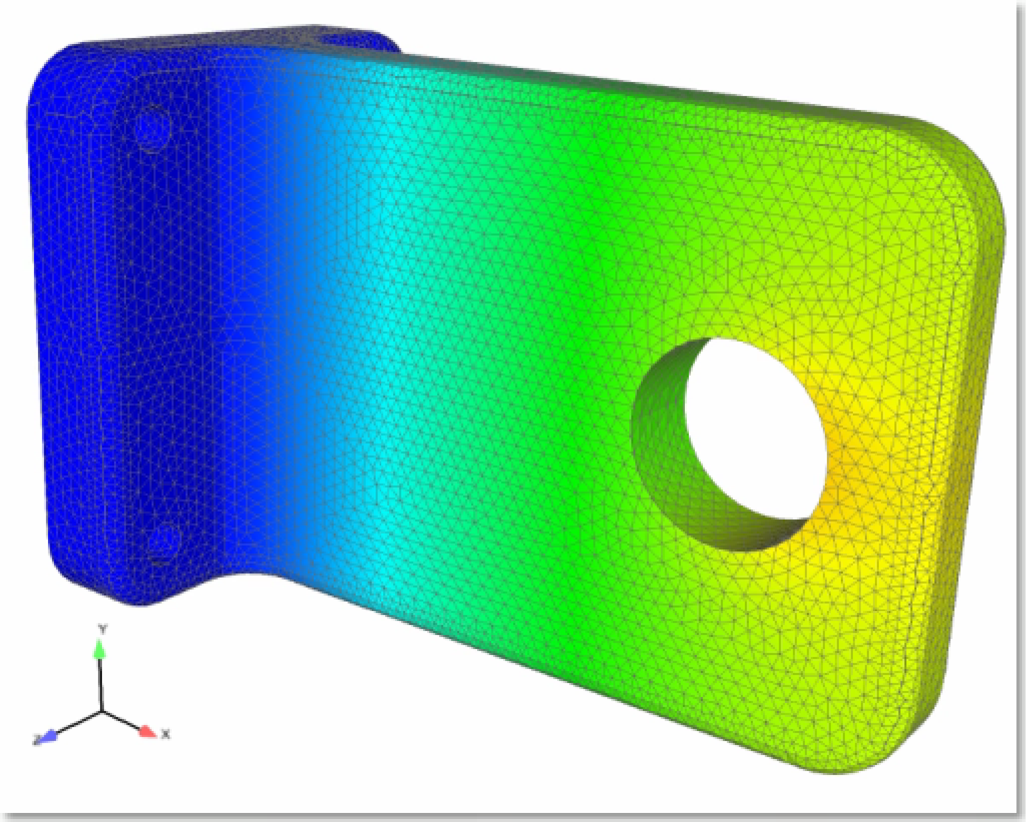
- Topology optimization explodes design space
- Take advantage of new materials with unique properties
- Enabled by HPC & high fidelity mod/sim
- Use additive manufacturing to realize organic designs

Example: satellite bracket design with increased stiffness, 40% weight reduction

PLATO Features:

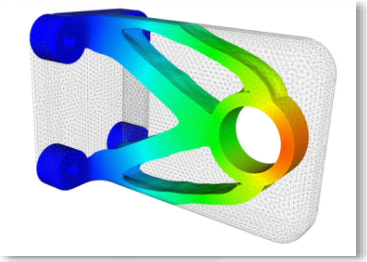
- Print ready design
- UQ-enabled designs
- Multi-material designs
- Designs with lattice metamaterials
- Automated conversion back to CAD surfaces

Incorporating the right physics is essential
Topology & Shape Optimization

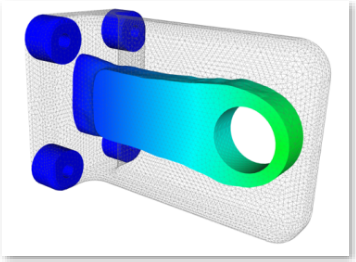


- GPU enabled solver package
- Optimized for stiffness and thermal conductivity

Mechanical Optimization Only



Thermal Optimization Only

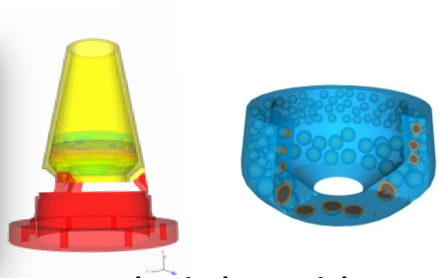


Inverse Optimization Methods & Metamaterials

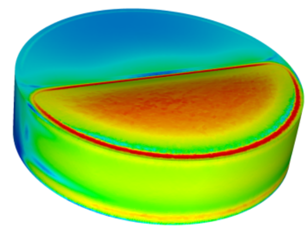
- A significant amplifier for Sandia computational simulation.
- Useful for analysis, engineering design, experimentation
- Essential in development of unique metamaterials

Wide range of use cases

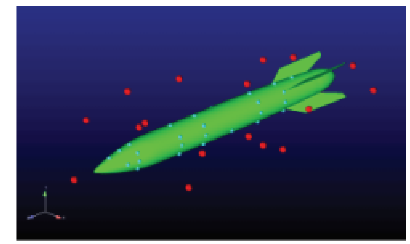
Flux boundary conditions



Thermo-mechanical material parameters, metamaterial design, Residual stress



Delamination/weld/bolted joint characterization



Ground-based acoustic/thermal tests

Source Reconstruction ↓

Material & residual stress Reconstruction ↓

Contact surface Reconstruction ↓

Design of Experiments ↓

Sierra-SD, Sierra-SM, Sierra-TF
with embedded sensitivities (adjoints, etc)

Goal: enable all Sierra apps to reconstruct forces, materials, contact surfaces, and assist in designing experiments

Uniqueness: CompSim-enabled inverse optimization that provides capabilities for the above use cases

New tools/platforms to make this work possible now and in the future

- Sandia's engineering missions are pushing us in new directions
  - Complex full-system engineering models that span a system's lifecycle
  - Explicit focus on how humans and computers interact to enable critical decisions
  - Adding automation, data-analytics, and intelligence throughout computational simulation
- But advances in computing overall are also important . . .
  - Exascale Computing Project—enabling 50x improvement in capability by 2021-23
  - Sandia's new ARM-based supercomputer prototype (Astra) helps open the door for future custom hardware options
  - Neuromorphic and quantum efforts also moving forward
- Along with novel diagnostics for elucidating phenomena and validating models.
- External partnerships and a diverse workforce are a must!

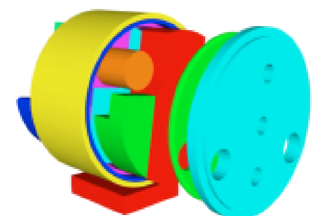
Computational Simulation Tools

Sierra: Structural Dynamics

Structural Dynamics – Linear, static, implicit dynamic & modal response

Shared mechanics capabilities

- small deformations, small-strain linear material behavior
- solid & structural elements, constraint elements
- transient–modal–modal transient solution switching, multi-sequence analyses
- non-linear pre-load transfer from Sierra/SM



shock response that includes Sierra/SM preloads

Time domain, statics & transients

- parallel scalable domain decomposition solver with many constraints
- joint models with dissipation
- material property inversion
- stochastic material (elastic) properties

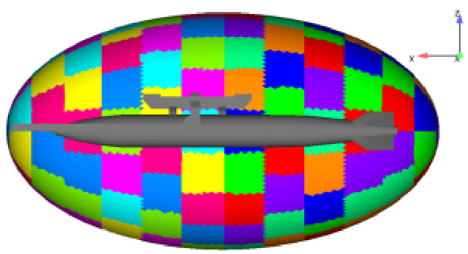
Frequency domain

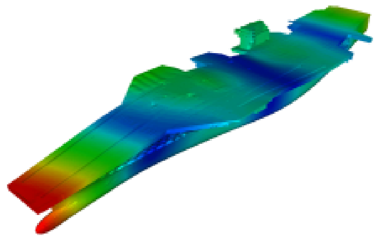
- Helmholtz solver, performance

Acoustics – linear

- absorbing boundaries
- acoustic pressure source inversion
- monolithic coupling with structural response

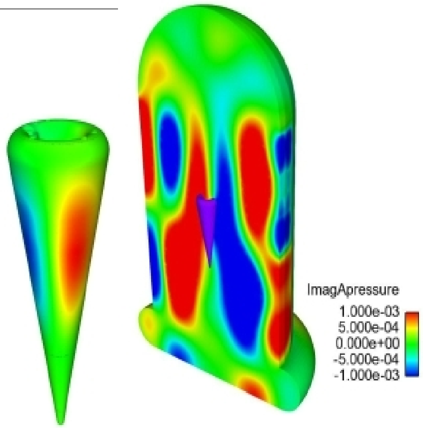
acoustic field modeling



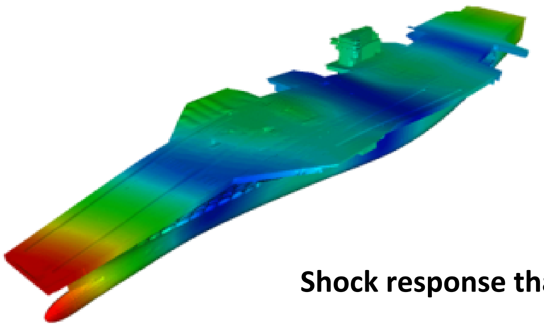


Sierra : Structural Dynamics

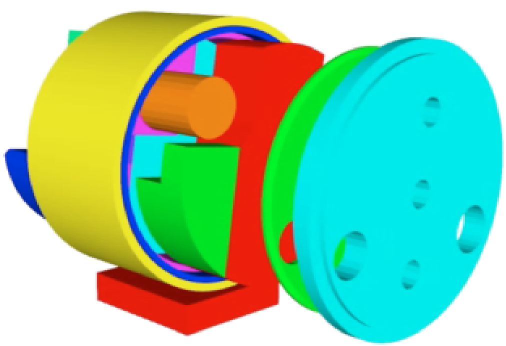
Acoustic → structural coupling



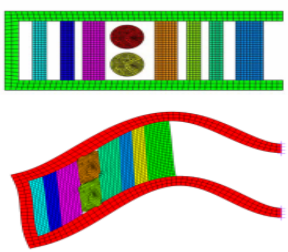
Time domain, modal transient



Shock response that includes Sierra/SM preloads

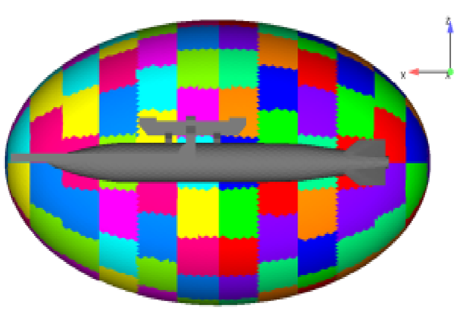


Preload → modal



linear stress analysis, (mechanical SM, SD)

Acoustic field modeling



Sierra - Solid Mechanics

Solid Mechanics – Quasi-static, implicit & explicit transient dynamic response

Shared capabilities

- large deformations, large-strain nonlinear material behavior
- implicit-explicit solution switching, multi-sequence analyses
- continuum & structural finite elements, particle methods
- parallel scalable accurate frictional contact
- common & unique material models: 100+
- geometric and temporal multi-scale methods

Implicit Solid Mechanics

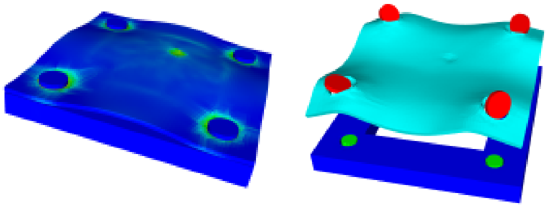
- coupled thermal-mechanical modeling, with failure
- preloads
- encapsulation & cure, incompressible material behavior

Explicit Solid Mechanics

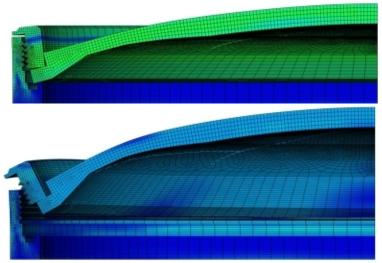
- energy-dependent material models
- fracture & failure modeling (cohesive zones, XFEM, remeshing)
- empirical blast pressure loads (CONWEP)
- coupled to CTH shock-hydro, Alegra EM

COMPSIM SOLID MECHANICS

Implicit→explicit switching



pressure & temperature loading
snap-thru & disassembly

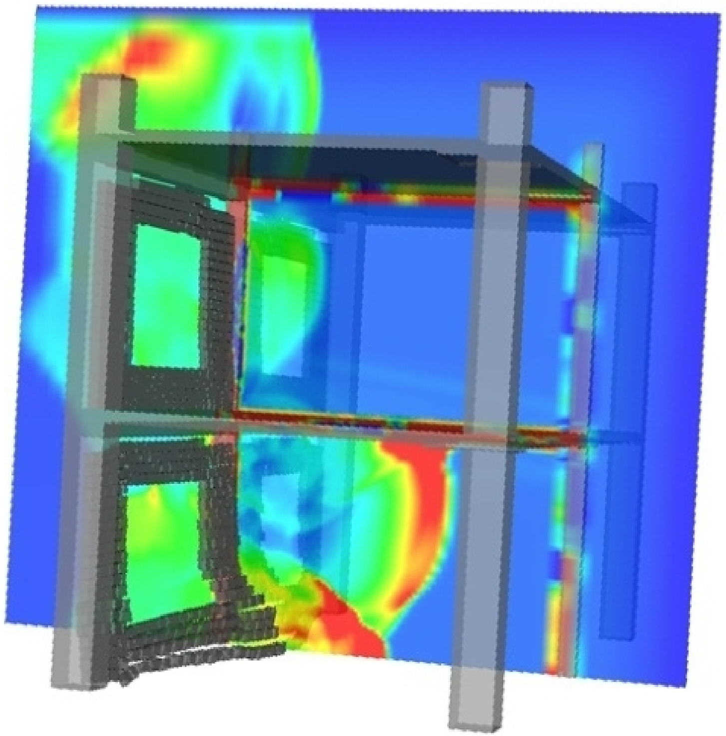


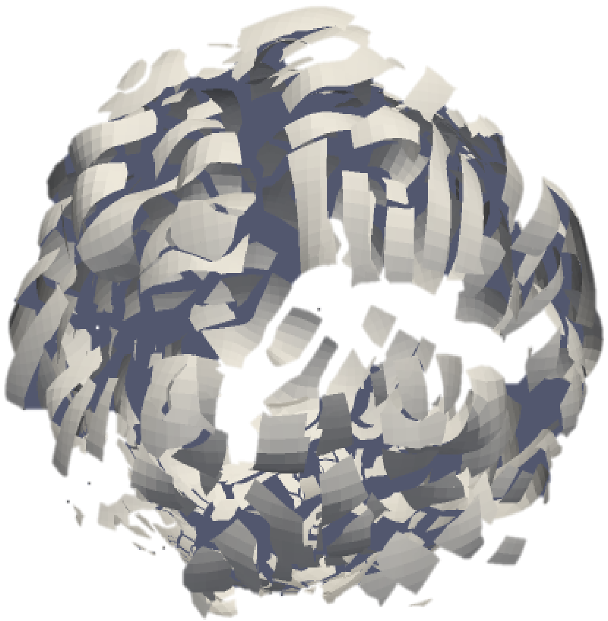
2D XFEM Fracture Simulation

Sierra - Solid Mechanics

COMPSIM
SOLID MECHANICS

Material failure modeling, Blast-on-Structure





Sierra – Thermal/Fluid/Fire

Thermal – Heat Transfer, Enclosure Radiation and Chemistry

- Conduction, Radiation, Convection
- Dynamic thermal radiation enclosures
- Element birth death, Contact

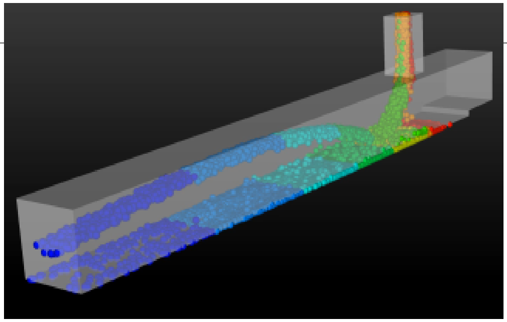
Multiphase – Non-Newtonian, Multi-physics, and Free Surface Flows

- Complex material response, Flexible coupling schemes
- Level sets for surface tracking

Fire/Combustion – Low Speed, Variable Density, Chemically Reacting Flows

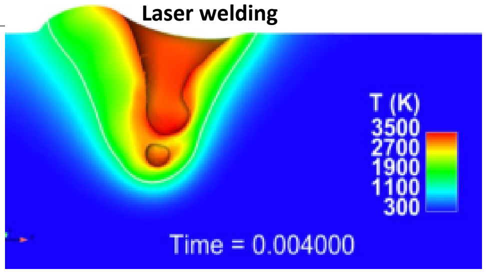
- Eddy dissipation and mixture fraction reaction models,
- Variable density
- RANS and LES based turbulence models, Unstructured Mesh, Pressurization models
- Coupling to Radiation transport code

Particles in crossflow



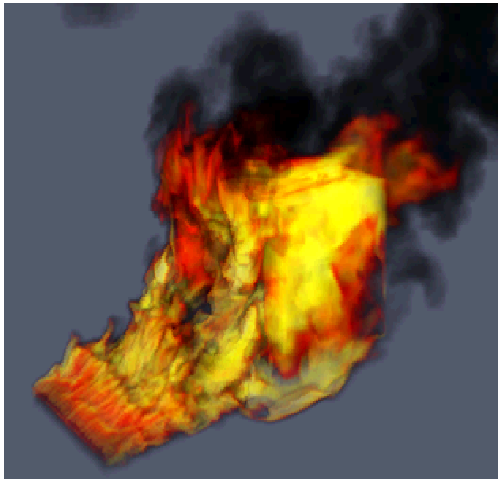
low-mach flows (thermal, fluids, participating media)

Laser welding



Manufacturing (thermal, fluids)

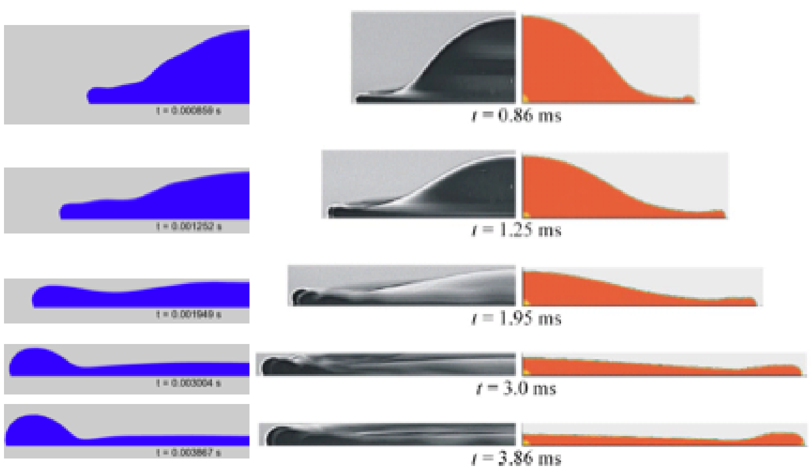
Fire modeling for subsequent weapon thermal response

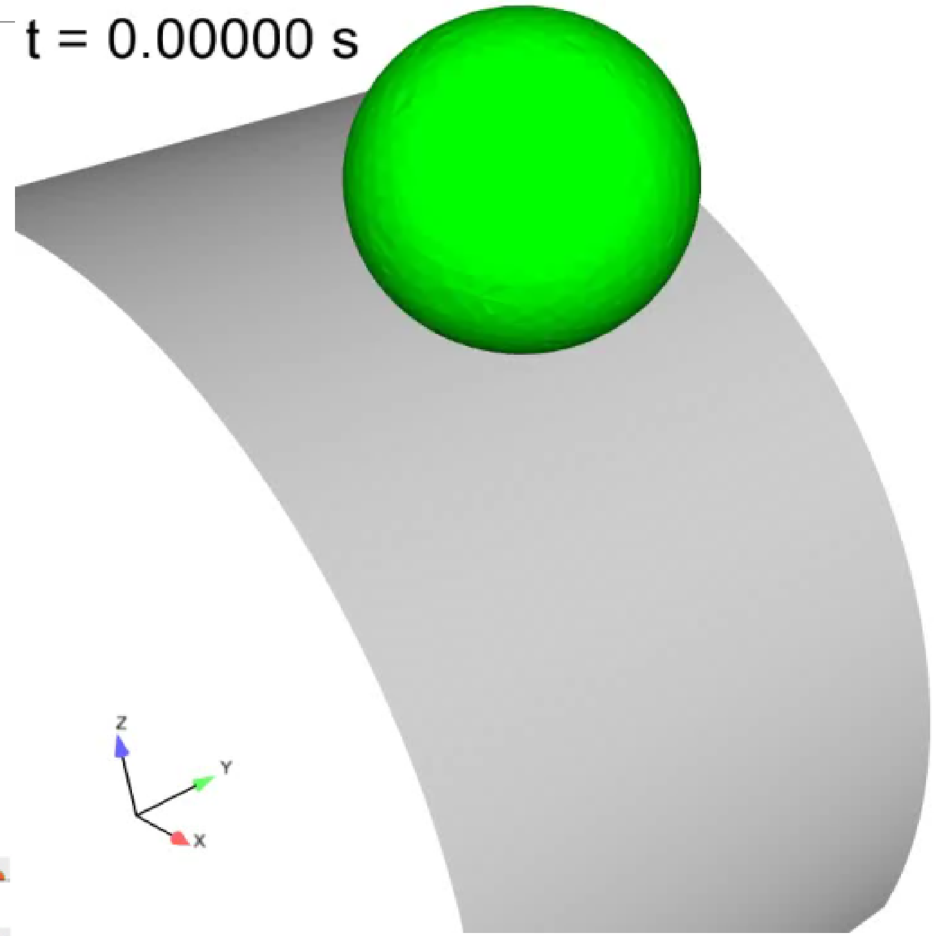


Aria: Drop impact

microscale drops impact solid surfaces

physics
- fluid dynamics
- interfacial dynamics
- energy transport



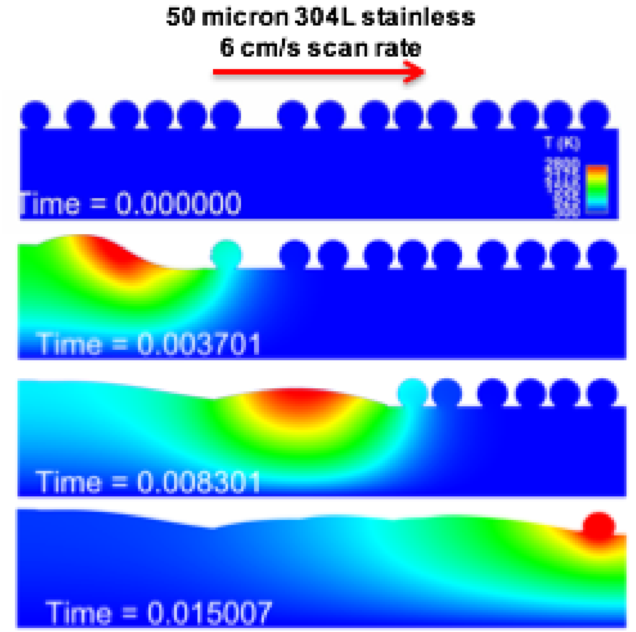


S. Roberts

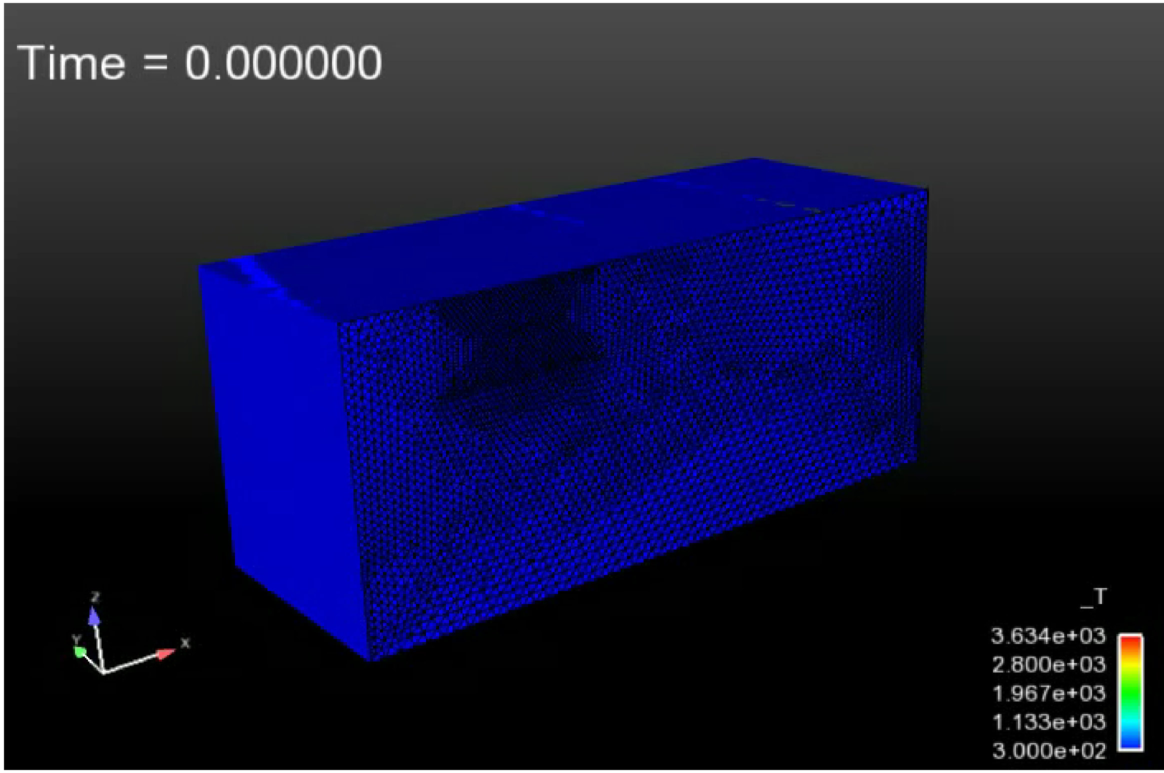
Aria: Laser Welding & Additive Manufacturing

Physics

- Selective Laser heating
- Nonequilibrium vaporization
- Conduction
- Capillary forces

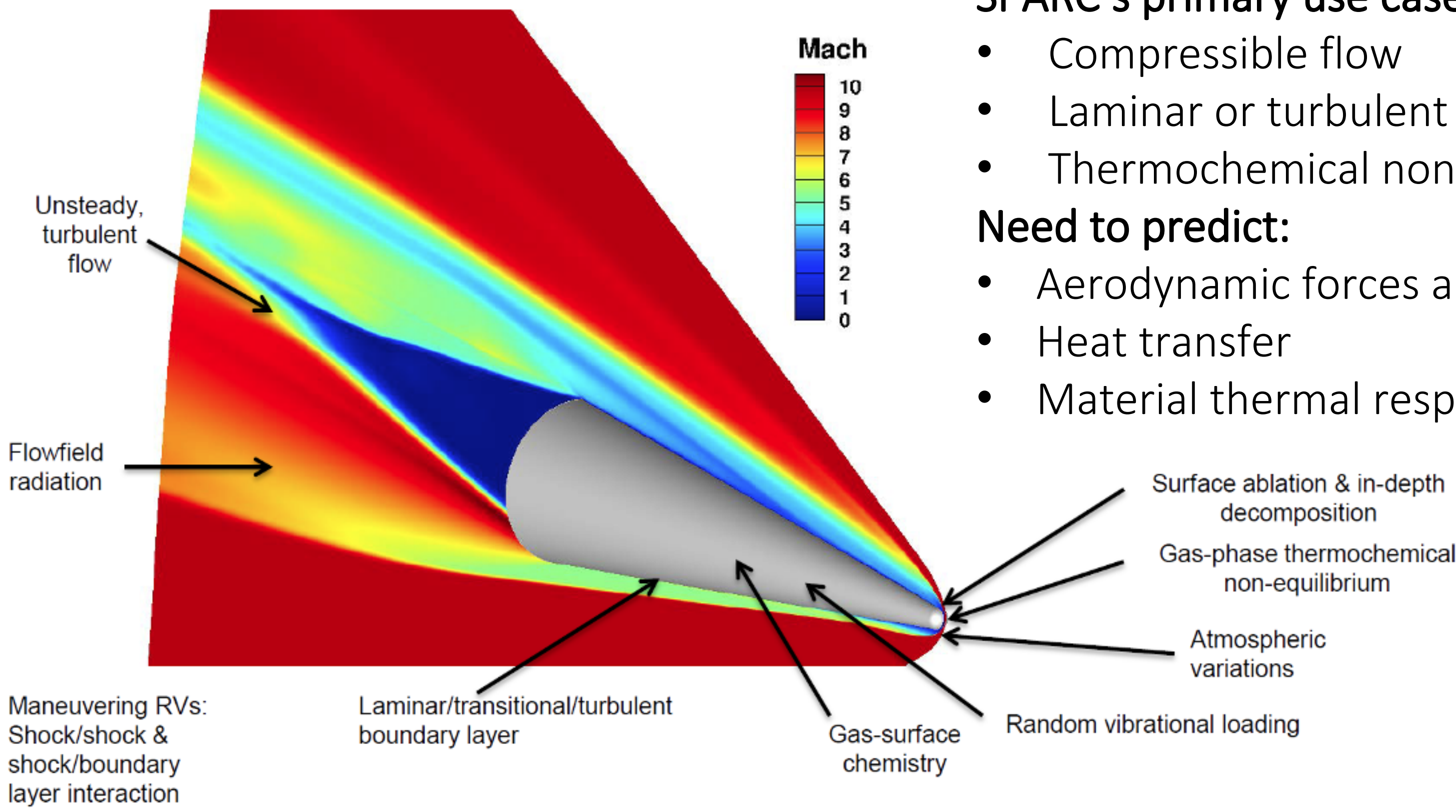


Additive Manufacturing via selective laser melting



D. Noble, M. Martinez

Sandia Parallel Aerodynamics and Reentry Code (SPARC)



SPARC's primary use case: atmospheric reentry
- Compressible flow
- Laminar or turbulent
- Thermochemical nonequilibrium

Need to predict:
- Aerodynamic forces and moments
- Heat transfer
- Material thermal response

State-of-the-art hypersonic CFD on next-gen platforms

Production: hybrid structured-unstructured finite volume methods

R&D: high order unstructured discontinuous collocation element methods

Perfect and thermo-chemical non-equilibrium gas models

RANS and hybrid RANS-LES turbulence models; R&D: Direct Numerical Simulation

Enabling technologies

Performance portability through Kokkos

Scalable solvers

Embedded geometry & meshing

Embedded UQ and model calibration

Credibility

Validation against wind tunnel and flight test data

Visibility and peer review by external hypersonics community

Software quality

Rigorous regression, V&V and performance testing

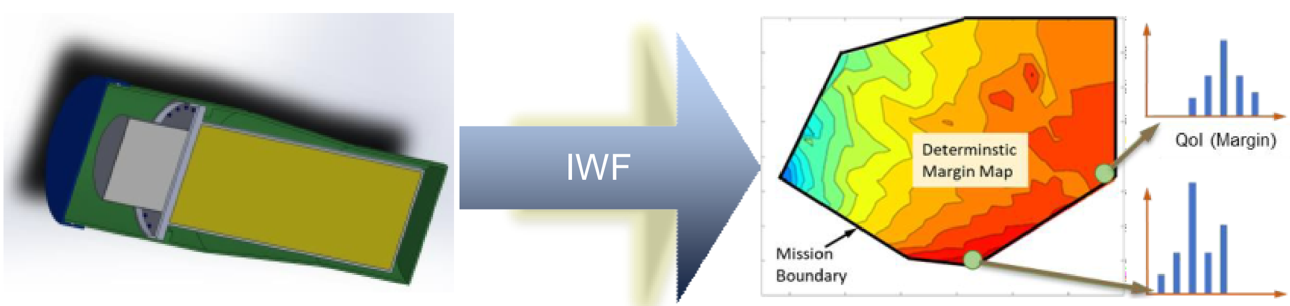
Integrated Workflow

Sandia Analysis Workbench (SAW) **Parametric** Analysis Workflow Platform

Next Generation Workflow: Integrated, Graphical, Automated, Self-Documented, Archived Process and Data

Transforming Engineering Science Analysis

- Demonstrates production-level analysis and credibility workflow to accelerate Turn-Around-Time (TAT)
  - **Current**: 1100 lines of opaque scripts/one year. **Future/Now**: reviewable visual workflow → one month
  - New visual process flow authoring paradigm; democratizes large scale ModSim integration
  - Weapons programs will see trade/uncertainty info in design phase to support early decisions
  - Impactful in the long-term (training, on-boarding, knowledge retention)
  - Relevant (supports real problems)
  - Non-trivial (requires significant development, stresses IWF infrastructure)



IWF will enable analysts to more easily perform intensive end-to-end high-consequence ModSim towards improved model credibility through clear communication and robust execution

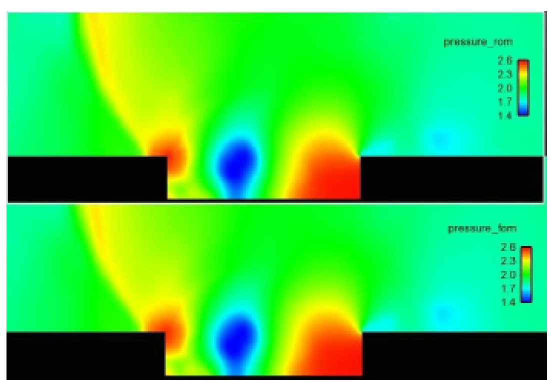
Reduced Order Models (ROMs)

Rigorous Surrogates for QMU

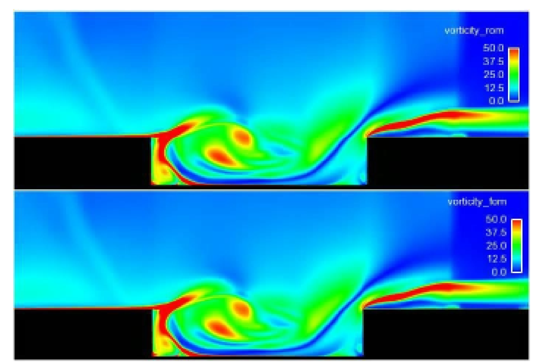
- **Motivation**:
  - *Goal*: better integrate **computational simulation** and **QMU**
  - *High-fidelity models*: expensive
  - *Typical surrogates:* physics-blind, not robust, poor epistemic UQ
- **Approach:** reduced-order modeling (ROM)
  - + orders of magnitude computational savings possible
  - + physics-based, robust, can post-process any QoI
  - + rigorous epistemic UQ and control
  - + Machine learning to quantify ROM-induced **epistemic uncertainty**

ROM
32 min, 2 cores

High-fidelity model
5 hours, 48 cores



Pressure field



Vorticity field

NASA Engagements
Summary of past interactions

- **NASA sites interested in Sierra Mechanics**
  - Langley, LaRC
    - 5+ years, training, research transition path, exploring co-development
  - JPL
    - Use of Sierra, joint projects
  - Kennedy
    - Flight Structures - Dynamic Environments, NASA Launch Services Program
    - Minor interactions
  - Johnson
    - Loads & Dynamics, NASA Engineering and Safety Center (NESC)
    - Minor interactions
  - Marshall
    - Inquiries, use of Sierra

NASA LaRC Interactions
Recent/Future

- **Yearly training visits, briefings, Sierra Mechanics**

- **Visit with Ed Glaessgen, 14 Nov 2019, joint briefings**
  - Michael Skroch, Miguel Aguilo, Tim Walsh, Sandia
  - Topology Optimization & Inverse Optimization
  - Results in many ideas, and desire for regular technical exchanges

- **NASA HPC Meeting, 18-19 Mar 2020 @ LaRC**
  - Tim Walsh, Sandia, invited speaker
  - Cara Campbell Leckey (LARC-D313), Lead – HPC Incubator

NASA LaRC Interactions
Potential Collaborations

- **Sierra Mechanics Use & Extension**
  - Transition for NASA Research, co-development, fracture mechanics
- **Non-destructive Evaluations**, Structural Health Monitoring, Delamination's, cracks, etc. (Inv Opt)
- **Techniques for Qualification**
- Establish periodic **Technical Exchange Meetings**
- **Microstructure code simulation,** SPPARKS (PLATO)
- **AM Process Simulation w/Chris Lang** (PLATO)
- **Design for Inspectability** (PLATO)
- **Design Under Uncertainty** (PLATO)
- **Material Property Characterization** of airframes and related structures (InvOpt)
- **Load Identification** (InvOpt)
- **Design of experiments** (InvOpt)
- **Thermal Inverse** (InvOpt)
  - Conductivity, flux estimations

Sandia National Laboratories

Exceptional service in the national interest

Sierra Suite of Tools

Sierra is ASC's engineering mechanics simulation code suite

Distinguishing strengths:

- Integrated workflow components
- *Application aware* development
- Scalability
- SQA and V&V
- Multiple scales
- Multi-physics coupling

Capabilities include:

- Solid Mechanics
- Structural Dynamics
- Thermal Mechanics
- Fluid Dynamics: Low-Mach
- Fluid Dynamics: High-Mach