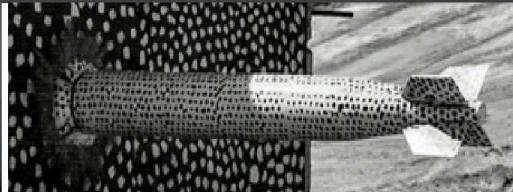


# Significant Advances in Computational Simulation Workflow for National Security Applications



ASSESS Congress  
October 29, 2019  
SAND #

*PRESENTED BY*

Dr. Walt Witkowsky

Sandia National Laboratories  
Computational Simulation Group

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.  
wrwitko@sandia.gov



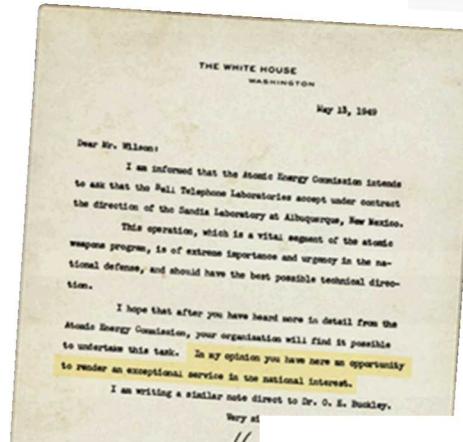
Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

# Sandia National Laboratories

## Then....

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

*Exceptional service in the national interest*

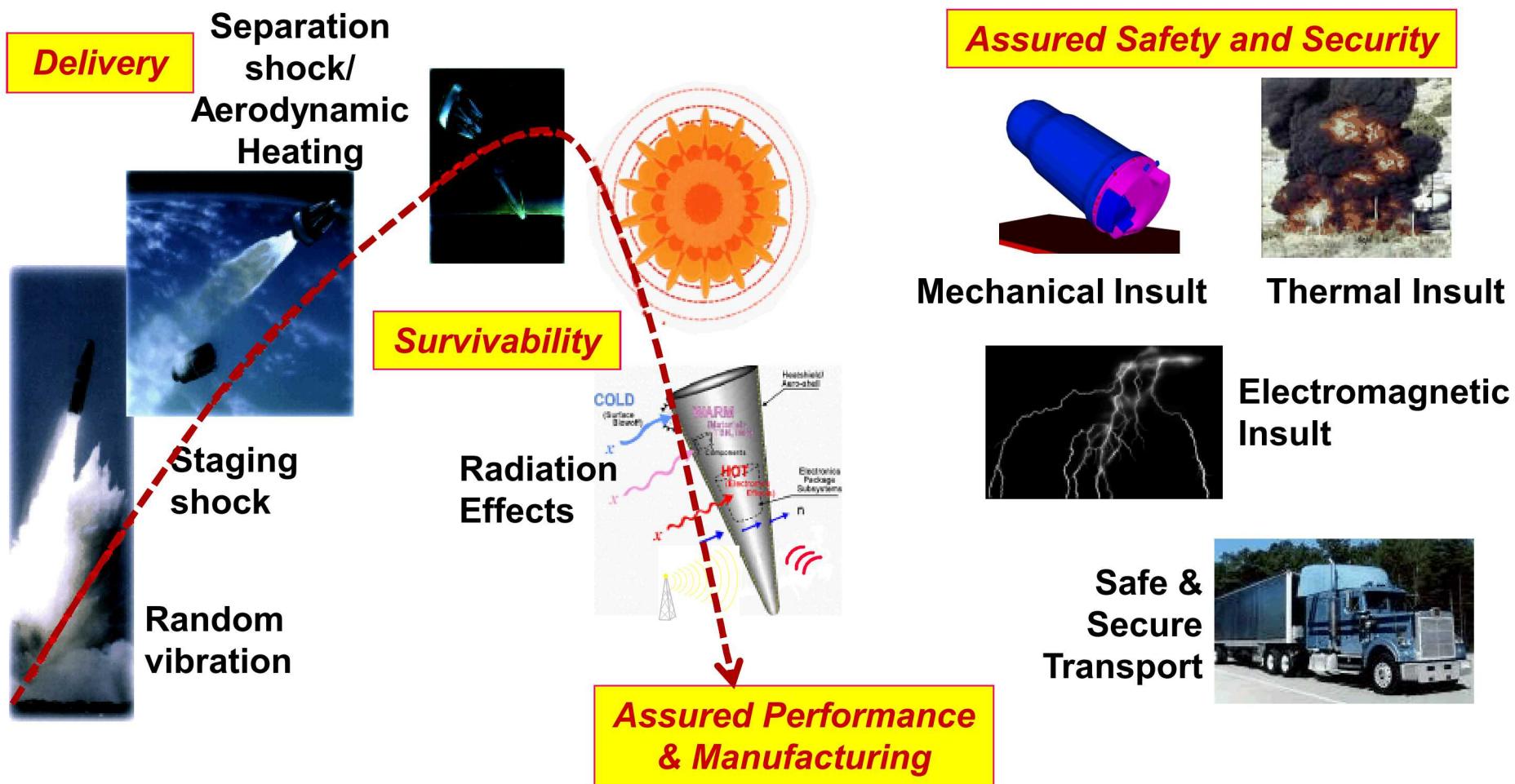


## Now....

- Core mission in Nuclear Weapons
- Addressing the nation's most critical 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 Minnesota (2007)
  - BP Deepwater Horizon Oil Spill (2010)
  - Aircraft Vulnerability (2013)
  - Waste Isolation Plant Leak (2014)



# SNL's Nuclear Weapons Program is the principal driver for Our Computational Simulation efforts



**SNL Engineering Codes are supporting the engineering needs of the complex**

# SNL's Growing Reliance on Predictive CompSim



- SNL nuclear weapon mission drivers:
  - Several systems including 2 current LEPs
  - Support annual assessment & certification that all weapon types are safe, secure & reliable
- Changing paradigm from testing dominated approach
- Few/no tests at the full system level;  
few/some/no tests at subsystem/component level:
  - not allowed, and/or (radiation effects tests)
  - too expensive, and/or (crash impact tests)
  - too environmentally unfriendly, and/or (fuel/propellant fire tests)
  - too few units available (annual surveillance)
  - Or ....just cannot perform the test at the application specs

## Are we 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



# Sierra Suite of Tools

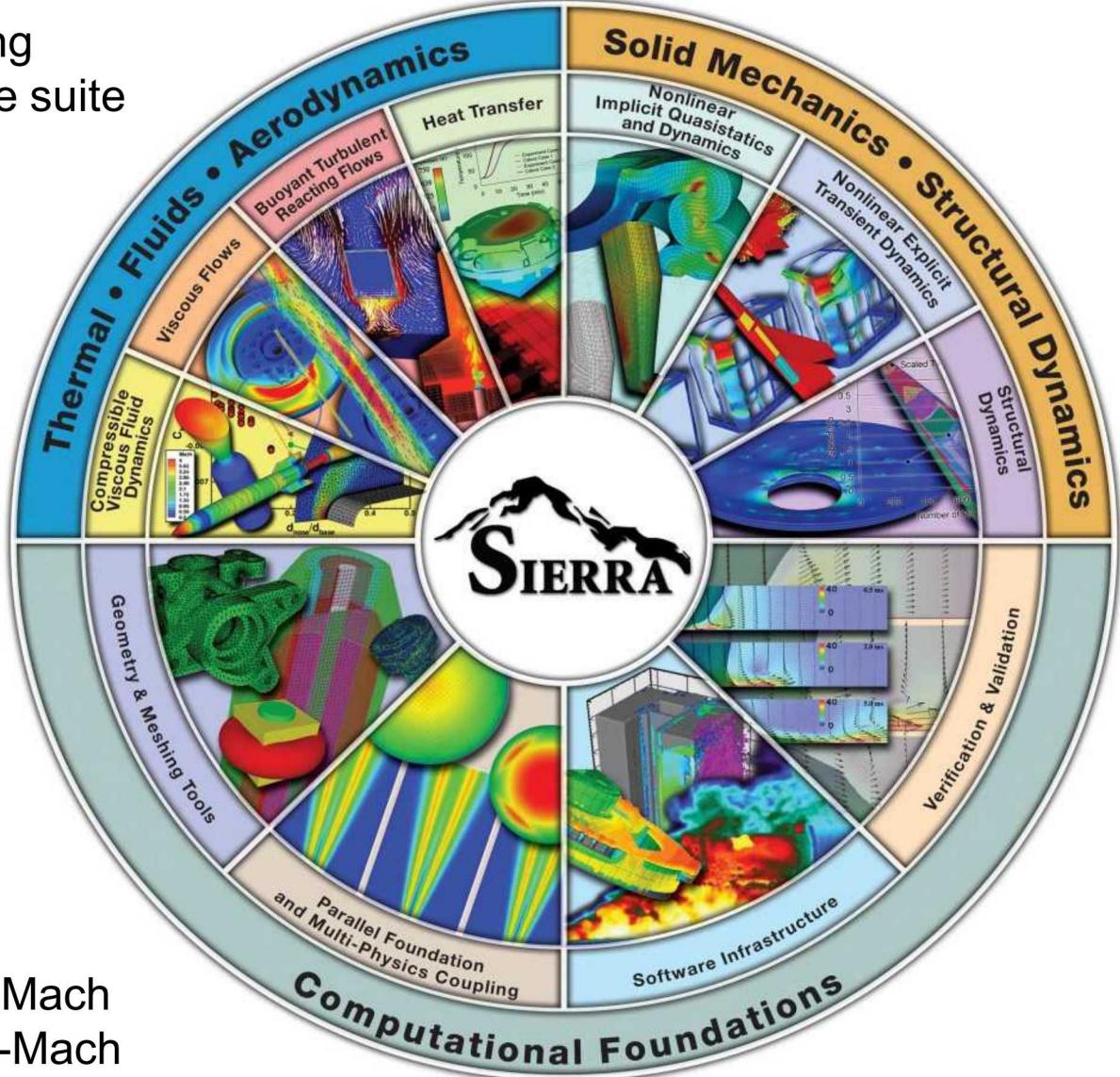
**Sierra** is ASC's engineering mechanics simulation code suite

Distinguishing strengths:

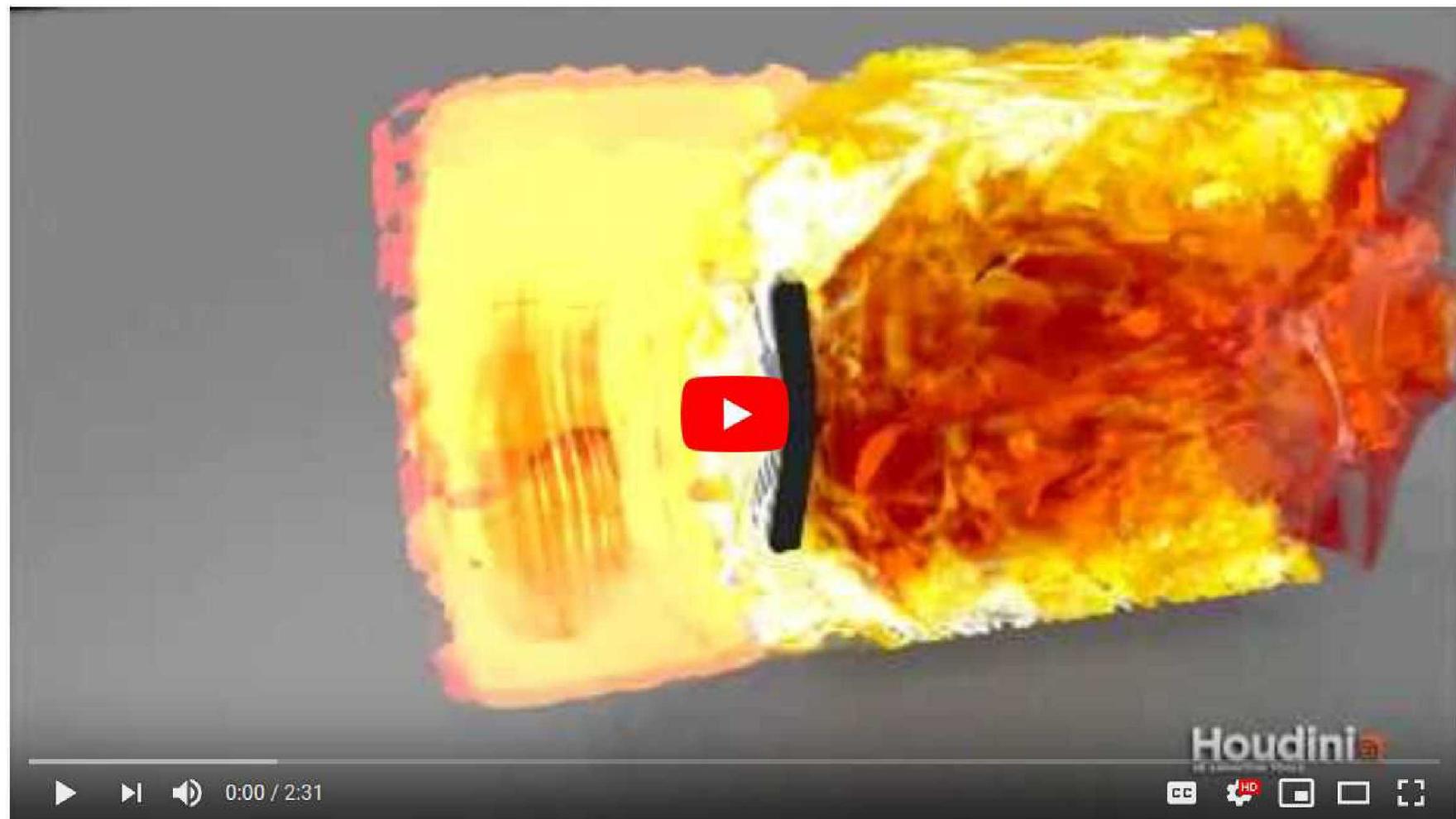
- Integrated workflow components
- *Application aware* development
- Scalability
- SQA and V&V
- Multiple scales
- Multi-physics coupling

Capabilities include:

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



# Engineering Sciences Video

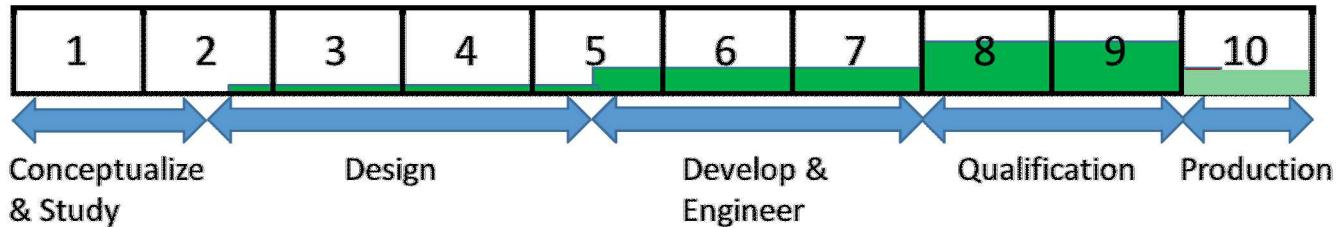


Engineering Sciences at Sandia Labs

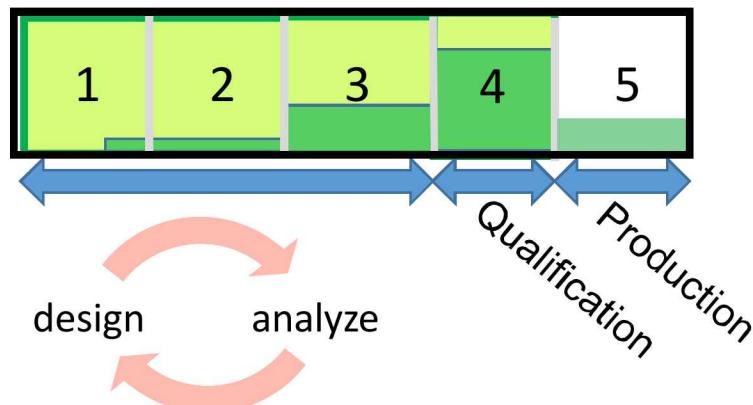
- <https://www.youtube.com/watch?v=o1qAjLSEvOA>

# Engineering Agility is a Lab-level/NNSA-level goal

Current Life extension program has a duration of 10 years:



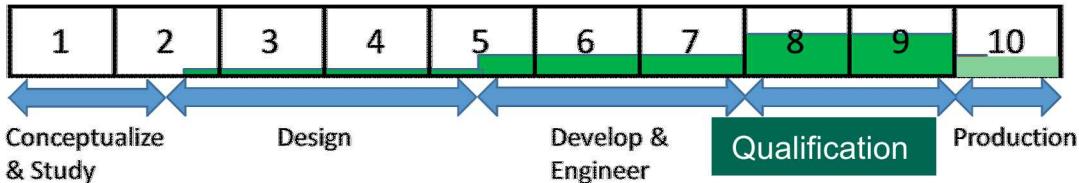
Enable and impact all facets of lifecycle



**10 → 5 yrs...  
...maybe 3 years!!**

**“Fast cycles of learning”  
with 100s of Virtual builds**

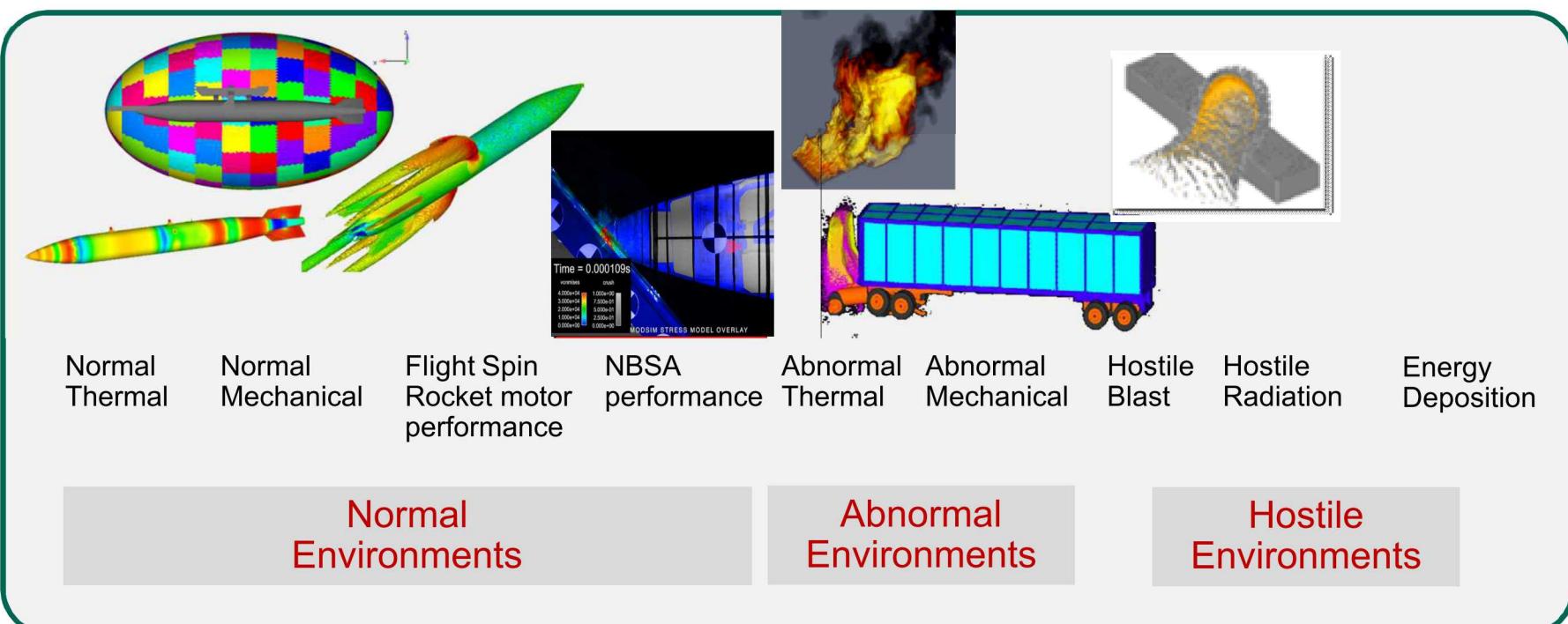
# ModSim impact on Qualification phase



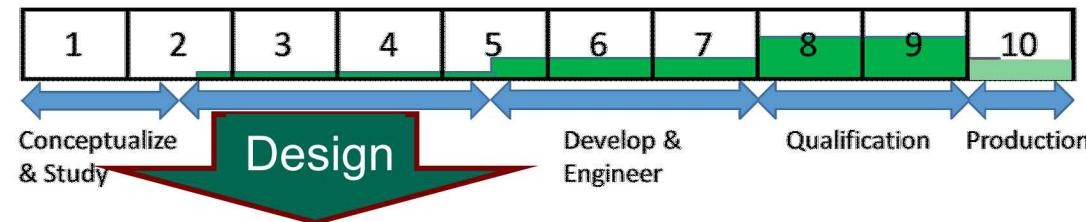
ModSim footprint across normal, abnormal & hostile environments

- ❖ 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



# ModSim impact on Design phase



Example:

- Stronglink component is a mechanism assembly of 30-40 parts
- Question: determine performance of various stronglink configurations in mechanical drop (shock) environment.
- Desired turn-around-time: **4 weeks**
  
- ❖ Actual turn-around-time: **8 months**  
**7 months all hex mesh model creation,**  
4 weeks analysis & reporting

## Challenge

Reduce the turn-around-time of model creation by 100x

# Lab Directed R&D (LDRD)

Targeting a 100X reduction from design to analysis:  
An agile, tetrahedral workflow for component design...

## Technical challenge

Hex formulation is ideal/optimal, but time-consuming to generate a mesh

Tet meshing is far more tractable, but formulations have historically all performed poorly

LDRD resulted in a breakthrough

A viable tet element formulation for each of the Sierra mechanics disciplines

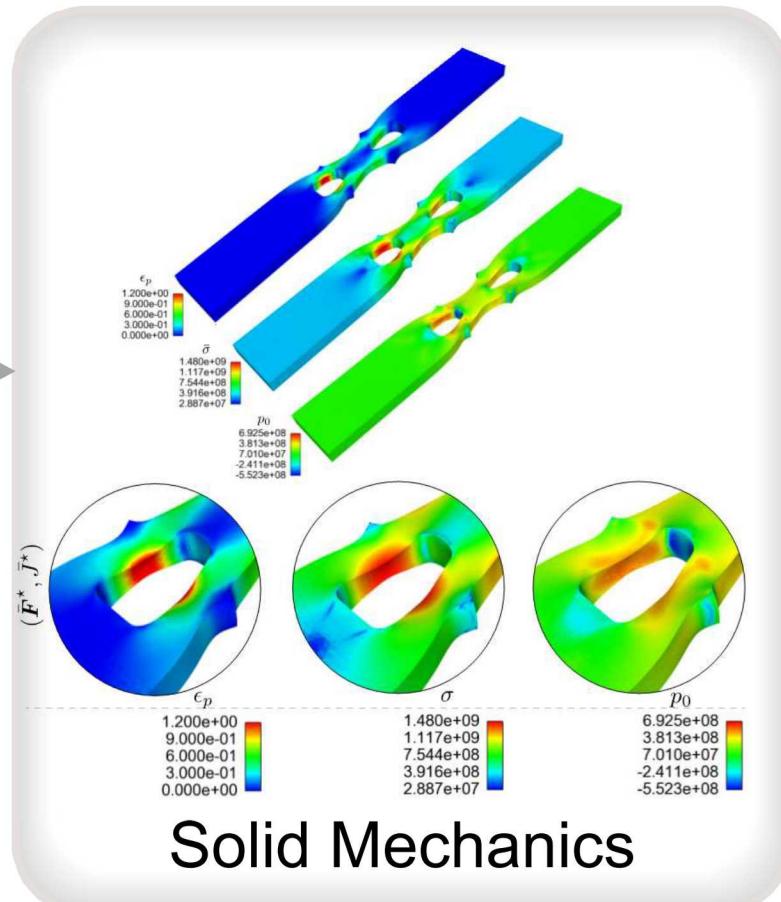
Tet4 standard simplex ele

Thermal Fluids

Tet4 with bubble function

Structural Dynamics

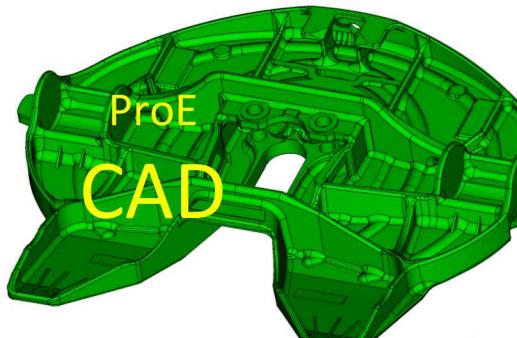
## Composite Tet10



# Next Generation Simulation Capability (NGS)



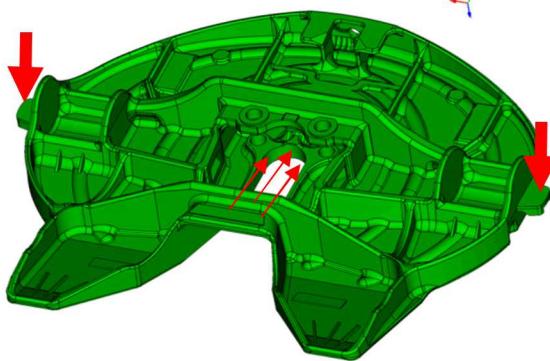
Perform analyses with known quality  
in minutes not months



**Efficient Model creation:**  
no CAD clean-up!  
Automated, parallel in-situ  
tet meshing



**With Credibility Evidence:**  
Solution verification,  
Quantity-of-interest & sensitivities,  
Reproducibility



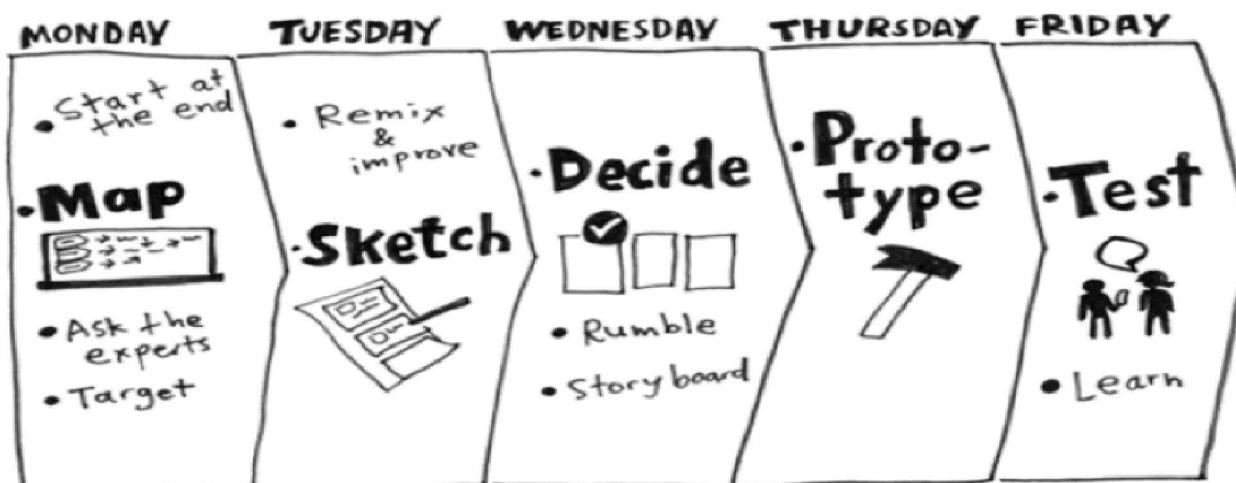
## Intuitive User Experience:

Context-specific workflows: conceptual design thru qualification  
Model attribution on geometry (not on mesh),  
Feature of interest selection

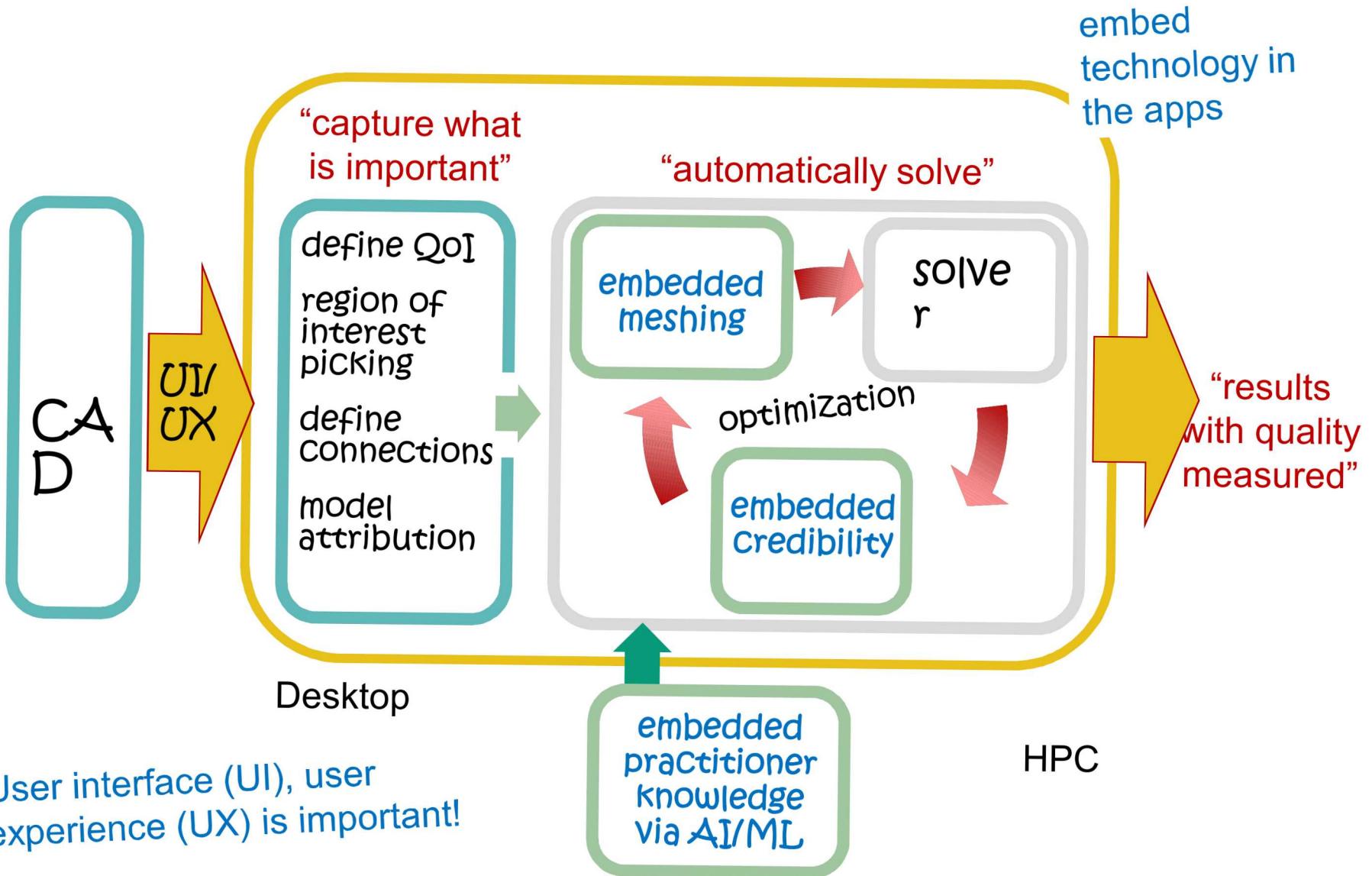
# Agile NGS Definition and Planning

## Google Venture Sprint Exercise

1. Embedded Discretization
2. Embedded Credibility
3. User Experience

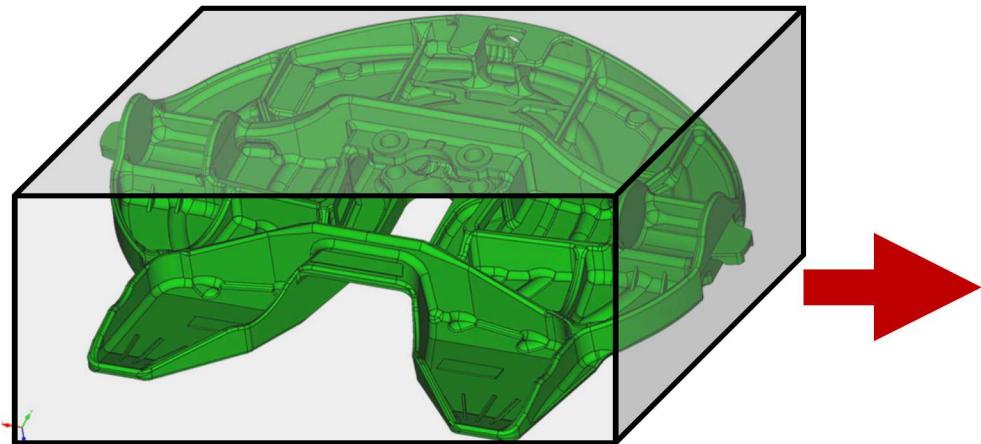


# NGS enables users to do engineering!



# NGS automated meshing

overlay grid encloses CAD geometry



grid nodes snapped to geometry

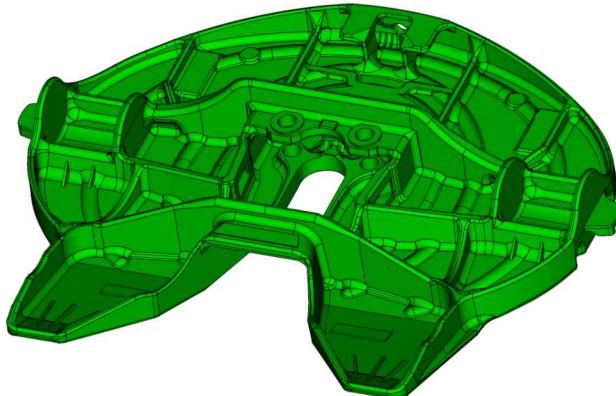
## Unique meshing algorithm:

- 1) no CAD clean-up !
- 2) parallel in-situ mesh generation algorithm, **Morph**  
Executes on desktop and HPC , MPI parallel
- 3) **guaranteed element quality**  
Iterative solution: move node to target + tet transformations

(Tet transformations are from Lagrangian shock modeling community)

# NGS automated meshing

**Tolerant to  
CAD issues**

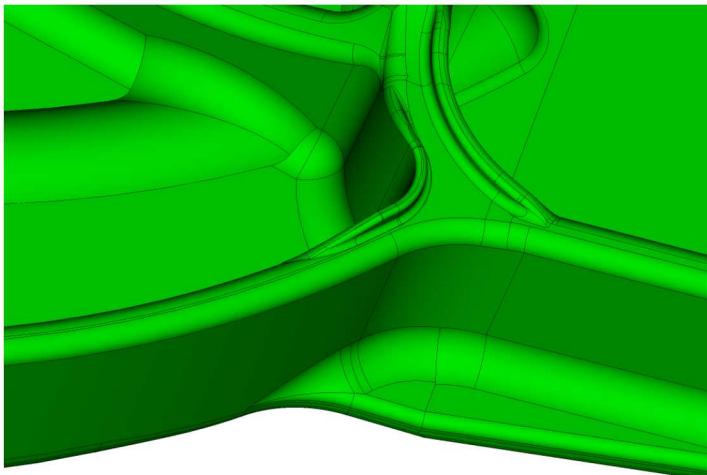


5<sup>th</sup> wheel part has  
> 10,000 curves & surfaces  
many with geometry issues

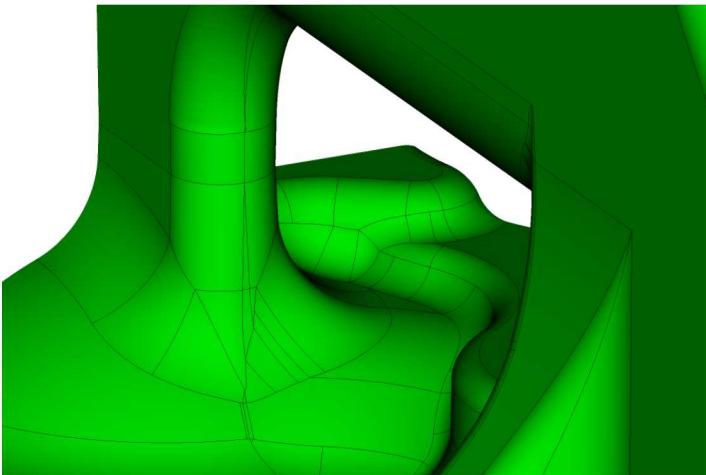
examples:



curve tangencies



zero-area surface

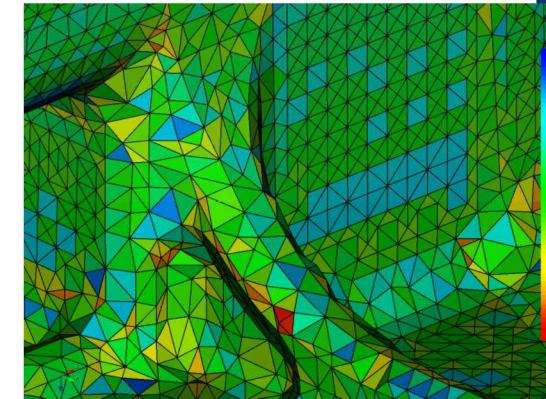
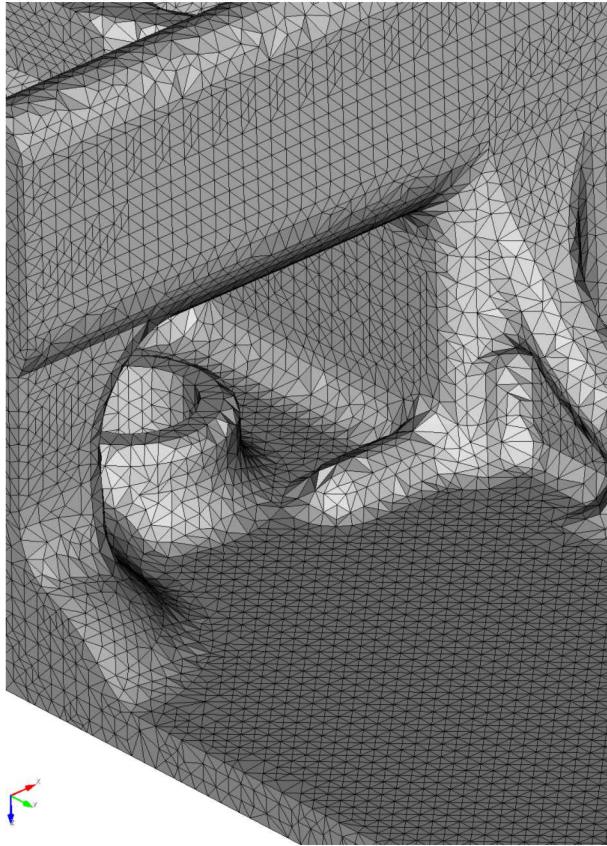
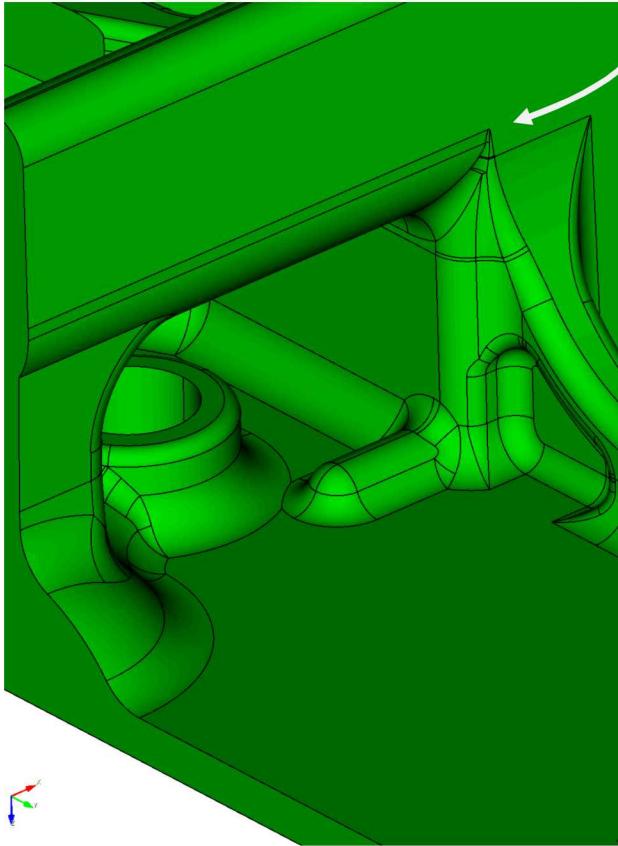


## Difficult to mesh parts:

Parts with complex geometry and/or small geometry features  
geometry with curve tangency points, acute angles between curves/surfaces  
Geometry with issues/errors (not water tight, topology errors, non-physical)

# NGS automated meshing

capture features larger than specified length-scale  
and “ gracefully ” ignores smaller features



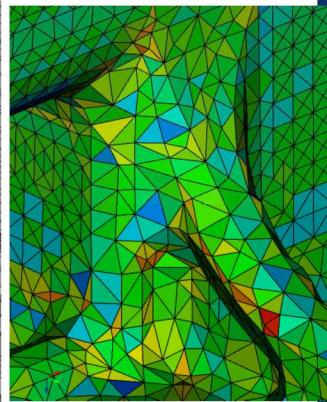
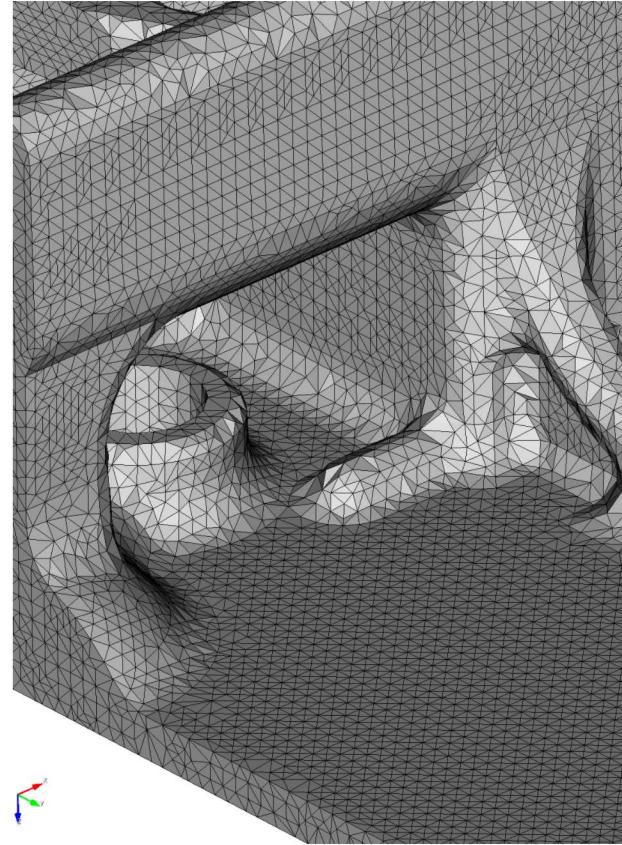
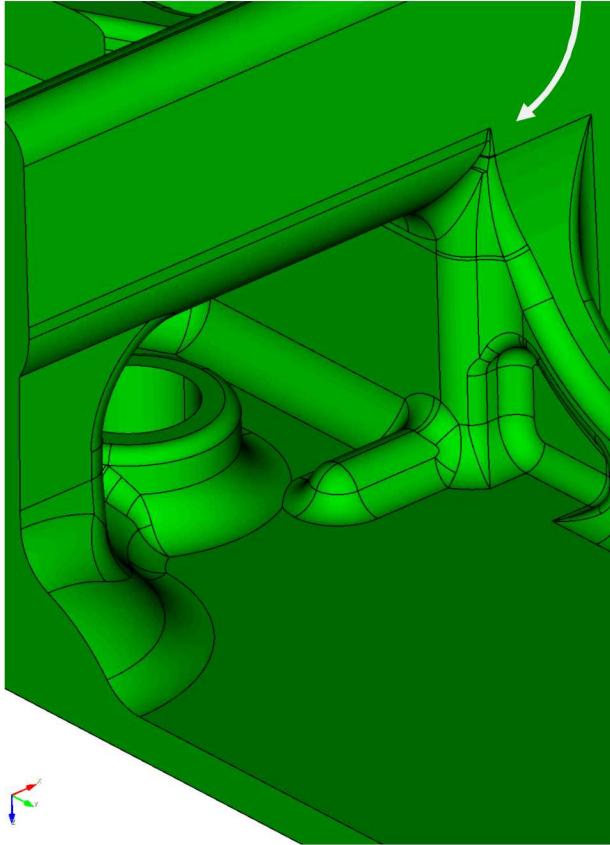
with guaranteed  
element quality

## Key algorithm step:

Geometry agglomeration (using graph theory) for too much geometry in a cell.  
Allows Nodes, edges and faces to straddle-over small geometric features

# NGS automated meshing

capture features larger than specified length-scale  
and “ gracefully ” ignores smaller features



## Key algorithm step:

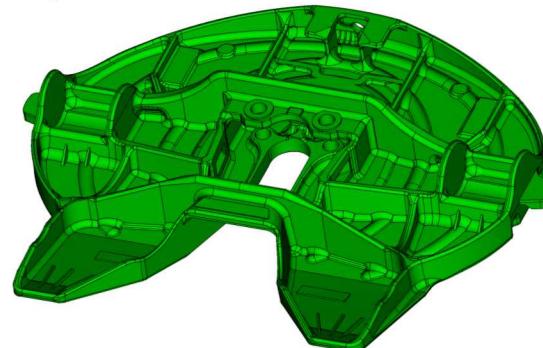
Geometry agglomeration (using graph theory) for too much geometry in a cell.  
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# NGS embedded credibility

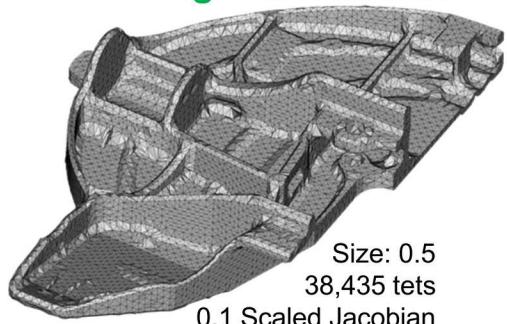


provide credibility evidence:

solution verification,  
quantity-of-interest & sensitivities,  
reproducibility

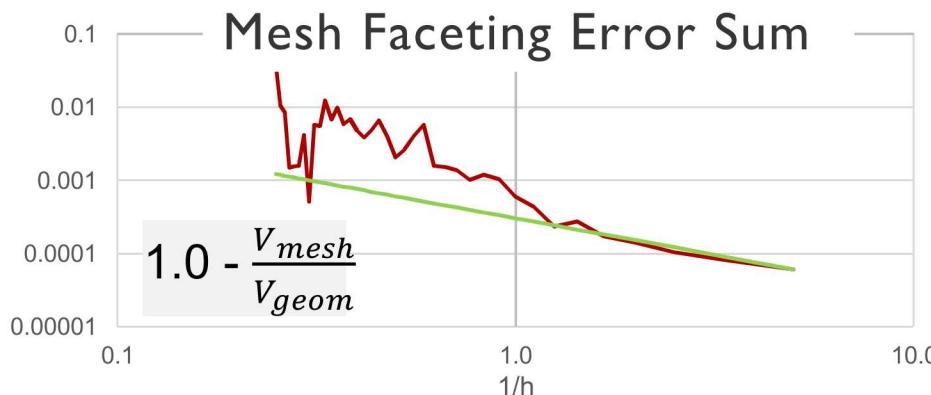
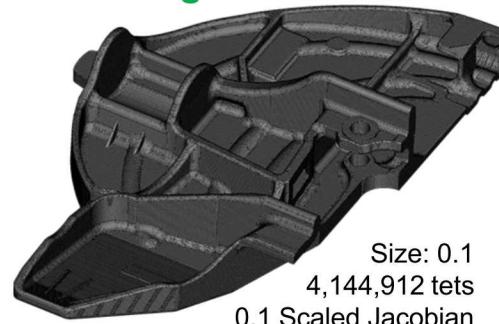


Meshing TAT: 3 minutes



Sequence of  
refined meshes  
➡

Meshing TAT: 50 minutes



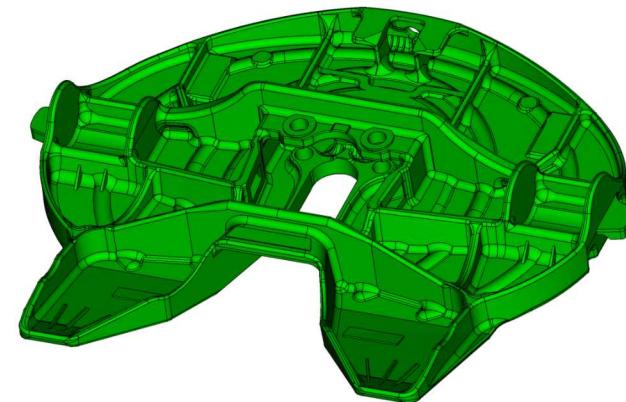
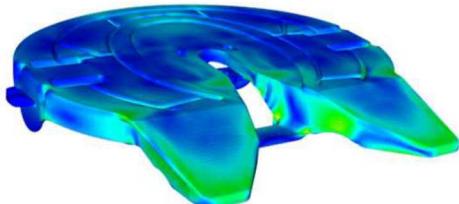
# NGS embedded credibility



## provide credibility evidence:

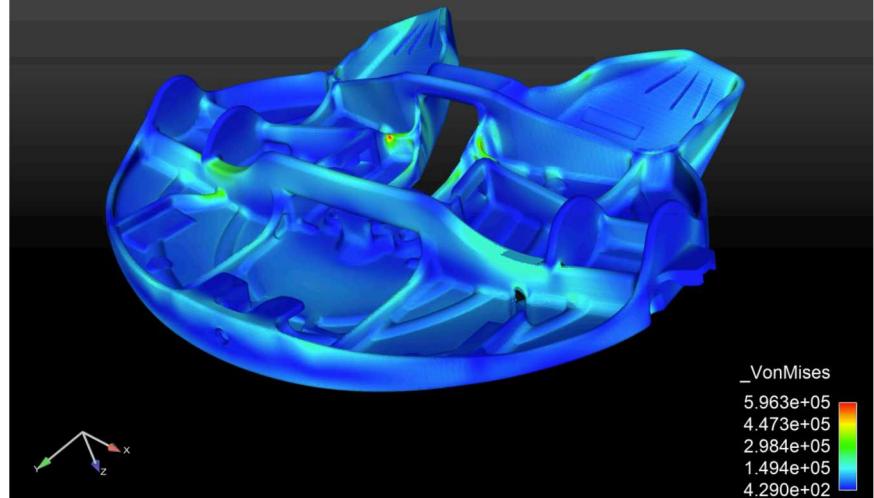
solution verification,  
quantity-of-interest & sensitivities,  
reproducibility

Thermal,  
Structural Dynamics and  
Solid Mechanics  
analyses supported



## Structural Dynamics modal analysis

Time = 30.068623

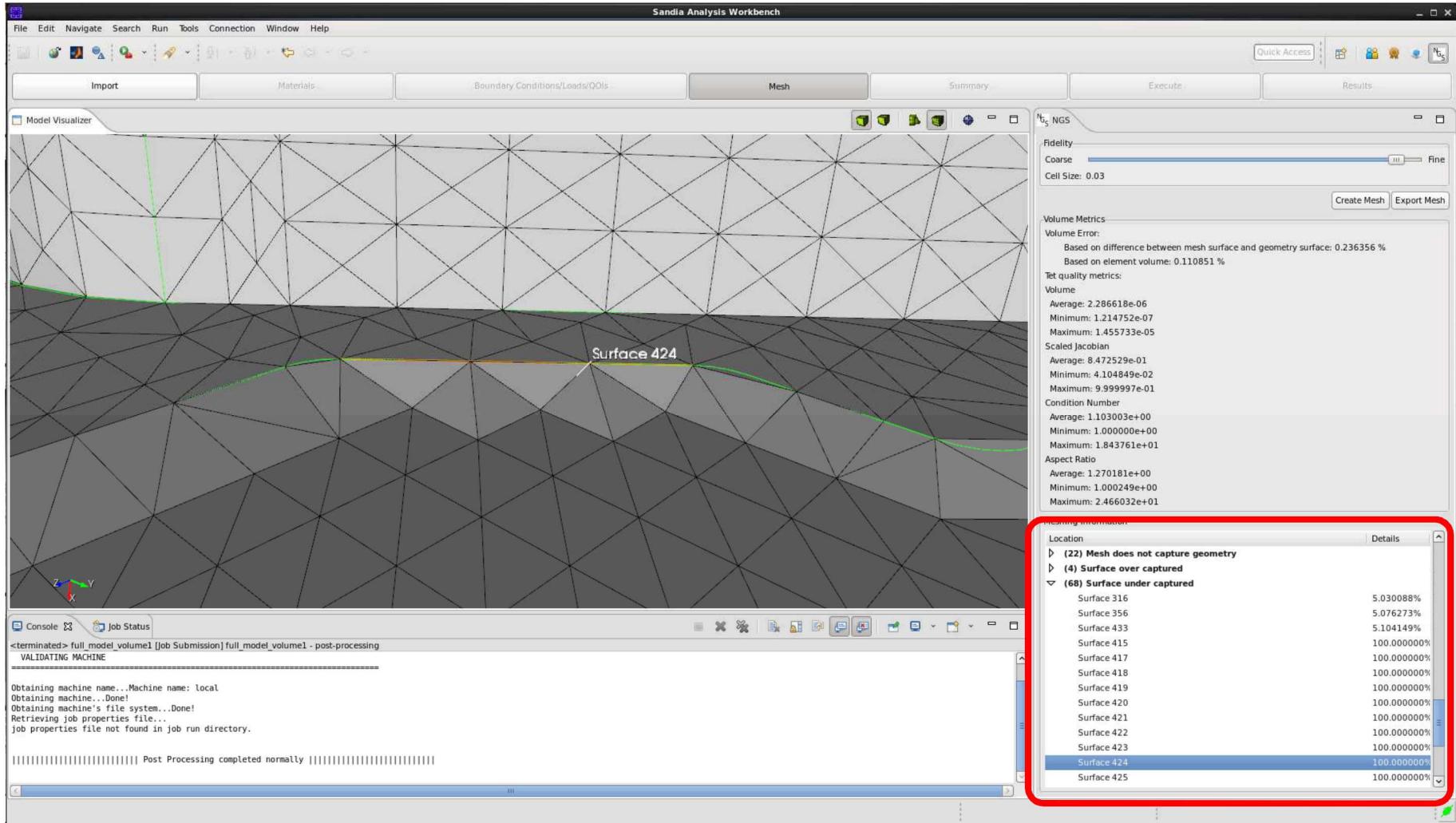


# NGS User experience

UI is simple, context-specific

Interaction with User is about 'Features of interest' (not on the mesh quality)

User attributes geometry directly

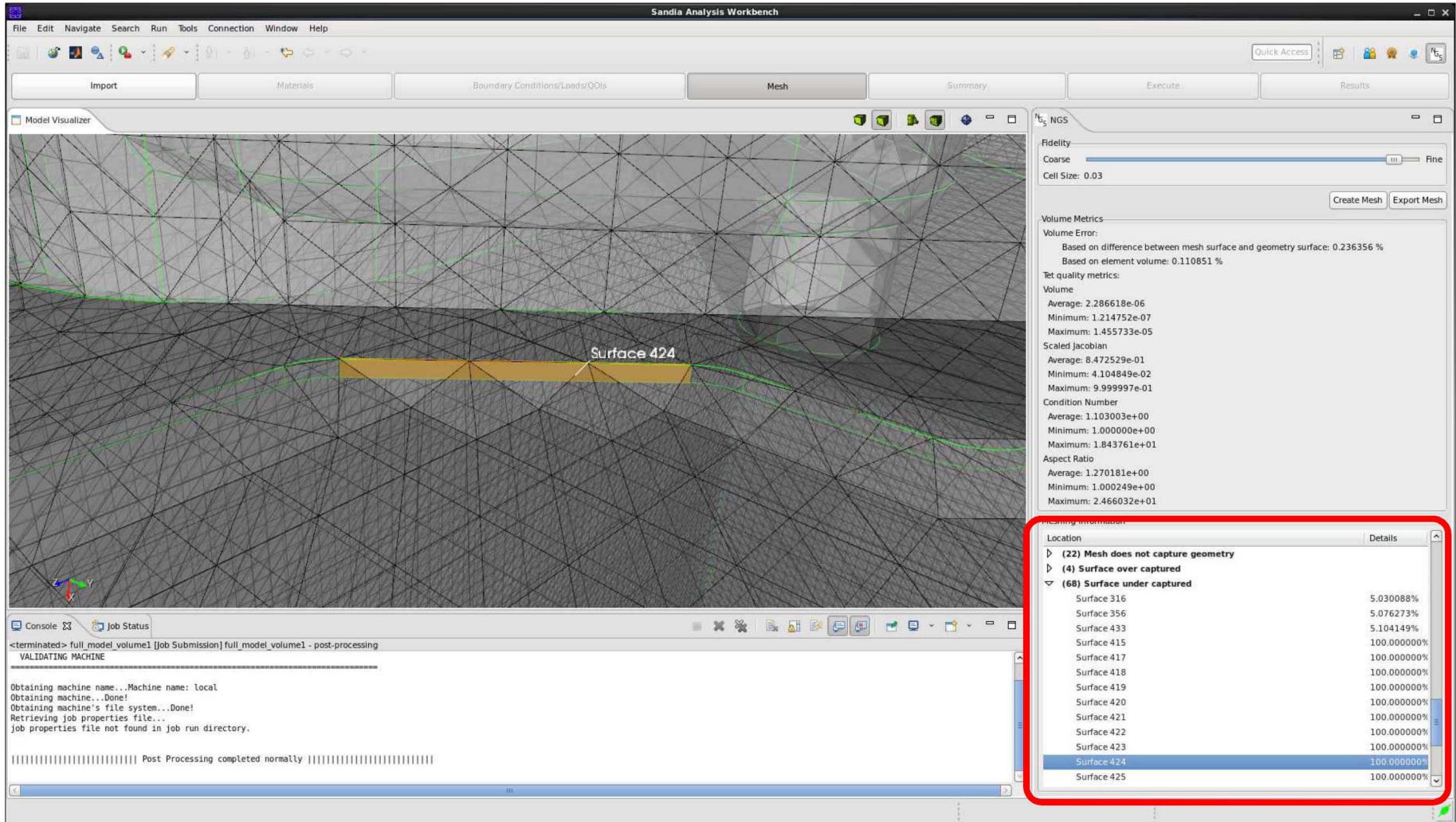


# NGS User experience

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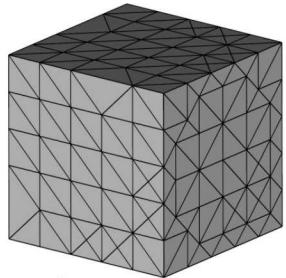


# NGS: current meshing directions

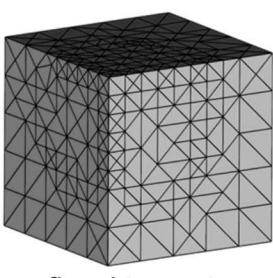


## Adaptivity

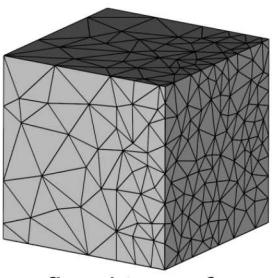
arbitrary overlay grids



uniform



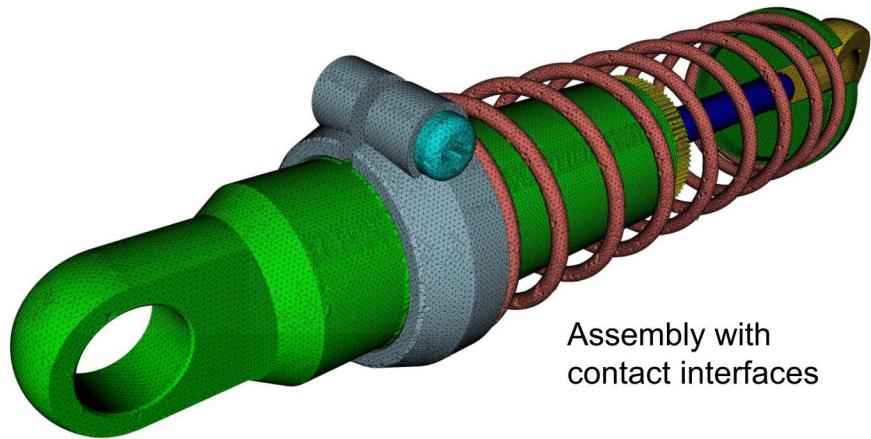
refined to vertex



refined to surface

## Assemblies

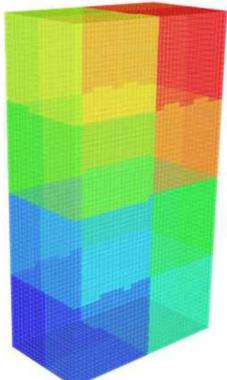
Interfaces, enclosures



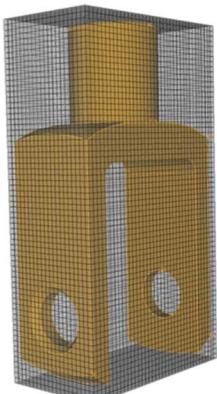
Assembly with contact interfaces

## Parallel

performance & scalability



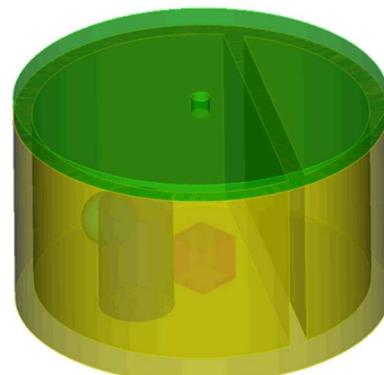
Overlay grid spread across processors



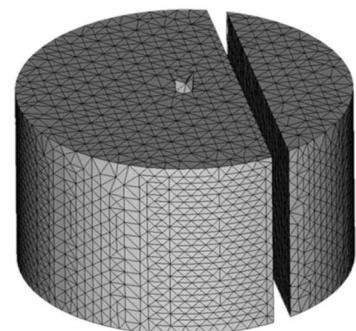
Parallel Morph algorithm



Re-balance for parallel physics simulation



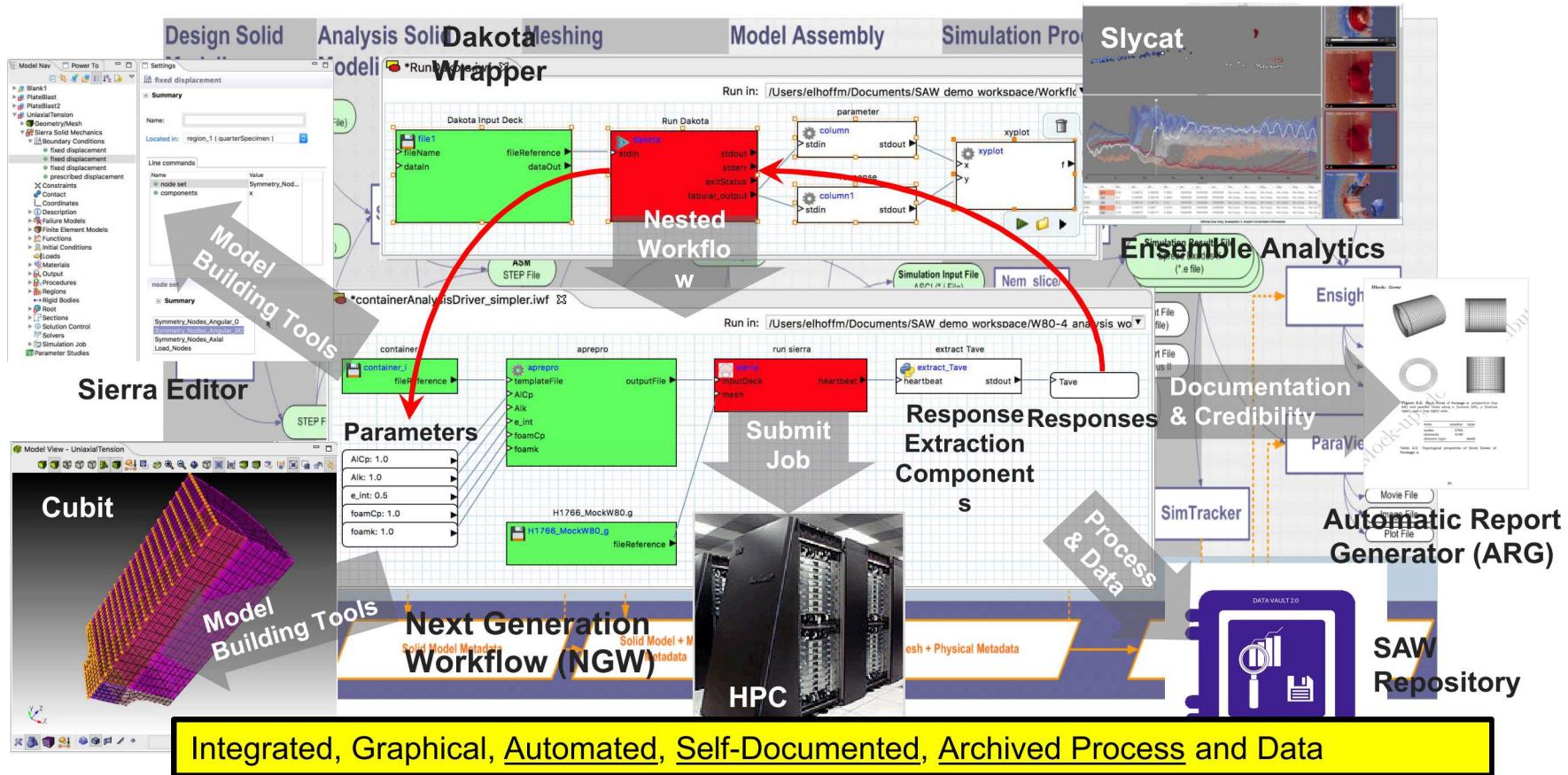
Can Assembly with Interior Enclosures



Mesh of Enclosure

# Integrated Workflow

Sandia Analysis Workbench (SAW) Parametric Analysis Workflow Platform



# Transforming Engineering Science Analysis

- Demonstrates production-level analysis and credibility workflow to accelerate T-A-T
  - 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:

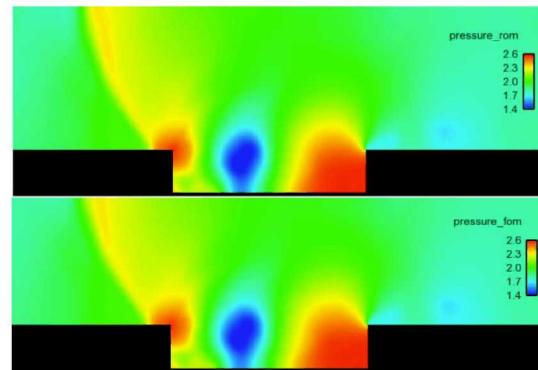
- *Goal:* better integrate **computational simulation** and **QMU**
- *High-fidelity models:* **expensive**
- *Typical surrogates:* **physics-blind, not robust, poor epistemic UQ**

### ■ 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**

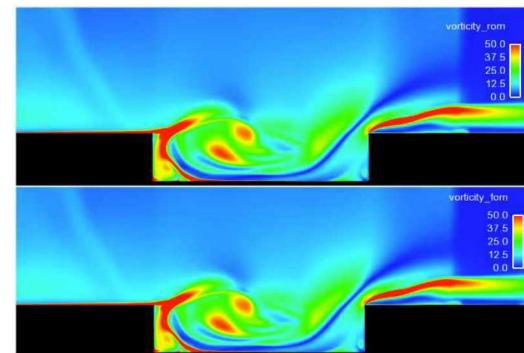
**ROM**

*32 min, 2 cores*



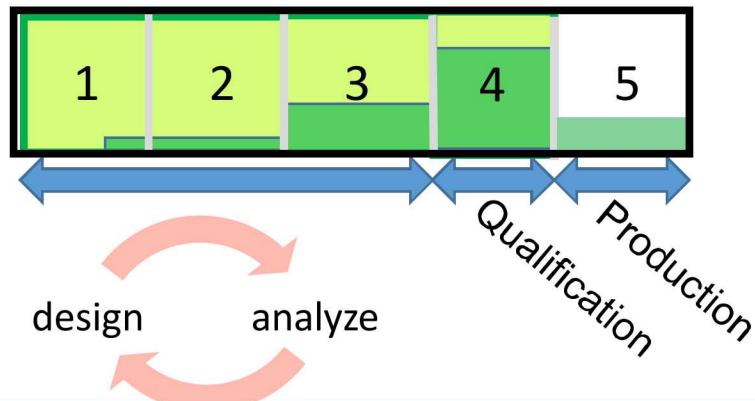
**Pressure field**

**High-fidelity model**  
*5 hours, 48 cores*



**Vorticity field**

# Summary: Meeting the **Challenge** of future agile Engineering Capability



Transform ModSim to *enable* Fast Cycles of Learning  
already in the conceptualization phase

- ② Tet meshing is automated & part of the FEM solver  
enabled by 100x LDRD break-thru discretization technology
- ② User focus is on the analysis goals!!..... not the meshing!!  
workflow usability, by today's standard
- ② Solution credibility is transparently known and easy to generate  
maintain & encourage expert judgement of our analysts

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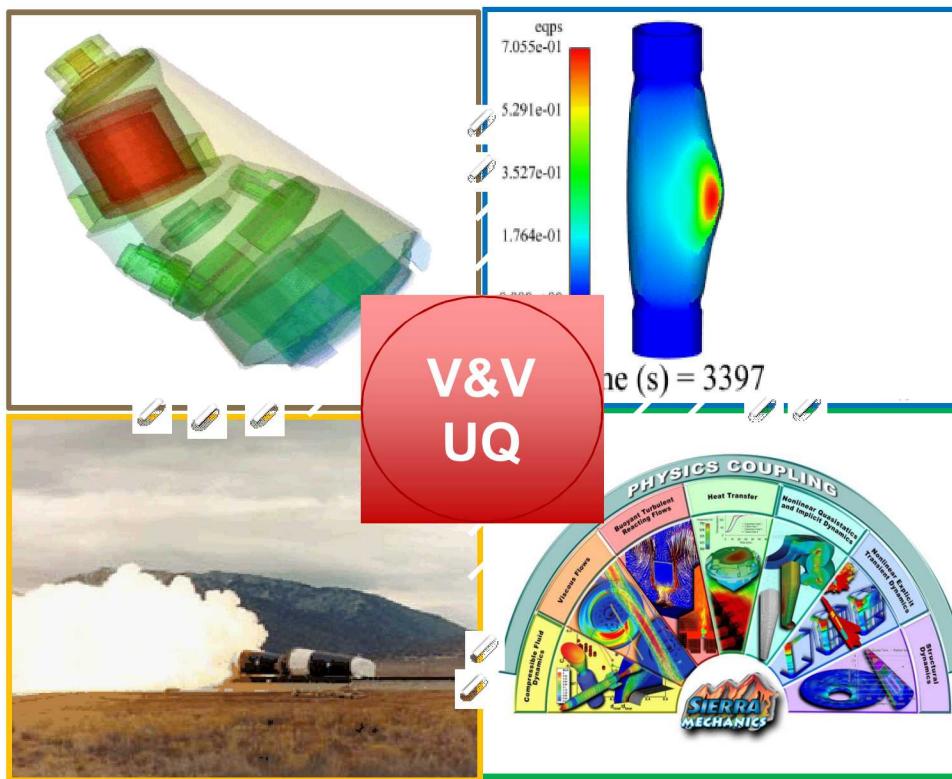
# THANK YOU

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# Environmental Tests and Computational Simulation *Capabilities Required to Design, and Qualify the Stockpile*

Integrated theory, computational simulation and experimental discovery/validation across length and time scales is critical to develop the technical basis for complex systems.

# Engineering Analysis



# Environmental Simulation & Test

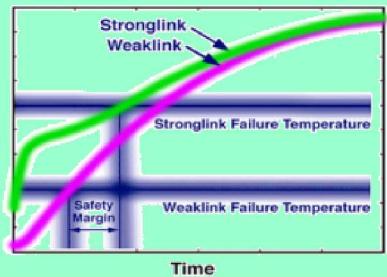
# Engineering Science Physical Phenomena

# Computational Simulation Technology

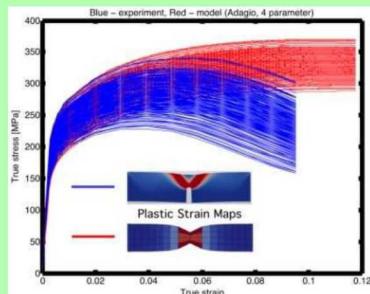
# The NNSA Advanced Simulation and Computing (ASC) program for Engineering Sciences capability development

## Defense Applications and Modeling

### Integrated Codes (IC)



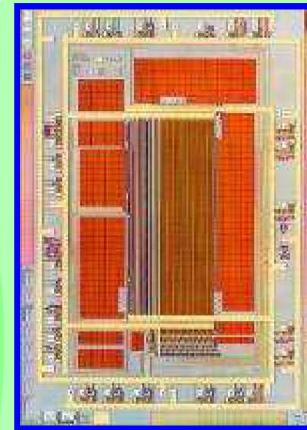
### Verification and Validation (V&V)



### Physics and Engineering Models (P&EM)

## Computing

### Computer Science and Software Engineering (CSSE)



### Facility Ops and User Support (FOUS)



## Advanced Technology Development and Mitigation (ATDM)