SAND2020-1365C

Sandia National Laboratories

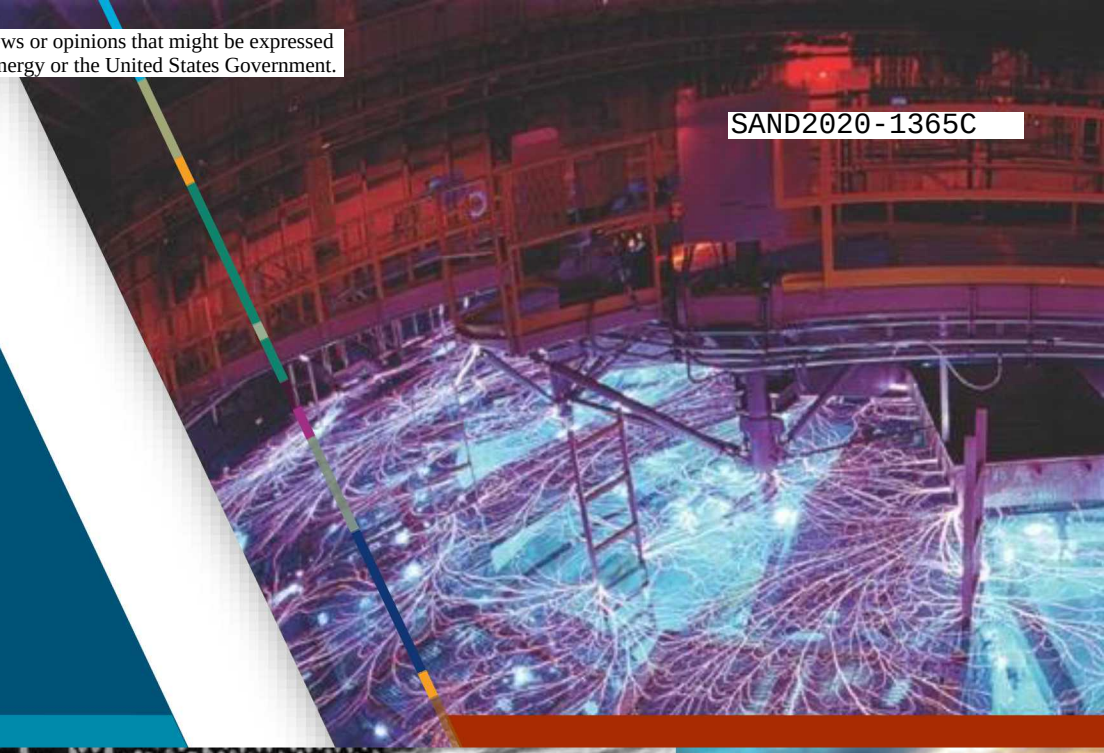
Exceptional service in the national interest

Artificial Intelligence for Scientific and High Performance Computing at Sandia

John Feddema, Sr. Manager, Enhanced Decision Making Group
Sandia National Laboratories
jtfedde@sandia.gov

ASC™

SAND2020-XXXX



ENERGY NNSA

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.

PURPOSE STATEMENT DEFINES WHAT WE DO

Sandia develops advanced technologies to ensure global peace

NUCLEAR DETERRENCE

Responsibilities form a critical mandate

Warhead systems engineering & integration

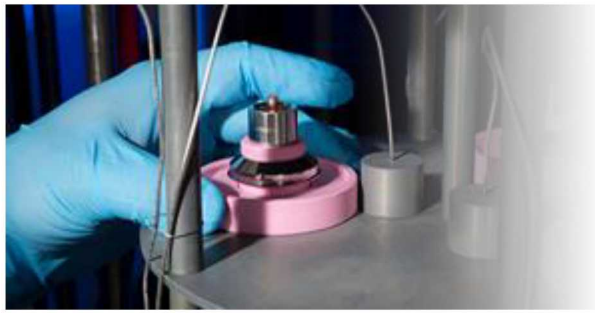
Design agency for nonnuclear components

- Gas transfer systems
- Radar
- Safety systems
- Arming, fuzing & firing systems
- Neutron generators

Multidisciplinary capabilities

Required for design, qualification, production, surveillance, computation/ experimentation

- Major environmental test facilities & diagnostics
- Materials sciences
- Light-initiated high explosives
- Computational analytics

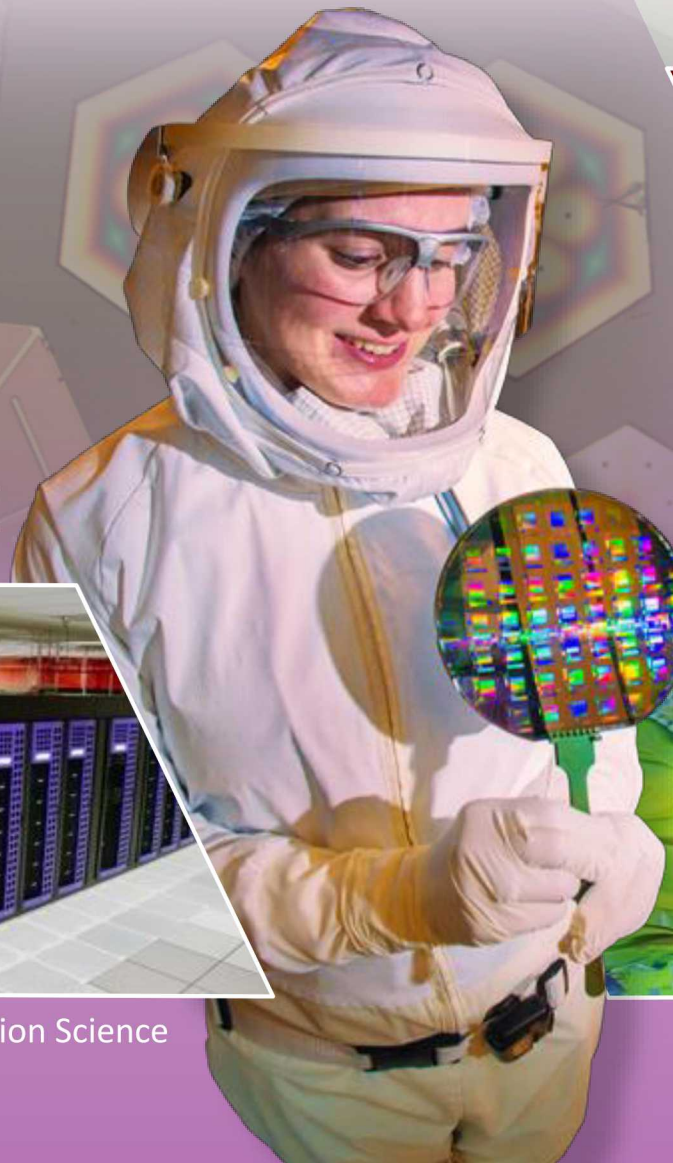


Production agency

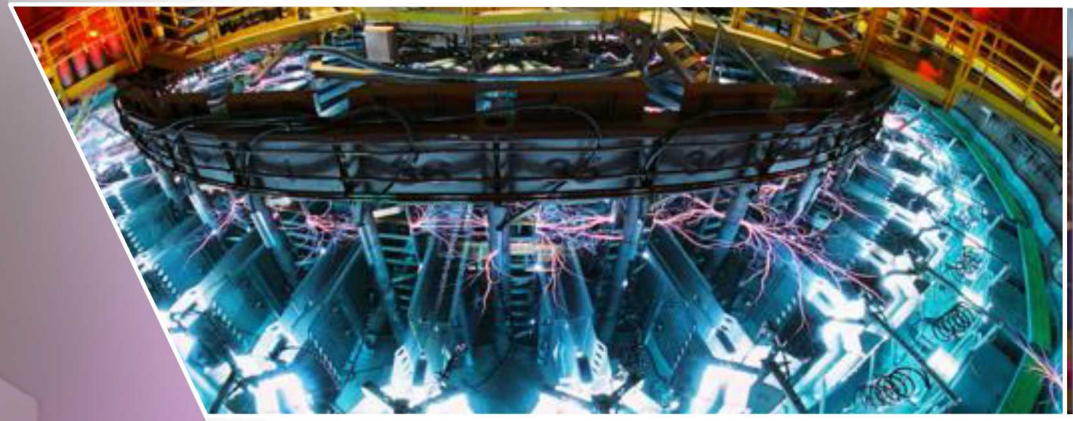
- Neutron generators
- Sandia external production
- Microelectronics
- Thermal battery backup

ADVANCED SCIENCE & TECHNOLOGY

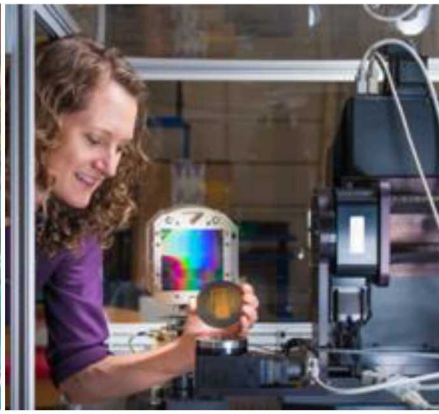
Research Foundations play an integral role in mission delivery



Nanodevices & Microsystems

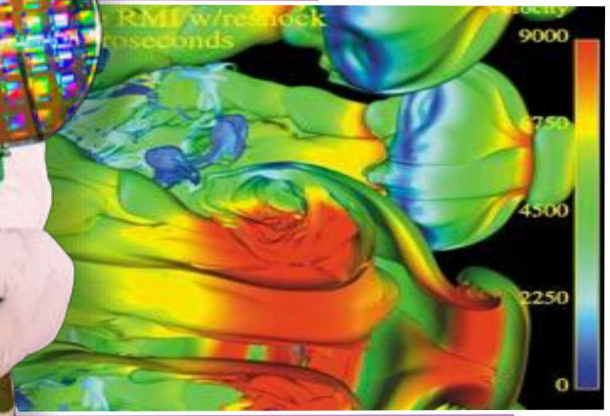


Radiation Effects & High Energy Density Science



Materials Science

Computing & Information Science

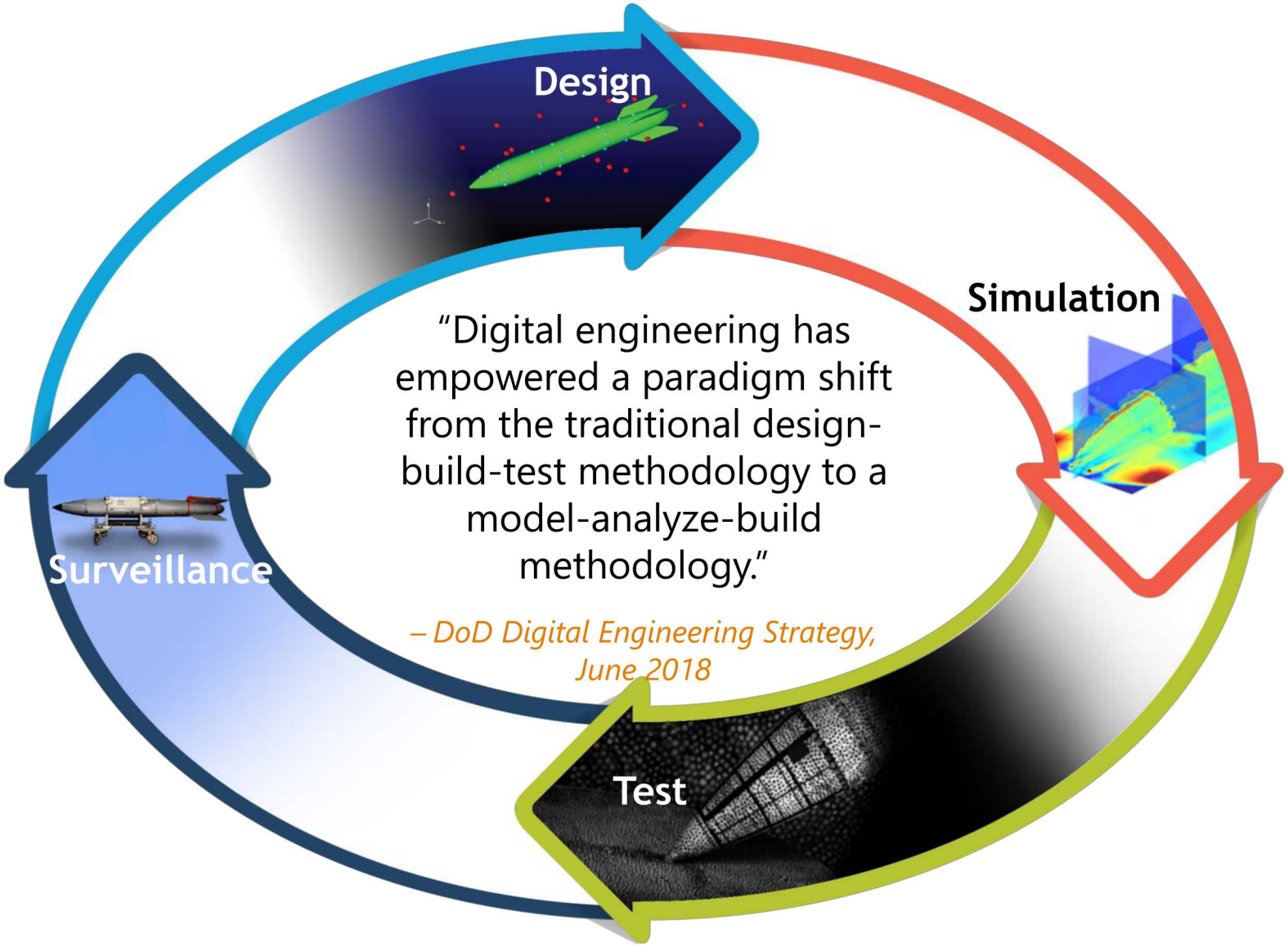


Engineering Science

Geoscience

Bioscience

A Digital Engineering Strategy will Enable Transformational Goals

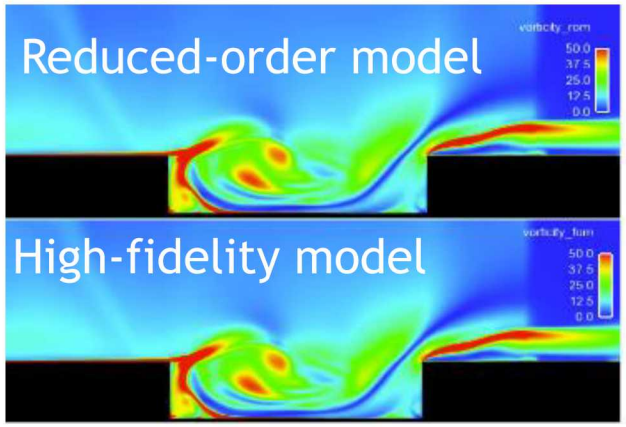


Transformative Goals

- Reduce the design cycle time
- Increased production throughput
- Re-think the surveillance program for the 21st century

Machine Learning will Enable Efficiencies

Faster Reduced Order Models

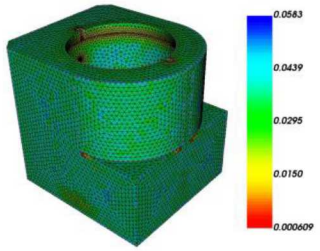


Turbulent flow vorticity field

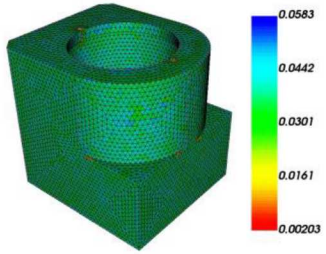
- Runtimes are 100-1000 times faster and are only 1% less accurate than the high-fidelity simulations
- Can predict errors with validated statistical properties

Automated Meshing of Components

Before ML = 1,45M tets



After ML = 215K tets



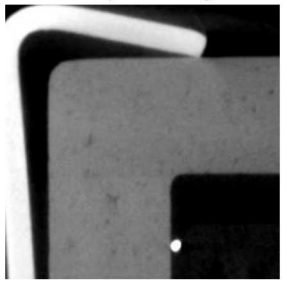
- ML techniques rank geometry-modification operations (defeaturing) by their likelihood of yielding a meshable model
- Reducing the number of tetrahedrons, reduces the execution time of the simulation

Diagnosing HPC Performance Variation

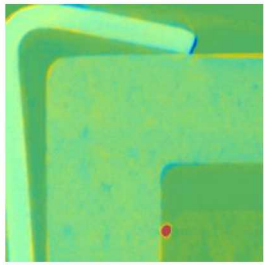
- ML algorithm based on CPU, memory, and network usage data outperforms existing methods
- Storage overhead reduced to less than 10%
- Computation overhead below 1% of a single core

Discovering Anomalies in High-Reliability Components

Query image



Anomaly detection



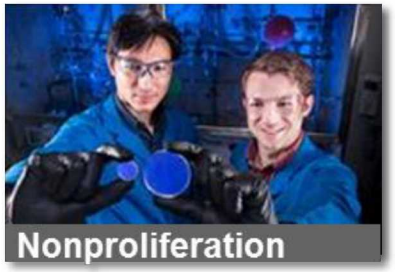
X-Ray CT scan of electronic component with defect

- Deep learning model finds anomalies in seconds that would take a human hours to find
- Entirely unsupervised anomaly detection

But is AI Trustworthy Enough for High Consequence National Security Applications?

Sandia's Unique Mission Needs

- **High-confidence decisions**
  - Typically designing to "Five 9's" of reliability
  - Need to assure trust in our solutions
  - Need to understand uncertainty of decisions
  - Algorithms need to be explainable
- **Applications may consist of large volumes of simulation data but often only small volumes of experimental data**
  - First principles physics may be known, or not
  - Multiple data sources – measured, observed and simulated – with limited, unknown, or no ground truth (no labeling and little to no positives).
- **Some Sandia national security missions require decisions to be made in a very short time frame (milliseconds to minutes) while other missions have longer time frames (hours to days)**
- **Need to account for potential adversarial issues**



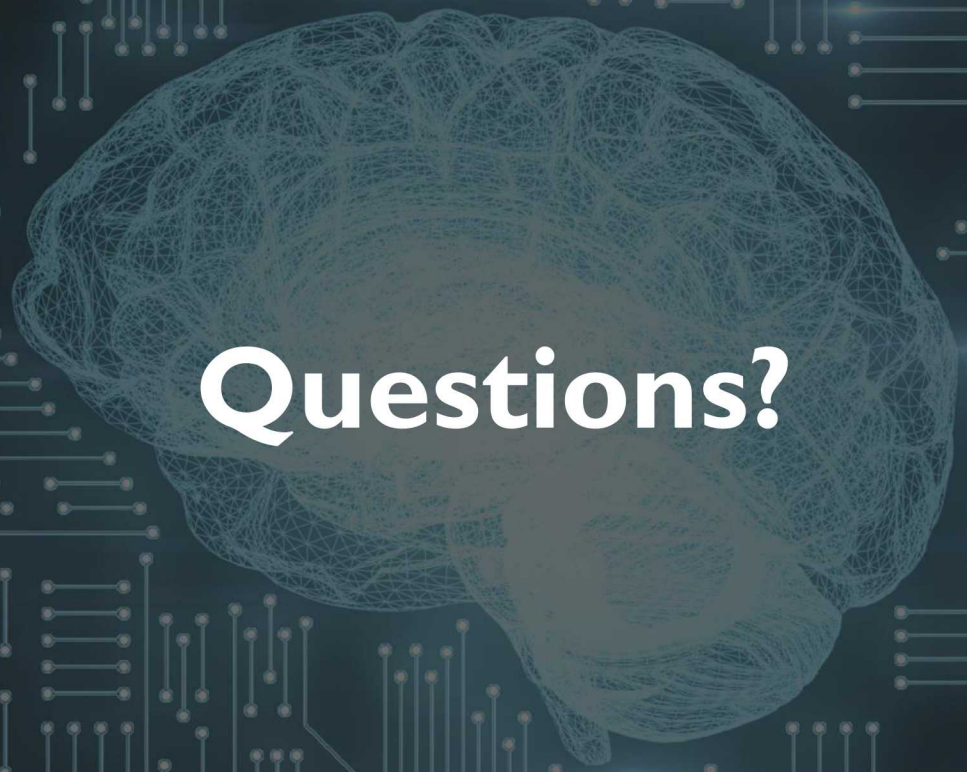
Sandia's 5-Year Trusted AI Research Initiative

Sandia is investing in the following research:

- ***Mathematical foundations of AI/ML*** – **mathematically rigorous** approaches **to understand high-consequence decisions**
- ***AI/ML Uncertainty Quantification*** – **uncertainty propagation and quantification at all stages** of the modeling and learning process (data uncertainties, labeling uncertainty, model selection, meta-parameter uncertainty, …).
- ***Domain-Informed AI/ML*** – mathematically rigorous and principled frameworks for **incorporating physics, engineering, and/or human expertise** into the AI/ML workflow; as well as **rigorous approaches to combine data from physical measurement** with predictive computational models.
- ***AI/ML with Limited or Poor-Quality Data*** – techniques that **enable learning from small, sparse, incomplete, noisy, unknown pedigree, or unlabeled datasets** Methods that enable extrapolation from previously observed data or can identify never-before seen patterns, rare events, or mathematical relationships.
- ***Adversarial AI/ML*** – understanding of mechanisms by which an adversary can tamper with data streams to commit obfuscation or sabotage. **Learning techniques to counter these attacks** that identify potential subversions or are **resilient to tampering**

Summary

- Machine learning will provide new capabilities for scientific and engineering applications
  - Reduced order surrogate models for scientific/engineering problems
  - For agility of application workflows (automating processes)
  - Ability to identify anomalies and regions of interest in inspection and surveillance data
  - Correlating and certifying simulation and experimental results
  - As a supplement for physics models, ML might help us learn what is wrong/missing in physics models and aid in experimental design
- Machine learning will provide new capabilities for HPC system administrators, facilities, and dev-ops
  - Help model complex behaviors (e.g., failures, degradation, energy)
  - Automate/adapt usage to comply with more complex policy (e.g., energy consumption)
- However, trusted AI research is needed to apply AI to high consequence national security applications, and Sandia is starting a new initiative in this area.



Questions?