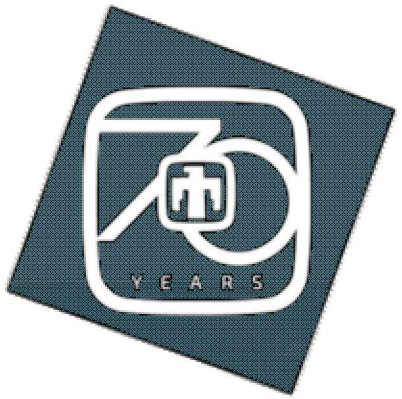
SAND2020-10970PE

# Overview of Sandia and ASC Program




PRESENTED BY

**S. Scott Collis,** Director Computing Research and Director Sandia ASC Program



Approved for Programmatic Release: 2020 PSAAP-III Kickoff Meeting, 8/14/2020

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.

# Outline

**Brief Introduction to Sandia**

- Budget, staffing, lab strategic priorities
- How does ASC fit in? Advanced Science & Technology

**ASC Program at Sandia**

- Integration across organizational lines
- Research areas, strategic initiatives, priority research directions

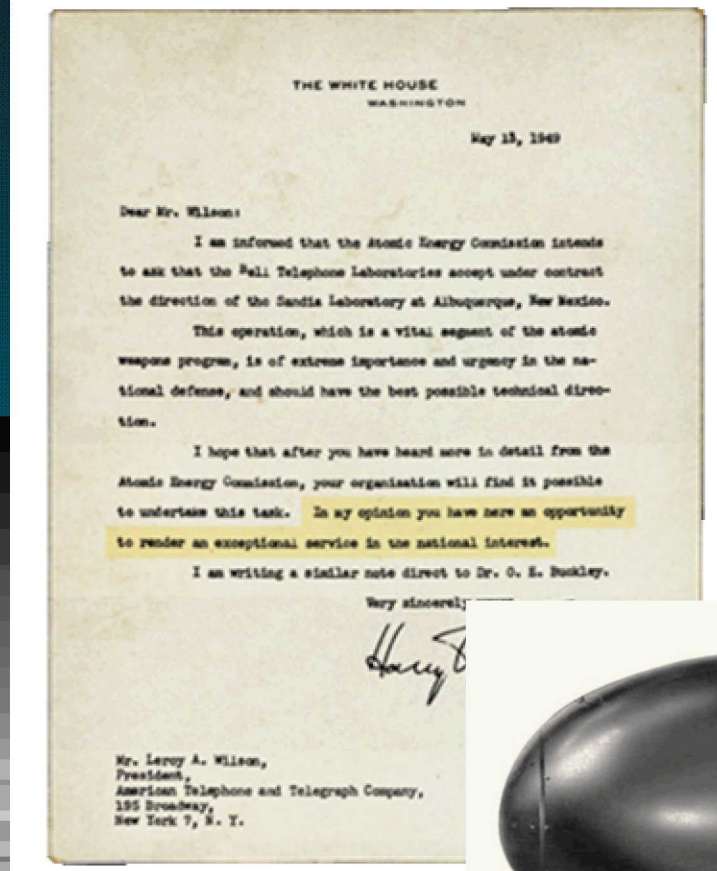
**PSAAP III**

- AST, CRT, TST and RT Members
- Thoughts on collaboration opportunities
- Sandia's Goals for PSAAP III

# SANDIA'S HISTORY IS TRACED TO THE MANHATTAN PROJECT

*…In my opinion you have here an opportunity to render an exceptional service in the national interest.*

- July 1945
  Los Alamos creates Z Division
- Nonnuclear component engineering
- November 1, 1949
  Sandia Laboratory established
- AT&T: 1949–1993
- Martin Marietta: 1993–1995
- Lockheed Martin: 1995–2017
- Honeywell: 2017–present



THE WHITE HOUSE
WASHINGTON

May 13, 1949

Dear Mr. Wilson:

I am informed that the Atomic Energy Commission intends to ask that the Bell Telephone Laboratories accept under contract the direction of the Sandia Laboratory at Albuquerque, New Mexico.

This operation, which is a vital segment of the atomic weapons program, is of extreme importance and urgency in the national defense, and should have the best possible technical direction.

I hope that after you have heard more in detail from the Atomic Energy Commission, your organization will find it possible to undertake this task. In my opinion you have here an opportunity to render an exceptional service in the national interest.

I am writing a similar note direct to Dr. O. E. Buckley.

Very sincerely

Mr. Leroy A. Wilson,
President,
American Telephone and Telegraph Company,
195 Broadway,
New York 7, N. Y.


# OUR PRIORITIES CREATE A VISION FOR THE FUTURE


- Deliver **quality engineering, science, and technology** in the most efficient way possible
- **Safety and security** are top of mind
- **Collaboration** is vital – inside and outside the Labs
- Sustain a **diverse and inclusive** Laboratories culture
- **Think strategically:** What might the world look like in 20 to 30 years?

# SANDIA HAS FACILITIES ACROSS THE NATION

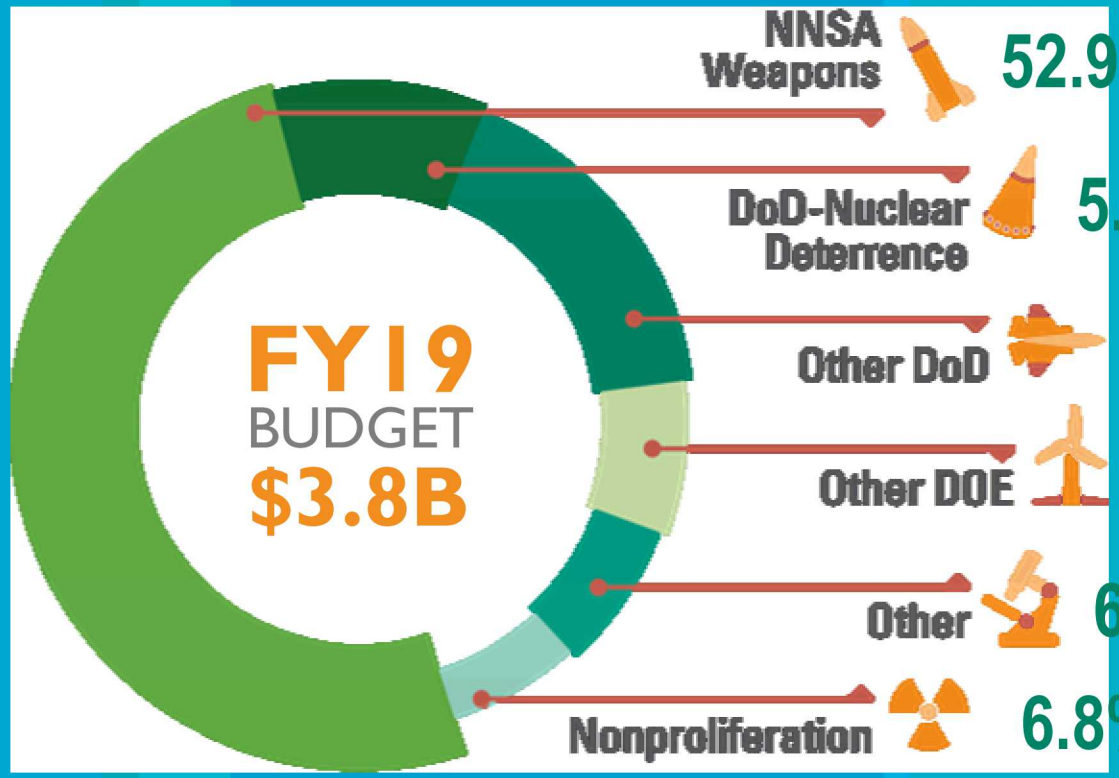
## Activity locations

- Kauai, Hawaii
- Waste Isolation Pilot Plant, Carlsbad, New Mexico
- Pantex Plant, Amarillo, Texas
- Tonopah, Nevada

## Main sites

- Albuquerque, New Mexico
- Livermore, California

# SANDIA'S BUDGET COVERS A BROAD RANGE OF GOVERNMENT AND OTHER WORK




**OTHER**

Department of Homeland Security
Other federal agencies | Nonfederal entities
CRADAs, licenses, royalties | Inter-entity work

**DoD**

Air Force | Army | Navy
Defense Threat Reduction Agency
Ballistic Missile Defense Organization
Office of the Secretary of Defense
Defense Advanced Research Projects Agency
Intelligence Community

**OTHER DOE**

Science
Energy Efficiency and Renewable Energy
Nuclear Energy
Environmental Management
Electricity Delivery and Energy Reliability
Other DOE

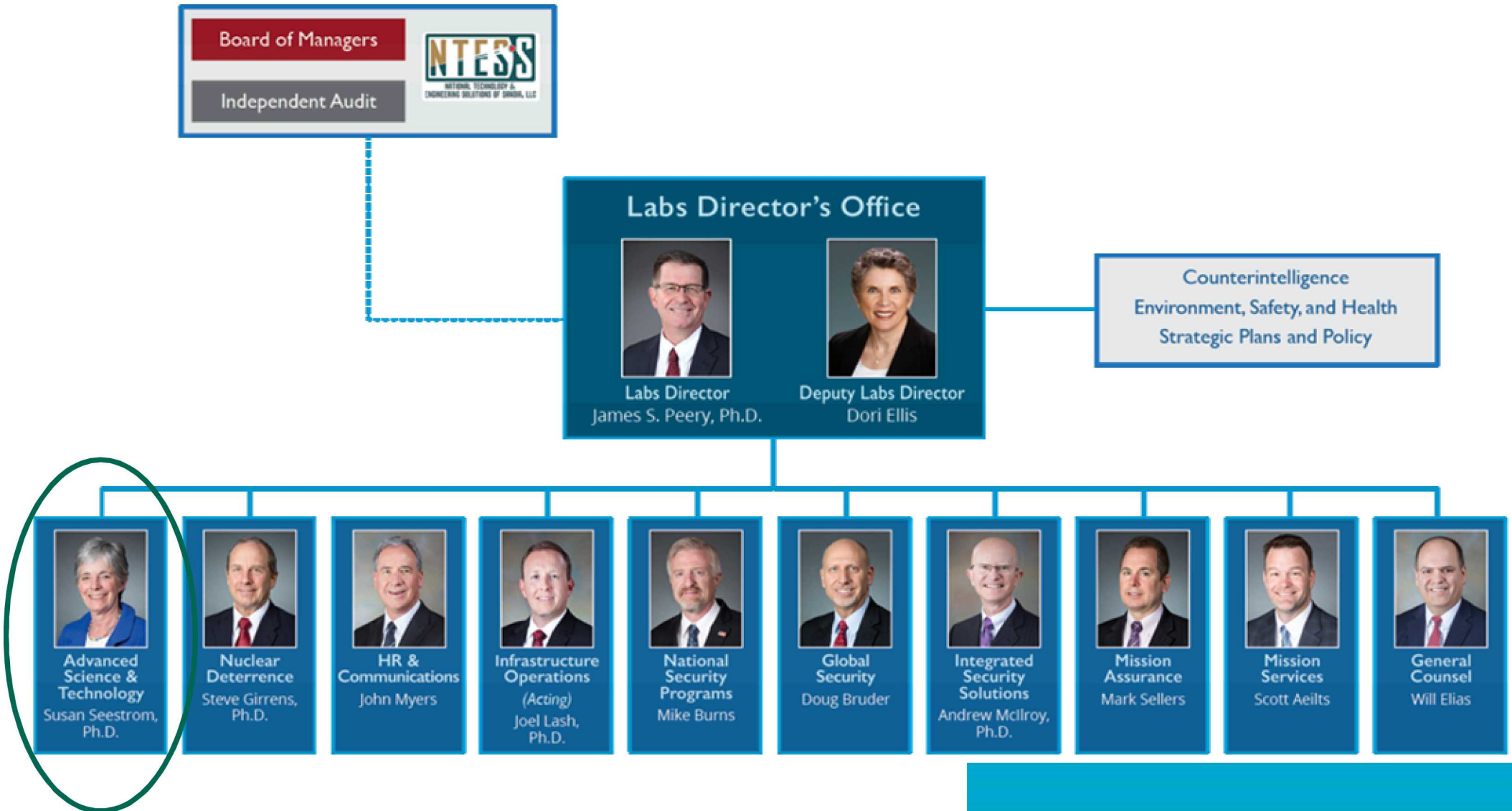
**NONPROLIFERATION**

NNSA/NA20 | State Department

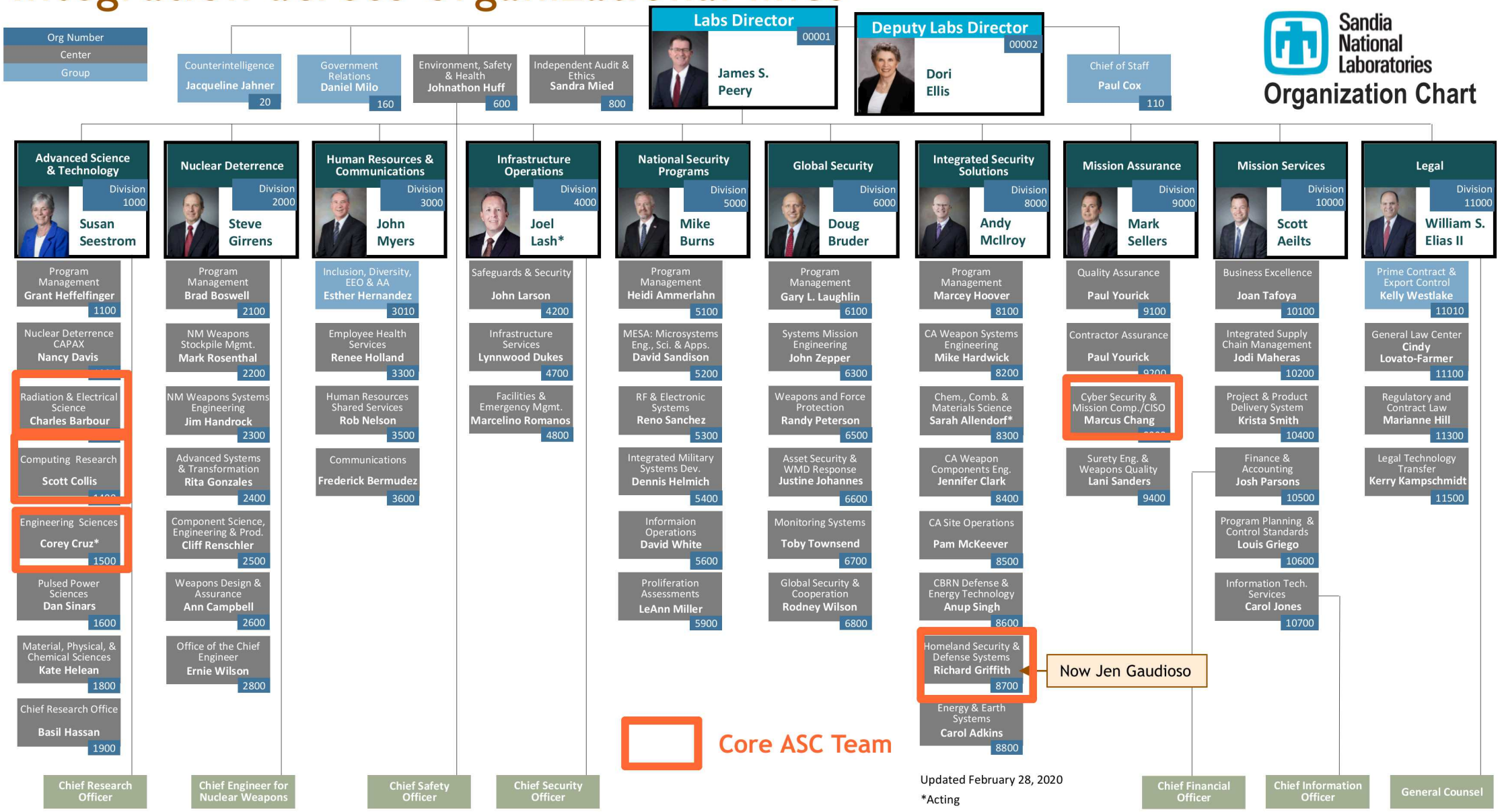
# SANDIA'S WORKFORCE

Staff has grown by over 5,000 since 2009 to meet all mission needs

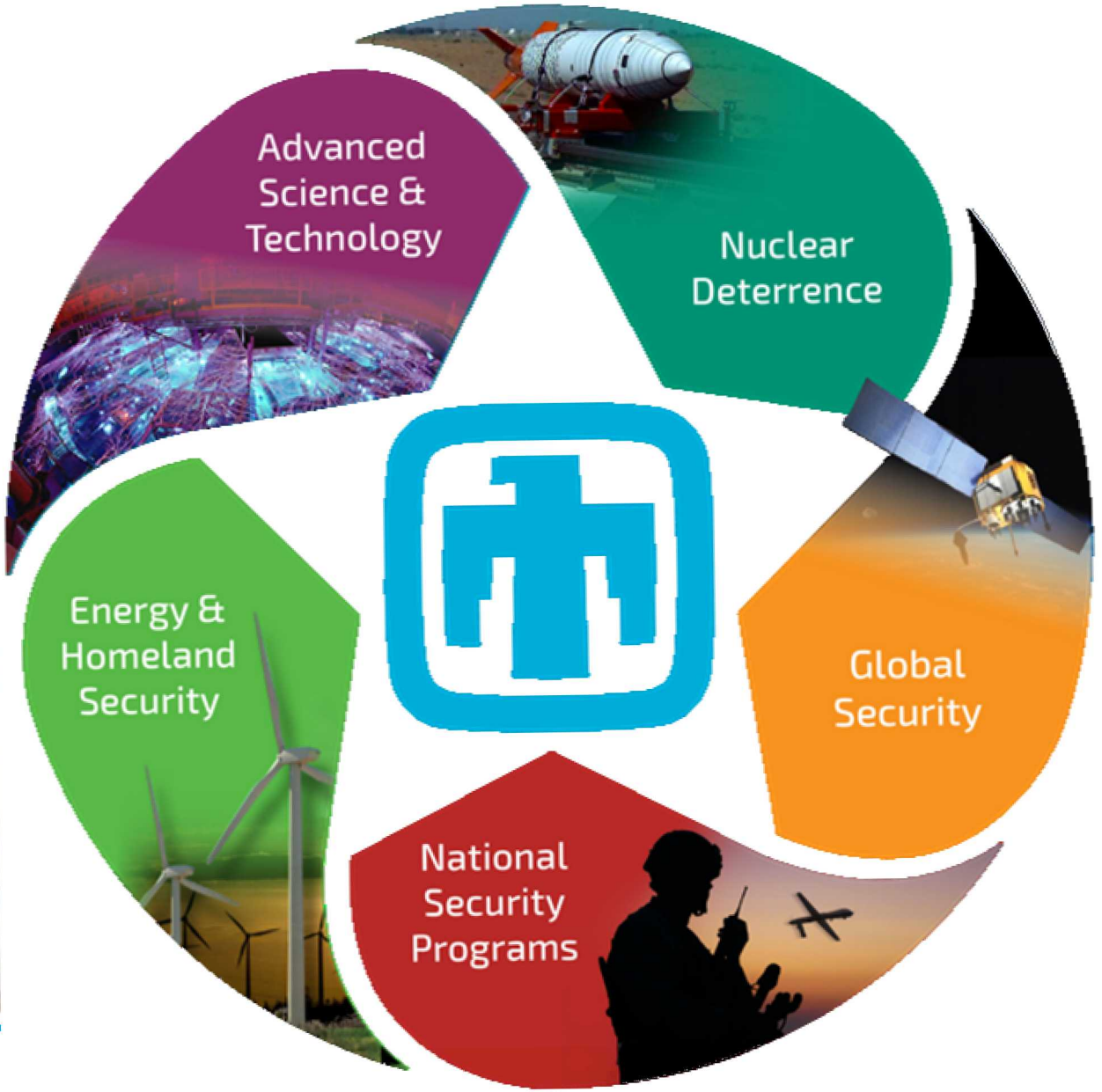
# THE LEADERSHIP TEAM BRINGS EXPERIENCE AND EXPERTISE IN MISSION AND MISSION-ENABLING DIVISIONS



# ASC Program
## Integration across organizational lines

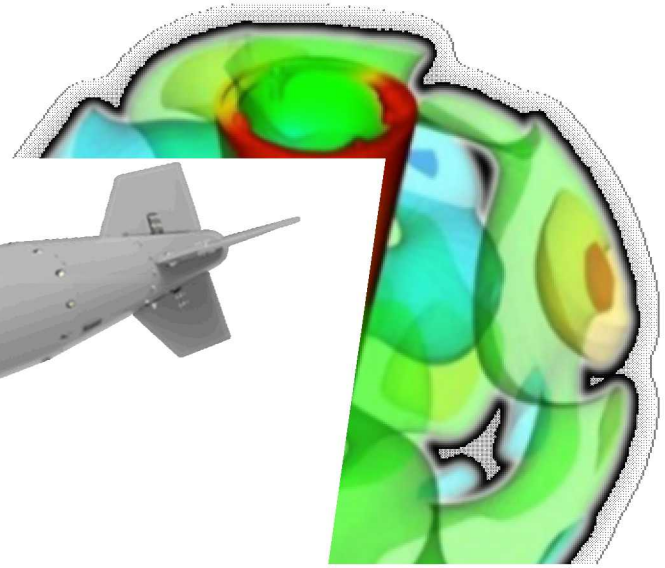


# SANDIA HAS FIVE PROGRAM PORTF




# NUCLEAR DETERRENCE

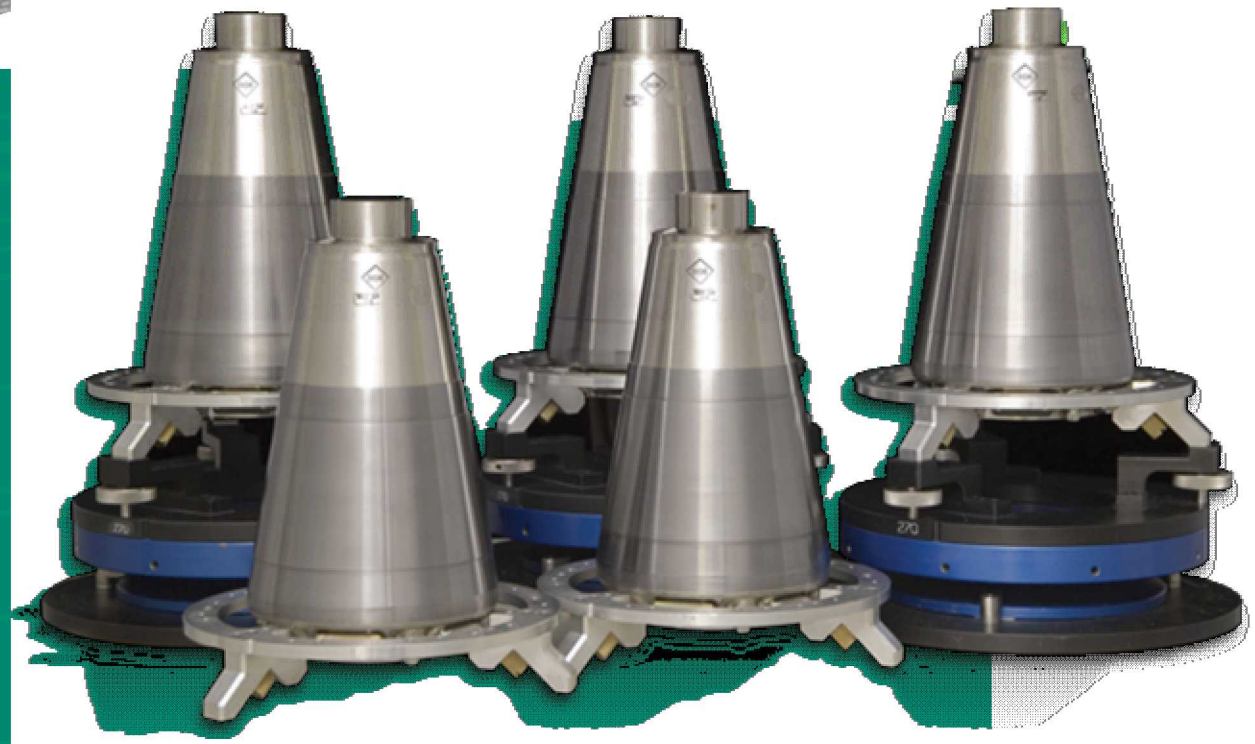
## Responsibilities form a critical mandate



### Warhead systems engineering & integration

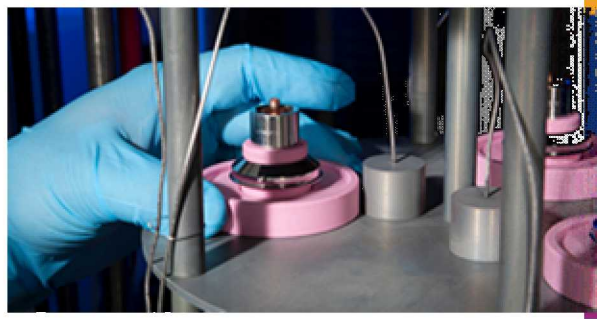
### tidisciplinary
### ıbilities

ired for design,
ication, production,
illance, computation/
imentation
ajor environmental test
ilities & diagnostics
aterials sciences
ght-initiated high explosives
mputation and Simulation



### Design agency for nonnuclear components

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



### Production agency

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

# GLOBAL SECURITY

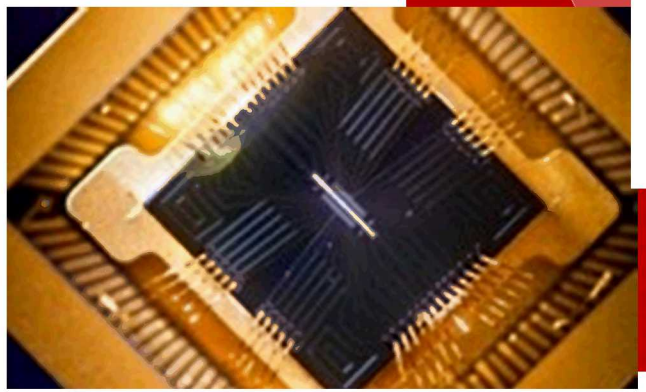
## Protect the nation from dangerous people and materials at home and abroad

- Develop space- and ground-based sensor systems for monitoring emerging threats
- Supply technology, crisis response, and training to respond to a crisis associated with weapons of mass destruction
- Provide capabilities for protecting U.S. nuclear weapons and materials at fixed sites and in transit
- Produce systems that deter proliferation and verify compliance with international agreements using space-borne and ground-based sensing technology
- Lead global technical engagement to prevent the misuse of nuclear, chemical, biological, and radiological materials

# NATIONAL SECURITY PROG

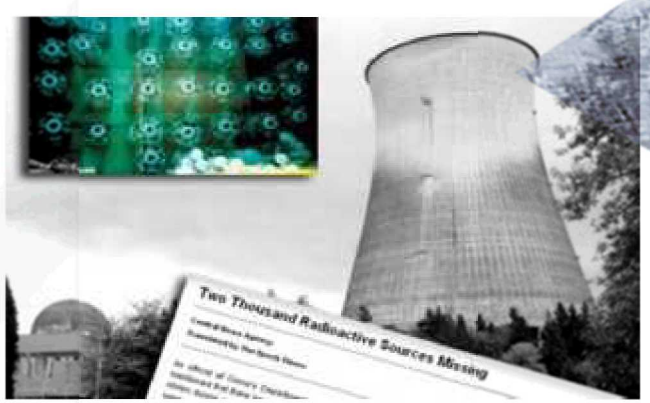
## Strengthens our nation's defenders

Information operations



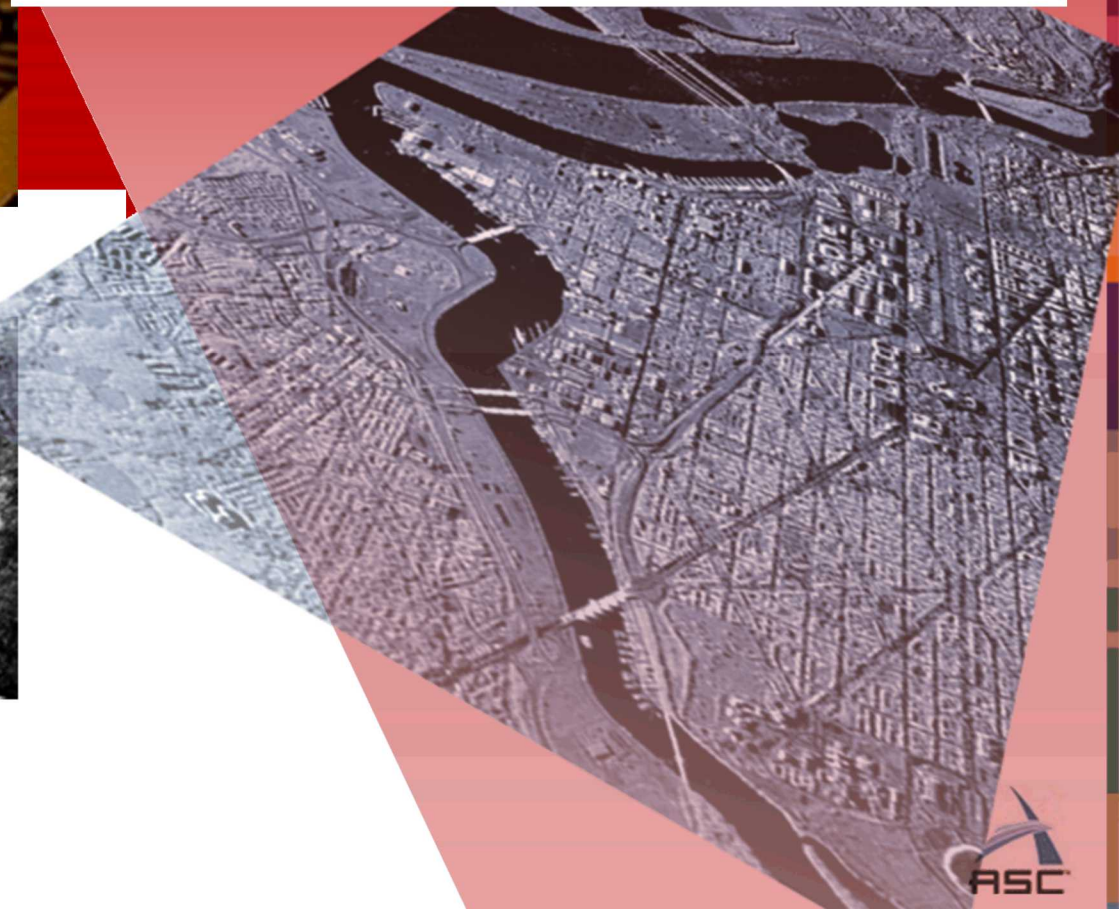
Science & technology products

Integrated military systems




Proliferation assessment

Surveillance &



# ENERGY & HOMELAND SECURITY

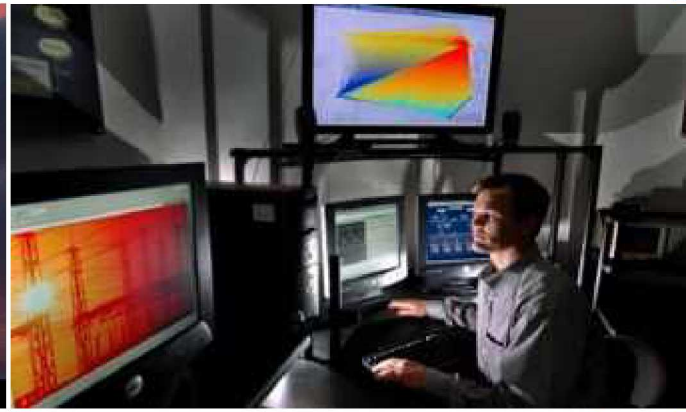
Innovates for a secure future

- Perform fundamental and applied R&D to support the resilience and security of the nation's energy system

Provide protection for our nation's digital and physical critical infrastructures

Reduce U.S. vulnerability to chemical, biological, radiological, and nuclear threats

Accelerate transformative innovations in the transportation sector through foundational physical and computational research



# ADVANCED SCIENCE & TECHNOLOGY (ALD: Susan Seestrom)

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

### WEAPONS SCIENCE & TECHNOLOGY

Provides Sandia with foundational science and engineering capabilities to ensure the nation's nuclear stockpile is safe, secure, and effective

AS&T Program Director: Grant Heffelfinger

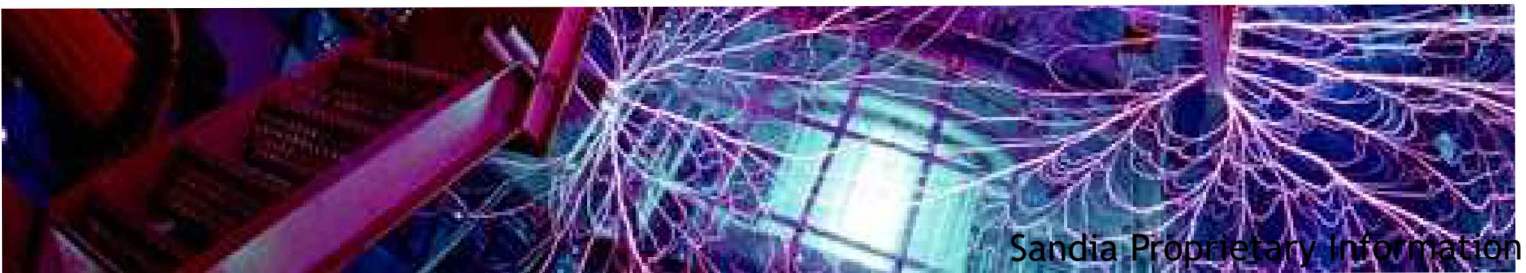
### OFFICE OF SCIENCE

Leads creative, hypothesis-driven inquiry in fundamental science to promote national security and international scientific leadership

### CHIEF RESEARCH OFFICER

Deputy CRO: Basil Hassan

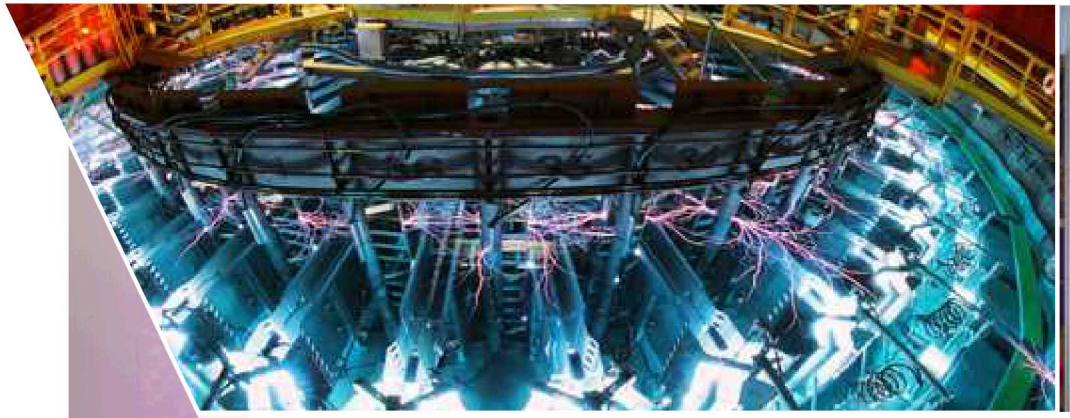
Governs and leads research strategy and stewardship of capabilities at Sandia, including the Laboratory Directed Research and Development program. Responsible for leadership of technology transfer and Sandia's partnerships with universities, industry, and the state of New Mexico.



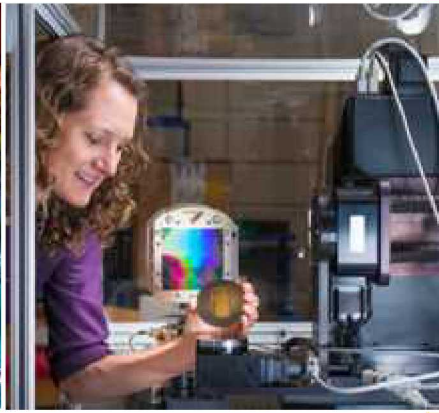
# Sandia's Seven Research Foundations Integrate Across Programs and Lines

## Research ... eraged development of capabilities

Nanodevices & Microsystems

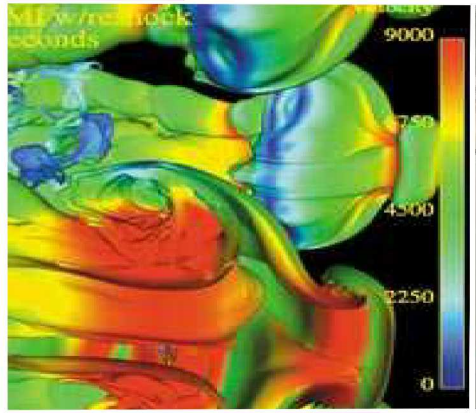


Radiation Effects & High Energy Density Science



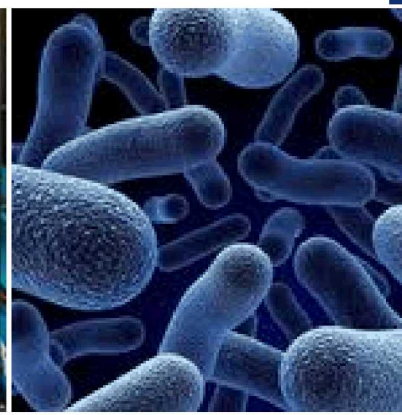
Materials Science

Computing & Informa...




Engineering Science

Earth Science



Bioscience

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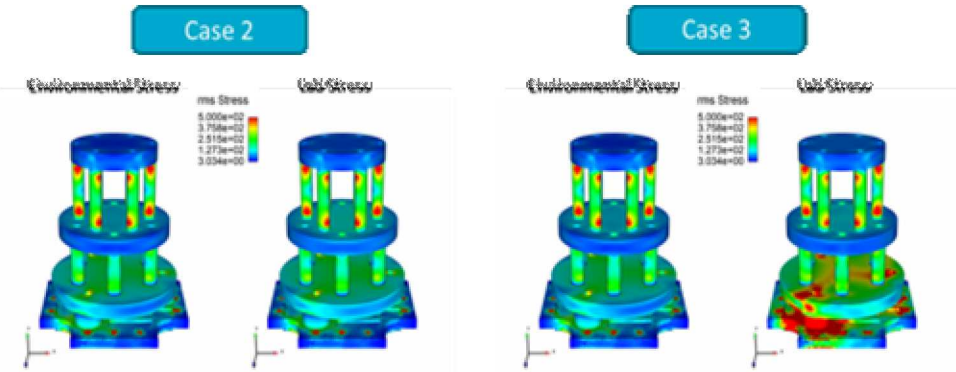
- Sandia's Goals for PSAAP III

# ASC Mission at Sandia

Support the current stockpile

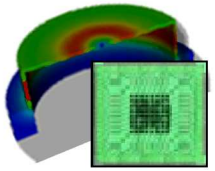
Support the modernization programs and enable an agile future deterrent



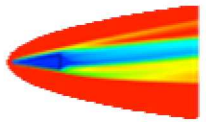

Develop next-generation HPC hardware and software for the deterrence mission

VANGUARD

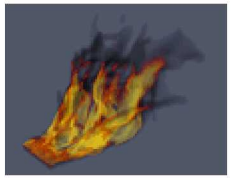
Help ensure the survivability and safety of weapon systems



Radiation / Electromagnetics

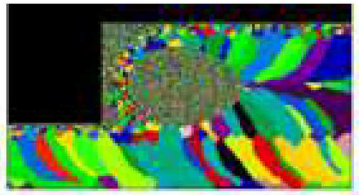


Re-entry

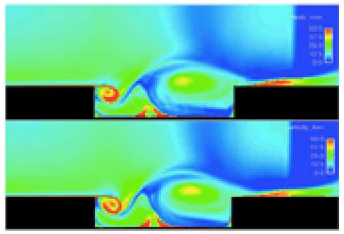


Safety

Perform pioneering research and development in support of the future deterrent



Production Science



Reduced Order Models

# Advanced Simulation & Computing (ASC)

*Sandia National Laboratories*

**Advanced Simulation and Computing**

The Advanced Simulation and Computing (ASC) Program develops, delivers, and supports high-performance computational simulation capabilities for the U.S. nuclear deterrence mission, including design, qualification, and assessment.

**Scott Collis**
Program Executive

**Erik Strack**
Program Manager & Deputy Executive

**Jeremy Templeton**
Deputy Program Manager

**John Feddema**
Predictive Science Academic Alliance Program (PSAAP)

**Scott Hutchinson**
Digital Engineering Integration

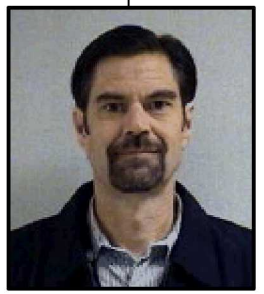
**James Stewart**
Advanced Technology Development & Mitigation (ATDM)
*Code Development and Applications (CDA)*

**Rob Hoekstra**
Advanced Technology Development & Mitigation (ATDM)
*Architectures and Software Development (ASD)*

**Tom Klitsner**
Facility Operations & User Support (FOUS)

**Rob Hoekstra**
Computational Systems & Software Environment (CSSE)

**Amanda Dodd**
Verification & Validation (V&V)



**Jeff Payne**
Physics & Engineering Modeling (PEM)

**Walt Witkowski**
Integrated Codes (IC)

# Sustain ASC impact on the entire weapon lifecycle

**Agile Design Tools** – Explore conceptual designs with quantified confidence

**Environment Specification** – Simulation of environments to define system and component requirements

**Design Analysis & Optimization** – Performance and margin assessment to support development build cycles

**Test Design** – Definition of test parameters to stress key elements needed for model validation and qualification

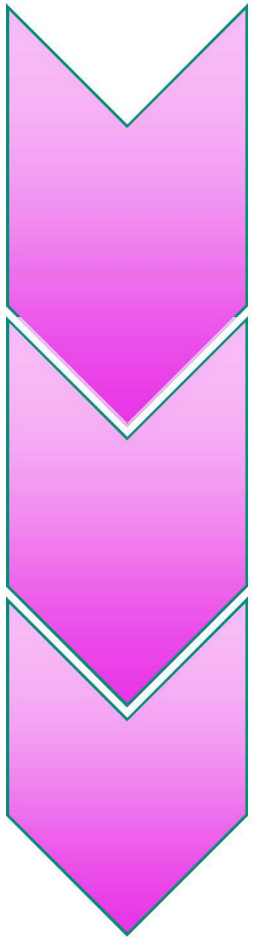
**Qualification** – Technical basis for asserting performance and safety requirements

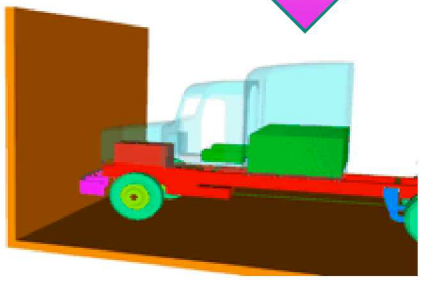
**Production** – Improve production processes for increased quality and efficiency

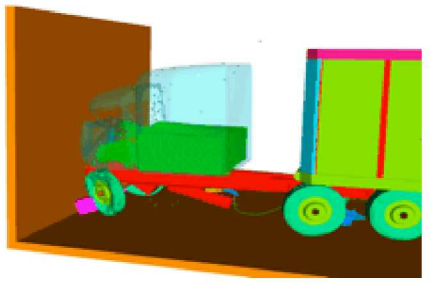
**Transportation** – Assess and mitigate threats

**Surveillance** – Provide technical basis to ensure the stockpile remains safe and reliable

**Dismantlement** – Retire systems while maintaining human and environmental health







# ASC Codes & Capabilities – Sierra Suite of Tools

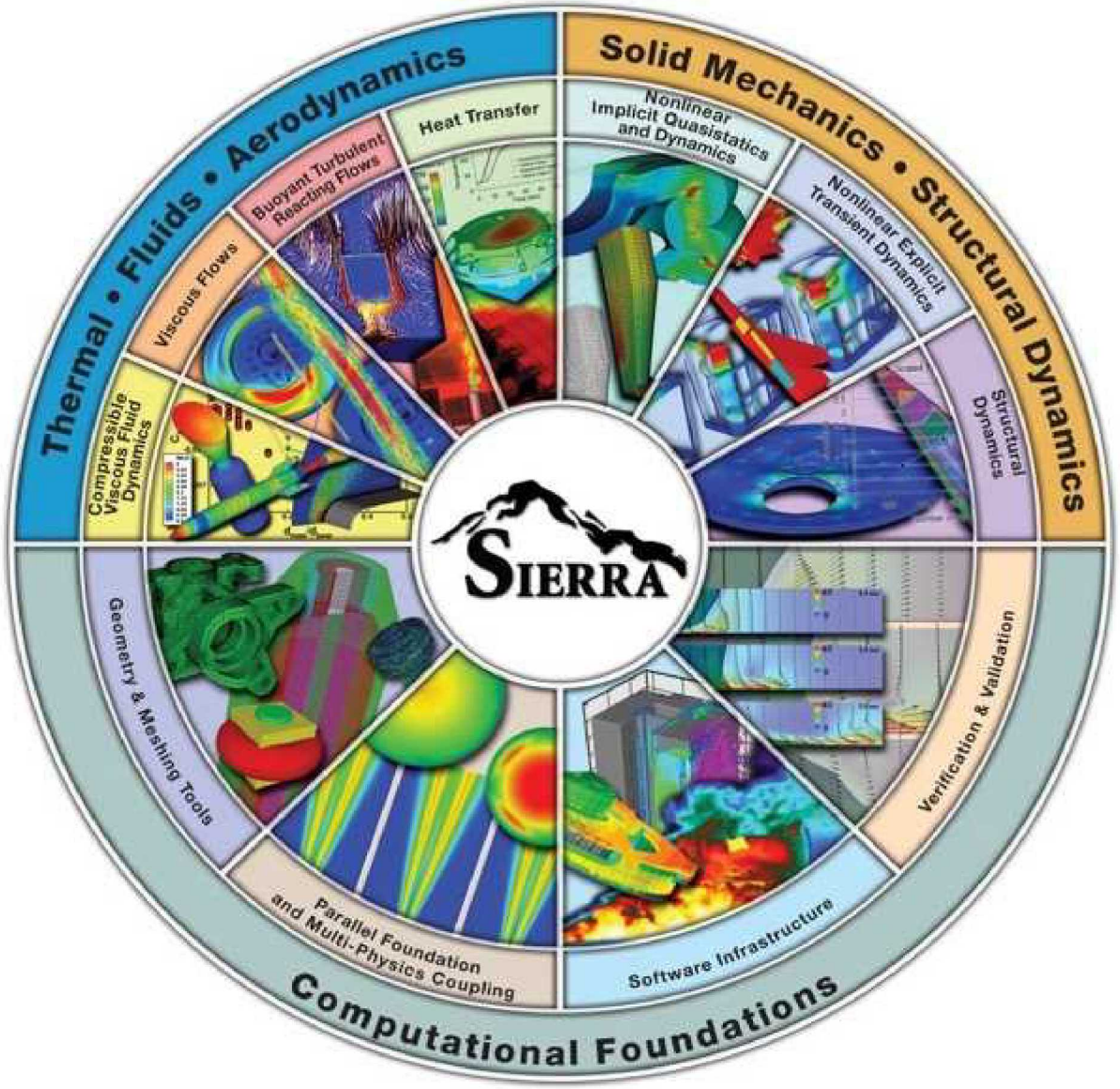
**Sierra** is ASC's engineering mechanics simulation code suite

**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



# ASC Codes & Capabilities – RAMSES Suite of Tools

**RAMSES** - Radiation Analysis, Modeling and Simulation for Electrical Systems:

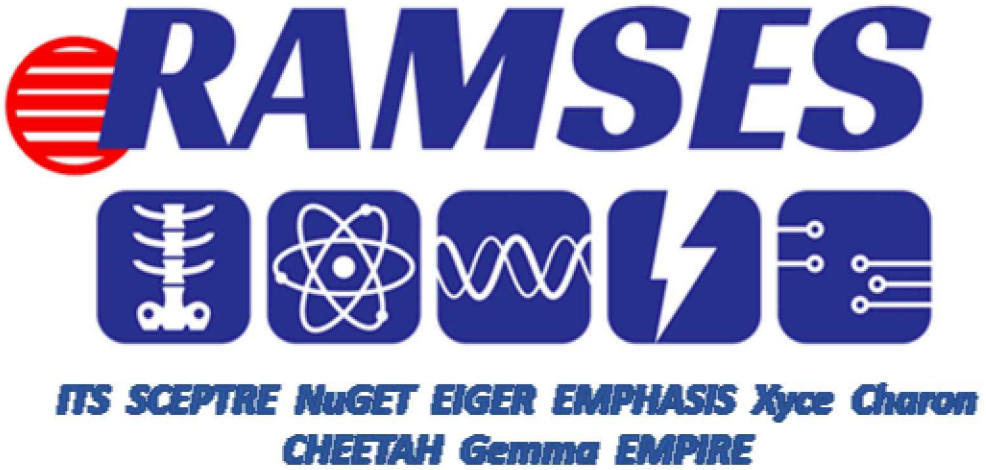
ASC code suite for design, assessment and qualification in electromagnetic and ionizing radiation environments

**Capabilities for circuit modeling:**

- Charon – Semiconductor Device Modeling
- Xyce – Electrical and Radiation-Aware Circuit Modeling

**Capabilities for electromagnetic and plasma environments:**

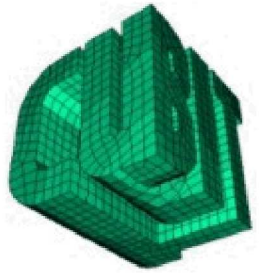
- EIGER/Gemma – Electromagnetics
- EMPHASIS/EMPIRE – Plasma




*RAMSES is used for simulating the electrical response of a system to electromagnetic and plasma environments.*

# ASC Codes & Capabilities – Computational Foundations & Tools

*Tools*



Meshing

DAKOTA

Explore and predict with confidence

Uncertainty Quantification and Optimization

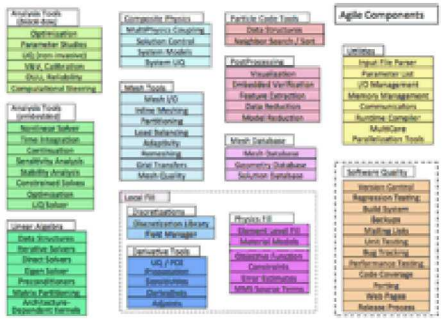
ParaView

Visualization

*Software Components*

TRILINOS

Mathematical Software (Solvers & Infrastructure)



Agile Components

kokkos

Performance Portability

TUCKERMPI

Data Compression

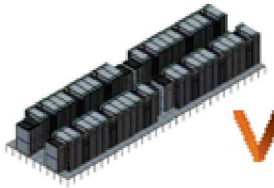
*Computing Foundation*

portals

Scalable Communication

SST

Computer Architecture Design

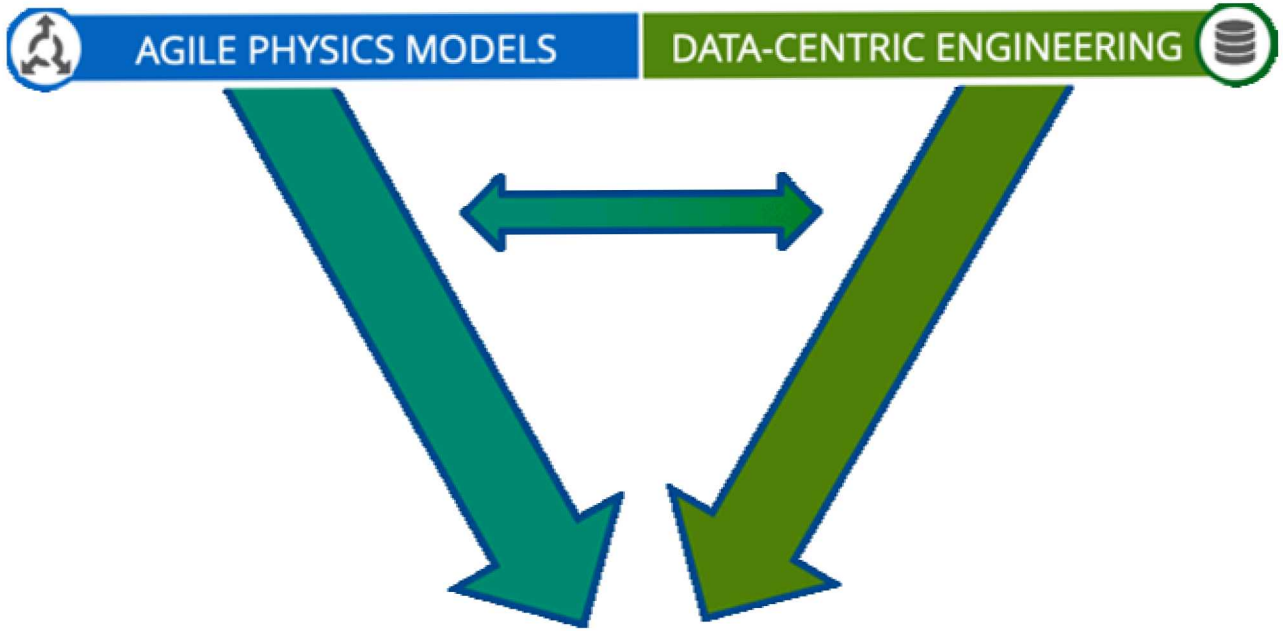


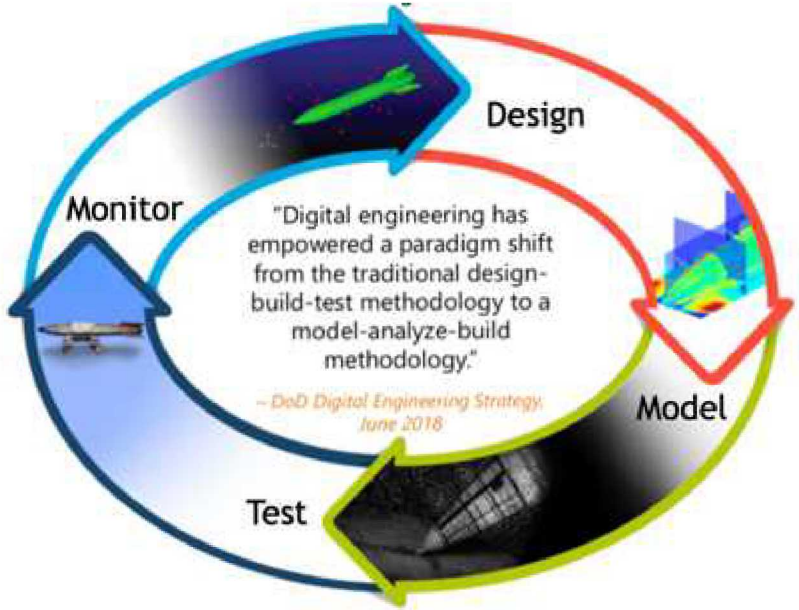
VAN

Astra

Computing Hardware, Facilities, Operations, and User Support

# ASC Vision


AGILE PHYSICS MODELS
DATA-CENTRIC ENGINEERING
Full System Lifecycle Models


Design
Monitor
"Digital engineering has empowered a paradigm shift from the traditional design-build-test methodology to a model-analyze-build methodology."
– DoD Digital Engineering Strategy, June 2018
Model
Test

# Sandia's Future: Full Life-Cycle Engineering Models

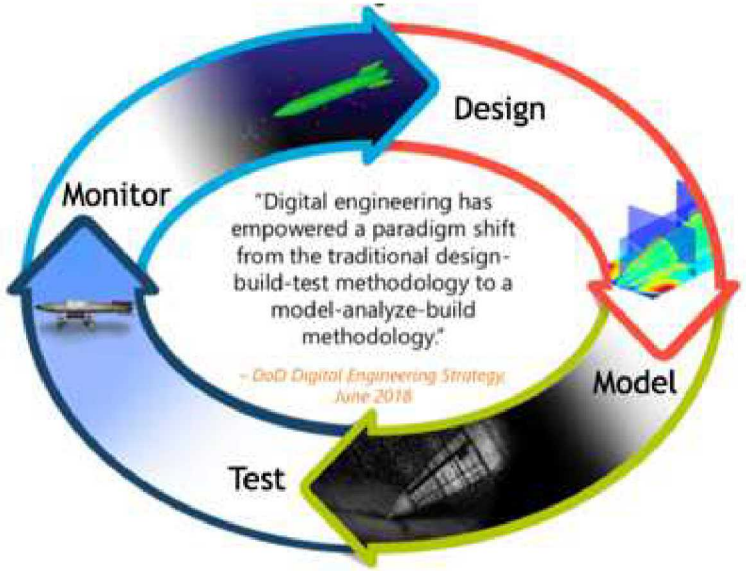
Single Physics → Code Linking → Tight Coupling → Full Physics

- Enhanced physics models with improved understanding and reduced uncertainty
- Workflow to automate model building and shorten time to solution
- Embedded UQ to identify critical sensitivities
- Conversion of CT Images to models to enable serial number based models (digital twins)

- Aging mechanisms into lifetime prediction
- Bridging length scales to embed local effects into global modeling
- Evolution of performance and safety assessments based on in-service conditions

- Combined environments drivers pushing to Exascale
- Multiphysics within components

- Data fusion techniques for integration of experimental and computational data
- Capabilities to assess large ensemble data sets to challenge our intuition
- Institutional efforts to create accessible cloud based data lakes



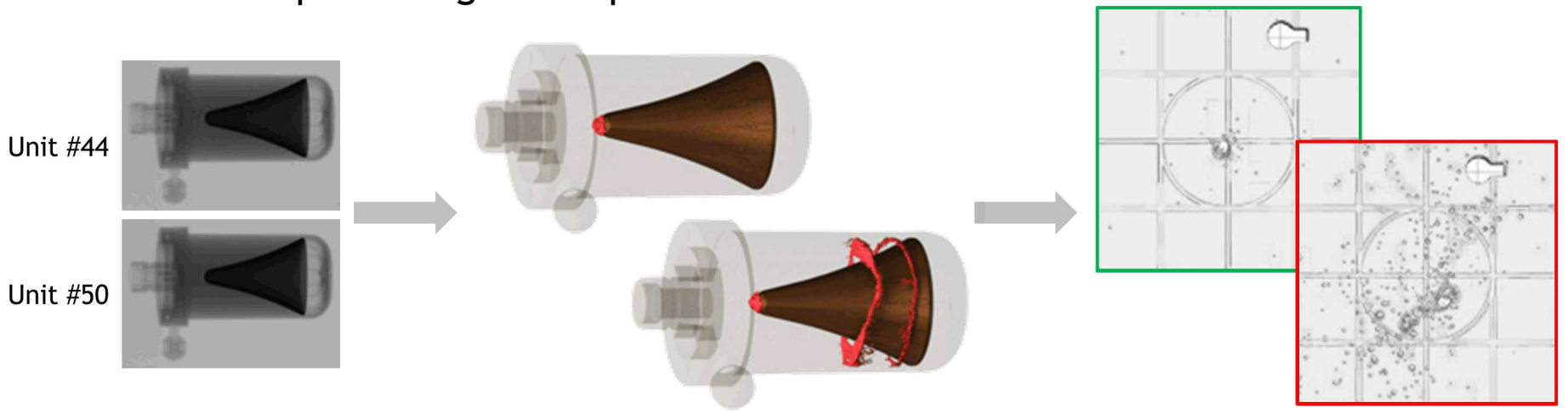
# Data-Driven Approach to Life-Cycle Management

## Digital Twin

Generate models from CT data for direct numerical simulation

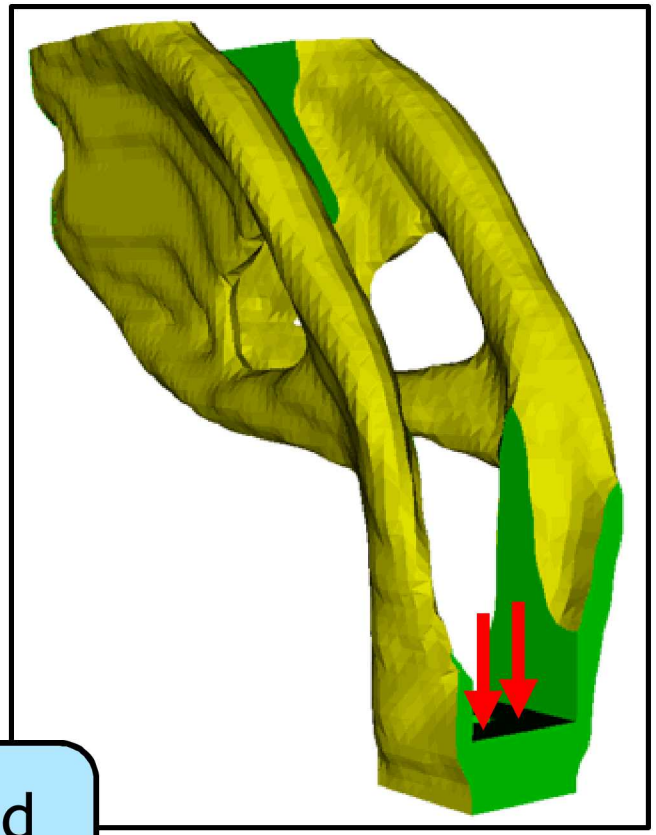
- Greatly simplifies analysis workflow
- Permits analysis of as-built systems
- Aging of each serialized unit can be studied
- Statistical lot acceptance can be replaced with individual performance acceptance

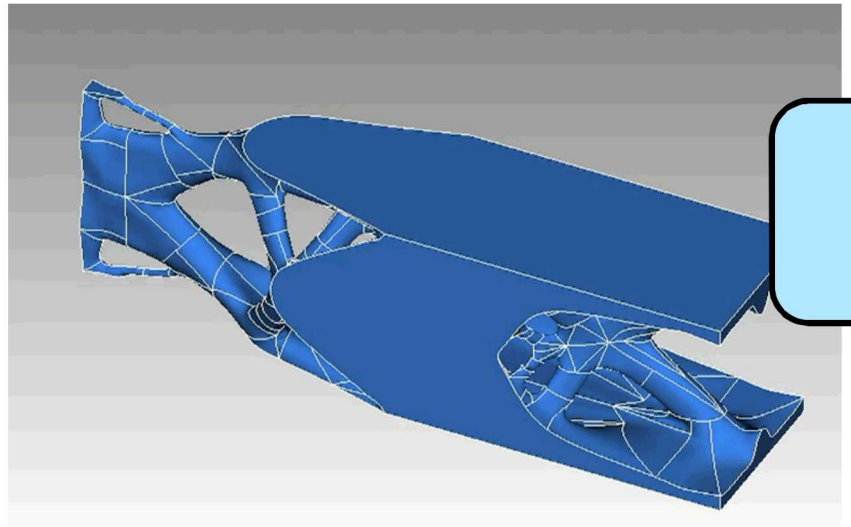
Commercial shaped charge example:



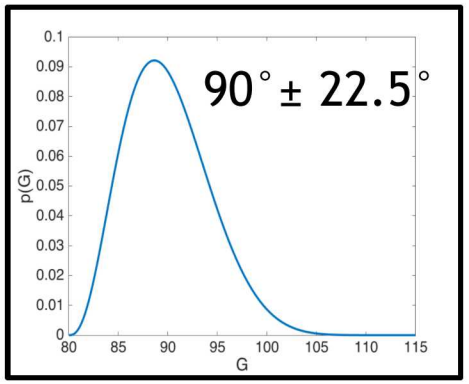
# Optimization Coupled with Multiphysics Simulation & UQ Lead to Next-Generation Designs

Adaptive Prune
Refine
(Good Results Fast)

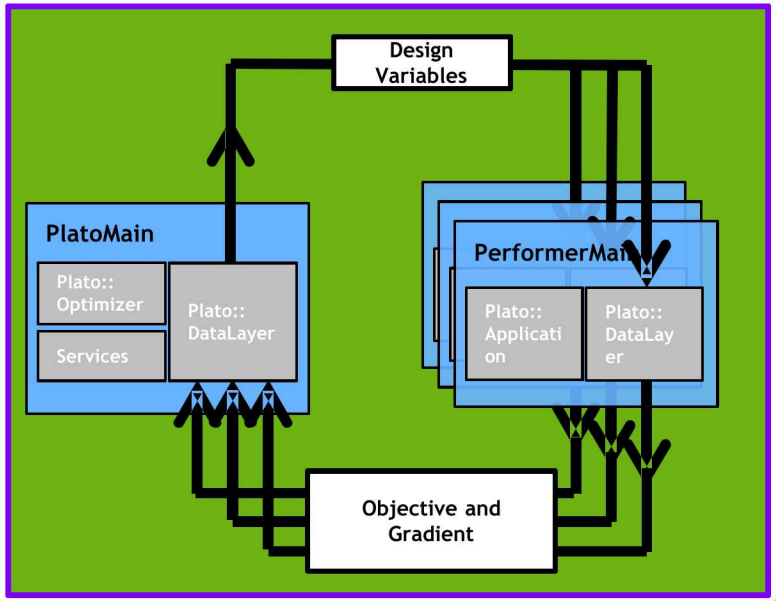




Automatic
Conversion to
CAD




UQ-Enabled
Optimization

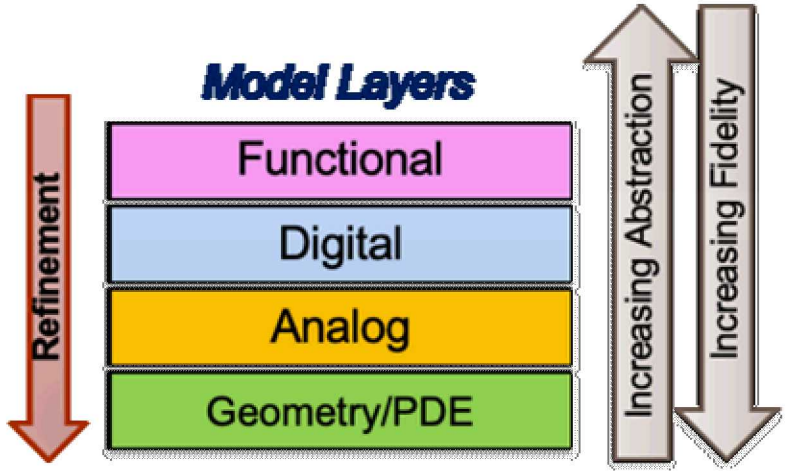


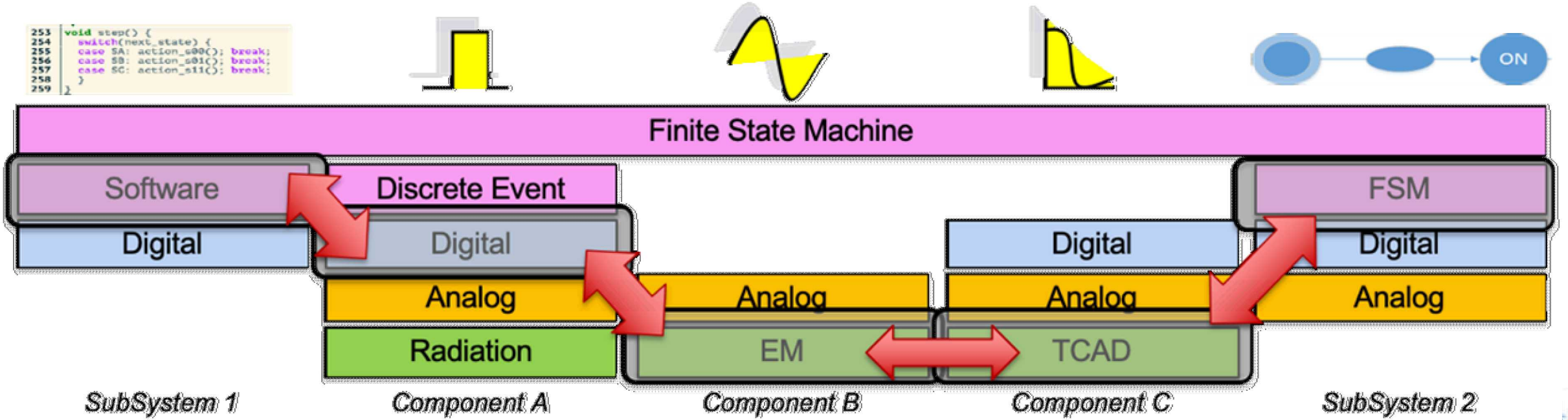

Multi-Physics
Platform

# Model-Based Design: Integrated Multi-Scale Electrical Simulation

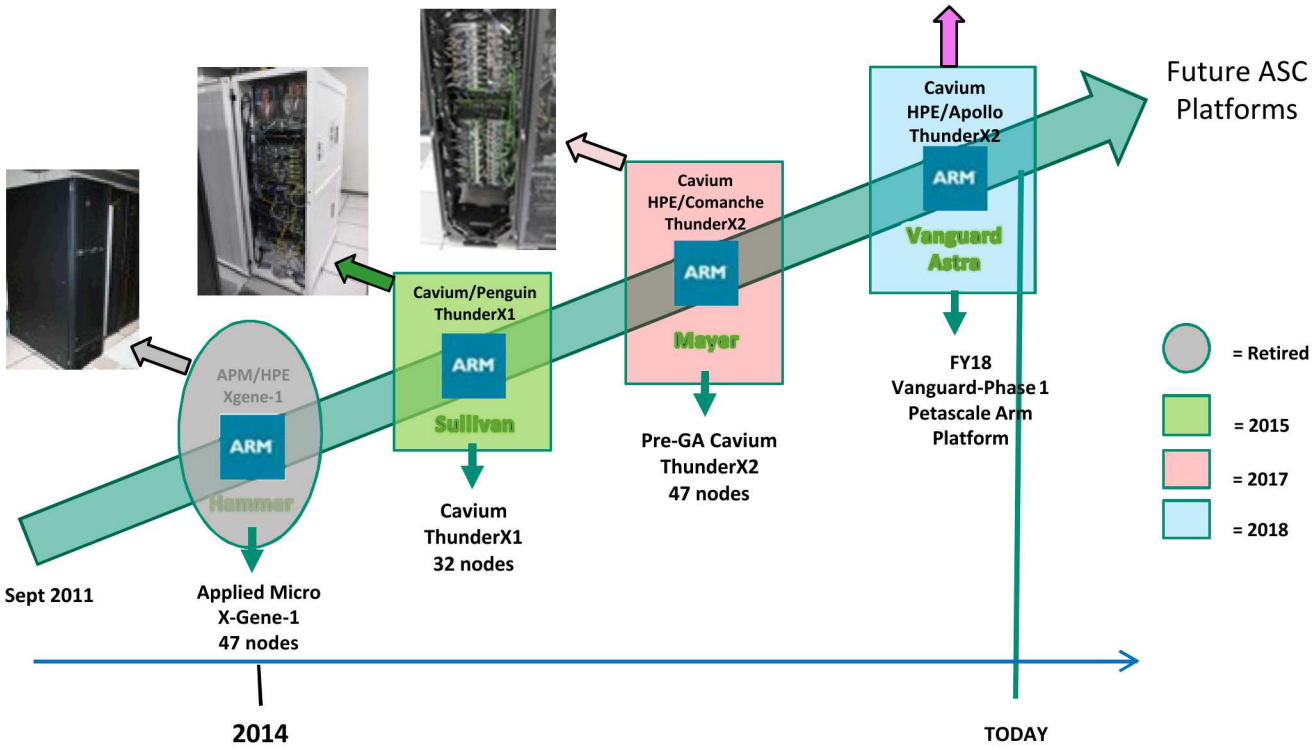
## Key Challenges

- Interfaces between distinct models and tools
- UQ and V&V for multi-scale, e.g., mixed analog-digital
- Model consistency, selection, and abstraction
- Leverage and integrate with design activities



# Enabling High-Fidelity Predictive Physics and Engineering Models


## Hardware – Software Co-Design

## Advanced Architecture Prototypes

Pathfinder systems at sufficient scale to demonstrate value to weapons codes

## Advanced Architecture Testbeds

Small, rack-sized systems of pre-release vendor hardware to evaluate potential future hardware options

VANGUARD

# Outline

**Brief Introduction to Sandia**

- Budget, staffing, lab strategic priorities
- How does ASC fit in? Advanced Science & Technology

**ASC Program at Sandia**

- Integration across organizational lines
- Research areas, strategic initiatives, priority research directions

**PSAAP III**

- AST, CRT, TST and RT Members
- Thoughts on collaboration opportunities
- Sandia's Goals for PSAAP III

# Sandia PSAAP-III: AST and CRT members

- **Alliance Strategy Team (AST)**
  - John Feddema, lead
  - Kathy Loeppky, assistant


- **Computer Resource Team (CRT)**
  - Joel Stevenson, outgoing lead
  - Heidi Uphoff, new lead
  - Kathy Amspaugh, Accounts
  - Lilia Garcia, SARAPE
  - Norma Chavez, SARAPE





# Sandia PSAAP-III: Tri-lab Support Team (TST) members

- **Univ. of Colorado Boulder**
  - Dan Bolintineanu
  - Jimmy Carleton


- **Univ. of Illinois at Urbana-Champaign**
  - Mike Glass
  - David Noble


- **Stanford**
  - Stefan Domino
  - Mike Eldred


- **Univ. Texas at Austin**
  - Tiernan Casey
  - Tim Wildey


- **University of Buffalo**
  - John Hewson, Chair
  - Greg Weirs


- **MIT**
  - Luke Shulenburger
  - Johnathan Vo


- **Univ. of Maryland**
  - Matthew Barone, Chair

- **Univ. of New Mexico**
  - Kevin Pedretti

- **Oregon State Univ.**
  - Kerry Bossler

# Sandia PSAAP-III: Review Team (RT) members

- **Univ. of Colorado Boulder**
  - Robert Clay
  - Jeremy Lechman


- **Univ. of Illinois at Urbana-Champaign**
  - Rob Hoekstra
  - Greg Weirs


- **Stanford**
  - Bill Rider, Chair
  - Michael Powell


- **Univ. Texas at Austin**
  - Shawn Pautz, Chair
  - Robert Knaus


- **University of Buffalo**
  - Bill Erikson
  - Travis Fisher


- **MIT**
  - Normand Modine, Chair
  - Patrick Blonigan


- **Univ. of Maryland**
  - Brian Freno

- **Univ. of New Mexico**
  - Ron Brightwell

- **Oregon State Univ.**
  - Brian Franke

# Sandia PSAAP-III: Motivating Ideas (perfect places for collaboration) [from 3yrs ago]

- **Revolutionize engineering systems**
  - Model-based and data-driven design
  - Advanced manufacturing – "born qualified"
  - As-built modeling
  - Virtual test – fusion of physical and computational simulation
  - Life-cycle models
- **Materials characterization & modeling**
  - Up-scaling micro/meso-scale information to macroscale
  - Thermal protection materials, energetics, turbulence modeling
- **Engineering in extreme environments**
  - Temperature, radiation, vibration
  - Material fracture analysis
- **High resolution diagnostics fused with computational models**

# HPC Machine Learning

From 3yrs ago…

- A new paradigm (and challenge) for UQ?
- Closure laws for turbulent flows (subgrid modeling)
- Prediction of complex dynamics (combustion)
- Model development (think optimized FEM, model-form)
- Adaptive algorithms
- HPC resource management
- Identifying patterns of interest (impact, failure, fracture, fragmentation, …)
- High-dimensional interpolation and preconditioning
- Application to engineered systems…

# Other Thoughts…

- Embedded Analysis – bake in optimization, UQ, ML, DA, ….
- Performance Portability – this is a polarity
- Production Prototypes – another polarity
- Stochastic Algorithms
- Dynamic task-based programming models
- Dynamic/optimized algorithms and numerics
- *Software engineering*

DAKOTA
Explore and predict with confidence

kokkos

# Sandia's Goals for PSAAP III

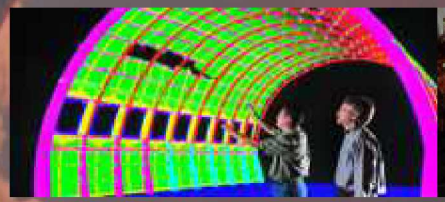
- **Build strong collaborations with PSAAP III Universities and across Tri-Labs**
  - Many shared technical areas of interest
- **Progress the science of Predictive Computational Simulation**
- **Progress on the underlying Computing and Computer Science**
- **Build a pipeline of future Computational Scientists**



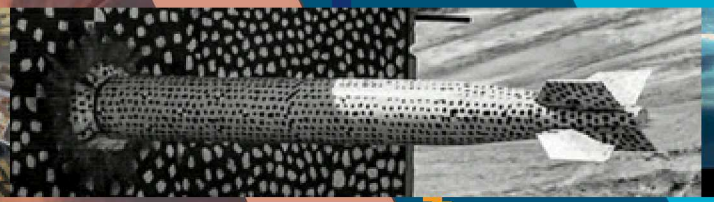
Outreach Institutes

**We look forward to working closely with you in PSAAP III!**

# Exceptional service in the national interest







# Sandia's Support of PSAAP III

- **CRT members are to help PSAAP III Universities with**
  - Access to DOE HPC computing resources
- **TST members are to help with**
  - Technical advice (e.g., UQ, software integration, DOE computing access, etc.)
  - Open source software (e.g., Dakota, Trilinos, etc.)
  - Establishing collaborations with University professors and students
  - Placing intern students at the National Laboratories
- **Review Team and AST members are to**
  - Evaluate progress on scientific milestones and deliverables
  - Provide programmatic and technical guidance