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Title: Nuclear Fundamentals Orientation Module 2: Nuclear Weapons Computational Physics

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Los Alamos NATIONAL LABORATORY

Nuclear Fundamentals Orientation
Module 2

Nuclear Weapons Computational Physics

Los Alamos NATIONAL LABORATORY

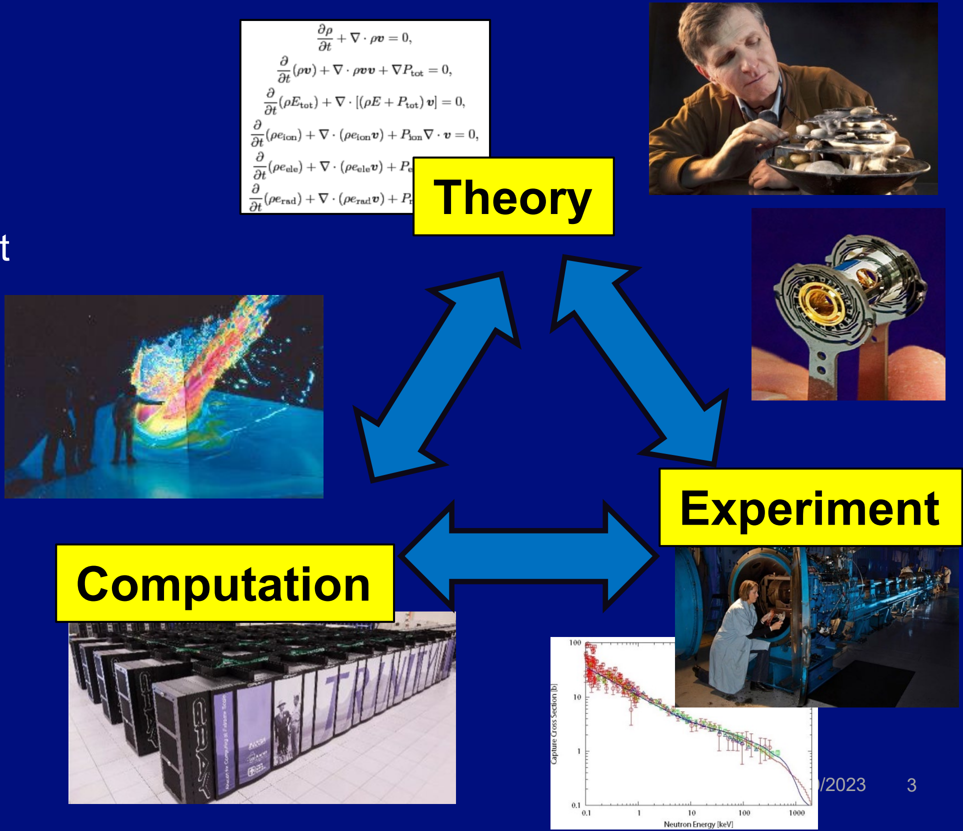
Computational Physics Overview

- Introduction
  - What is computational physics, and why is it important?
  - What role did LANL play in the history of computational physics?
  - How does computational physics differ at LANL vs other places?
- Computational physics in the LANL weapons program
  - What role does computational physics play in the weapons program: Past, present and future?
  - What role do experiments play in computational physics?
- How is computational physics structured at LANL?

Computational physics is an important part of the overall investment in National Security Science at LANL

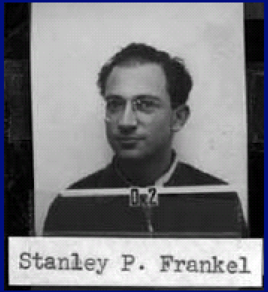
- Per Wikipedia:
  - Computational physics is the study and implementation of numerical analysis to solve problems in physics for which a quantitative theory already exists
  - Historically, computational physics was the first application of modern computers in science

- Three key elements to computational physics:
  - Mathematical models of physical phenomena and conservation equations
  - Computer codes that implement these models
  - Computer platforms that execute the code instructions and manipulate the data

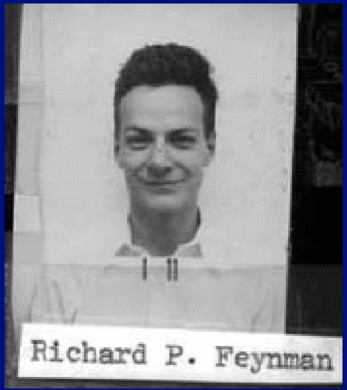


Los Alamos is the birthplace of computational physics

- LANL played critical roles in the history of computational physics and computing
- Names you should know: The first "computer geeks"



They worked out the neutronics equations (1942) and invented the first parallel computing method on the IBM Punch Card Accounting Machine



They led the operations of the computing center

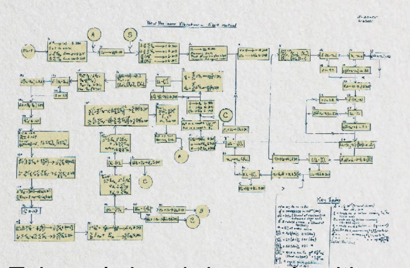
First thermonuclear calculation (with Frankel) on the ENIAC (1945)

See Bill Archer's excellent talk:
"A History of Los Alamos Scientific Computing" LA-UR-20-24471

Women played important roles in early computational physics at Los Alamos

Mary Tsingou Menzel

Developed the code to solve the “Vibrating String Problem” on the MANIAC computer in 1955. The results are considered foundational work in nonlinear systems theory.



Tsingou’s hand-drawn algorithm

Ref. Virginia Grant,
National Security Science, Dec 2020

Arianna Wright Rosenbluth

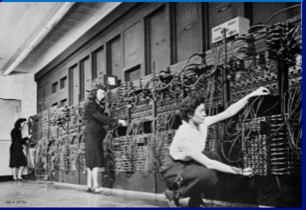
Developed the code for the first Markov Chain Monte Carlo method on the MANIAC computer in 1953. Co-authored the resulting paper “Equation of State Calculations by Fast Computing Machines.” This algorithm is foundational to the field.

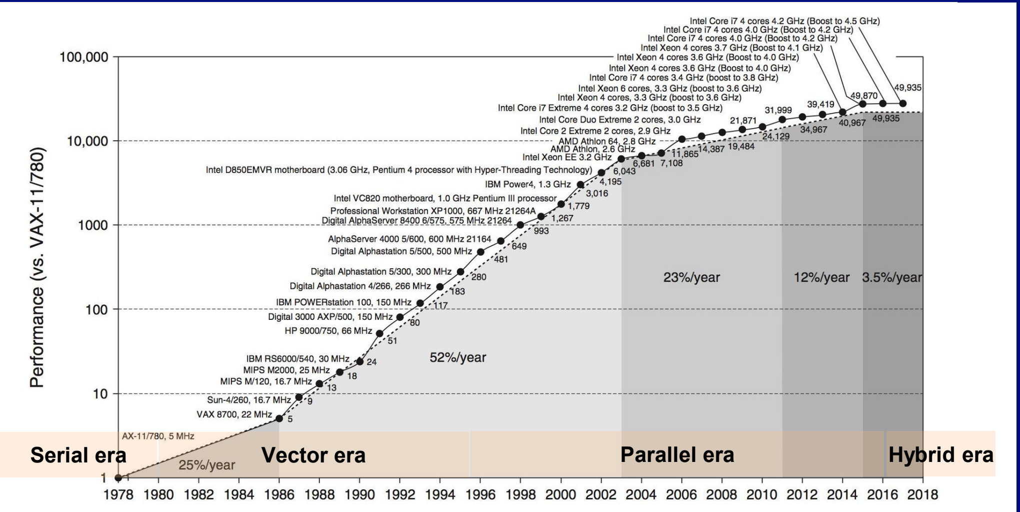
Ref. Madeline Whitacre,
LA-UR-21-22305

Los Alamos has been at the forefront of high-performance computing since 1943

1943: Calculator
3 operations per sec

1945: ENIAC
385 multiplications per second





researchgate.net

Los Alamos has driven and taken advantage of increased computing capability to solve computational physics problems.

A 16 order-of-magnitude increase in capability in 70 years! (Compare the size of a virus to the orbit of the moon.)

2018: Trinity: 40 PFLOPS

2008: Roadrunner: LANL first to 1 Petascale (10^{15})

1976: CRAY-1
200 MFLOPS

From: Archer LA-UR-20-24471

Typical points of emphasis in computational physics differ between universities, industry, and LANL

University

research | user applications | collaboration

- More emphasis on research
- Less emphasis on user applications
- Extensive external sharing & collaboration

Industry

research | user applications | collaboration

- More emphasis on user applications
- Less emphasis on research
- Little external sharing & collaboration

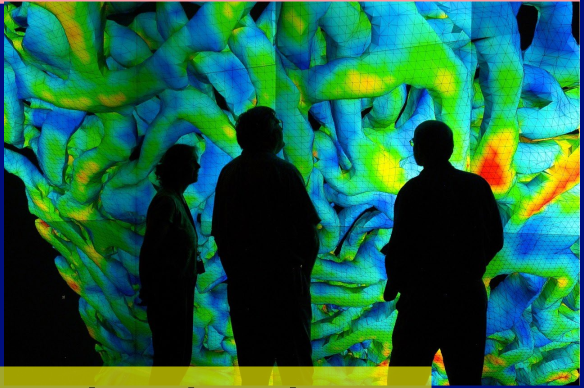
LANL

research | user applications | collaboration

- Balanced investment in research & applications
- Mostly develop our own codes
- Some external sharing & collaboration

The role of computational physics in the weapons program has changed over the decades

1992		2025
Designers with test experience	mentoring	2^{nd} and 3^{rd} generation designers
Nuclear tests	understanding the data	Archived nuclear test data
Experiments	range and fidelity	Experiments
Calibration-heavy simulations	removing calibrations increasing fidelity	Science-based simulation

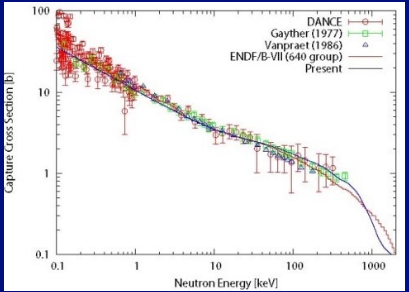


Stockpile stewardship **requires physics and engineering insight enabled by experiment, computation, and theory**

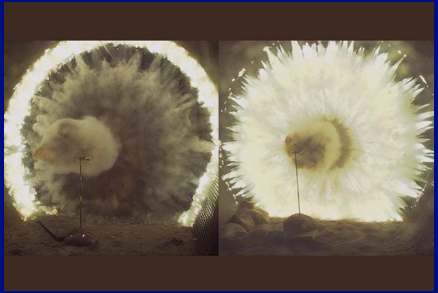
Computational physics will be important in our future

- Developing for portability, quality, capability, and performance
- Addressing an aging stockpile
- Designing for a future stockpile
- Partnering for experiments, engineering and production
- Contributing to national and global security

Fundamental and single-physics experiments help to validate our computational physics capabilities



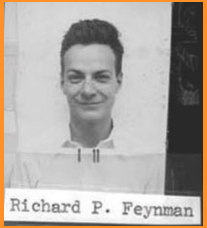
Nuclear Data Measurements



High Explosives

Extreme material dynamics

Nuclear Criticality

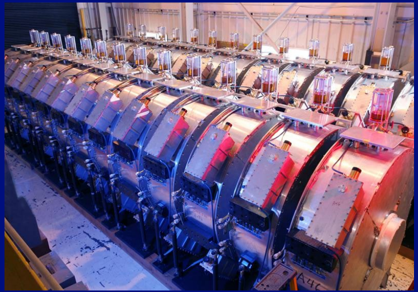
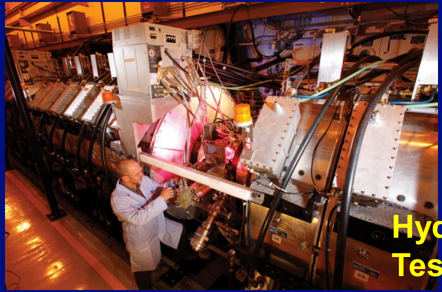


"It doesn't matter how beautiful your theory is, it doesn't matter how smart you are. If it doesn't agree with experiment, it's wrong."

Integral experiments have always played a vital role in validating our computational physics capabilities

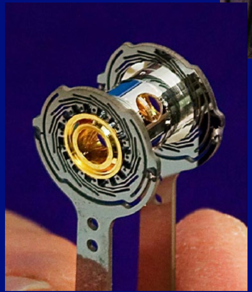


Nuclear Testing

Hydrodynamic Testing

Subcritical experiments

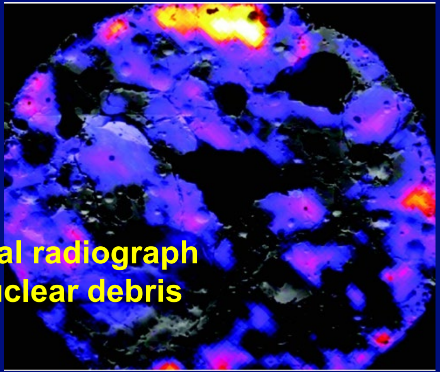
High Energy Density (HED) Experiments

Precision laser measurements

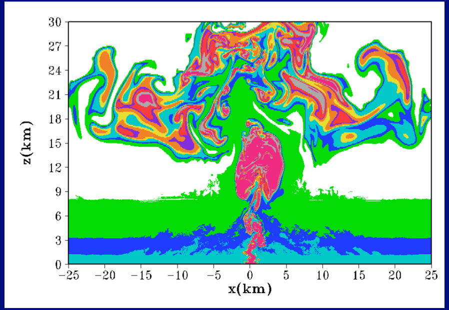
LANL's computational physics capabilities support key mission areas in Global Security

- Emerging global threats
- Nuclear nonproliferation
- Nuclear emergency response
- Weapons effects
- Nuclear forensics

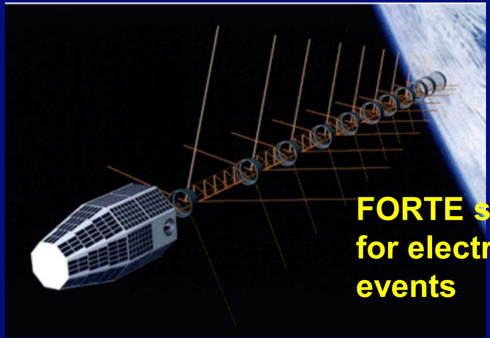
Fire growth and spread



Digital radiograph of nuclear debris

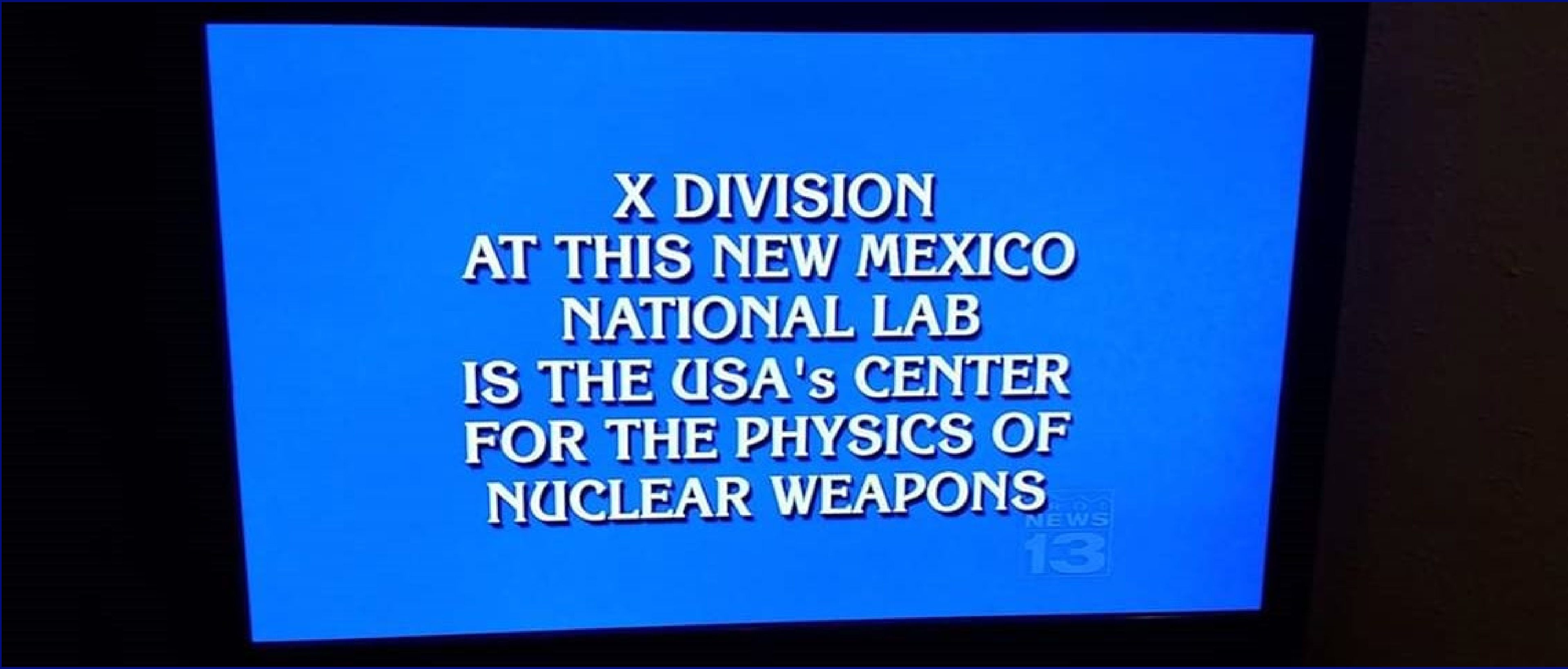


Nuclear emergency response



FORTE satellite to monitor for electromagnetic pulse events

X is a reminder of the division's history!



X: A reminder of the division's history, our responsibilities, and our critical, lead role within the core of Los Alamos National Laboratory's national security mission space

1943	Bethe, Mark	Theoretical (T) Division		
1971	Thorn	Theoretical Design (TD)		Theoretical (T)
1979	Selden	Applied Theoretical Physics (X)		
1993	Juzaitis	Applied Theoretical and Computational Physics (X)		
1999	Weisheit, Bernardin	Applied Physics (X)		
2010	Chadwick	X-Computational Physics (XCP)	X-Theoretical Design (XTD)	Theoretical (T)

> "When we couldn't come up with a good idea, we decided on a temporary expedient—put in X as a place holder … because of constant other interruptions, the acronym meeting was never held. For lack of a better idea, X stuck."
>
> — Buck Thompson

Computational Physics: we develop physics models, numerical methods, and computational modeling and simulation tools for complex, multi-physics applications.

Today, XCP is an internationally recognized leader in computational physics, at the national laboratory where computational physics was pioneered.

Our mission is to develop, integrate, and deliver LANL's mission-critical, modeling, and simulation software.

- XCP *develops* weapons-relevant physics theory and models, numerical methods and algorithms, and verification, validation, and uncertainty quantification processes.

- XCP *integrates* these capabilities with complimentary capabilities from our partnering line organizations.

  XCP is the "managing partner" responsible for capability integration and the production of the computational modeling and simulation tools designed for and used by the Weapons Program.

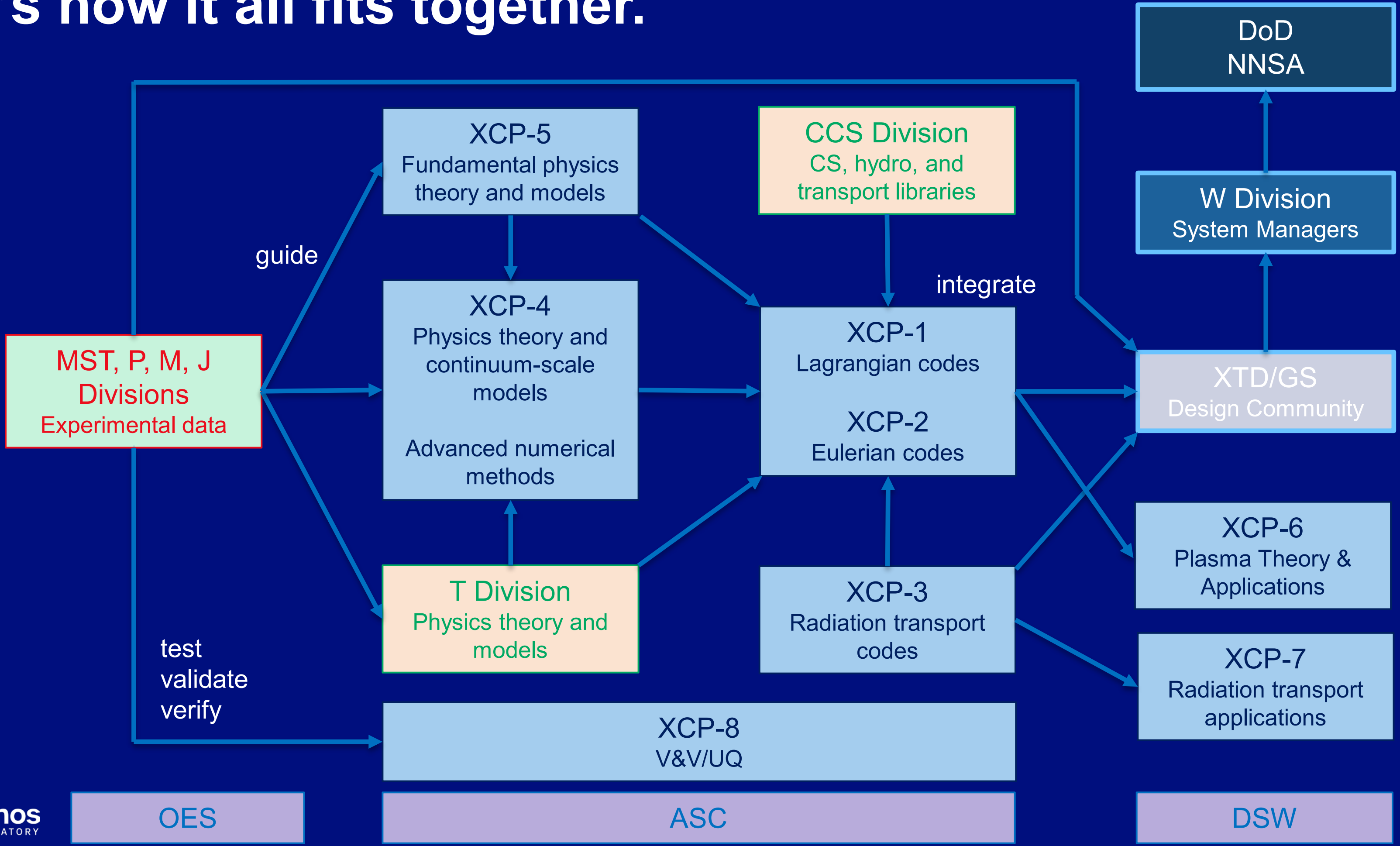
- XCP *delivers* the evolving suite of modern, multi-physics, modeling, and simulation software to our colleagues in XTD, the broader Weapons Program, and the Global Security Directorate to address challenges across a spectrum of national security applications.

  XCP partners with the X-Theoretical Design (XTD) Division, and others, to provide the physics, methods, and code expertise required to successfully execute the Laboratory's directed stockpile work and global security missions.

"The beauty of computation is that it lies at the intersection of theory & utility."

— Charlie McMillan, June 2018

Here's how it all fits together.



Here is our laboratory leadership.

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"We are one team, dedicated solely to the success of our Laboratory's national security mission."

—Thom Mason, Laboratory Director

Here is the leadership team for the Computational Physics Division.

Mark Schraad

Division Leader

Jimmy Fung

Deputy Division Leader

Rob Ward

XCP-1
Lagrangian Codes
Group Leader

Brandon Smith

XCP-2
Eulerian Codes
Group Leader

Jeremy Sweezy

XCP-3
Monte Carlo Methods, Codes, and Applications
Group Leader

Angela Herring

XCP-4
Methods and Algorithms
Group Leader

Abby Hunter

XCP-5
Materials and Physical Data
Group Leader

Paul Bradley

XCP-6
Plasma Theory and Applications
Group Leader

Josh Spencer

XCP-7
Radiation Transport Applications
Acting Group Leader

Brandon Wilson

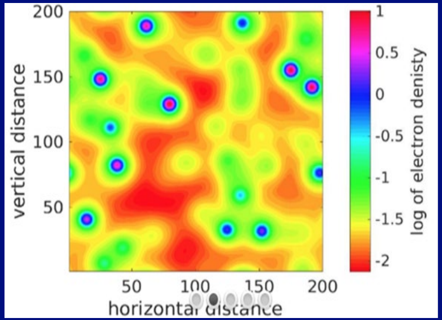
XCP-8
Verification and Analysis
Group Leader

Materials and Physical Data, XCP-5

Abby Hunter

Group Leader

- **Group Leader: Abby Hunter**
- **Hallmark**: The trusted source for materials physics expertise and equation-of-state, nuclear, and atomic opacity data for national security applications.
- **Mission**: To develop models for material strength, damage, spall, and phase-transition kinetics; and physical datasets for equations of state, nuclear cross sections, and atomic opacities for implementation and use in multi-physics simulation codes, with an emphasis on national security applications.
- **Capabilities**
  - Fundamental materials physics
  - Mechanics of materials
  - Thermodynamics and statistical mechanics
  - Electronic structure
  - Nuclear physics and reaction data
  - Atomic physics and opacities
  - Multi-physics simulations



Electron density in liquid Al

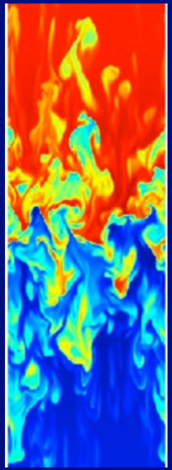
Developing and delivering the critical physics theory, models, and data sets for national nuclear security and global security missions.

Continuum Models and Numerical Methods, XCP-4

Angela Herring

Group Leader

- **Hallmark:** Providing comprehensive cross-linked physics and advanced algorithmic expertise for the development of advanced multi-physics modeling and simulation tools.
- **Mission**: Development of advanced numerical methods for high-speed multi-material flow and models for turbulence and multi-component reactive flow.
- **Capabilities**
  - Numerical Methods for Computational Hydrodynamics
    - Advanced higher-order methods
    - Adaptive mesh refinement (AMR) techniques
  - Modeling and Simulation of Turbulent Mixing at Extremes
    - Turbulence models (RANS, LES, hybrid RANS-LES)
    - Advanced closure model development
    - Fluid flow instabilities
  - High Explosives Modeling and Simulation
    - Reactive burn model development and implementation
    - High Explosives Equation of State Development
  - Code-to-code linking and simulation management



RT-driven fluid instabilities

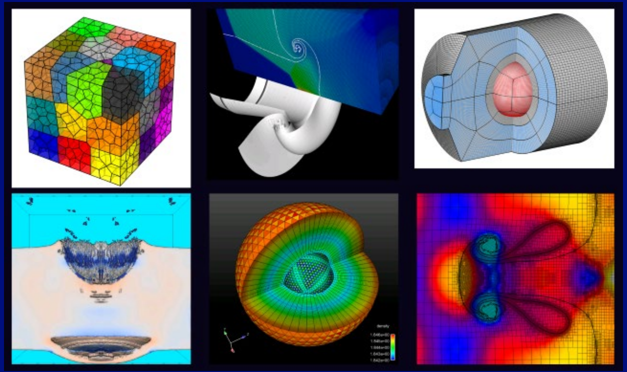
Developing and delivering physics models and numerical methods for national nuclear security and global security missions.

Lagrangian Codes, XCP-1

Rob Ward

Group Leader

- **Hallmark**: Developers of the FLAG multi-physics ALE hydrocode and the INGEN and CROSSLINK mesh generation codes.
- **Mission**: Stewards the Laboratory's capabilities in mesh generation, advanced methods development, and the development of Lagrangian and Arbitrary Lagrangian–Eulerian (ALE) multi-physics modeling and simulation software.
- **Core Capabilities**
  - Lagrangian and ALE hydrodynamics methods development
  - Multi-physics coupling considerations
  - Modern software design and development practices
  - Geometry modeling, mesh generation, and mesh optimization
  - Software development for advanced computer architectures
- **Cross-Cutting Capabilities**
  - Computational fluid and solid mechanics
  - High energy density and nuclear physics
  - Plasma physics and radiation hydrodynamics
  - High explosives and materials science
  - Turbulence/multi-phase flow and particulate damage



Hydrodynamics Method Development

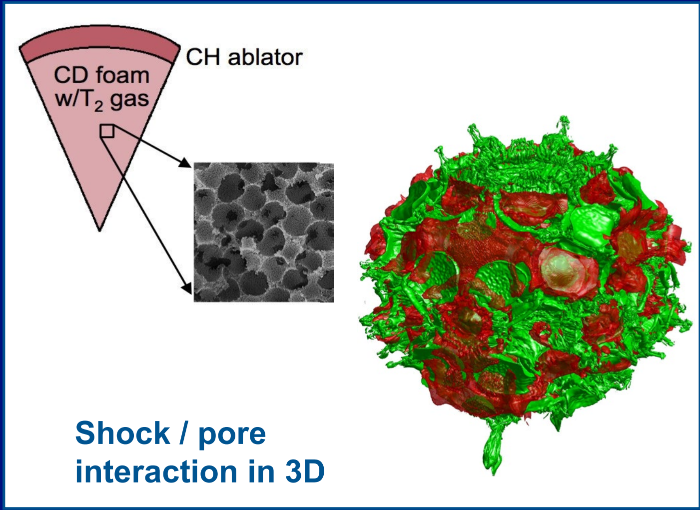
Developing and delivering the computational simulation tools required for modeling highly coupled multi-physics applications within Lagrangian and ALE frameworks.

Eulerian Codes, XCP-2

Brandon Smith

Group Leader

- **Hallmark**: Development of the xRage multi-physics Eulerian Adaptive Mesh Refinement (AMR) hydrocode
- **Mission**: Stewards the Laboratory's capabilities in advanced methods development and multi-physics modeling and simulation software development for Eulerian AMR hydrocodes.
- **Core Capabilities**
  - Compressible Eulerian AMR hydrodynamics methods
  - Advanced 3-D modeling and simulation
  - Coupled/multi-physics code development
  - Modern software design
  - Software development for advanced computer architectures and massively parallel computing
- **Cross-Cutting Capabilities**
  - High-explosive modeling and algorithm development
  - Material modeling in Eulerian frameworks
  - Thermonuclear burn



Developing and delivering the computational simulation tools required for modeling highly coupled multi-physics applications within Eulerian frameworks.

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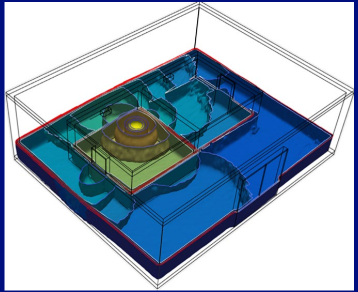
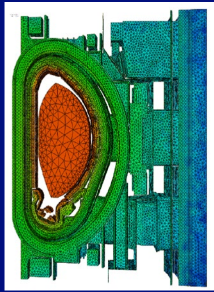
Monte Carlo Codes, XCP-3

Jeremy Sweezy

Group Leader

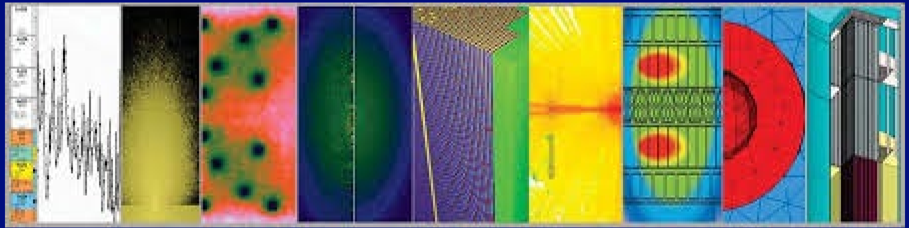
- **Hallmark**: Development of the MCNP and MCATK Monte Carlo particle transport codes
- **Mission**: Stewards the Laboratory's capabilities in Monte Carlo particle transport to meet the radiation transport modeling needs of the Laboratory, the Department of Energy, and the nation.
- **Core Capabilities**
  - Nuclear Criticality methods development
  - Monte Carlo variance reduction methods development
  - Software development for massively parallel computing and GPU accelerators
  - Modern software design
- **Cross-Cutting Capabilities**
  - Nuclear Reactor simulation
  - Criticality Safety
  - Radiation Protection and Shielding
  - High-energy physics modelling





High-energy Physics Modelling

MCNP6



Verification and Analysis, XCP-8

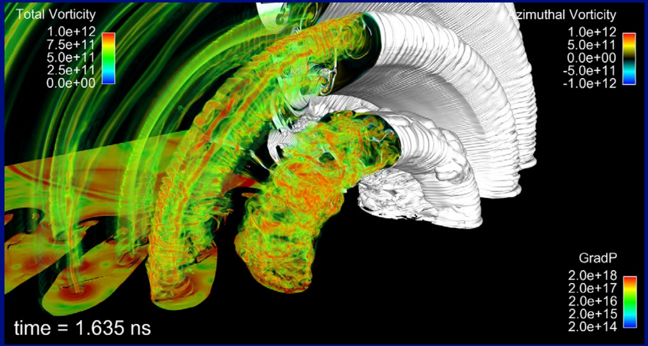
Brandon Wilson

Group Leader

- **Hallmark**: Ensuring that XCP modeling and simulation tools are pedigreed, verified, and validated before delivery to the user community.

- **Mission**: Code verification, model validation, data analysis, and uncertainty quantification to improve the predictive capability of our nuclear weapons modeling and simulation tools.

- **Capabilities**
  - The development and application of advanced code and solution verification tools and methods, to support suites of verification and validation tests.
  - Estimation and propagation of physical uncertainty bounds for the purposes of code validation and experimental design.
  - The development and application of tools for the interpretation of simulations of complex systems to provide support for decision making.
  - Data analysis, including modern machine learning algorithms and their application.



Advanced Code Verification Tools

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Improving the user community's confidence in the science-based predictions of our multi-physics and multi-component modeling and simulation tools.

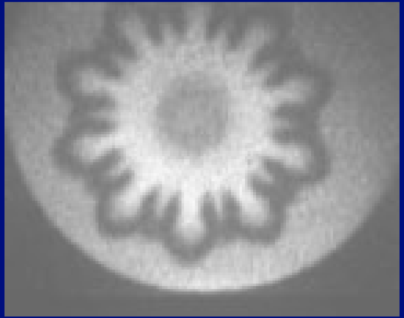
Plasma Theory and Applications, XCP-6

Paul Bradley

Group Leader

- **Hallmark**: The home of plasma physics theory, modeling, and simulation at LANL.
- **Mission**: Provide confidence in plasma physics of Los Alamos codes; model ICF and HED experiments fielded at facilities around the nation; advance experiments that will achieve ignition and high yield.
- **Capabilities**
  - High-energy density science
  - Charged particle beam generation
  - Plasma acceleration and transport
  - Magneto-hydrodynamic phenomena
  - Laser-plasma interactions
  - Space plasmas
  - Directed-energy research
  - Pulsed-power physics
  - Inertial confinement fusion
  - Thermonuclear ignition
  - Fast ignition concepts
  - X-ray radiographic simulation
  - Particle-in-cell code simulations

Radiograph of cylindrical Rayleigh-Taylor experiment

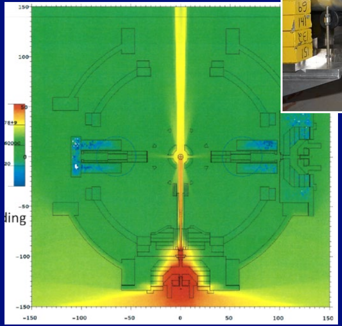


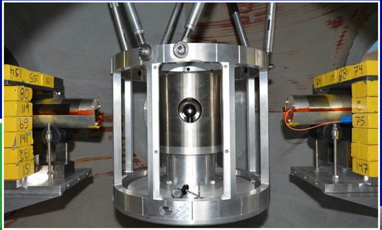
Responsible for plasma physics theory, model and algorithm development, and implementation in our multi-physics modeling and simulation tools.

Radiation Transport Applications, XCP-7

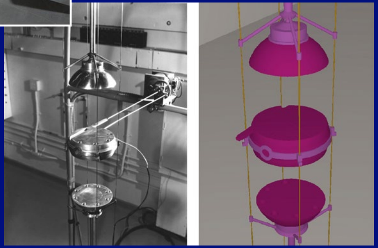
Tim Goorley
Group Leader

- **Hallmark**: We are the radiation transport and analysis experts.
- **Mission**: Our teams apply a wide variety of state-of-the-art tools to simulate neutron, gamma and other radiation transport to understand challenges and find solutions for weapons and global security issues. Frequently we are involved in, sometimes even lead, experiments that help inform our analysis or demonstrate the solutions we find.
- **Capabilities**:
  - modern and historic experimental diagnostics
  - X-ray & neutron radiography
  - intrinsic radiation
  - shielding design
  - criticality safety
  - radiation detection and measurement
  - nuclear threat reduction and response
  - nuclear counter terrorism and counter proliferation
  - nuclear non-proliferation and arms control
  - nuclear forensics
  - nuclear weapons effects





Experimental Diagnostic Tools



We bring together weapons code development teams, designers, engineers, and experimentalists to solve problems for national security.

Any questions?

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