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Title: Welcome to Computing Research Leadership Council

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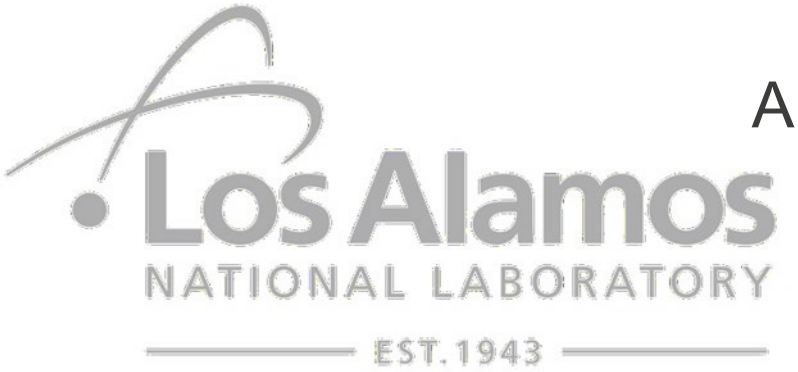
# Welcome to Computing Research Leadership Council




**Irene Qualters**
ALD, Simulation and Computation

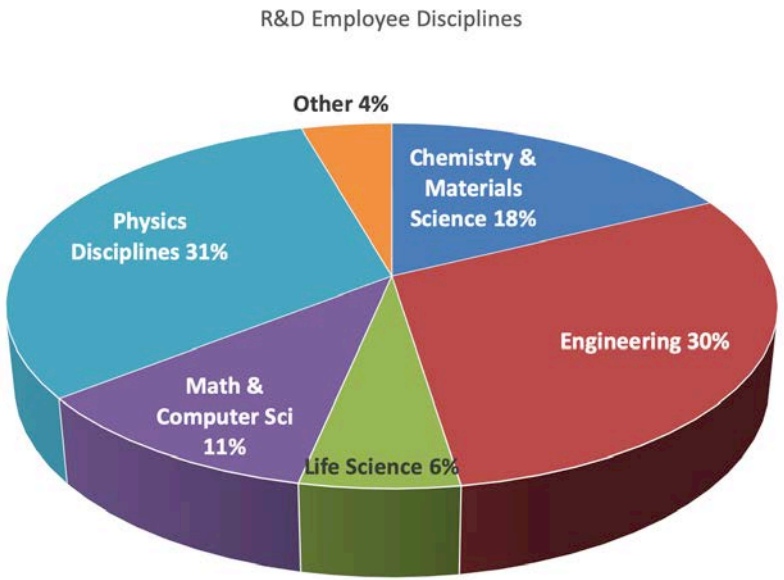
March 3, 2020

NNSA
National Nuclear Security Administration
Managed by Triad National Security, LLC for the U.S. Department of Energy's NNSA

# Los Alamos National Laboratory

*Delivering science and technology to protect our nation and promote world stability*

- The senior DOE Federally Funded Research and Development Center (FFRDC) and operated by Triad National Security, LLC under contract to the National Nuclear Security Administration (NNSA)
- People: >12,800; >1,800 students and > 450 post-docs; 19% PhD.; 43% minorities; 36% female
- Budget: $2.92B
- Location: 1,000 buildings on 35 acres 35 miles NW of Santa Fe, NM



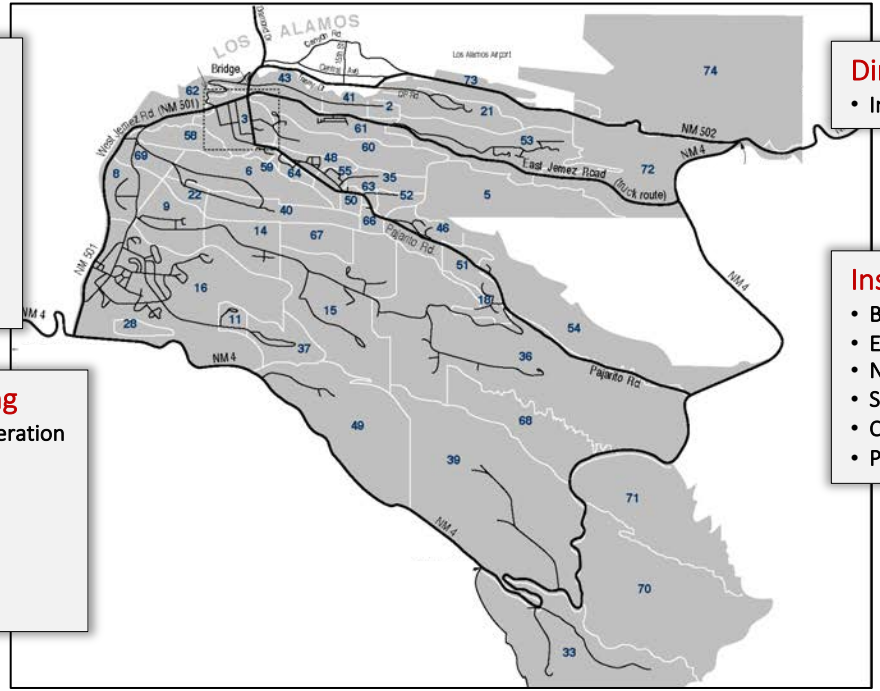
# The Laboratory is a complex, dynamic system of people, facilities, materials, and services

## Weapons Programs

- Weapons Physics Design and Computation
- Weapons Engineering
- High Explosives
- Plutonium
- Tritium/GTS
- Uranium, Beryllium, Salts, Metals
- Detonators
- Component Fabrication and Assembly

## Science, Technology & Engineering

- Nuclear Nonproliferation & Counter-Proliferation
- Emerging Threats
- Intelligence Community
- National Defense and Homeland Security
- Chemistry, Earth and Life Sciences
- Materials and Physical Sciences
- Theoretical and Computational Sciences




## Director's Office

- Institutional Management

## Institutional Operations

- Business Services
- Environmental, Safety, and Health
- Nuclear & High Hazard Operations
- Security and Mission Assurance
- Capital Projects
- Project Management Services

40 square miles 47 technical areas 1,280 buildings/ 9M sq ft 11 nuclear facilities 268 miles of roads

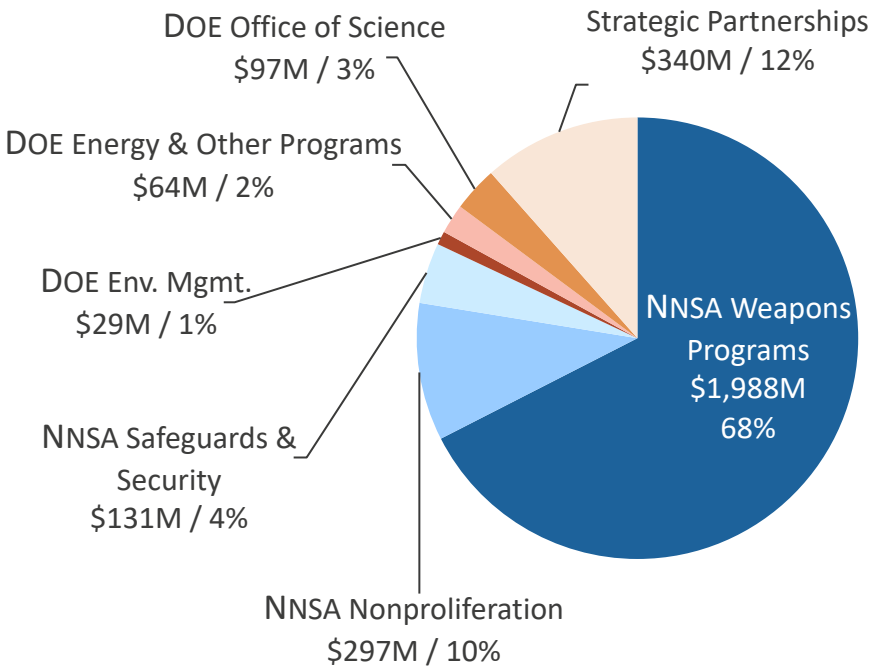
8,400 career employees/12,800 workers on site 2,500 R&D staff 1,100 veterans 460 postdocs 1,850 students

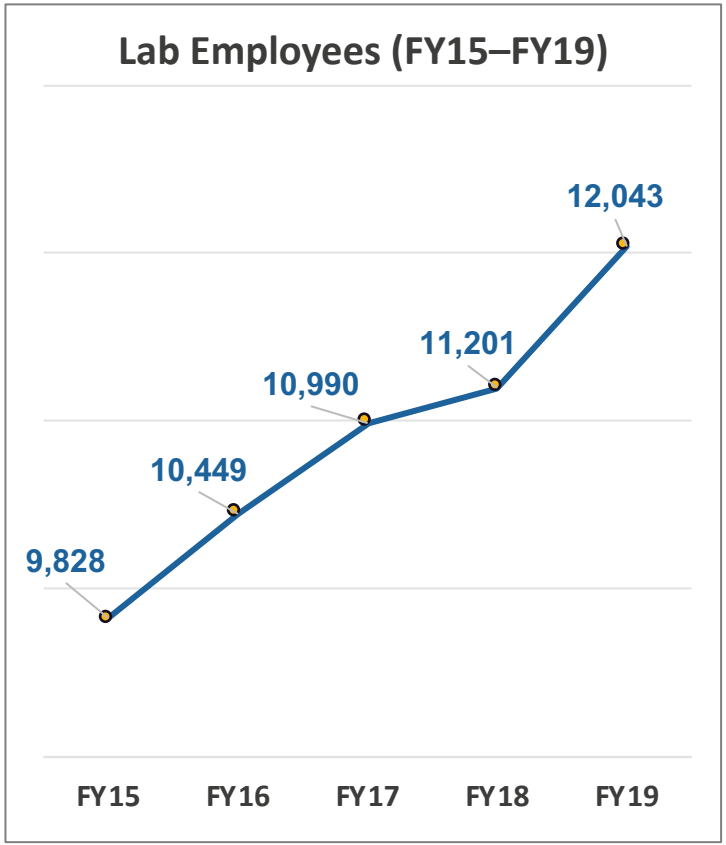
$2.9B budget 4,700 projects 600 B&R codes

11 Directorates 60 Divisions

# LANL has a steady budget and a growing staff

## FY20 Programmatic Portfolio: $2.946M (Est.)



# Lab Agenda: Simultaneous excellence

*Mission, Vision, and Culture*

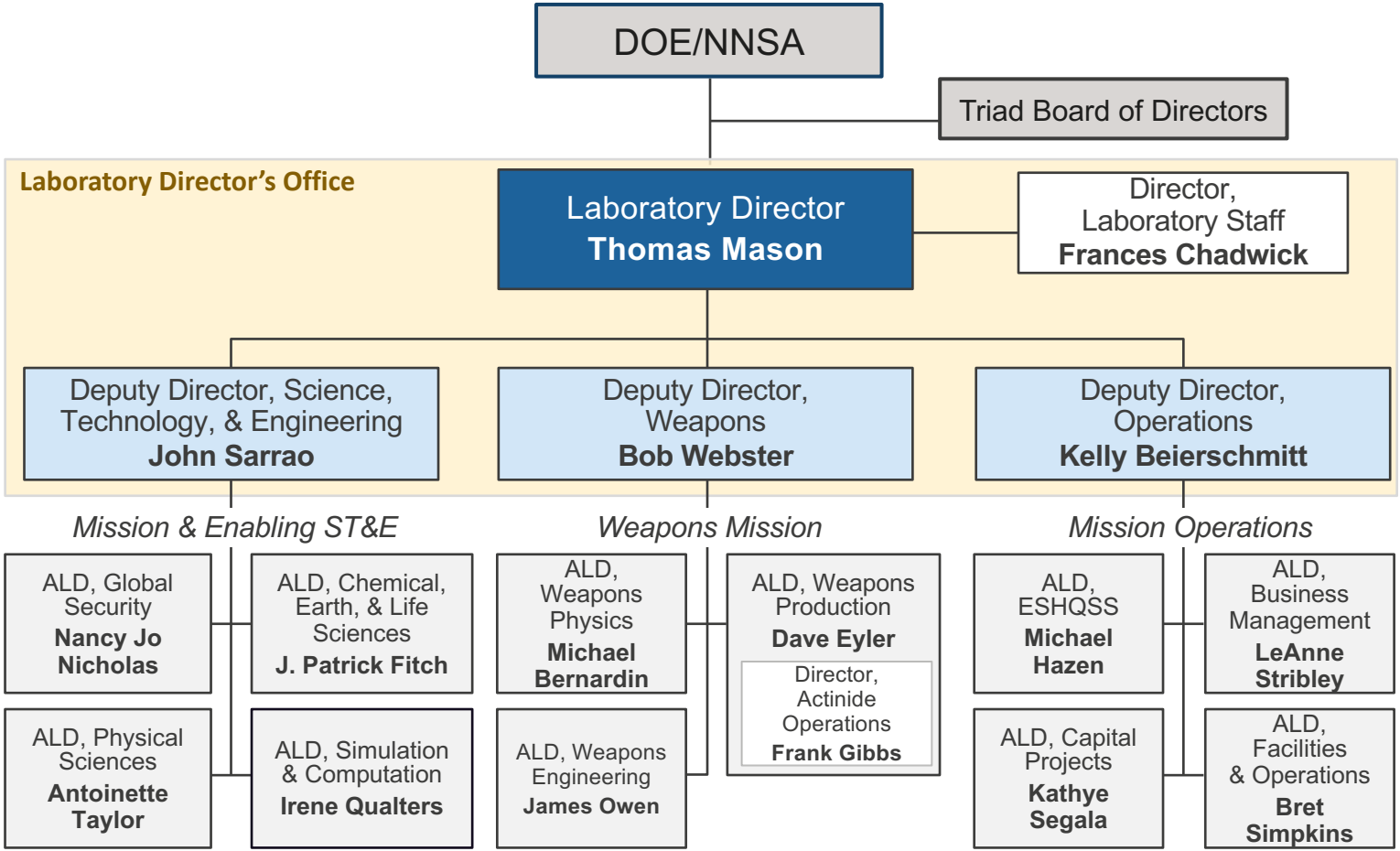
**Design, produce, and certify current and future nuclear weapons and reduce global nuclear threats**

**Deliver scientific discovery and technical breakthroughs that support DOE & NNSA missions**

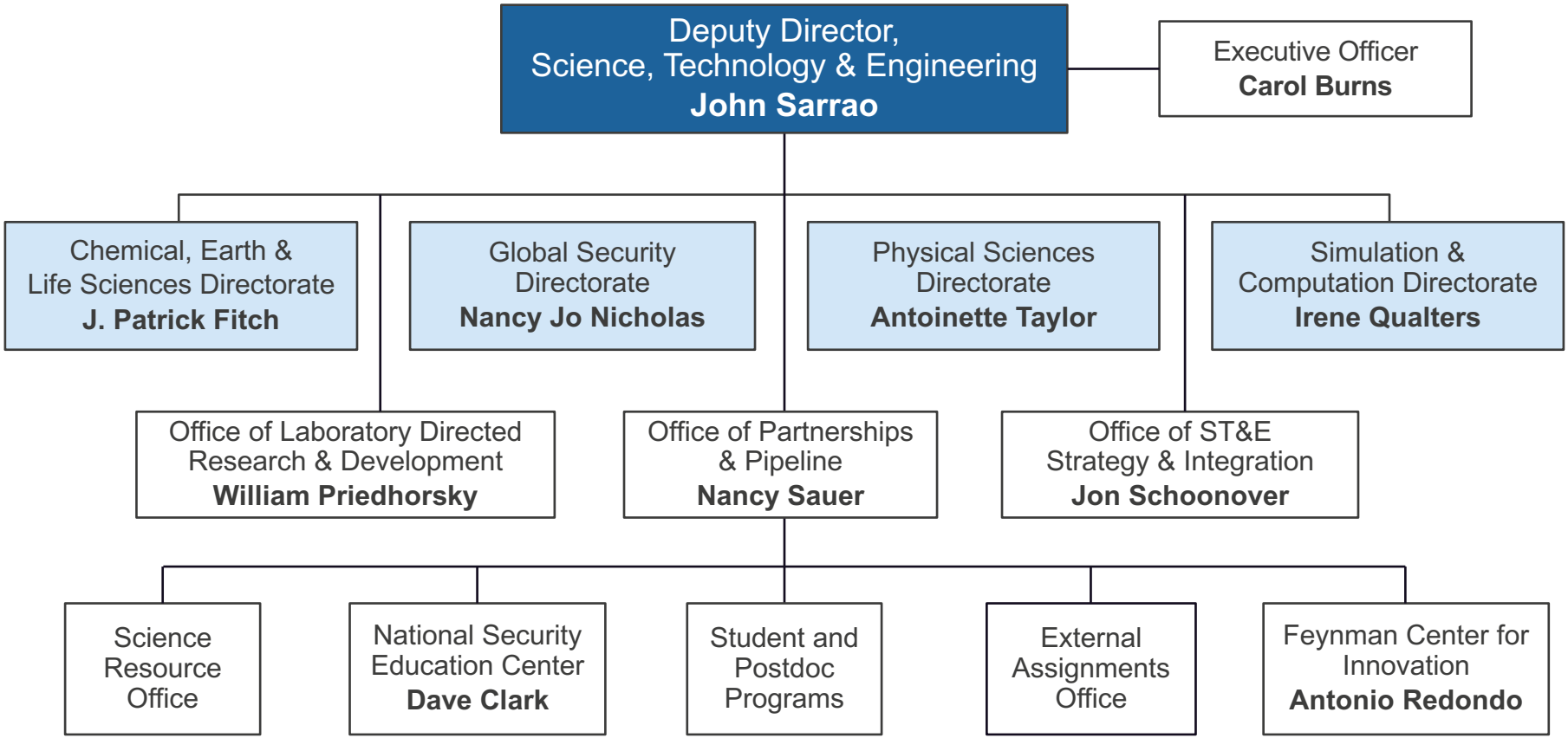

**Execute sustained operations that are reliable and responsive to mission needs**

**Sustain and enhance LANL's partnership with the community across Northern New Mexico**

# Los Alamos National Laboratory Organizational Structure



# DDSTE organization



# Partnerships & Pipeline Office (PPO) was formed at transition to enhance our internal coordination and external outreach

Pipeline

Partnerships

## Pipeline Mechanisms:

- **Student Programs:** Education opportunities for high school, undergraduate, and graduate students
- **Postdoctoral Programs:** Postdocs contribute to research efforts, enhance our STE capabilities

## Partnership Opportunities:

- **National Security Education Center Strategic Centers:** Scientific centers of excellence with high international visibility that innovate strategic new science and education programs
- **New Mexico Consortium Coordination:** Creative mechanisms for collaboration with NM research universities through joint appointments and unique facilities
- **Feynman Center for Innovation:** From “tech transfer”’ to innovation asset stewardship with strategy driven through Innovation Asset Strategic Council

# Our student and postdoc pipeline is crucial for recruiting the workforce of the future

- 1,850 students and 460 postdocs were part of our workforce in FY19
- Conversion of postdocs to technical staff is our most highly utilized early-career pipeline

**Percentage of total LANL population who were former students or postdocs**

| 36% | 61% | 33% |
|---|---|---|
| **All LANL employees** (Reg, TRMA) | **All R&D scientists & engineers** | **Managers** |

Summer Physics Camp for Young Women

Supercomputing Challenge

29% of regular/term employees have at least 1 degree from a NM college/university

41% of Los Alamos employees are native New Mexicans

# ALDSC Organization

## Associate Laboratory Directorate for Simulation & Computation

**Deployed Support**

- **Kerry Mandril,** *Financial Business Manager (FA-STE)*
- **Melanie Vigil,** *Human Resources Generalist (HR-FCS)*
- **Christine Doyle,** *Human Resources Generalist (HR-FCS)*
- **Dan Schmidt,** *Deployed Security Officer (EMD-DS)*
- **Mary Lou Holmes,** *Senior Cyber Security Advisor (OCIO)*
- **Vanessa Richardson,** *ES&H Subject Matter Expert (DESH-UIS)*

**Antonya Sanders**
*Administrative Officer*

**Irene Qualters**
*Associate Laboratory Director*

**Paul Dotson**
*Chief Operating Officer*

**Beth Kaspar**
*Project-Program Director*

**Candace Culhane**
*Project-Program Director*

**Steve Poole**
*Scientist 6*

### Computer, Computational and Statistical Sciences Division

**Anita Casteneda**
*Chief of Staff*

**Ed Dendy**
*Division Leader*

**Aric Hagberg**
*Deputy Division Leader*

**Markus Berndt**
*Group Leader*
*Computational Physics and Methods*

**Linn Collins**
*Group Leader*
*Applied Computer Science*

**Patrick Kelly**
*Group Leader*
*Information Sciences*

**Mike Lang**
*ASC CSSE Program Manager*

**Michael Fugate**
*Group Leader*
*Statistical Sciences*

### High Performance Computing Division

**Patty Molina**
*Chief of Staff*

**Gary Grider**
*Division Leader*

**Rand Rheinheimer**
*Deputy Division Leader*

**Cindy Martin**
*Group Leader*
*Environments*

**Jim Lujan**
*ASC Platforms Program Manager*

**Jeff Johnson**
*Group Leader*
*Systems*

**Paul Weber**
*IC Program Manager*

**David Morton**
*Group Leader*
*Design*

**Jason Hick**
*ASC FOUS Program Manager*

### Theoretical Division

**Eleanor Alarid**
*Chief of Staff*

**Joel Kress**
*Division Leader (acting)*

**James Colgan**
*Deputy Division Leader (acting)*

**James Colgan**
*Group Leader*
*Physics & Chemistry of Materials*

**Anna Hayes-Sterbenz**
*Group Leader*
*Nuclear & Particle Physics, Astrophysics & Cosmology*

**Kim Rasmussen**
*Group Leader*
*Fluid Dynamics & Solid Mechanics*

**Avadh Saxena**
*Group Leader*
*Physics of Condensed Matter & Complex Systems*

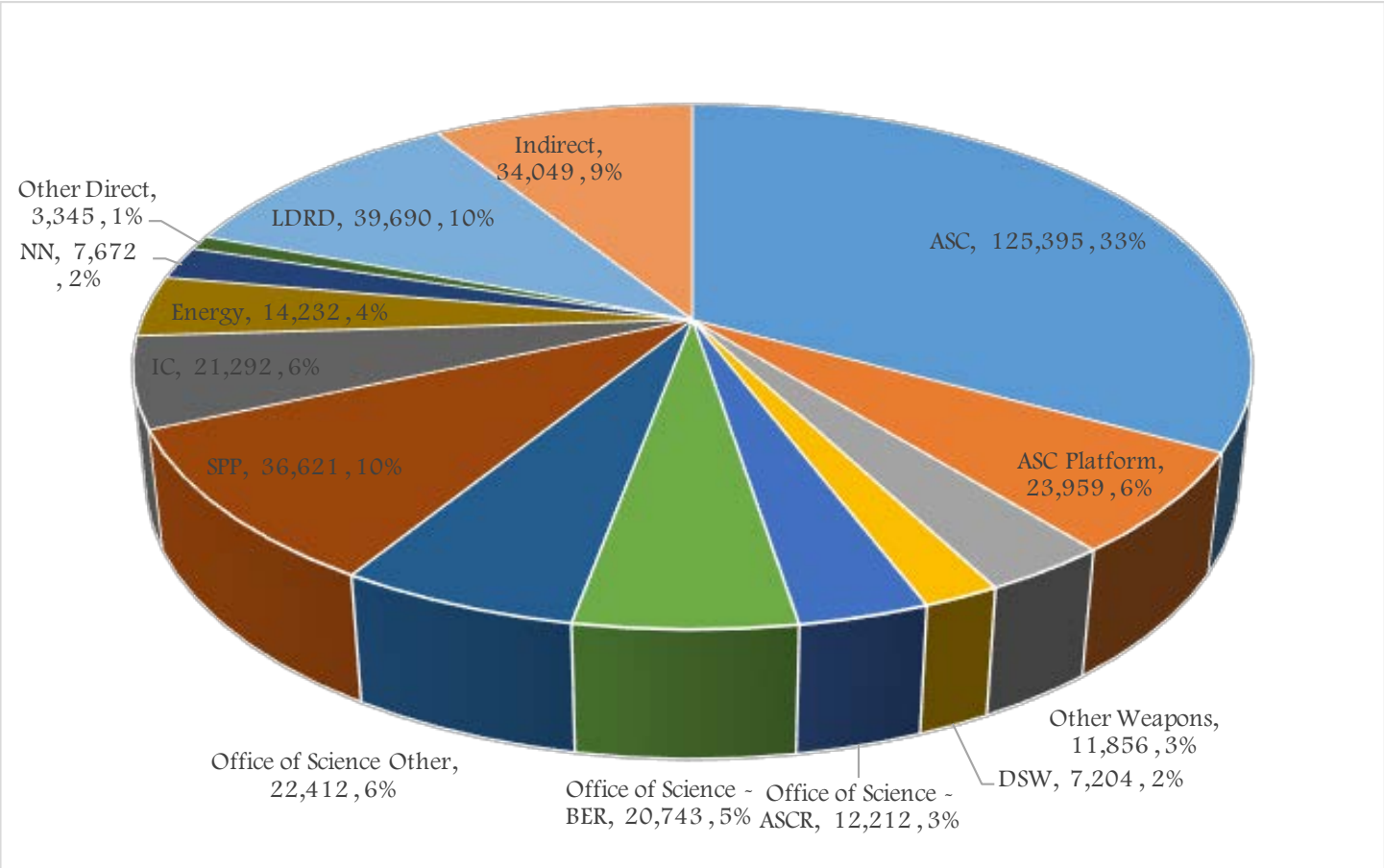
**Pieter Swart**
*Group Leader*
*Applied Mathematics and Plasma Physics*

**Nicolas Hengartner**
*Group Leader*
*Theoretical Biology & Biophysics*

**Angel Garcia**
*Center Leader*
*Center for Nonlinear Studies*

1/14/20

# FY19 Year-End ALDSC-wide Operating Budget of $380.7M Mirrors Lab Funding Diversity *Excludes Capital Funding*



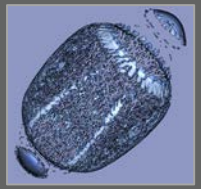
# LANL's long term capability areas ("Pillars") define science, technology & engineering areas in which we must lead/invest

## Materials for the Future

- Defects and Interfaces
- Extreme Environments
- Emergent Phenomena

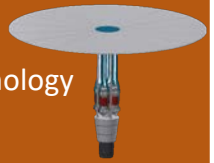
## Science of Signatures

- Nuclear Detonation
- Nuclear Processing, Movement, Weaponization
- Natural and Anthropogenic Phenomena



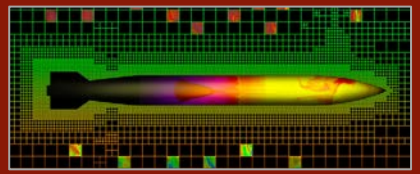
## Nuclear and Particle Futures

- High Energy Density Physics & Fluid Dynamics
- Nuclear & Particle Physics, Astrophysics & Cosmology
- Applied Nuclear Science & Engineering
- Accelerator Science & Technology



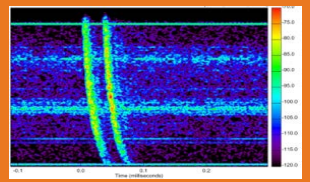
## Weapons Systems

- Design
- Manufacturing
- Analysis



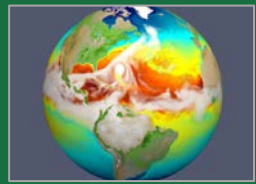
## Integrating Information, Science, and Technology for Prediction

- Complex Networks
- Computational Co-Design
- Data Science at Scale



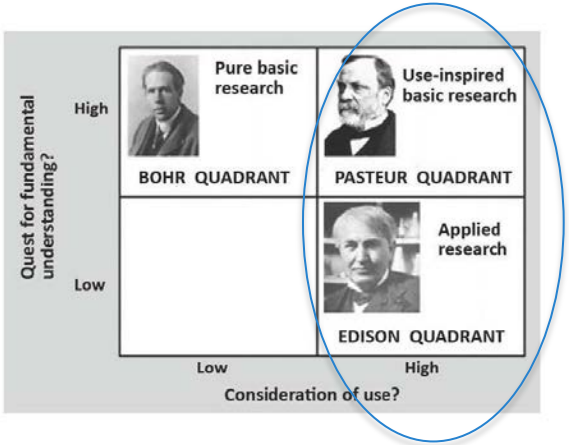
## Complex Natural and Engineered Systems

- Human–Natural System Interactions: Nuclear
- Engineered Systems
- Human–Natural System Interactions: Non-Nuclear

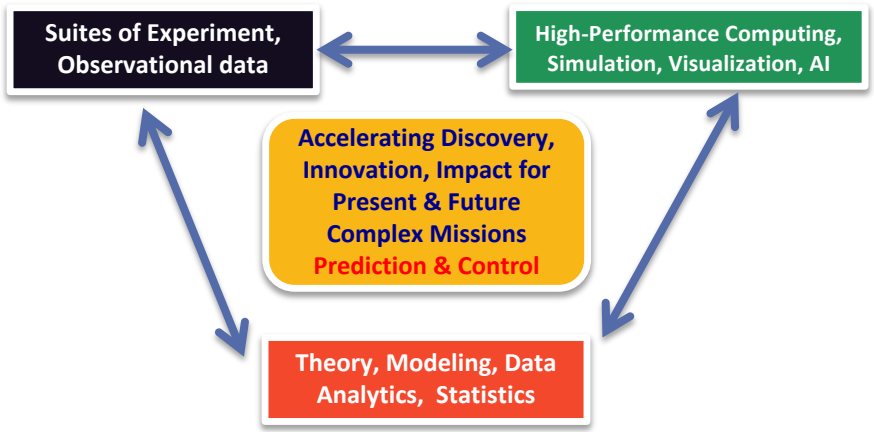


# Co-design: our enduring approach and organizing principle to accelerate and advance discovery (insight, prediction, control)

- Co-design is a *process*, not a goal unto itself
- Directly underpins our broad national security mission
- Crosscuts a wide swath of LANL scientists from STE, Weapons, Global Security



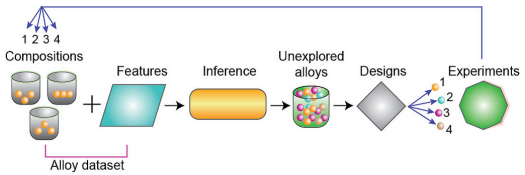

***Co-design … it's in our DNA***



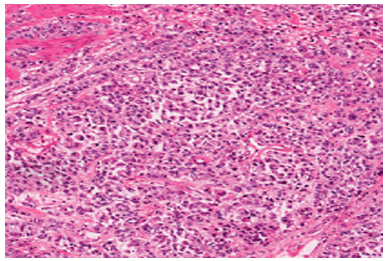
# Leaning forward: LANL's strategic computing priorities

- **Data science for mission**
  - AI/Machine learning, complex work and data flows (sensors, instruments)
  - **Current Focus: Domain science-informed machine learning**
    - Experimental-facility-centric data streams, including sparse data
    - Informed by theory; integrated with simulation; trustworthy
    - Cyber-physical systems; optimization methodology
- **Novel system architectures, technologies**
  - Quantum, Neuromorphic, …
  - Hybrid and heterogenous
  - "Semi-custom"
- **Revolutionary approaches to efficient extreme scale computing platforms**
  - Blurring the boundaries of applications, algorithms, software & ASICs post-exascale ("Co-Design on steroids")
  - 3D methods; multiphysics/multiscale approaches
  - Engineering agility into the software platforms

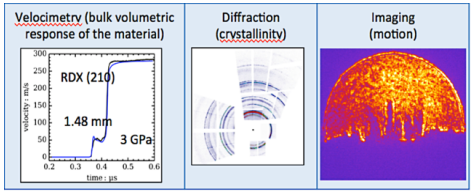
# Data science (machine learning, visualization) is evolving a critical part of today's scientific methodology at LANL



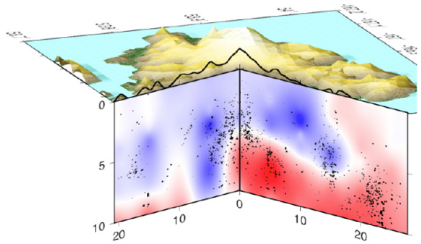

**Machine Learning Accelerating Discovery of New Materials**



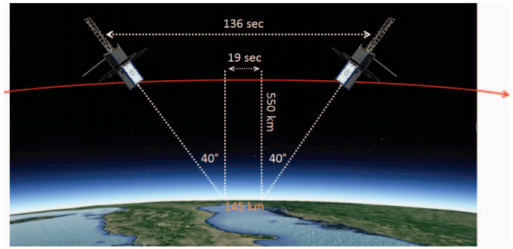
**Bioinformatics/ Emergent Diseases**



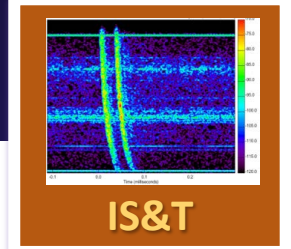

**Real-time Adaptive Acceleration of Dynamic Materials Data Analysis**



**Critical Stress in Subsurface Energy Dynamics and Earthquakes**




**Constellation of CubeSats Carrying Ultra-Compact Spectral Sensors**



# Example of co-design: MELT (LDRD) – ML for Turbulence

*Accelerate hydroclosure, preserving relevant physics and accuracy*

- **Diagnostics** of ML solutions
  - sequence of tests

- Physics-**Free** ML -> Physics **Informed** ML
  - correct objective
  - modify the class of NN functions
  - learn multi-body GM
  - construct NN with physical layers

- Physics Informed **Tuning** -> PIM **Learning**
  - NN interpretation of turbulence
  - learn closure models
  - learn Lagrangian models

- **Synthesis** of PIT -> PIML & PFML -> PIML

- Static to dynamic maps
  - e.g. GANs to ConvLSTM

- PFML->PIML, construct NN with physical layers

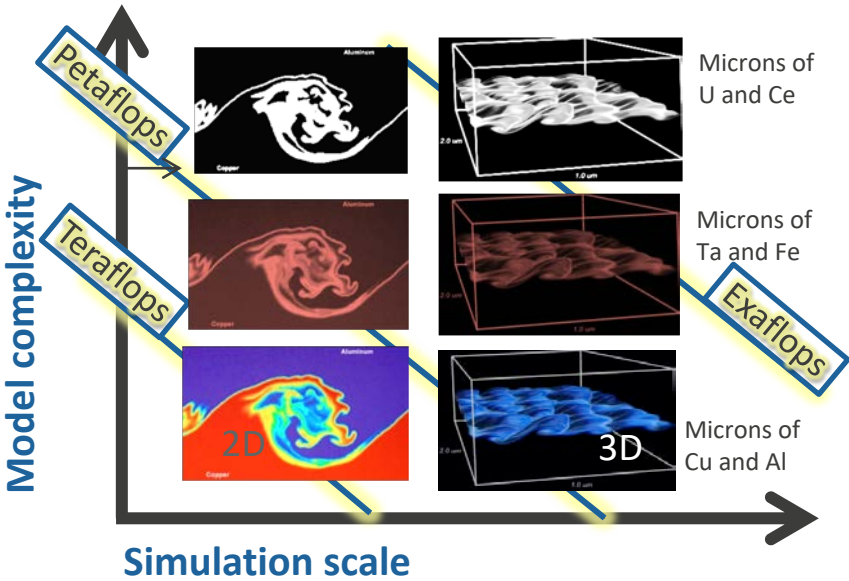
- PIT-> PIML
  - RANS & LES, NN-empowered
  - tetrad model

- Turbulence Applications
  - scalar turbulence
  - HIT
  - variable density turbulence
  - Rayleigh-Taylor turbulence

- Applications in astrophysics and climate

# Advances in predictive modeling, simulation, and computation are required to address both urgent and longer-term NNSA needs

- **Urgent national security drivers:**
  - Aging and manufacturing challenges in current stockpile systems
  - Changing threat environment for both current and future systems
- **Longer-term national security issues requiring higher resolution include:**
  - Nuclear device disablement
  - 3D assessment of surety options
  - Understanding plutonium
  - Determining the effects of hydrodynamic mixing on performance
- **Similar motivations exist for many science fields and DOE programs**
  - e.g., seismic, astrophysics, ….

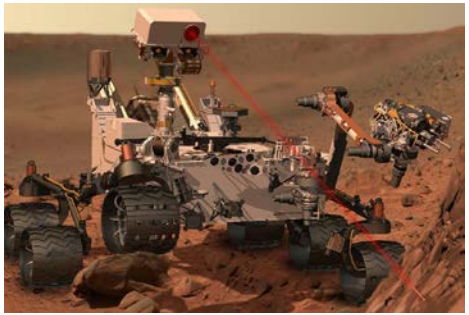


# The Laboratory continues to be essential to the nation's security

## Los Alamos delivers national security mission solutions

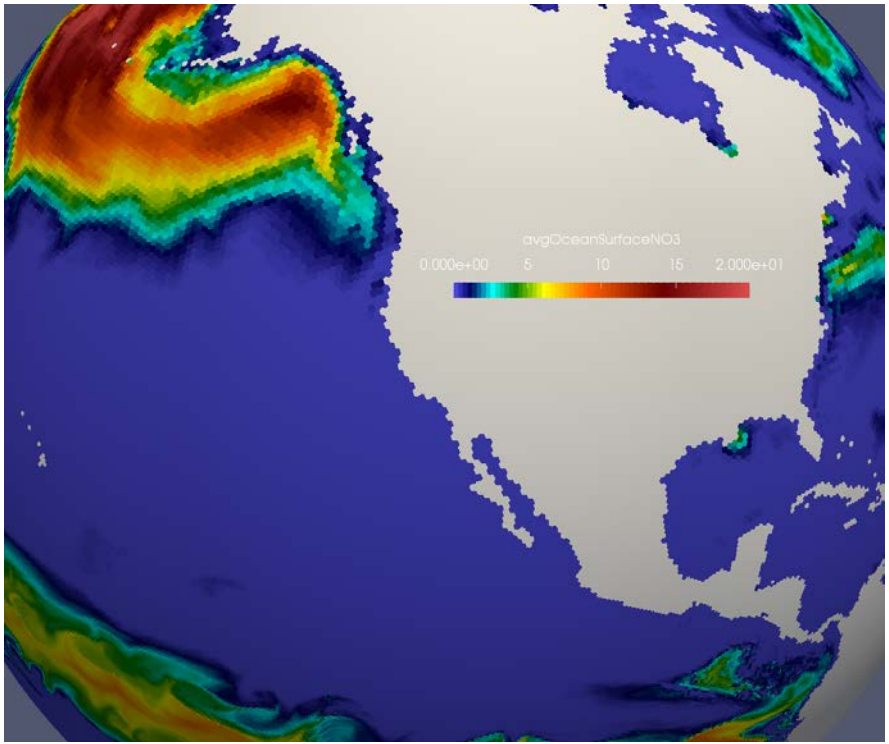
- By applying multidisciplinary science, technology & engineering capabilities, in unique experimental, computational, and nuclear facilities
  - With an agile, responsive, and innovative workforce
    - Dedicated to addressing complex national security issues and the world's most difficult challenges



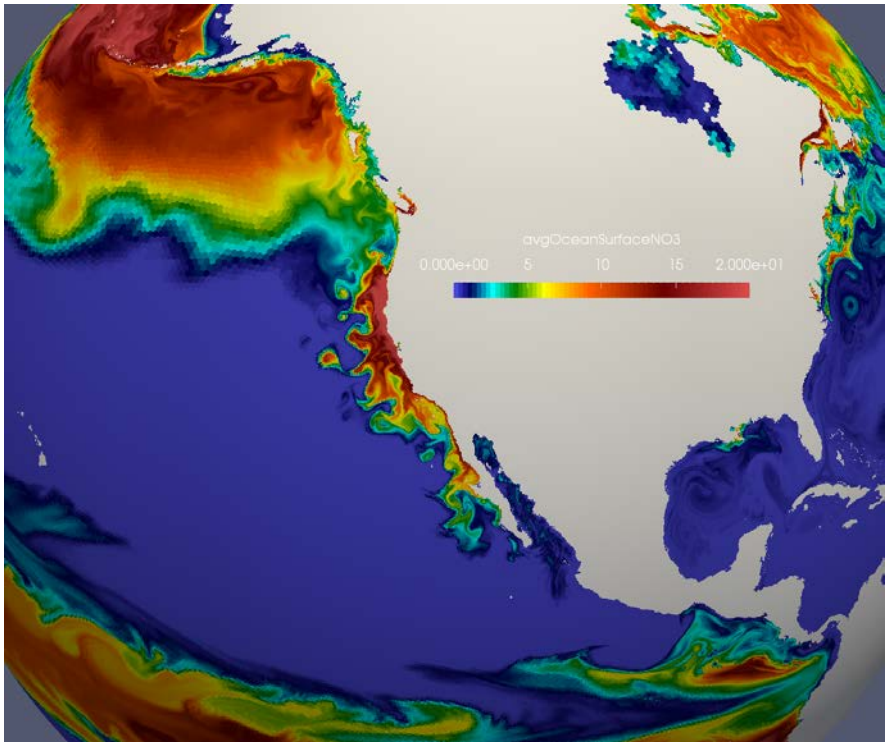



# Advances in high resolution 3D multiphysics coastal simulations are fundamental to  to DOE's Energy Exascale Earth System Model  (E3SM)

## Average Ocean Surface Nitrate




Low resolution




Enhanced resolution along North American coasts

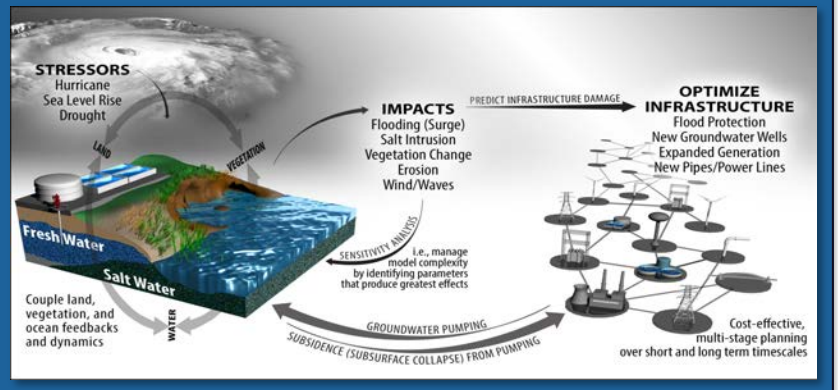
# Predictive understanding of human and environmental coastal dynamics for society and national security

CLIMATE @LANL

LANL's Coastal Grand Challenge

LDRD

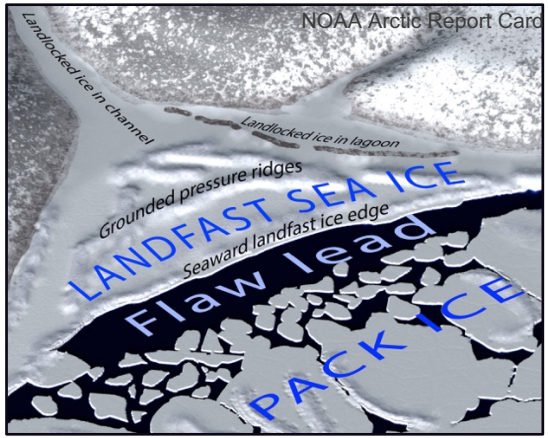
New Science for Multisector Adaptation (NeMSA)

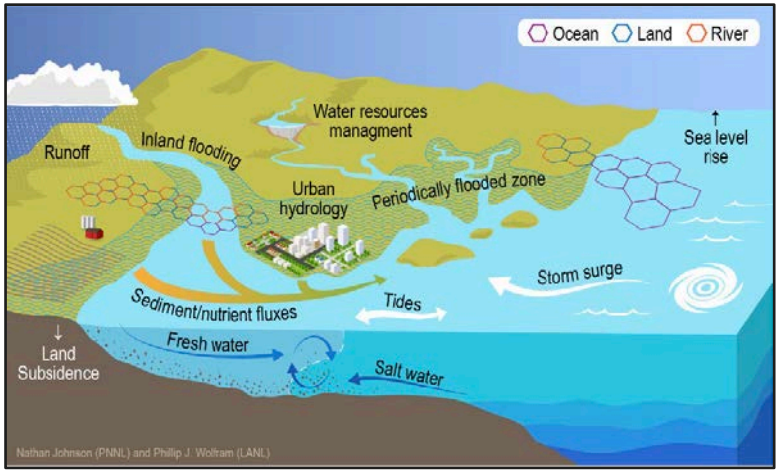




New DOE projects

## Interdisciplinary Research for Arctic Coastal Environments (InteRFACE)

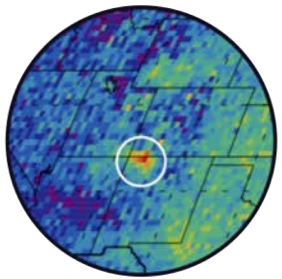

## Integrated Coastal Modeling (ICoM)

***Joint research across DOE/BER, National Laboratories, Academia***

# Climate impacts on national security

- Climate moving toward a “no analog” future
- Threats to civilian and defense infrastructure and operations
- Threats to the stability of countries


Coastal Resilience


Geoengineering


The New Arctic


First Offset


Regional Stability

Data Analytics

Infrastructure Analysis and Adaptation

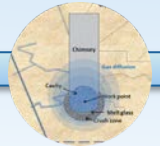
Flexible Computing

# The integration of science, engineering, and mission enables agile responses to national security challenges

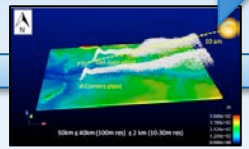
PAST → FUTURE

## SUBSURFACE

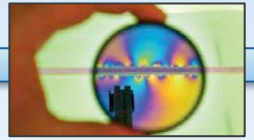
Containment
(Large events)



Nonproliferation and verification



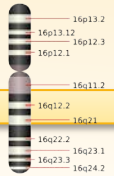
Environment:
Atmospheric & subsurface



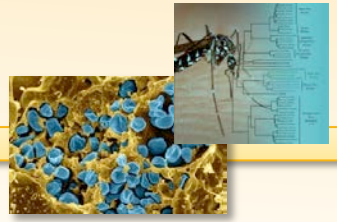
Small event detection,
Fracture formation,
Weapons performance

## BIOSECURITY

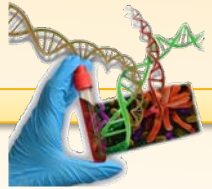

Radiation
health effects




Human Genome
Project



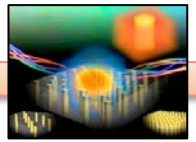
Biosurveillance,
Disease tracking



Bioinformatics, Cancer research,
Data science at scale

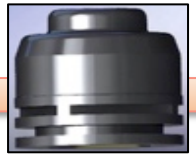
## NANOSCIENCE

Foundational nanoscale
materials research



Metamaterials

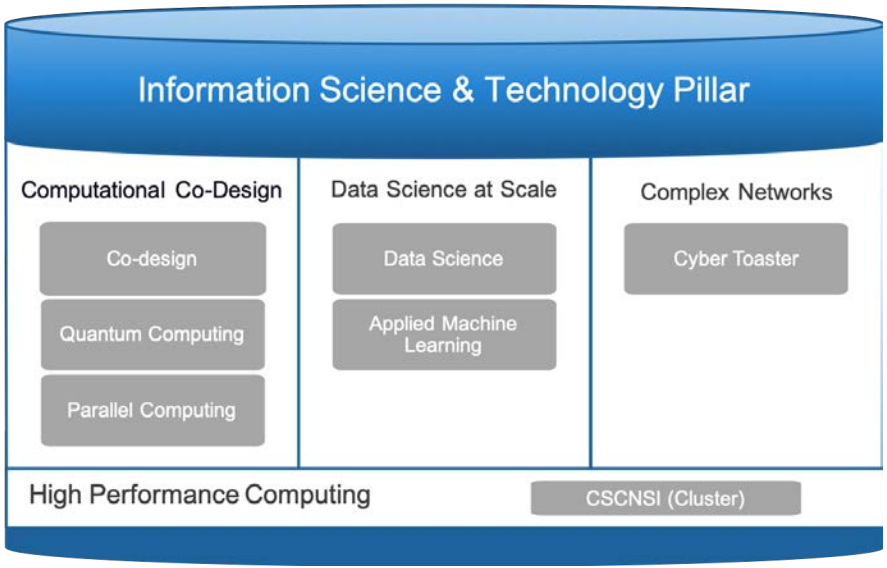
Nanocrystal quantum dots,
Energy applications



Engineered materials with
controlled functionality

# Supplemental Slides

# ISTI Summer Schools address strategic areas within the IS&T Pillar to fill recruiting pipelines




***Co-sponsors***

- Advanced Simulation and Computing Program
- Center for Nonlinear Studies
- Center for Space and Earth Science
- Office of the Chief Information Officer

***Summer School Program***

- 2nd Quantum Computing Summer School
- 3rd Applied Machine Learning Research Internship
- 3rd Cyber Toaster
- 4th Parallel Computing School
- 9th Computational Co-Design School
- 9th Data Science at Scale School
- 13th Computer Systems, Clusters, and Networking Summer Institute
- Computational Physics Summer Workshop (affiliate)

# Summer Schools: What and Why?

- "A summer school exhibits most or some of the following characteristics":
  - Student presence at LANL 10 – 12 weeks (in summer)
  - Structured environment (lectures, presentations)
  - Unifying technical topic relevant to LANL mission space
  - Led by school lead(s) who assemble a dedicated mentor team
  - Physical colocation of students

- Rationale:
  - Recruiting pipeline
    - School structure increases chances that students return to LANL
    - Exposing students to LANL National Security challenge overcomes recruiting disadvantages

  - In some LANL-unique technical areas, externally-offered courses simply do not exist or are not common

# Parallel Computing Research Internship (PSCRI)


## SYNOPSIS

The Parallel Computing Summer Research Internship is an intense 10 week program aimed at providing students with a solid foundation in modern high performance computing (HPC) topics integrated with research on real problems encountered in large-scale scientific codes. Students will collaborate in teams to identify and investigate different computational problems and implement solutions with guidance from mentors with scientific and computational expertise.

## STATISTICS

| | |
|---|---|
| Started: | |
| # Students per year | 2016 |
| # Applicants per year: | 12-16<br>50 - 100+ |
| # Students total: | 57 |
| # Universities (FY19): | 10 |
| # Mentor Groups (FY19): | 8<br>~30% |
| # Returnees to LANL: | SC, SIAM, |
| Posters | LANL Student Symposium |

## EXAMPLE PROJECTS

- Quantifying Uncertainties in Vector Particle-In-Cell (VPIC)
- Runtime Examination of Kokkos
- Enabling Performance Portable Exascale Atmospheric Simulations: HiGrad GPU Port and Performance Analysis
- Statistical Estimation via Variational Inference using MPI and GPUs
- Numerical Method for the Computation of Synchrotron Radiation in the Near-Field
- Impact of a Stencil Kernel's Radius and Loop Tiling on Performance

# Supercomputer Institute

**SYNOPSIS**

Supercomputer Institute is a 11 week technical summer school program offering hands-on experience building and operating state-of-the-art and next-generation computer clusters, high-speed networks, extreme-scale filesystems, containers, security, and more. Students work in small project teams to execute real-world projects on computer clusters that they have assembled and configured.

**STATISTICS**

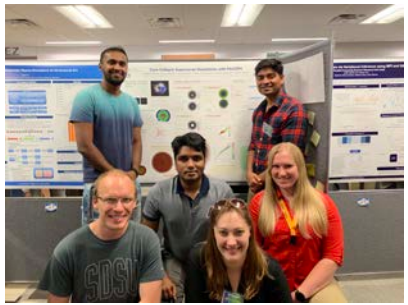
| | |
|---|---|
| Started: | 2007 |
| # Students per year: | 9-12 |
| # Applicants per year: | 40-50 |
| # Students total: | 151 |
| # Universities (FY19): | 11 |
| # Returnees to LANL: | ~50% |

Comment: recruited to HPC, NIE, XIT; Strong record of SC posters

**EXAMPLE PROJECTS**

- Exploring Computational System Health Monitoring and Reporting Solutions
- sFlow Monitoring for Security and Reliability
- LayerCake Workflow: Incorporating Containers into an HPC Environment
- An Analysis of the Effects of the Spectre and Meltdown Patches on the Lustre Parallel File System

# Codesign School



**SYNOPSIS**

The Codesign School recruits 6-8 graduate students from varying backgrounds (usually computer science, computational physics, and mathematics) to work on a computational codesign topic, such as novel programming models, on a specific application, such as hydrodynamics. The work usually results in research papers and posters.

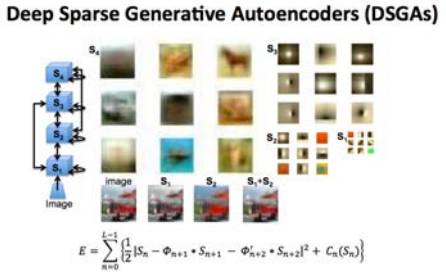
**STATISTICS**

Started: 2011
# Students per year:6
# Applicants per year: 40-50
# Students total: 56
# Universities (FY19): 6
# Mentor Groups (FY19): 5
# Returnees to LANL: ~25%
Comments: co-sponsored by ASC since 2014

**EXAMPLE PROJECTS**

- 2012: Scale-Bridging Approach to a Steady-State Neutron Transport
- 2013: Materials in Extreme Environments
- 2014: Adaptive Mesh Refinement for Hydrodynamics Simulations
- 2015: Quantum Molecular Dynamics
- 2016: Astrophysics – Neutron Star Mergers
- 2017: Accelerated Molecular Dynamics
- 2018: Equation of State: Caching and Balancing Tables
- 2019: Performance and Stack Portability of FleCSPH- Core Collapse Supernovae

# Applied Machine Learning (AML) Research Internship




## SYNOPSIS

The Applied Machine Learning Research Internship is an intense 10-week program is aimed at providing students with a solid foundation in modern machine learning (ML) topics combined with research on real problems encountered in national laboratory missions.

## STATISTICS

Started: 2017
# Students per year: 12-24
# Applicants per year: 100+
# Students total: 53
# Universities (FY19): 13
# Mentor Groups (FY19): 4
# Returnees to LANL: ~25%
# Publications: ICCV, AGU, plus others, Best Paper Award at LANL Symposium (2019)
Comments: Additional funding provided by CNLS and in FY18 also CSES as well as two individual LDRD projects

## EXAMPLE PROJECTS

- High-Resolution Velocity Model Estimate via Data-Driven Full Waveform Inversion- Generalization and Robustness Study
- Diagram Image Retrieval using Sketch-based Deep Learning and Transfer Learning
- Tensor Factorization Model for Asymmetric Pairwise Relationship: Application to Export Data
- Preconditioned ADMM on (Convolutional) Sparse Coding
- Image Segmentation for River Channel Analysis
- Visual Data: Technical Diagram Feature-Based Image Retrieval

# Cyber Security School


<cyber.toaster>

## SYNOPSIS

The Cyber Summer School (“Cyber Toaster”) prepares students for careers in cyber security. The school has two tracks: incident response to learn the necessary concepts and skills to investigate cyber security incidents, or research to develop innovative solutions to help address national cyber threats.

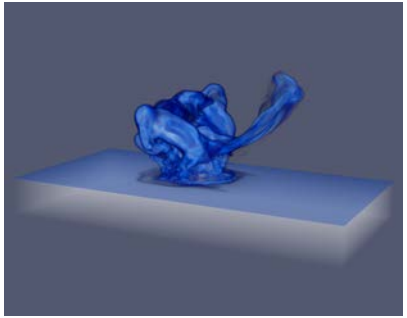
## STATISTICS

Started: 2017
# Students per year:9
# Applicants per year: 80-100
# Students total: 27
# Universities (FY19): 7
# Mentor Groups (FY19): 2
# Returnees to LANL: ~40%
# Publications: LANL Student Symposium Poster Winner
Comments: Additional funding provided by OCIO and the Cyber Fire Program.

## EXAMPLE PROJECTS

- Robust Detection of Computer Generated Text
- Detecting Fake (AI Generated) Text vs Real (Human Written) Text
- CAP: Classifying Audio Perturbations
- SNNzkSNARK: An Efficient Design and Implementation of a Secure Neural Network Verification System Using zkSNARKs
- Coordinating Incident Response to Advanced Threats

# Data Science at Scale School



**SYNOPSIS**

The Data Science School studies topics in data science as relevant to the Los Alamos National Laboratory mission. A key focus is placed on using big data technologies to gain insights from science data.

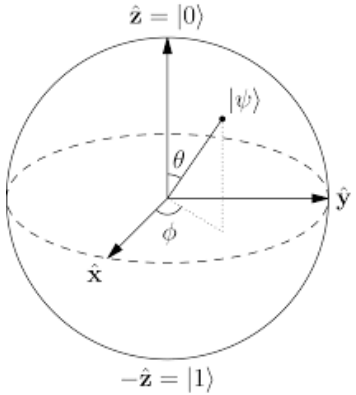
**STATISTICS**

Started: 2013
# Students per year: 10-25
# Applicants per year: 50-65
# Students total (FY19): 3 (funded by ISTI)
# Universities (FY19): 3
# Mentor Groups (FY19): 2
# Returnees to LANL: 3 (of ISTI funded students)
Comments: ISTI is one of many sponsors of the school supporting 3-5 students each year

**Example Projects**

- Exploring Feature Extraction and Semantic Interaction Techniques for Uncertainty Quantification of Image-based Simulation Ensembles
- Extending Visualization Task Taxonomies for Scientific Users
- Project Feigenbaum: Poking Hole in P0037R5 with Simple Physics Simulations
- In-Situ-Dashboard: Enable Scientific Simulation and Data Visualization of HPC Data
- Finite-time Saddles from Particle Origin and Destination

# Quantum Computing School




**SYNOPSIS**

The Quantum Computing School is an immersive 10-week curriculum focused on the theory, applications, and hands-on programming of quantum computers. In the first 2 weeks, students will attend lectures given by world-leading experts, from both academia and industry. In the following 8 weeks, each student will be paired with a mentor to work on a cutting-edge research project in quantum computing.

**STATISTICS**

Started: 2018
# Students per year: 10-15
# Applicants per year: 150+
# Students total: 22
# Universities (FY19): 11
# Mentor Groups (FY19): 6
# Returnees to LANL: ~15% (based on last year)
# Publications (FY19): 2 currently on ArXiv
Comments: Distinguished lecture series with guest lectures from world renowned people such as John Martinis, Peter Shor and many more.

**Example Projects**

- Quantum Algorithms for Lattice Gauge Theories
- Efficient Quantum Algorithms for Computing Renyi Entropies
- The Neutrino Many-body Problem on a Quantum Computer
- Variational Quantum Linear Solver
- Noise Resilience of Variational Quantum Compiling

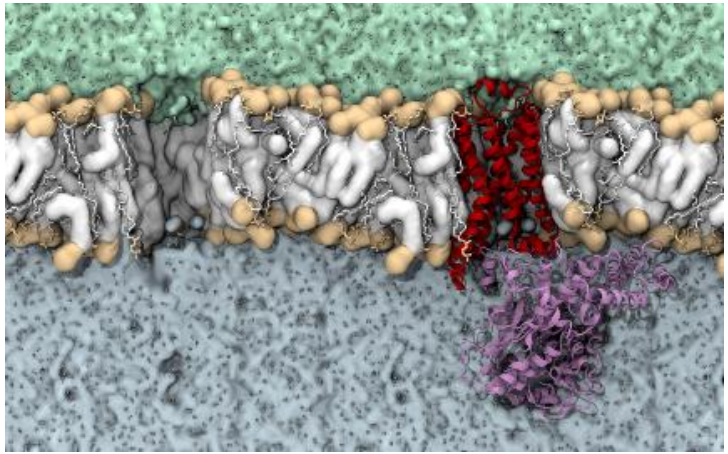
# Center for Nonlinear Studies (CNLS) - Approach

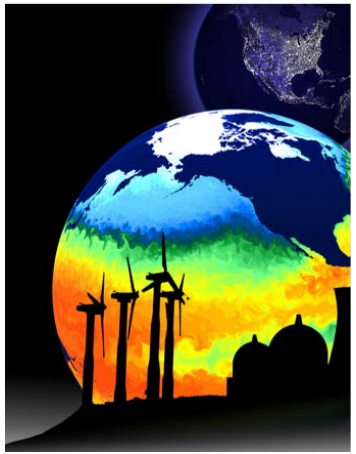
## CNLS meets its goals by maintaining:

- A robust and diverse **postdoctoral fellowships** that pairs postdoctoral fellows with laboratory staff
- A **graduate student** program during the calendar year and a summer student program (27 in 2015; 25 in 2016; 24 students in 2017, 23 in 2018)
- A large **visitors** program (~200 visitors/ year from academia and industry)
- Active **colloquium and seminar series** (Colloquium, Q-mat seminar, Quantum lunch, Postdoctoral fellows seminar, and other visitors seminars)
- Organization of international **conferences** that explore science at the interfaces
- The Ulam Scholar program that hosts long term (**sabbatical**) visitors at CNLS

# CNLS - Current Cross-cutting Scientific Themes

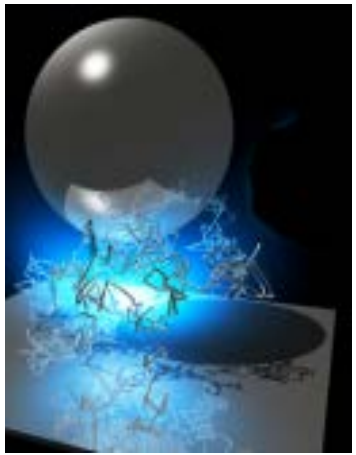
**Mechanistic Studies of Human Disease**

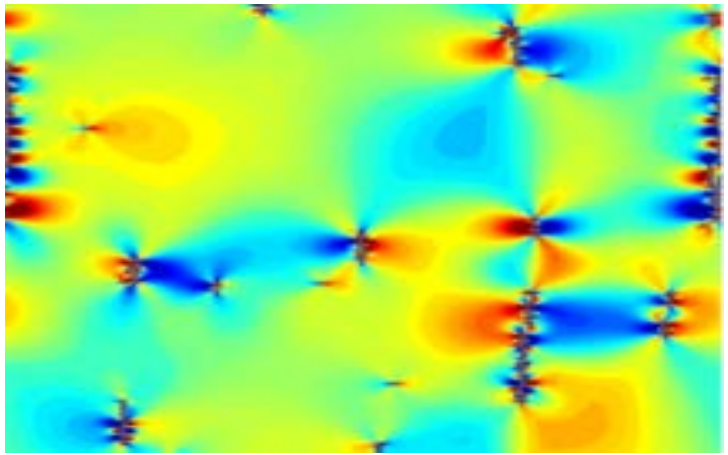




**Machine Learning Enhanced Modeling**

**Theory and Computation of Quantum Systems**





**Dynamics of Systems Far From Equilibrium**