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Title:	Update of Science, Technology and Engineering at Los Alamos
Author(s):	Terry C. Wallace and Janet A. Mercer-Smith
Intended for:	LLNS/LANS Science and Technology Committee Meeting Livermore, CA, USA July 12, 2011

Los Alamos
NATIONAL LABORATORY
EST. 1943

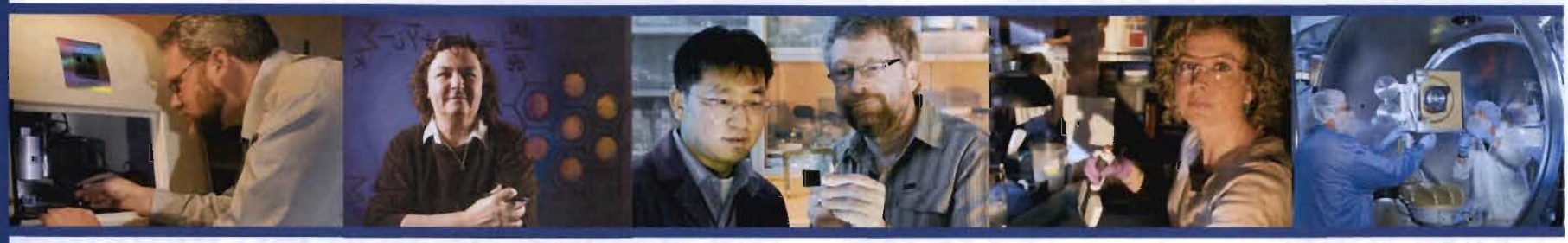
Form 836 (7/06)

Update of Science, Technology and Engineering at Los Alamos

Terry C. Wallace and Janet A. Mercer-Smith

The Laboratory provides science solution to the mission areas of nuclear deterrence, global security, and energy security. The strength of LANL's science is at the core of the Laboratory. The Laboratory addresses important science questions for stockpile stewardship, global security, and energy security.

Science at Los Alamos



Update of Science, Technology and Engineering at Los Alamos

Terry C. Wallace
Principal Associate Director for
Science, Technology and Engineering

July 12, 2011

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LANL Mission

***Our mission as a DOE national security science laboratory* is *to* develop and apply science, technology, and engineering solutions to:**

- Ensure the safety, security, and reliability of the U.S. nuclear deterrent
- Reduce global threats
- Solve Energy Security and other emerging national security challenges

Our vision is to be the premier National Security Science Laboratory.

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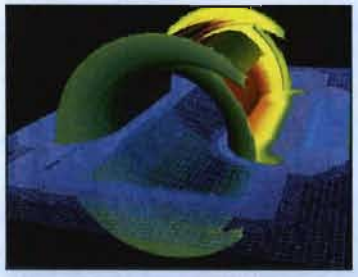
Mission

LANL Mission: National Security Science

Stockpile Stewardship

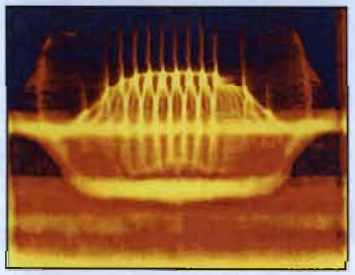


Large-Scale Simulation
Stockpile Stewardship

Pit Manufacturing

B61-7/11 Strategic Bomb

W76, W78, W88
for Trident &
Minuteman III

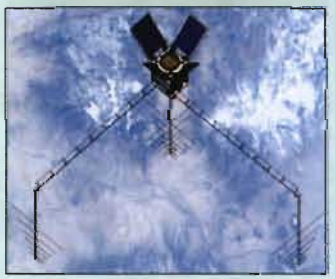


Proton radiography

Global Security

Non Proliferation

Intelligence Analysis

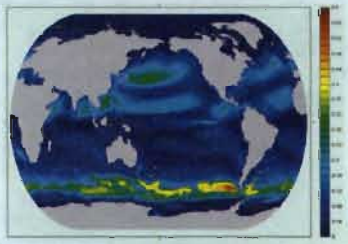


Space Systems
Six other product lines

Energy Security

Materials and Concepts
for Clean Energy

Nuclear Energy



Climate Energy Nexus

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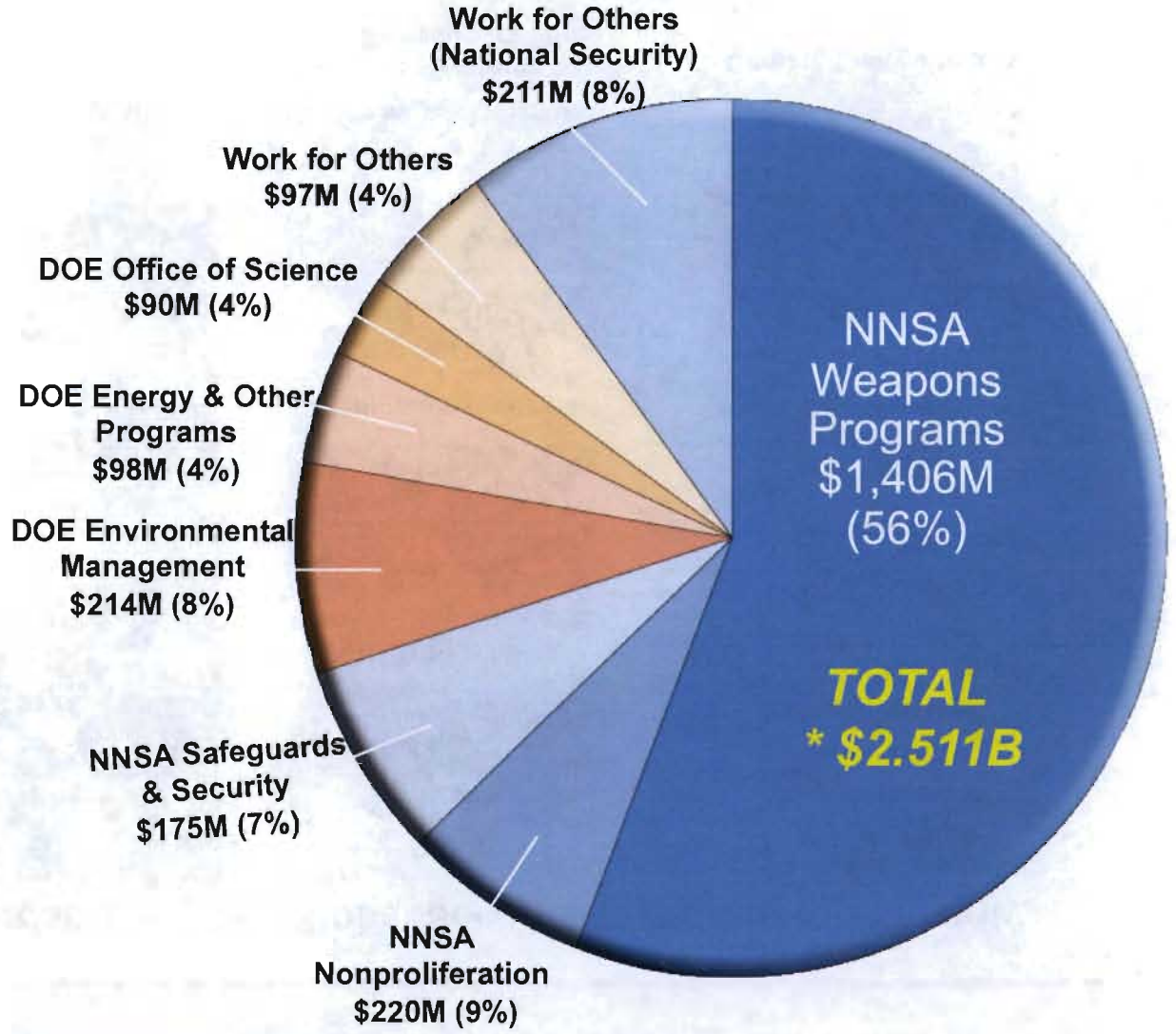
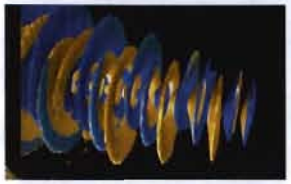
Lab Budget

*The Laboratory's FY11 annual budget is approximately $2.5 billion.



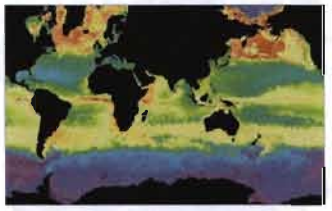
Capabilities

The capabilities of the Laboratory serve program.



Computational Physics & Applied Mathematics

Accelerators & Electrodynamics



Information & Knowledge Science

Nuclear Physics, Astrophysics & Cosmology

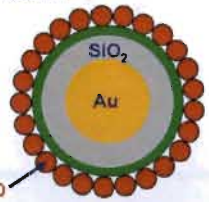
Weapons Science & Engineering

Sensors, Remote Sensing & Sensor Systems

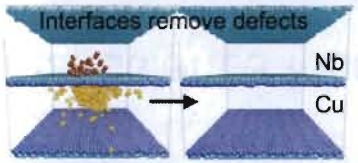
Biosciences

Computer & Computational Sciences

High-Energy Density Plasmas & Fluids



Chemical Science



Materials

Nuclear Engineering and Technology

Earth & Space Sciences

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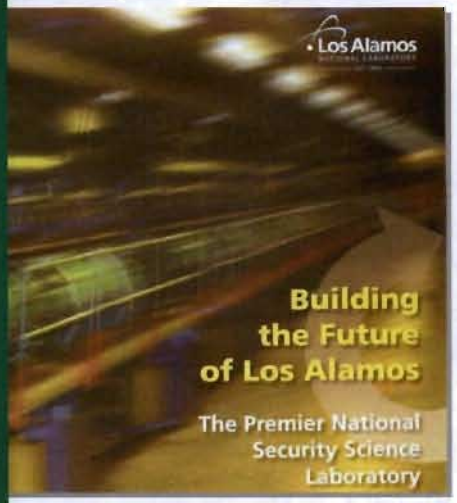
UNCLASSIFIED

Capability pillars define areas we must sustain.



- Experimental science focused on materials for the future
- Information science and technology enabling integrative and predictive science
- Science of Signatures for enduring national needs

Materials for the Future

Information Science and Technology for Integrative and Predictive Science

Science of Signatures

Controlled Functionality
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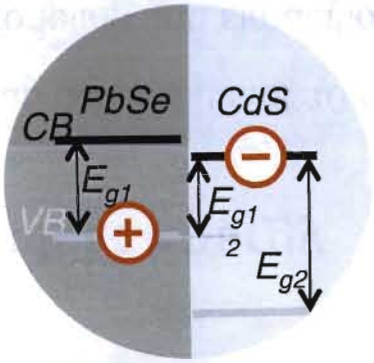
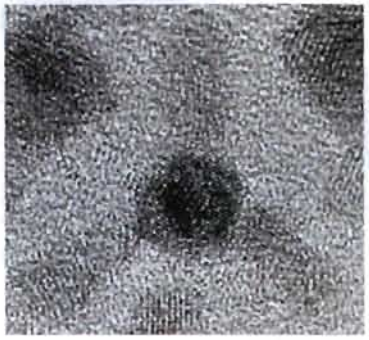
Center for Advanced Solar Photophysics

Novel Materials for Next-Generation Solar Cells

Nanoscale Heterojunctions

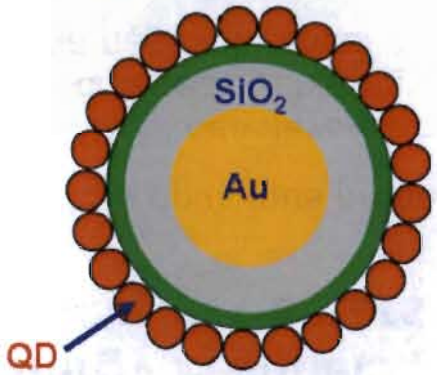
- Spatially indirect" gap (E_{g12}) tunable through infrared
- Pulls charges apart
- Increases time to extract and transport
- Potential use in photocatalysis and photovoltaics

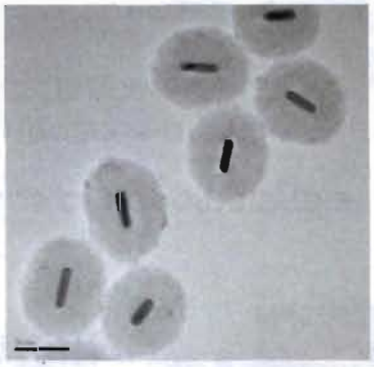




Semiconductor-metal hybrids

- Increased sunlight absorption
- Enhanced non-linear processes, such as two-photon absorption and carrier multiplication
- Potential use in ultrathin solar cells





Energy Security

Los Alamos forms collaborations to address major energy security science issues.

Biofuels

- National Alliance for Advanced Biofuels and Bioproducts Consortium
- National Advanced Biofuels Consortium
- LANL leads algal strain development, harvesting, extraction, catalyst development, commercialization.

Energy Frontier Research Centers

- Focus on unique properties of nanomaterials
- CMIME: nanolayered composites provide increased strength and enhanced radiation damage tolerance.
- Center for Advanced Solar Photophysics: nanoscale structures boost solar-energy conversion efficiency.

Green House Gas Information System

- Global climate models
- Monitoring and verification
- Infrastructure analysis

Nuclear Energy

- Hub consortium of 10 principal partners
- Modeling and simulation to improve performance of nuclear power plants
- LANL leads material science and models and numerical methods areas.

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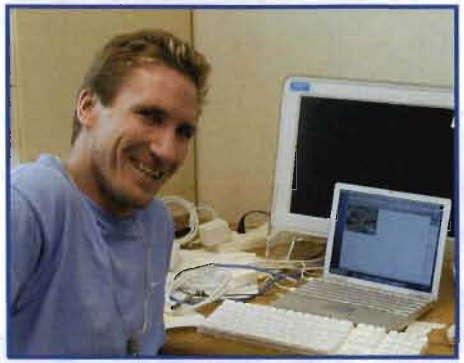
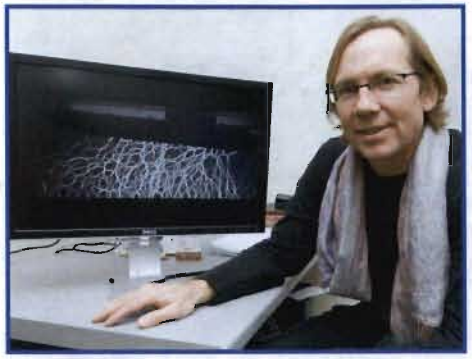
External awards recognize LANL researchers.

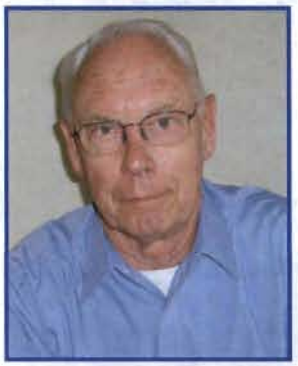


William Higdon
Fellow of the American Statistical Association



Paul Johnson
Fellow of the American Geophysical Union

Christine Anderson-Cook
Outstanding New Mexico Woman
Governor's Award

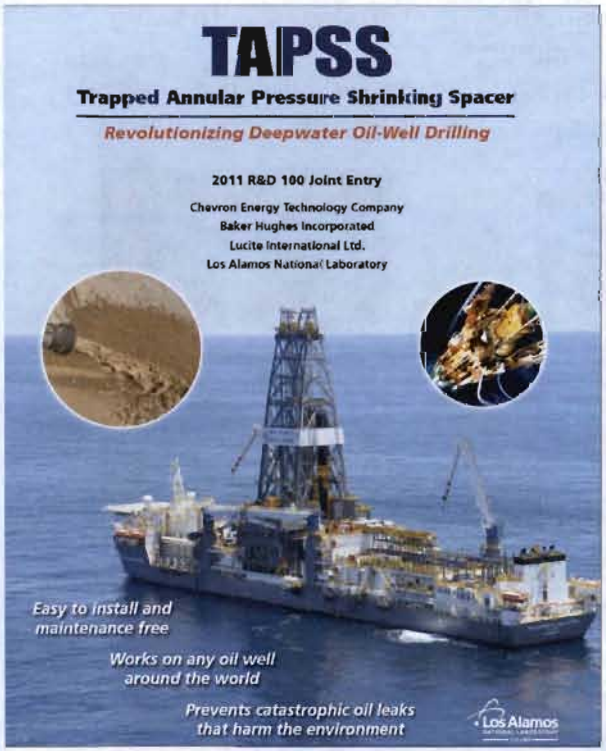


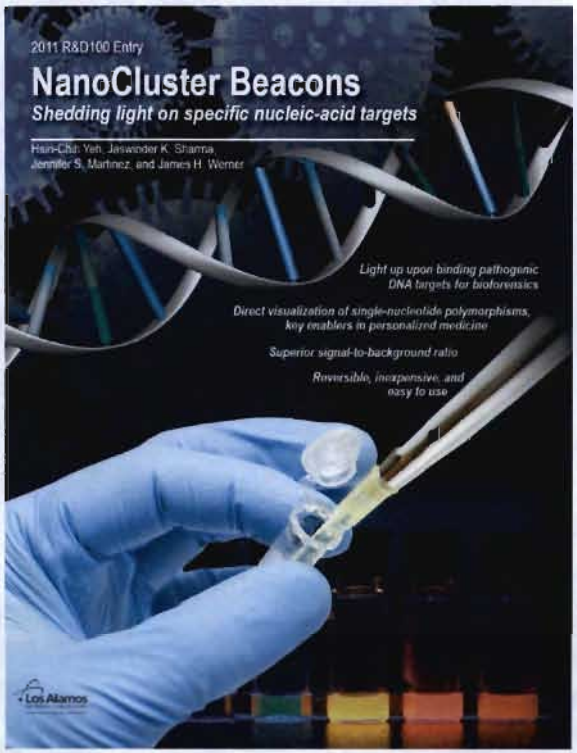
James N. Johnson
George E. Duvall Shock Compression Science Award
American Physical Society

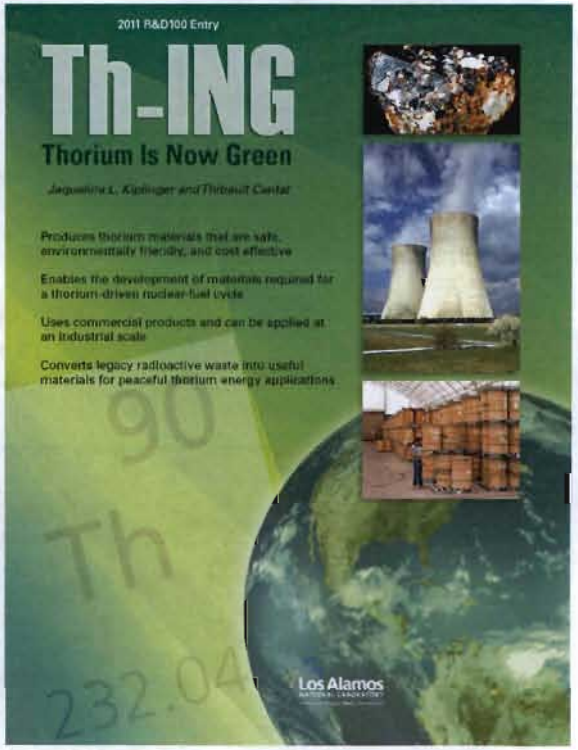
Bill Press
President
American Association for the Advancement of Science

Joanne Wendelberger
Chapter Service Recognition Award
American Statistical Association

R&D100 Awards recognize innovation.







In response to DOE's guidance, we are developing a pre-conceptual design proposal for MaRIE.

LANS Contract Transition

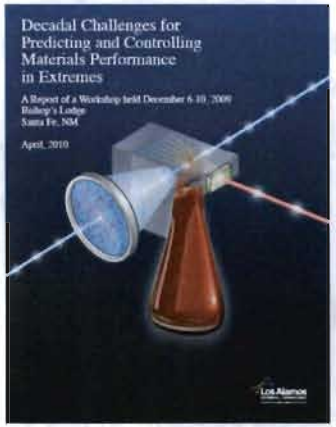
Concept Definition/Internal Competition

MaRIE selection

2006 - 2008

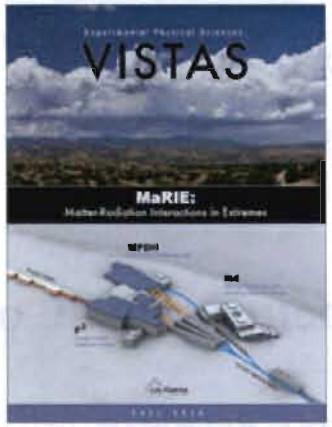
Pre-MaRIE

Science Need



2009

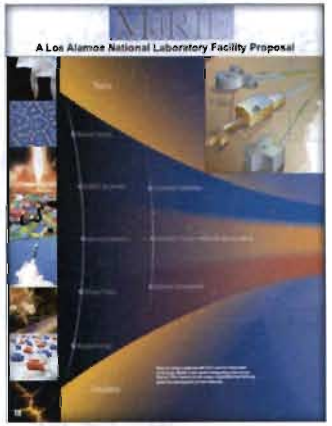
Facility Definition



2010

Today

Pre-conceptual Proposal



2011

Current activities with NNSA and NE are key steps down the path:

LANSCE→ Linac Risk Mitigation → MTS → MaRIE

MaRIE

Introduction and Summary

- **DOE/NNSA has affirmed its commitment to LANSCE for the next decade.**
  - *Letter from 3 Under Secretaries recognized role of LANSCE at LANL.*
  - *Requested LANL to develop strategy for long term science facility development.*
- **LANL has identified a clear scientific need: prediction and control of materials in extreme environments.**
  - *The broader community has validated the science opportunity via workshops.*
  - *The workshop process identified needs and gaps relative to today's capabilities.*
- **A facility concept has been developed to meet this need: Matter-Radiation Interactions in Extremes (MaRIE).**
  - *The proposed set of capabilities is unique.*
  - *Ongoing investments at LANSCE are an important base for this strategy.*
- **The science case and facility concept for MaRIE are complete: next step is CD-0.**
  - *Mission need crosses DOE, including NNSA, SC (BES, FES), and Energy (NE).*
  - *Developing a plan and budget profile requires active engagement from these offices*

We request your support to pursue a broad, DOE-wide CD-0 under the leadership of S-4.

NNSA has launched a "New Facilities Committee" somewhat emulating the Orbach 2003 SC Facility Plan.

Dear Dr. Anastasio:

The Office of Defense Programs is developing a strategy for construction of new experimental science facilities. This strategy builds on the framework laid out in the Stockpile Stewardship and Management Plan and will be included in the next submission of this Plan to Congress. The goal of the strategy is to ensure that NNSA and its national laboratories will have the capabilities to address future national security needs and to provide premier scientific user facilities for recruiting and retention. The strategy will also guide budgetary planning.

To prioritize construction of new facilities, a formal call for proposals will be announced. Submitted proposals will be presented to a review panel in a meeting

This process will focus on large facilities. Roughly, a large facility investment is taken to be one with costs exceeding $100M. Smaller scale facilities that would be part of a technical roadmap for development of a large facility will also be considered.

send the name of the nominee to Dr. Christopher Deeney. As NNSA would like to send out the proposal call by mid-summer, the Committee's work should be completed within the next two months.

Sincerely,

DONALD L. COOK
Deputy Administrator

New Facilities Committee

- Jason Pruet, NNSA
- Melissa Marggraff, LLNL
- Julia Phillips, SNL
- John Sarrao, LANL

Meetings

- LLNL, 6/28
- Washington, DC, 7/14

Output

- Define values, criteria, proposal content, review process.
- (NOT to perform actual review)

MaRIE

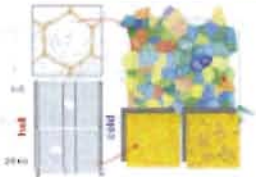
Recent efforts to integrate theory and experiment through co-design for materials in extremes are succeeding and build on LDRD investments.

MaRIE

Center for Defect Physics

EFRCs

CMIME
Center for Materials at Irradiation and Mechanical Extremes



Center for Materials Science of Nuclear Fuels

LDRD-DR: Dennis-Koller

CASL

ExMatEx

LDRD-DR: Germann

LDRD-DR: Beyerlein

OSTP "Materials Genome Initiative"

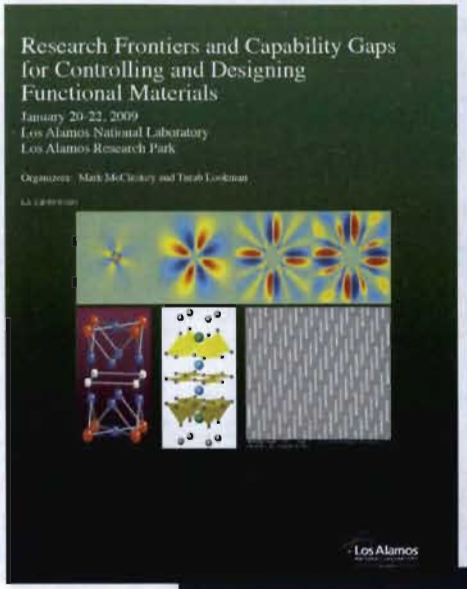
Materials in Extremes/Irradiation Resistant Materials (BES/FES/ASCR)/NNSA/NE

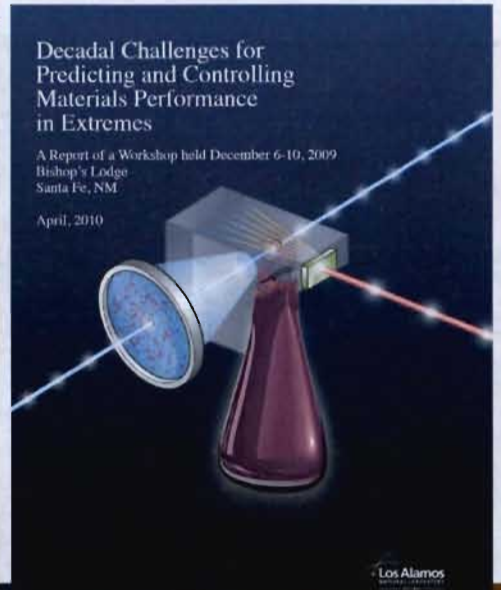
FY11 LDRD Reserve investments (~$2.5M) targeted on materials in extremes accelerate science underlying MaRIE first experiments.

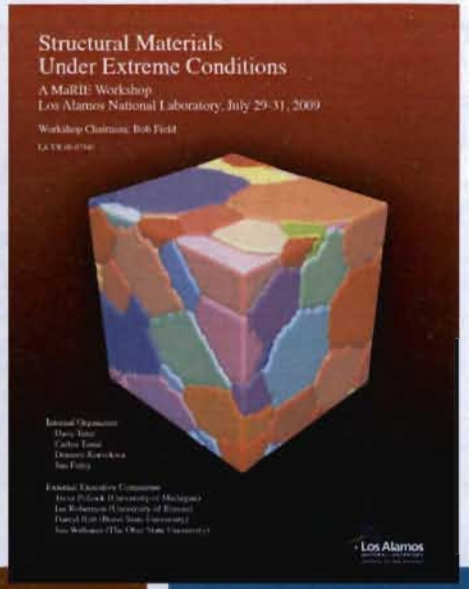
MaRIE

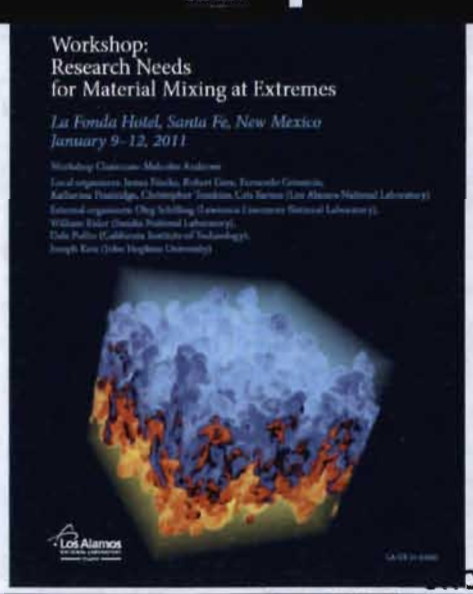
XFEL physics	Coherence Effects in X-ray Diffraction Imaging	Quinn Marksteiner John Barber
	Control of XFEL-Radiation Focusing through Electron-Beam Manipulation	Kip Bishofberger
APS expts	Synchrotron X-ray Laue Diffraction and Phase Contrast Imaging of Fe and Explosive Simulants under Shock Loading	Shengnian Luo
	In-Situ Probing Monitoring of Microstructure Evolution During Annealing of Radiation Damage with High Energy Synchrotron X-ray Diffraction	Donald Brown
Advanced pRad	Three Dimensional Quantification of Metallic Microstructures in the Presence of Damage	Curt Bronkhorst
	Achieving the Ultimate Spatial and Density Resolution of 800 MeV Proton Radiography	Alexander Saunders
Synthesis science	Developing and synthesizing epitaxial nanocomposites with controlled defect landscapes and desired functionalities	Quanxi Jia
	Fluid Flow Imaging of Alloy Melts and In-situ Fundamental Solidification Experiments at Temperature Extremes	Amy Clarke
Materials certificatio n	Microstructure Analysis for Extreme Events: A Stochastic Modeling Framework for Microstructure Datasets	John Bingert
	Accelerating Materials Certification	John Sarrao

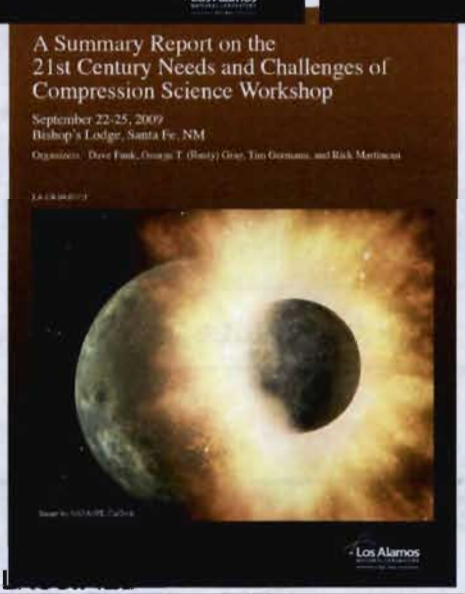
In 2009 we engaged more than 225 scientists from 80 institutions in 7 countries in a MaRIE-inspired dialogue (we continue to host workshops).

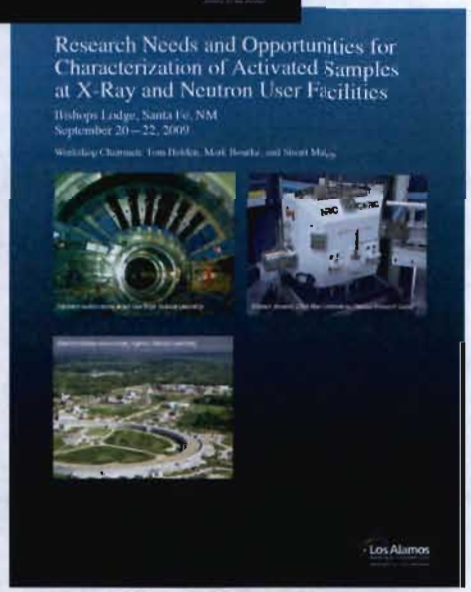












Thanks to our external colleagues who contributed to workshop leadership.

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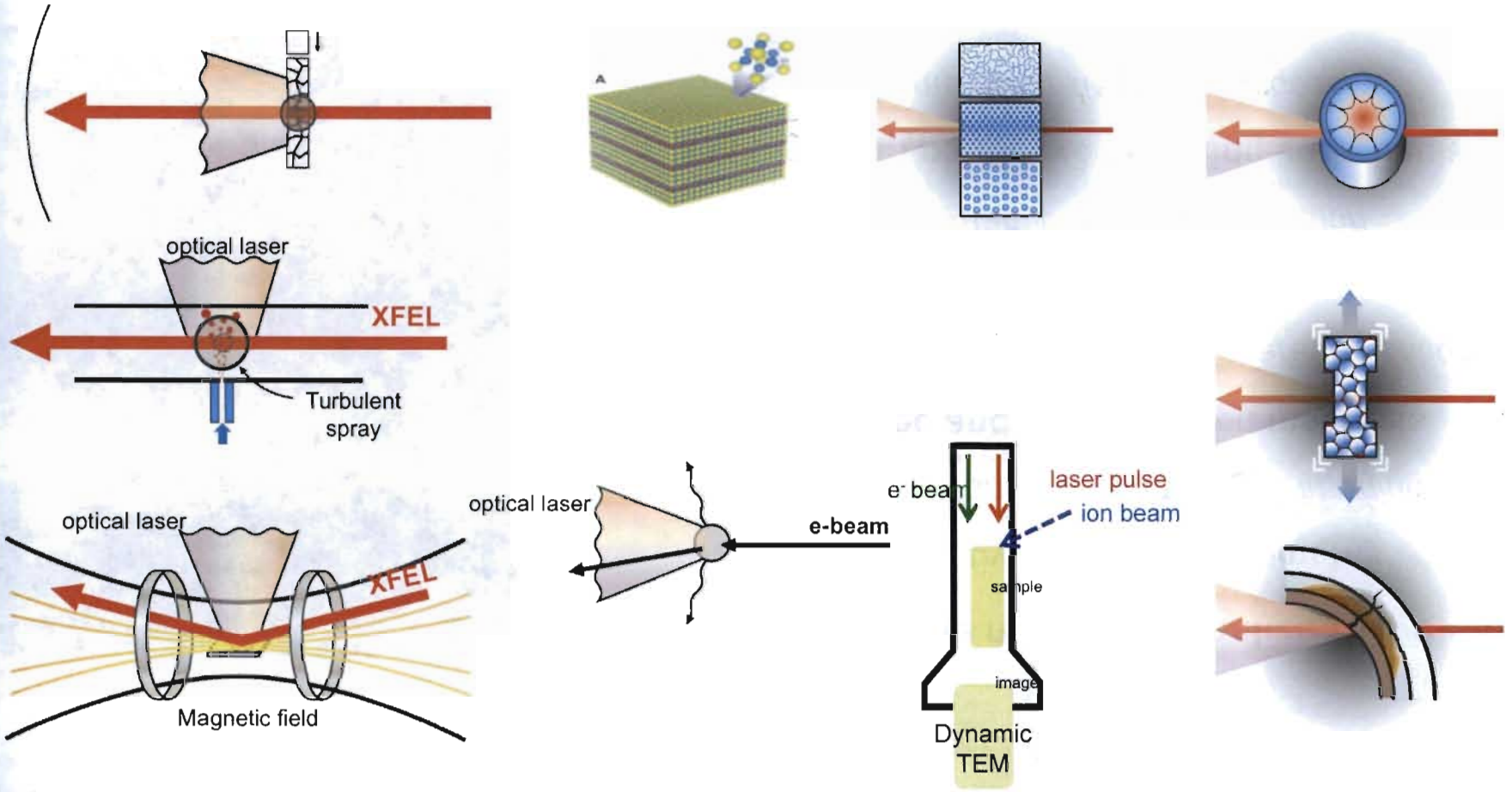
MaRIE

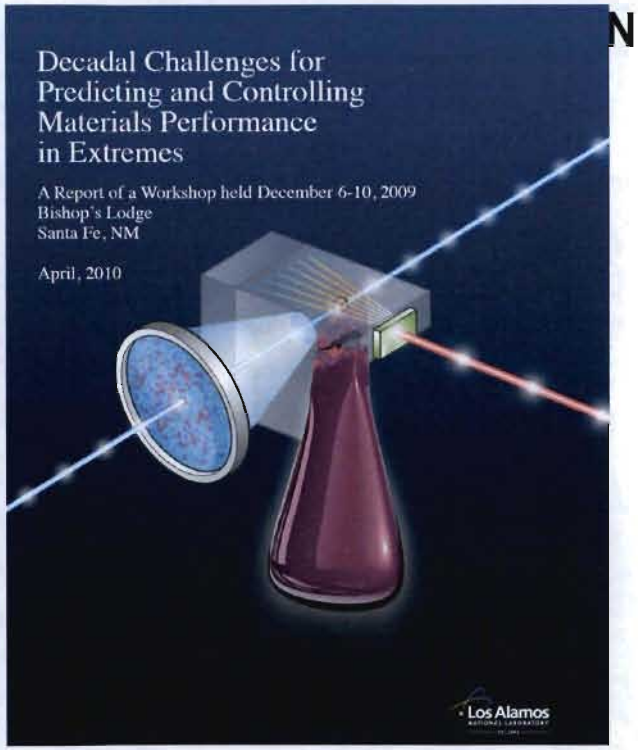
First experiment teams include ~170 scientists from ~ 60 institutions in 10 countries.



We are laying the foundation for a robust MaRIE user community.

Materials research is on the brink of a new era – moving from observation of performance to control of properties.

The confluence of improved experimental capabilities (e.g. 4th generation light sources, controlled synthesis and characterization, …) and simulation advances are providing remarkable insights at length and time scales previously inaccessible.



New capabilities will be needed to realize this vision:

In situ, dynamic measurements

simultaneous scattering & imaging

of well-controlled and characterized materials

advanced synthesis and characterization

in extreme environments

dynamic loading, irradiation

coupled with predictive modeling and simulation

materials design & discovery

MaRIE

MaRIE builds on the LANSCE facility to provide unique experimental tools to meet this need.

First x-ray scattering capability at high energy and high repetition frequency with simultaneous charged particle dynamic imaging

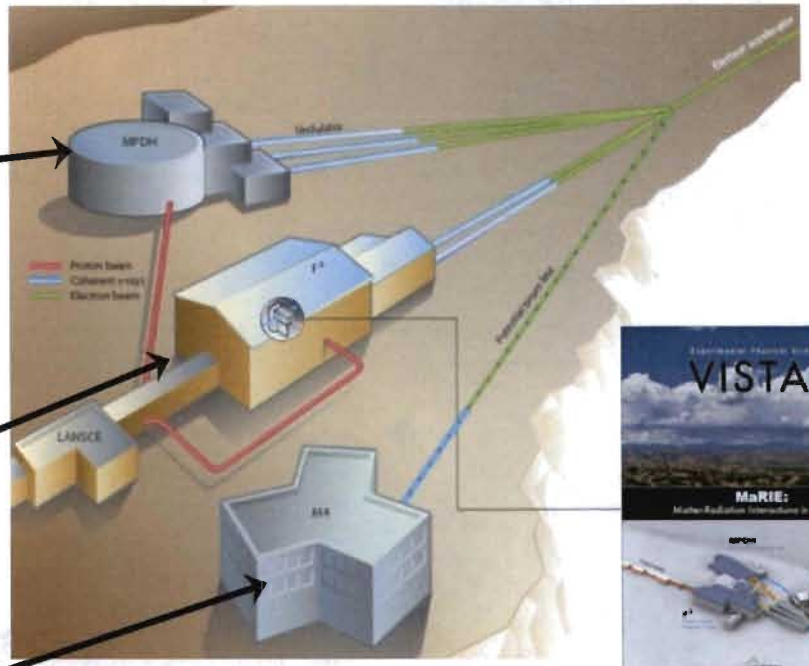
(**MPDH**: Multi-Probe Diagnostic Hall)

Unique in-situ diagnostics and irradiation environments beyond best planned facilities

(**F^3**: Fission and Fusion Materials Facility)

Comprehensive, integrated resource for materials synthesis and control, with national security infrastructure

(**M4**: Making, Measuring & Modeling Materials Facility)



- **Unique very hard x-ray XFEL**
- **Unique simultaneous photon-proton imaging measurements**
- **Unique spallation neutron-based irradiation capability**
- **Unique in-situ, transient radiation damage measurements**
- **Unique materials design and discovery capability**

MaRIE will provide unprecedented international user resources.

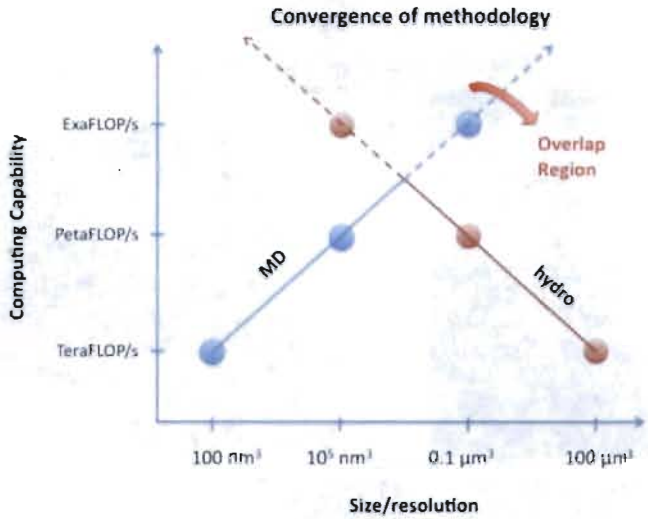
Co-design objective of the ExMatEx Center

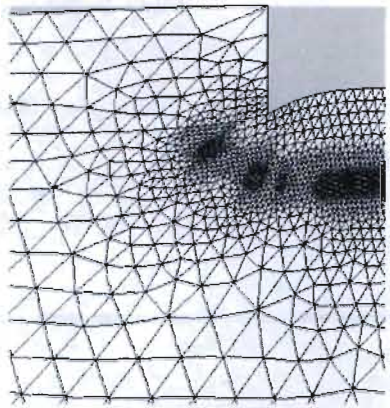
- **We will develop a multiphysics exascale simulation framework for modeling materials subjected to extreme *mechanical* and *radiation* environments.**
- **Our strategy is a UQ-driven *adaptive physics refinement* in which coarse-scale simulations spawn sub-scale direct numerical simulations as needed.**

•This *task-based* approach leverages the extensive concurrency and heterogeneity expected at exascale while enabling fault tolerance within applications.

•The programming models and approaches developed to achieve this will be broadly applicable to a variety of multiscale, multiphysics applications.

ExMatEx





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Co-design objective of the ExMatEx Center

- **We will establish and execute a continuous (i.e., throughout the project lifetime) algorithm/hardware modeling, evaluation, optimization, and synthesis loop, including optimization for performance, memory and data movement, power, and resiliency.**

Agile Development "Scrum"

- Both single-physics (e.g. petascale QMD and MD) applications and scale-bridging multi-physics materials science applications will be co-designed with candidate exascale hardware and software stacks.
- Proxy applications and performance models/simulators will be used to introduce a realistic domain workload into the exascale hardware and software stack development process at an early stage, and enable real scientific applications ready when exascale platforms become available.

Exascale Co-Design Center for Materials

We are planning the Exascale Co-Design Center for Materials in Extreme Environments ("ExMatEx")

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Lawrence Livermore National Laboratory

OAK RIDGE National Laboratory

Sandia National Laboratories

STANFORD UNIVERSITY

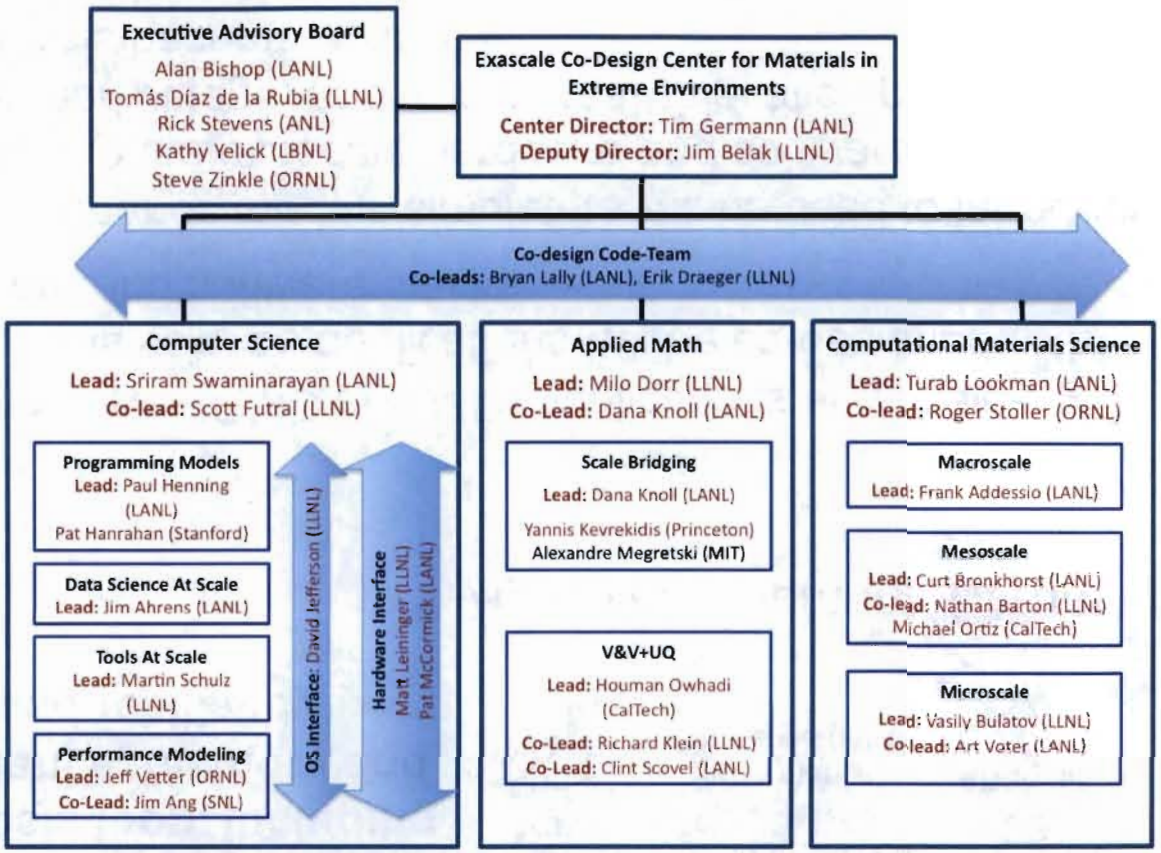
PRINCETON UNIVERSITY

California Institute of Technology 1891

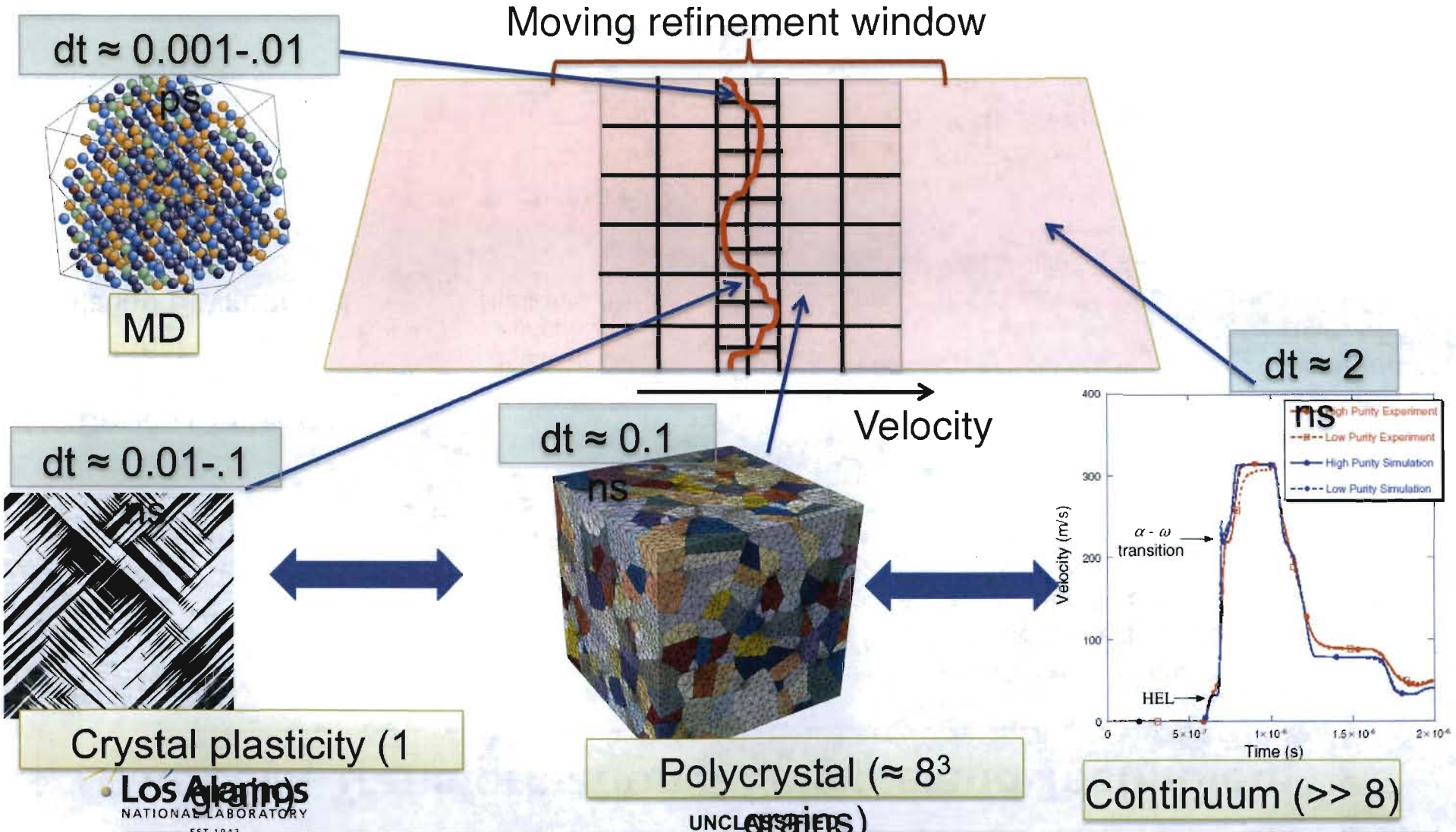
Massachusetts Institute of Technology

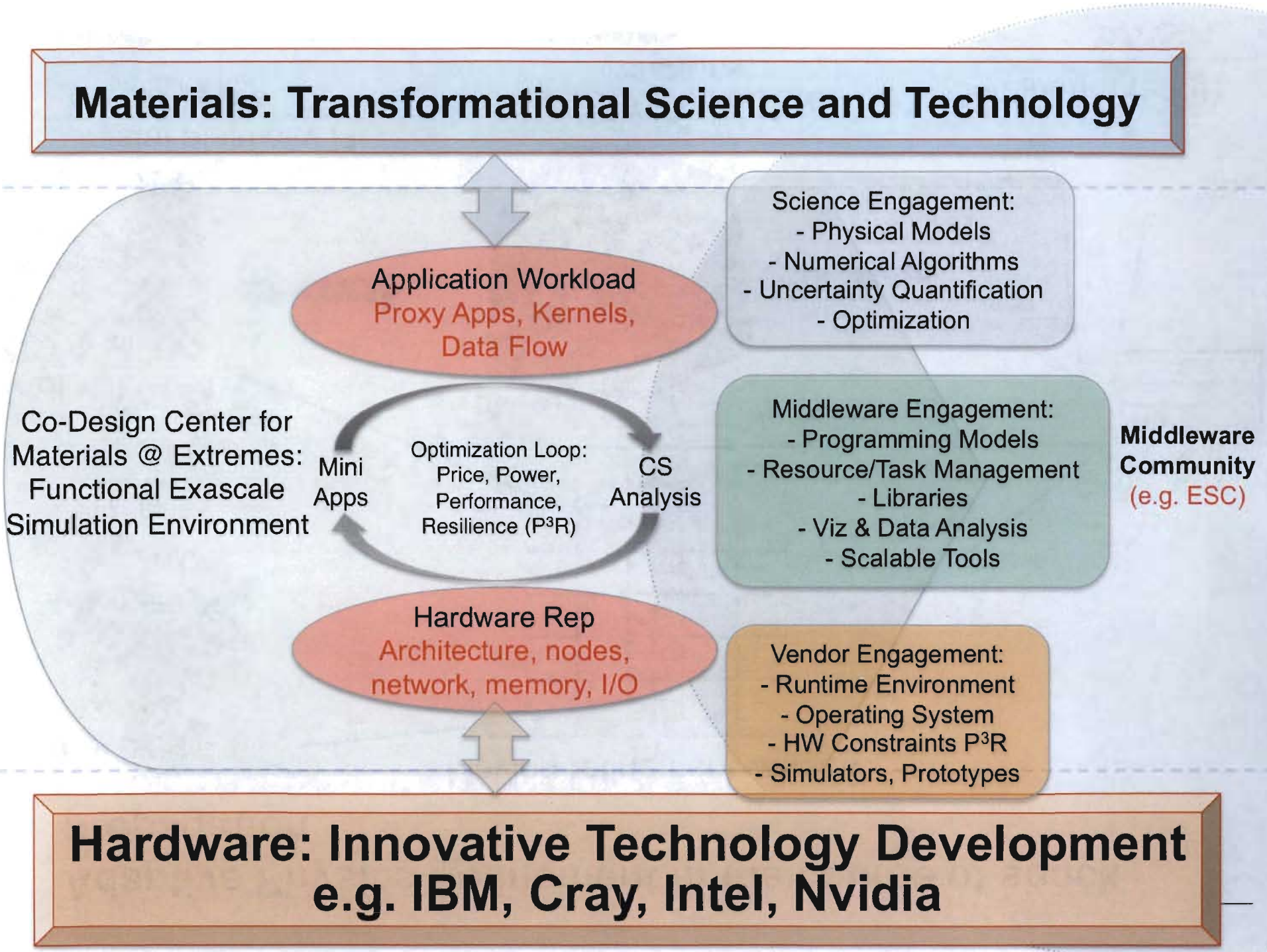
CRAY THE SUPERCOMPUTER COMPANY

intel

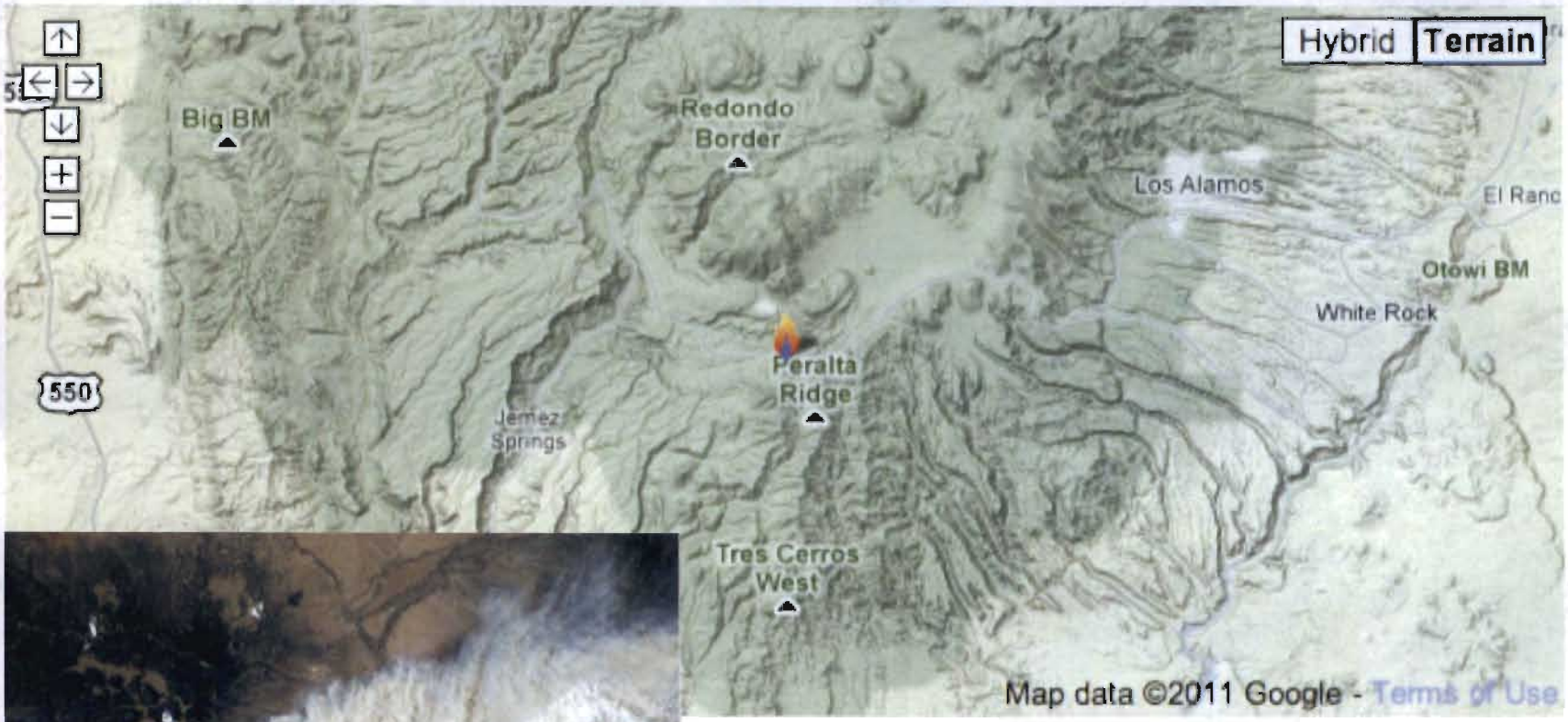


Adaptive Physics Refinement in the course of shock propagation




Materials: Transformational Science and Technology
Science Engagement:
- Physical Models
- Numerical Algorithms
- Uncertainty Quantification
- Optimization
Application Workload
Proxy Apps, Kernels,
Data Flow
Co-Design Center for
Materials @ Extremes:
Functional Exascale
Simulation Environment
Mini
Apps
Optimization Loop:
Price, Power,
Performance,
Resilience (P3R)
CS
Analysis
Middleware Engagement:
- Programming Models
- Resource/Task Management
- Libraries
- Viz & Data Analysis
- Scalable Tools
Middleware
Community
(e.g. ESC)
Hardware Rep
Architecture, nodes,
network, memory, I/O
Vendor Engagement:
- Runtime Environment
- Operating System
- HW Constraints P3R
- Simulators, Prototypes
Hardware: Innovative Technology Development
e.g. IBM, Cray, Intel, Nvidia

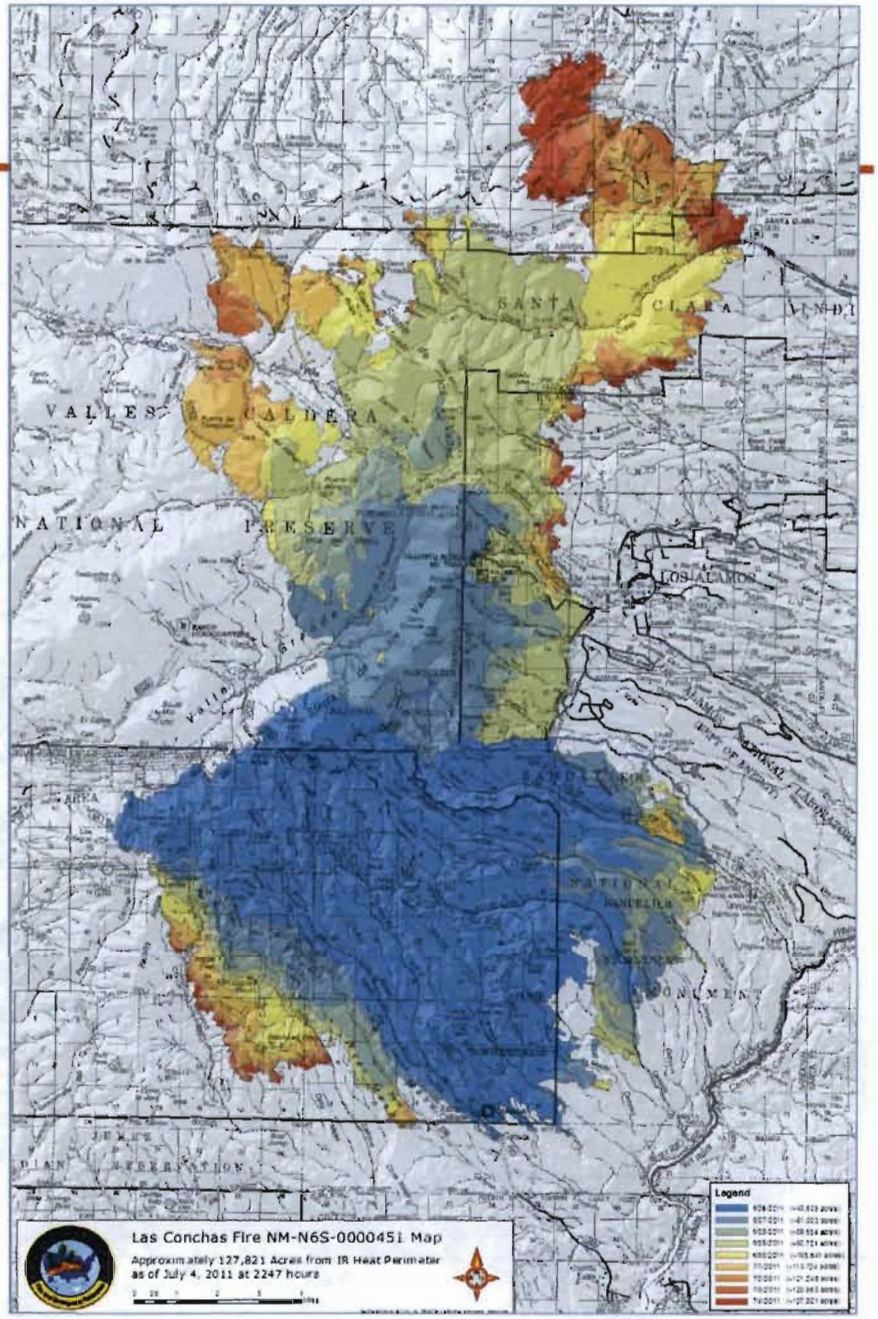
Early Stages of the Fire



Las Conchas Fire

Fire Statistics as of July 6

- Acres burned: 130,691
- Percent contained: 30%
- Total Personnel: 2,557 includes 63 crews
- Resources
  - Helicopters: 20
  - Engines: 91
  - Water Tenders: 35
  - Dozers: 14
- Residences
  - Threatened: 410
  - Destroyed: 62
- Commercial Property
  - Threatened: 45
  - Destroyed: 0
- Outbuildings
  - Threatened: 110
  - Destroyed: 32



Los Alamos NATIONAL LABORATORY EST.1943

The fire formed an enormous smoke plume.

Aerial View of LANL, Los Alamos Townsite, and Fire Extent