SAND2007-4670P

Sandia's Computer and Information Sciences

A Context and Overview for the CIS External Advisory Board

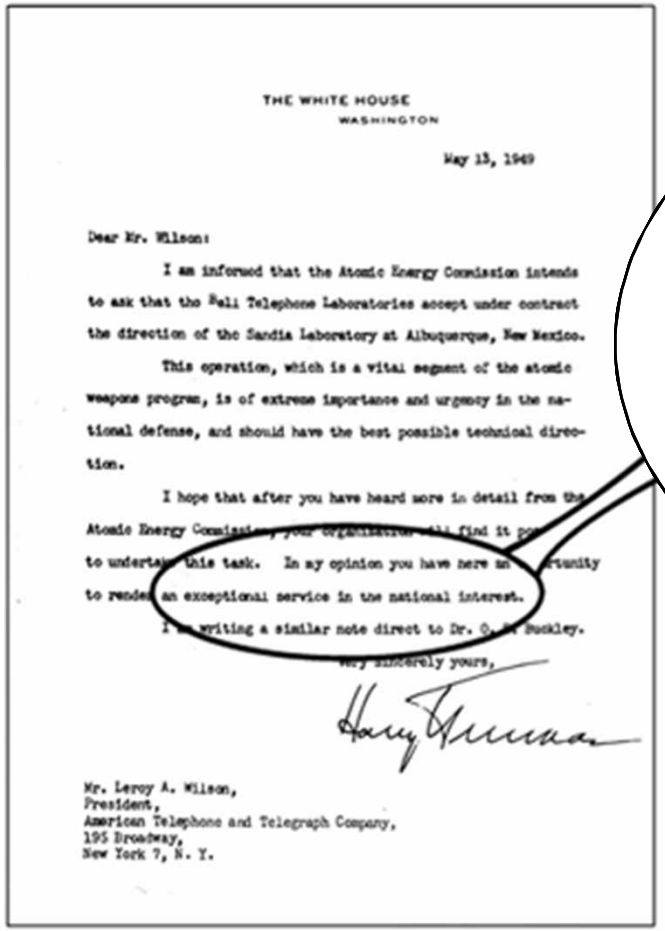
Dr. Leonard M. Napolitano, Jr.
Director
Computer Sciences and Information Technologies Center

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. **ENTER SAND # HERE**

Agenda

- **CIS Context and Overview**
- **Technical Talks**
- **CIS Strategic Direction**

Our Business is National Security



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 yours,

Harry Truman

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

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in detail from the Atomic Energy Commission,

your organization will find it possible to undertake this task.

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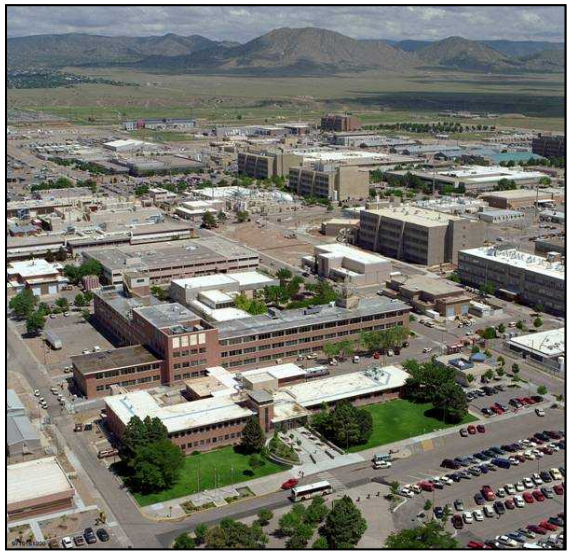
Two Major Laboratory Sites Anchor Our Set of Distributed Facilities



Albuquerque, New Mexico

Tonopah Test Range, Nevada

Kauai Test Facility, Hawaii

Yucca Mountain, Nevada

WIPP, New Mexico

Pantex, Texas

Livermore, California

National Nuclear Security Administration

July 2007

Sandia National Laboratories

We are a Mission-Driven Laboratory

We serve many agencies of the US Government with:

- Design and development: nonnuclear portions of US nuclear weapons
- Production: advanced components
- Safety, security, use control
- Treaty verification, nonproliferation, counterproliferation
- Advanced military technologies
- Energy and environment
- Homeland security, countering weapons of mass destruction

Four Mission Areas

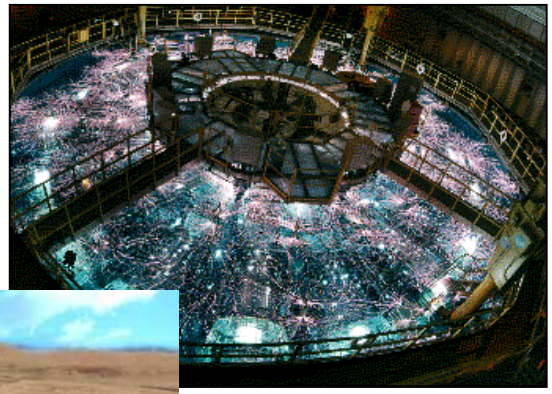
- Nuclear Weapons
- Defense Systems and Assessments
- Energy, Resources, and Nonproliferation
- Homeland Security and Defense

Nuclear Deterrence for National Security

Our Defense Programs Mission

Credible deterrence built on both a safe, secure and reliable nuclear weapons stockpile that is capable of meeting all military requirements – now and in the future – and a science-based engineering infrastructure capable of responding to national security needs whenever they arise.

B83 Modern Strategic Bomb



Sandia's Z Pulsed Power Machine

Microsystems, Engineering Sciences and Applications (MESA) complex

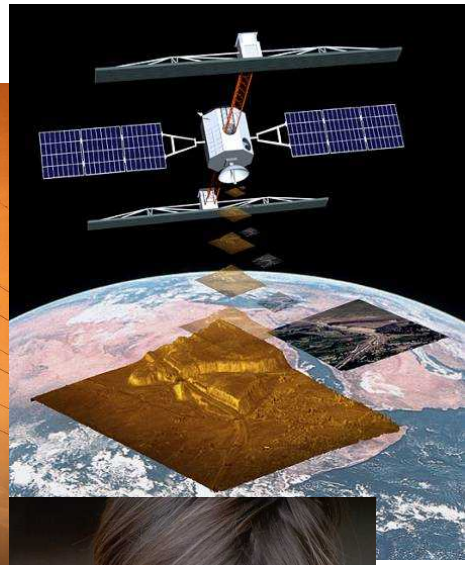
Defense Systems & Assessment Programs

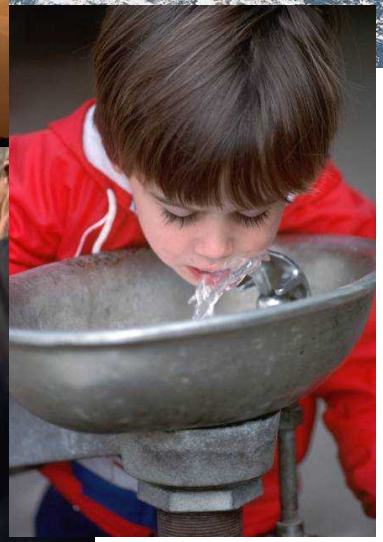
- Proliferation Assessment
- Information Operations
- Remote Sensing and Verification
- Space Missions
- Surveillance and Reconnaissance
- Integrated Military Systems

Energy, Resources, and Nonproliferation

Energy, Water, and Security Enabled by Science & Technology

- Secure energy supplies for national security
- Clean, abundant, and affordable energy
- Water research
- Infrastructure protection
- Technologies for detecting proliferation activities
- Cooperative international security programs
- Hydrogen research
- Nuclear power research
- Science, technology, and engineering base

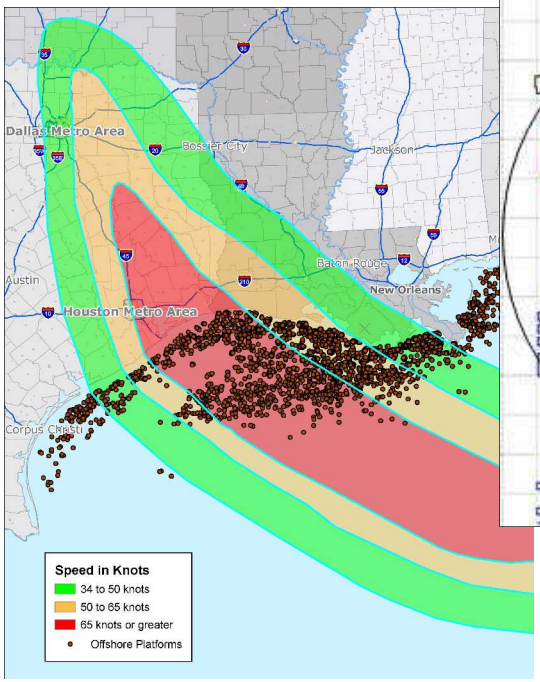


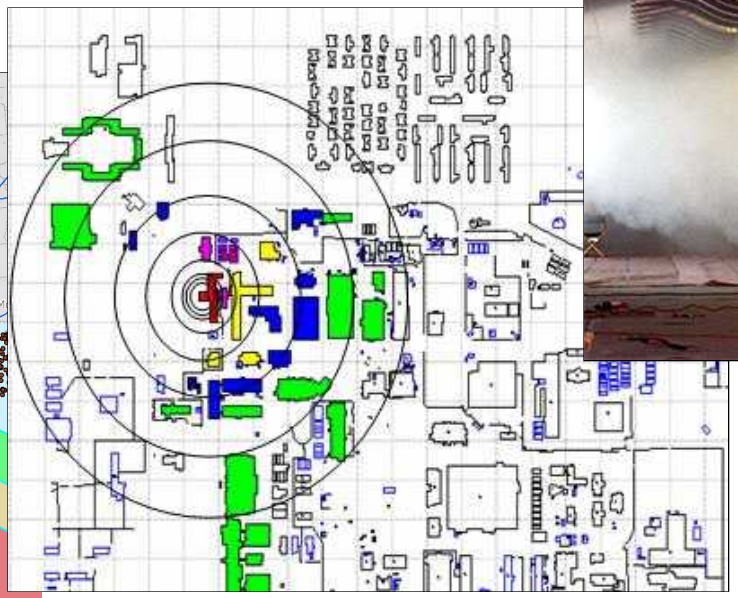


Homeland Security and Defense

Mitigating the risk of catastrophic events and enhancing the nation's ability to respond and recover

Risk Management and Infrastructure Protection





Homeland Defense and Force Protection

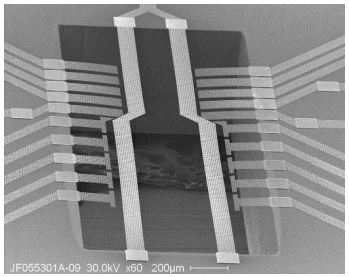
Catastrophic Event Mitigation

Technologies for National Security

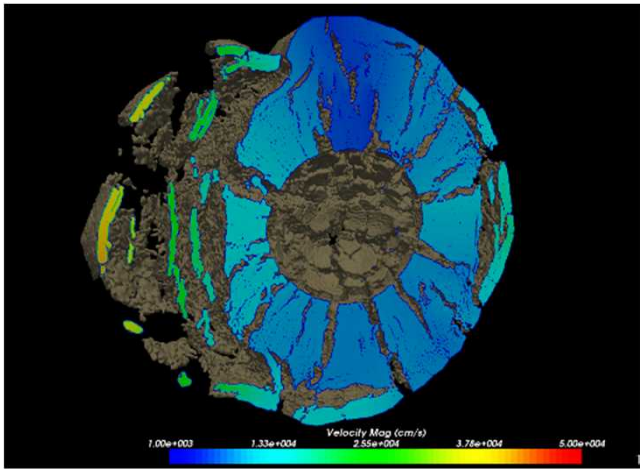
We develop technologies to:

- Sustain, modernize, and protect our nuclear arsenal
- Prevent the spread of weapons of mass destruction
- Provide new capabilities to our armed forces
- Protect our national infrastructures
- Ensure the stability of our nation's energy and water supplies.
- Defend our nation against terrorist threats

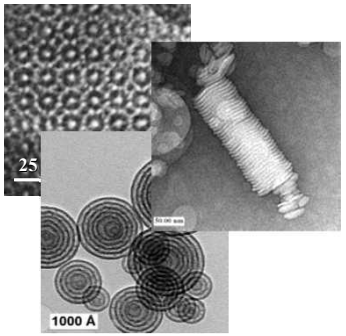
Computer and Information Sciences is One of the Six Core Technical Capabilities



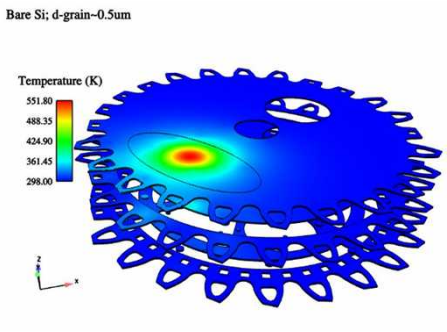
Microelectronics and Photonics



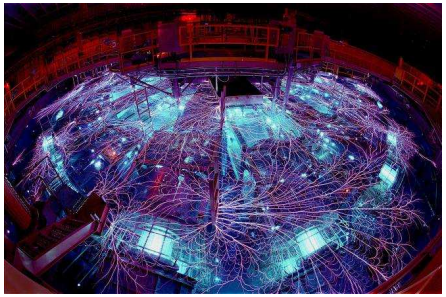
Computational & Informational Sciences



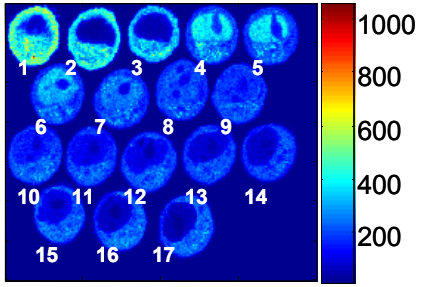
Materials Science & Technology



Engineering Sciences



Pulsed Power



Bioscience

CIS Mission

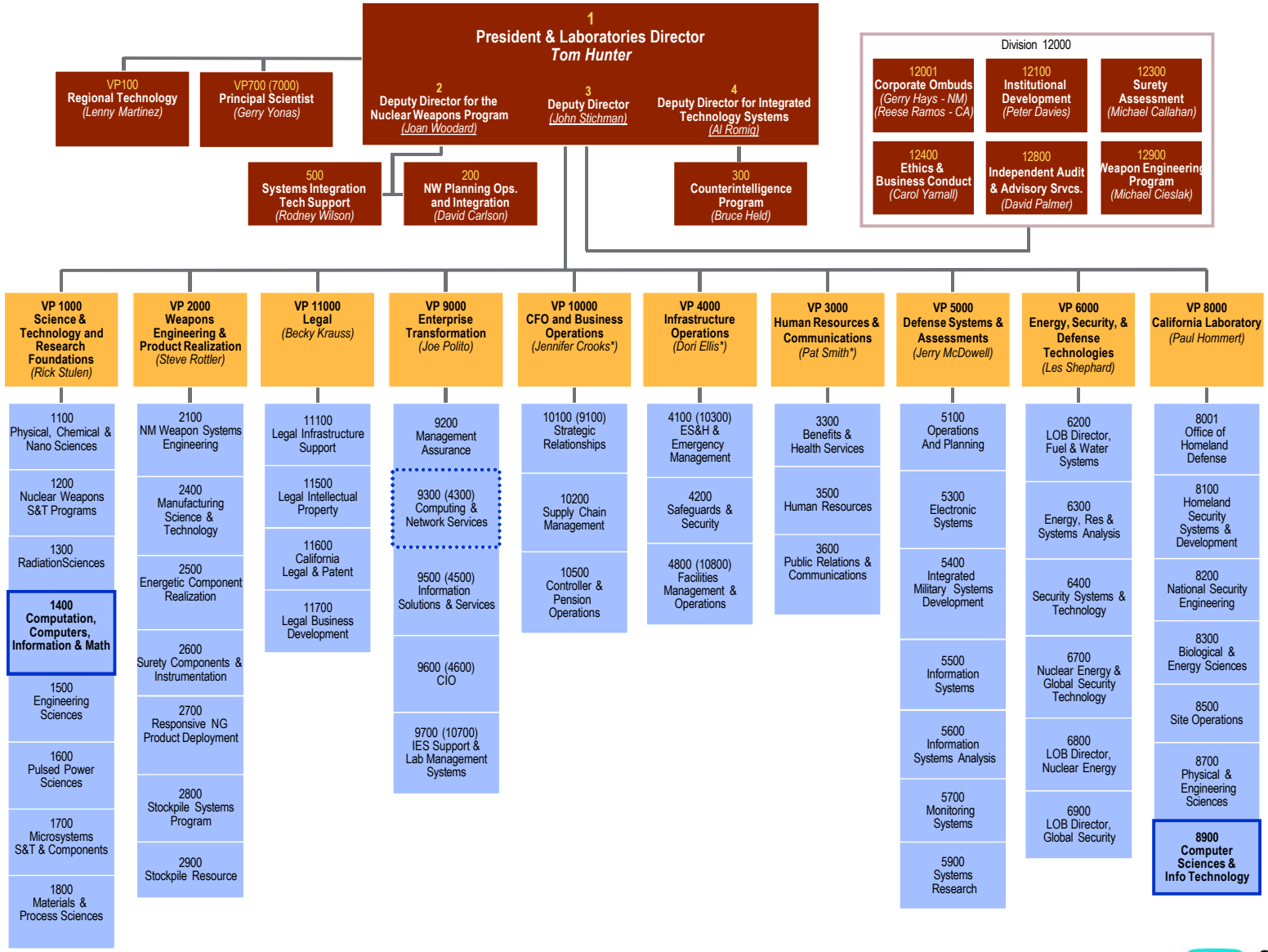
To Enable High Performance Computing by:

- **Providing SNL with the computational and informational science tools and the platforms they need to carry out the labs science and engineering missions at the leading-edge compared to our competitors**
- **Being a seed for new lab science initiatives – for example:**
  - Informatics and computing for intelligence
  - Applying cognitive science to our missions
  - Building modeling & simulation capabilities to support nanoscience and global nuclear energy initiatives
- **Helping disseminate new CIS technologies throughout the lab**
- **Being a high-tech corridor from academia into Sandia, and from Sandia into industry (spin-in and spin-out)**
- **Being a national resource in computing and informatics for America's national security missions**

CIS Mission in Relation to National Needs

- **CIS is a national R&D resource for mission agencies**
  - NNSA
  - DOE Office of Science
  - DOE Energy Missions
  - EPA
  - Intelligence Community
  - Department of Defense
- **CIS aims to enable solution of the most challenging problems facing the nation in highest-end computing and informatics**
- **To do so, CIS brings a focus on scientific and engineering disciplines together with broad capabilities in computing, information, and knowledge generation**

Sandia's Organization Structure



Sandia's CIS Organization Structure

Computation, Computers, Information & Math (NM) – ***James Peery****, Director*

Computer Science & Mathematics – David Wombie, Sr. Mgr.

- Optimization & Uncertainty Estimation
- Computational Biology
- Computational Mathematics & Algorithms
- Discrete Algorithms & Math
- Applied Computational Methods

Computer & Software Systems – Sudip Dosanjh, Sr. Mgr.

- Computational Modeling Sciences
- Scalable Computer Architectures
- Scalable Systems Software
- Data Analysis & Visualization

Computational Sciences R&D – Jennifer Nelson, Sr. Mgr.

- Computational Shock & Multiphysics
- Exploratory Simulation Technology
- Multiscale Dynamic Materials Modeling
- Electrical & Microsystem Modeling

Computer Sciences & Info Technologies (CA) – ***Len Napolitano****, Director*

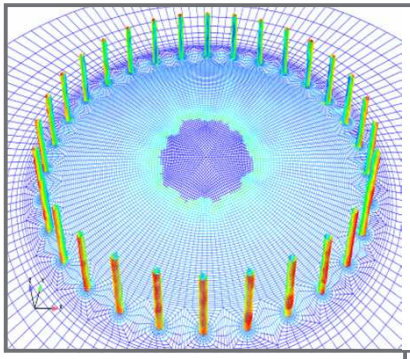
Computer Sciences – Howard Hirano, Sr. Mgr.

- Scalable Computing R&D
- Math, Information & Decision Sciences
- Visualization & Scientific Computing
- Advanced Software R&D
- Computer Network Security

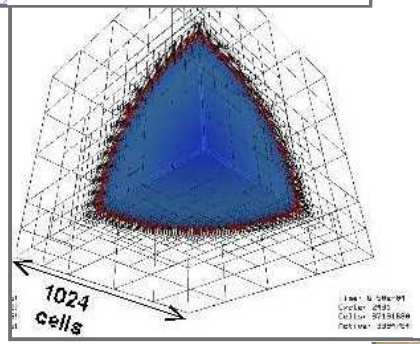
Information Technologies – Chuck Oien, Sr. Mgr.

- Collaborative Applications: Dev & Integration
- Information Systems & Services
- Videoconferencing & Collaborative Technologies
- Engineering Design Services
- Communication & Network Systems

Components of a CIS Capability



Computational Science Applications



Algorithms & Enabling Technologies

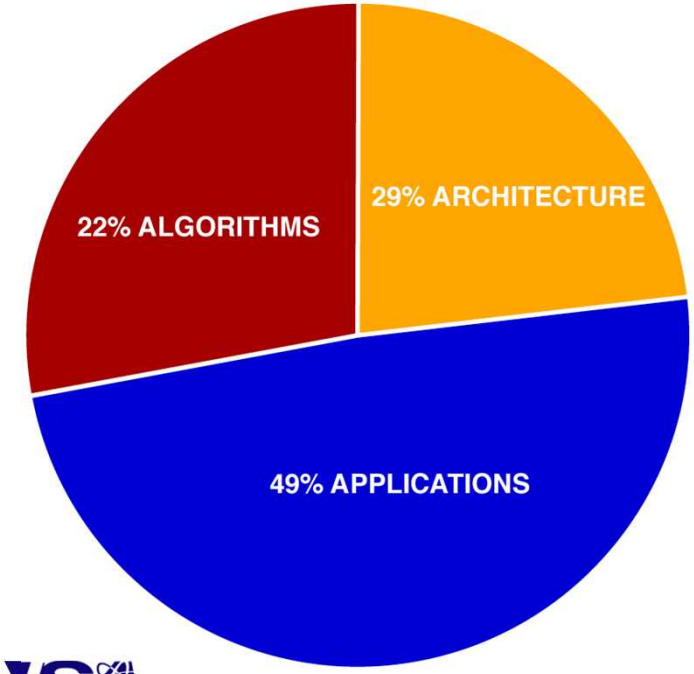
Computing Architectures & Hardware Systems

We Manage R&D Funds for LDRD and CSRF Projects

Computational & Information Sciences LDRD

Focus Areas Support Our Principal Customers and Major Programs

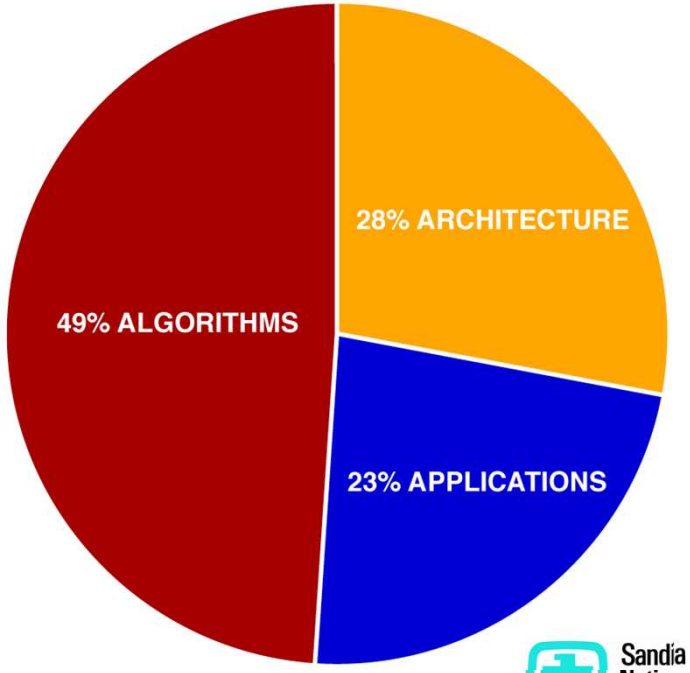
$7M Portfolio



Computer Science Research Foundation

Focus Area, Strategic Initiatives, and Advanced Technology R&D for NW Mission

$9.5M Portfolio



Our History of Leading-Edge Computing *(1977 - 1987)*

1977 1979 1981 1983 1985 1987

Cold War build up

1981 SNL decides to purcahse HPC

Aggressive MIRV

KARP Challenge issued

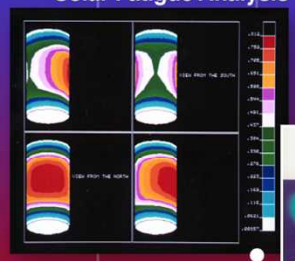
SNL creates HPC R&D capability

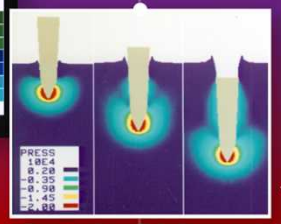
APPLICATIONS

B83 nose crush 3D simulation

2D simulation

Solar Fatigue Analysis





2D very low fidelity model of weapon details

Gordon Bell Award

Beat Karp Challenge (500x)

ALGORITHMS

CRAY 1-S

nCUBE

ARCHITECTURE

Vector »

MPP »

1977 1979 1981 1983 1985 1987

Our History of Leading-Edge Computing *(1987 - 1997)*

1987 1989 1991 1993 1995 1997

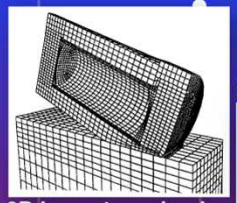
APPLICATIONS

Collapse of USSR

Underground Test Ban

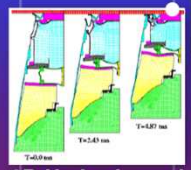
Formation of ASCI

3D coupled physics demonstration

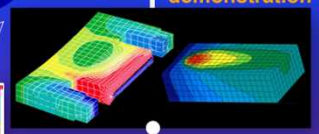


3D impact mechanics

Structural mechanics



2D Hydrodynamics



Dense solvers » » »

Iterative solvers (Aztec) » » » 2000

Load balancing (Chaco) » » »

Dynamic load balancing (Zoltan) » »

ALGORITHMS

Optimization (Dakota) » » » 2002

Parallel molecular dynamics » » » 1998

Parallel sorting & searching » » » 1998

Reorganization of computing at SNL:
» NM capability systems
» CA to distance computing

Paragon: Gordon Bell Award

DAISy

ASCI RED

ARCHITECTURE

MPP »

« Vector

Cluster »

1987 1989 1991 1993 1995 1997

National Nuclear Security Administration

July 2007

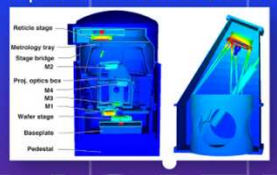
Sandia National Laboratories

Our History of Leading-Edge Computing *(1997 - 2007)*

1997 1999 2001 2003 2005 2007

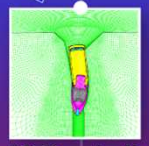
APPLICATIONS

System thermal model using parallel implementations of COYOTE & JAS3D

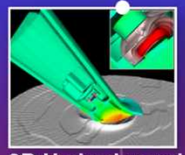


Low fidelity

Intelligence community



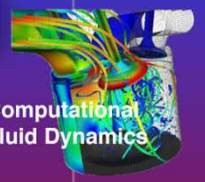
3D Penetration modeling



3D Hydrodynamic

V&V QMU Info assurance

High fidelity



Computational Fluid Dynamics

Agent-oriented software

Logistics modeling » » »

1995 « « « Dynamic load balancing (Zoltan) » » »

ALGORITHMS

Multithreaded architectures » » »

1994 « « «

Optimization (Dakota) » » »

Optimization + UQ (Dakota) » » »

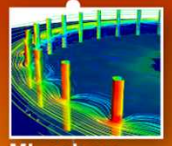
Integrated QMU » » »

Parallel graph algorithms » » »

Decision support informatics » » »

Compute process allocation

Trilinos solver framework » » »



ML solvers

ARCHITECTURE

Commodity:
» LINUX
» Multi-vendor
» Open source

MPP:
High-fidelity
quick
response

Visualization corridors

CPLANT

ICC

Catalyst

MPP »

Red Storm

Thunderbird

Cluster »

1997 1999 2001 2003 2005 2007

National Nuclear Security Administration

July 2007

Sandia National Laboratories

Technical Presentations to Follow

Computer & Software Systems

- **OpenFabrics & Infiniband: A Commodity Open-Source Architecture for HPC** – *M. Leininger*
- **System Software** – *R. Brightwell*

Algorithms & Enabling Technologies

- **Trilinos and Solver Research** – *P. Bochev*
- **Uncertainty Quantification Algorithms & Deployment in Dakota** – *M. Eldred*
- **Verification, Validation, and Uncertainty Quantification Towards a Predictive Simulation Capability for High-Consequence Applications** – *M. Martinez-Canales*

Applications Development

- **Graph-Based Informatics for Decision Makers** – *B. Hendrickson*
- **Applications of Agent-Oriented Software Engineering to Simulation and Optimization** – *J. Siirola*
- **Charon** – *R. Hoekstra*
- **A Mathematical Theory for Peridynamics** – *R. Lehoucq*

Emerging Issues

- Decline of NW funding
- Rise of other mission areas
- How to support capability?

Charge to the Panel

Measure the quality, appropriateness, and innovation of our R&D programs within the context of Sandia's missions and in the context of the national R&D enterprise.

Evaluate our strengths & weaknesses, as well as a holistic assessment of our place in the international community in HPC and technical informatics, using the metrics below:

- Quality & quantity of work
- Value for the dollar
- Innovation, creativity & originality
- Successful application of our R&D to SNL, DOE, other U.S. government agencies, and industrial needs
- Peer evaluation of the work measured by publications & citations to them
- Recognition of leadership in HPC through awards, invited talks & papers, and key committee membership/leadership roles
- Effectiveness in utilizing research funding to set a foundation for the future

Charge to the Panel

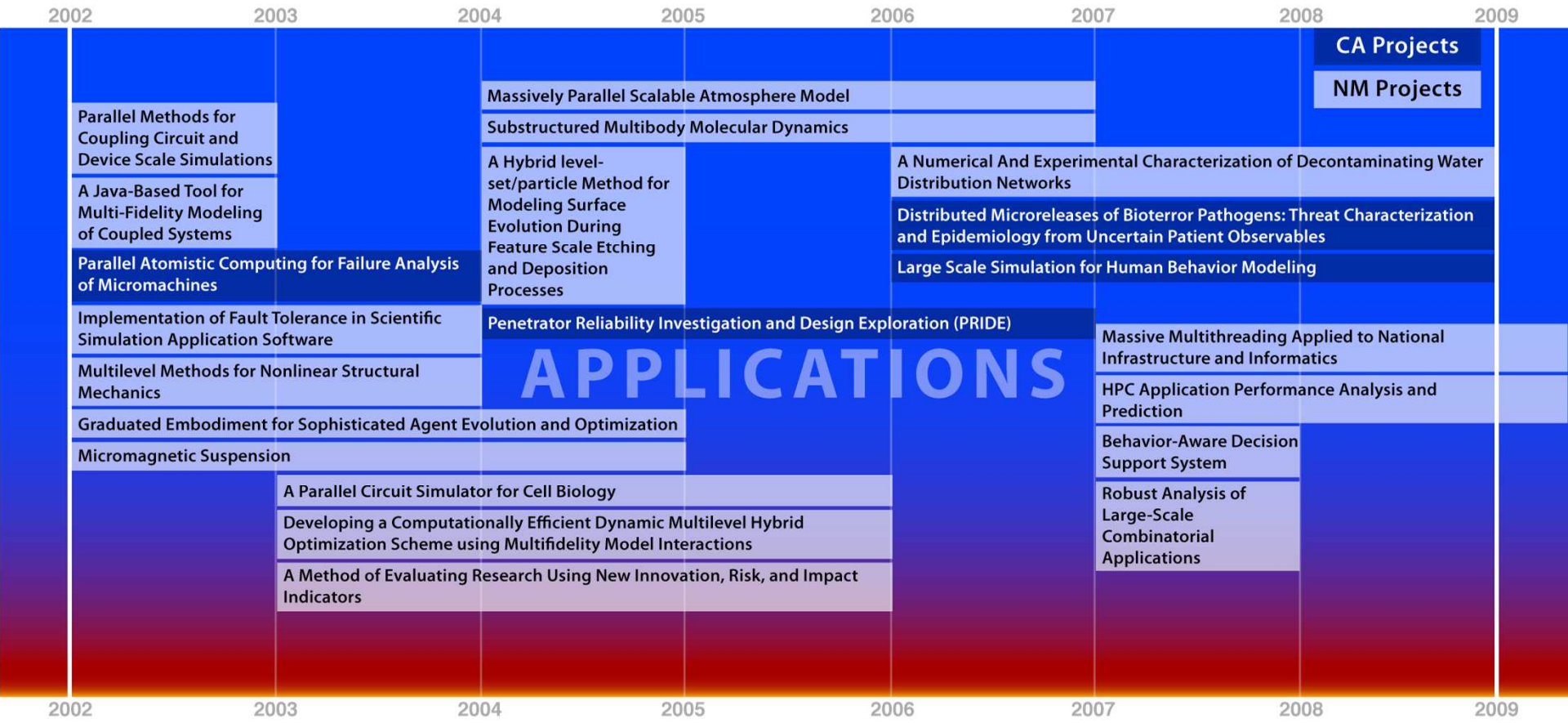
Advise us on the following in relation to the new strategic plan:

- National and international trends
- Opportunities to be explored
- Culture and environment (i.e., innovation, creativity, collaboration, etc.)
- Strengths & weaknesses

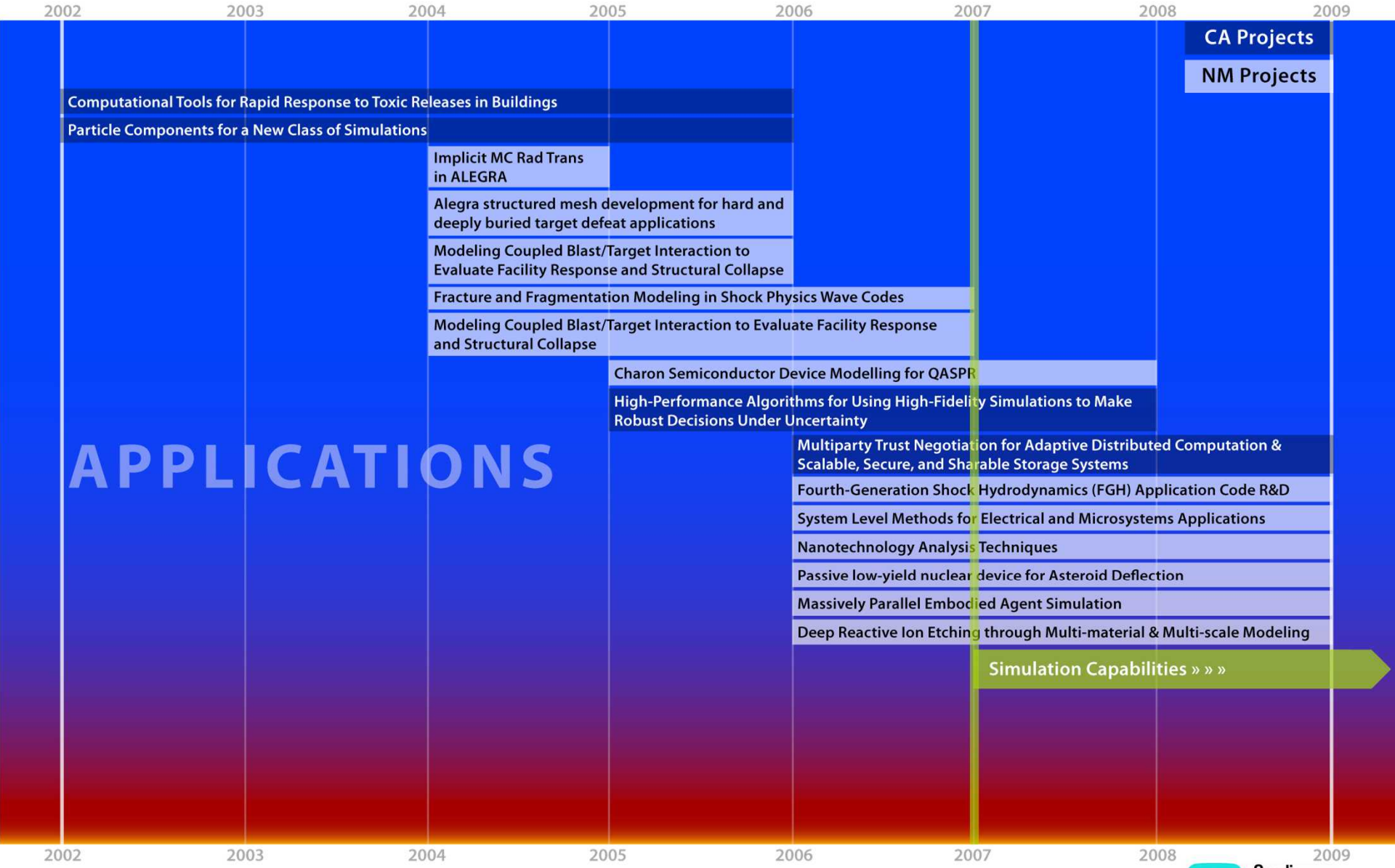
Requested Deliverable:

An out briefing to our upper management and the set of slides from that briefing, preferably with annotations on the 'notes' pages.

CIS LDRD Project Portfolio *(2002 – 2007)*



CIS CSRF Project Portfolio *(2002 – 2007)*



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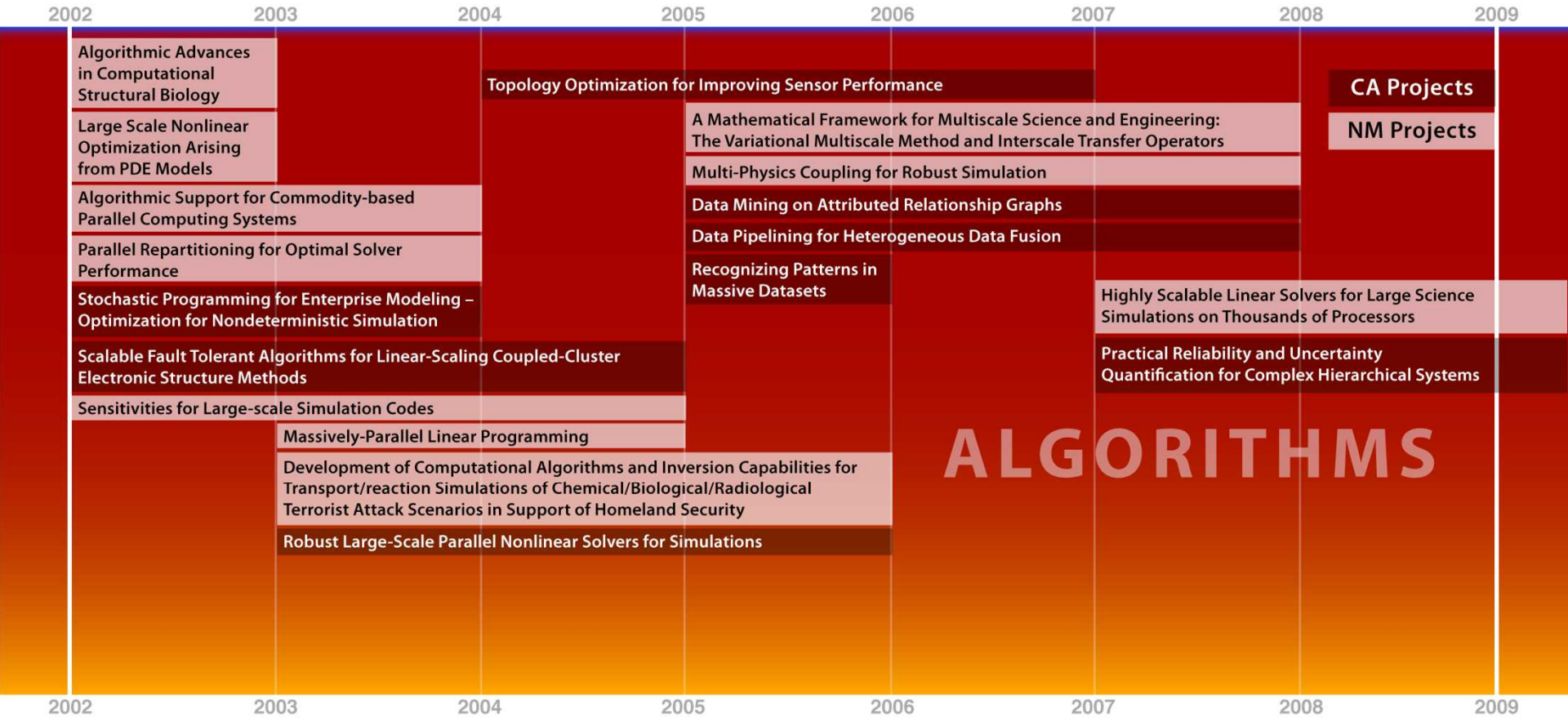
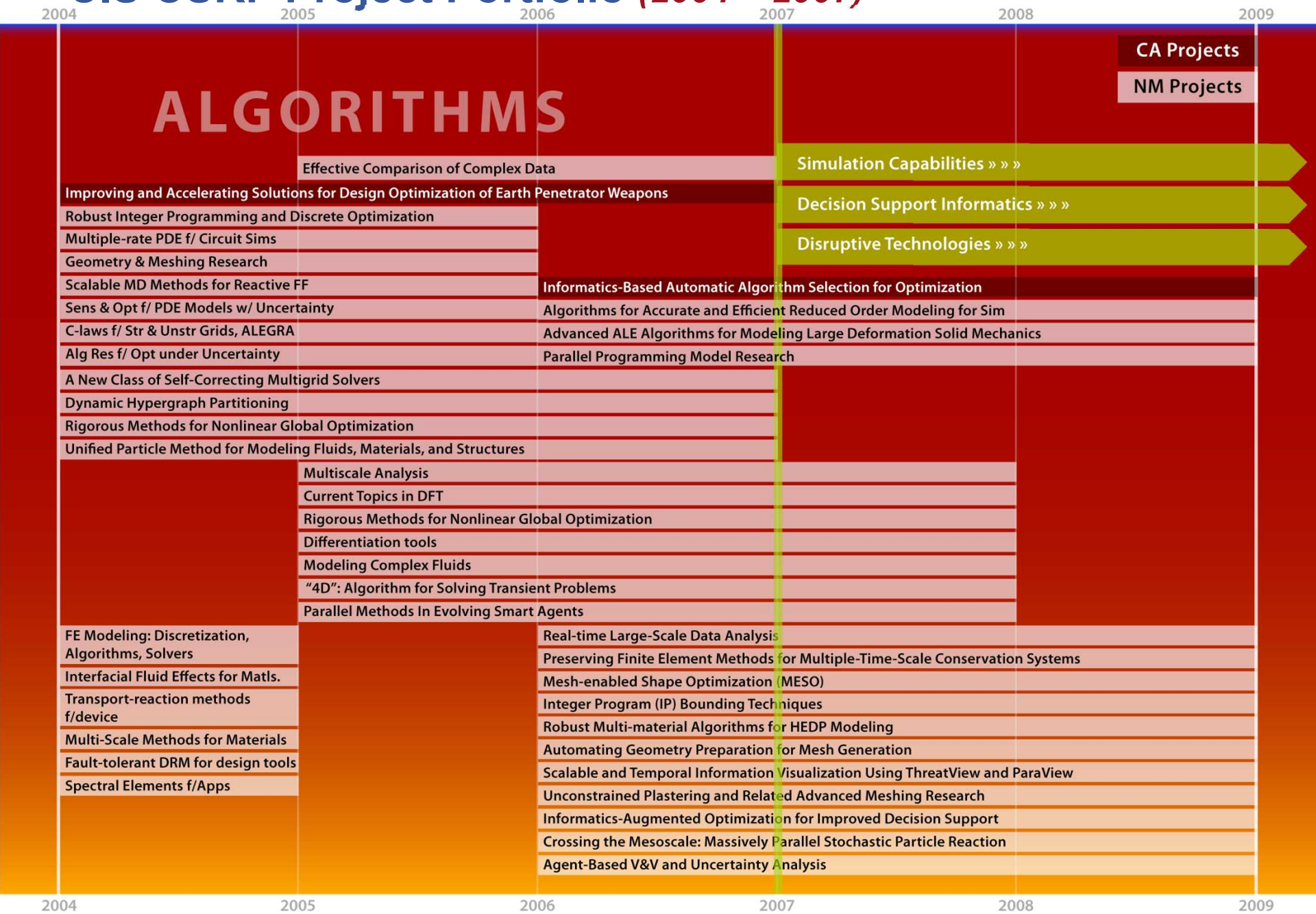
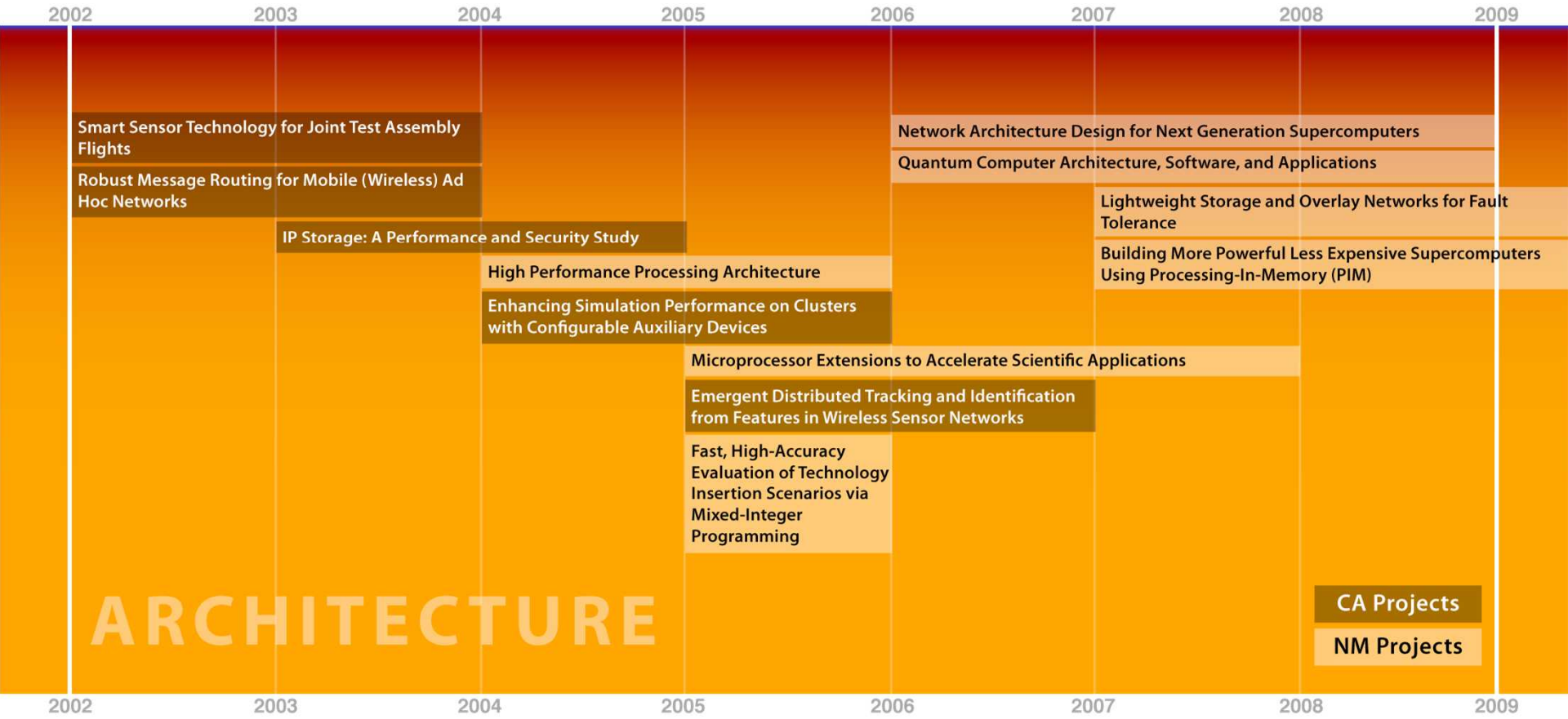


CIS CSRF Project Portfolio *(2004 – 2007)*



CIS LDRD Project Portfolio *(2002 – 2007)*



CIS CSRF Project Portfolio *(2003 – 2007)*