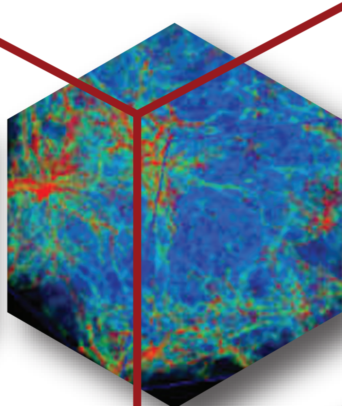
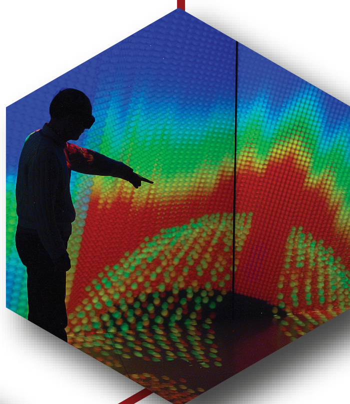
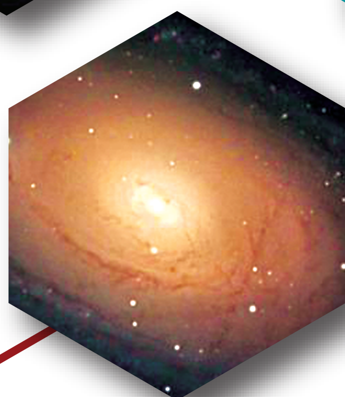
Theoretical Division's *Portfolio and Strategic Plan*

The Theoretical Division has been an intellectual resource to the Los Alamos National Laboratory since 1943.







T Theoretical Division

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Los Alamos NATIONAL LABORATORY

Theoretical Division's *Portfolio and Strategic Plan*

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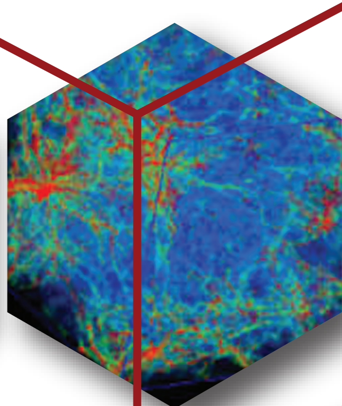
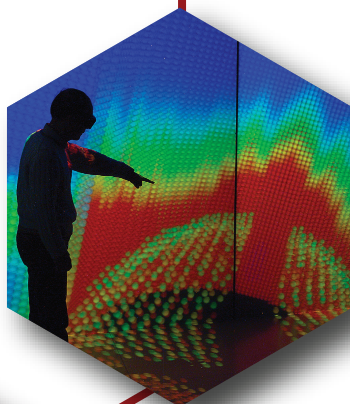
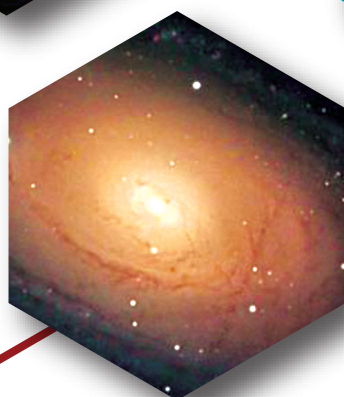






Theoretical Division

LA-UR-06-2453

Los Alamos NATIONAL LABORATORY

Theoretical Division Portfolio and Strategic Plan
Table of Contents

1.0 Executive Summary 1
1.1 Vision 1
1.2 Mission 1
1.3 Core Competencies, Business, and Future Directions 1

2.0 Technical Program Portfolio 2
2.1 Goals, Strategies, and Objectives 2
2.1.1 Melding Theory, Modeling, and Simulation with Experiment 2
2.1.2 Modeling Complex Systems via Computational Science 3
2.2 Programs and Initiatives 3
2.2.1 National Security 4
2.2.1(i) Nuclear Weapons 4
2.2.1(ii) Threat Reduction and Homeland Security 5
2.2.1(iii) Emergent National Security Programs: Energy Security 6
2.2.2 Frontier Science 6
2.2.3 Strategic Thrusts 7
2.3 Innovation and Partnering 8
2.3.1 Innovation: Individual Initiatives—The Entrepreneurial Spirit 8
2.3.2 Partnering for Success 8
2.4 Alignment with Institutional Technical Goals 9
2.5 Key Deliverables 10
2.5.1 Weapons Program 10
2.5.2 Laboratory Directed Research and Development 11
2.5.3 Office of Science 11
2.5.4 Other DOE 12
2.5.5 Reimbursables/Work for Others 13
2.6 Honors, Awards, and International Recognition 14

3.0 Organization, Workforce, and Operations 16
3.1 Organizational Structure 16
3.2 People and Capabilities 17
3.3 Culture 19
3.4 Facilities and Business Systems Infrastructure 20
3.5 Security, Environment, Safety, and Health 21

4.0 Customer and Sponsor, Funding, and Collaborations Profiles 22
4.1 Customers and Sponsors 22
4.2 Funding Portfolio 22
4.3 Collaborations 23

5.0 Transition Issues 26

Appendices

A. Scientific Thrust Descriptions A1
 1. Science-Based Prediction for Complex Systems A2
  a. Innovative Science in Support of Stockpile Stewardship A4
  b. Predictive Science and Technology for Threat Reduction and Homeland Security A8
  c. Innovative Science and Technology for Energy Security A11
 2. Hard, Soft, and Biological Matter A13
  a. Understanding and Design of Complex Materials A13
  b. Modeling Biological Processes A16
 3. Fundamental Processes A19
  a. Particle and Nuclear Astrophysics and Cosmology A21
  b. T Division Support of the LANL Quantum Institute A23
 4. High-End Computing Research A26
B. List of Laboratory Strategic Goals B1
C. T Division FY06 Laboratory Directed Research and Development Portfolio C1
D. Technical Descriptions of Groups D1
E. Management Position Descriptions E1
F. Quick Reference Guide of T Division Capabilities F1
G. List of Referenced Documents G1
H. Acronym List H1

Theoretical Division Portfolio and Strategic Plan

1.0 Executive Summary

1.1 Vision for T Division

Frontier Science for Laboratory Missions: The Theoretical (T) Division is a major intellectual resource to the Laboratory and the nation, providing creative scientific and technological solutions to challenges in national security and other problems of national and global importance. The Division pursues a robust portfolio of fundamental research at the frontiers of science, fostering a stimulating environment that attracts exceptional scientists and creates new skills and programs to benefit Los Alamos National Laboratory (LANL) missions.

1.2 Mission

Foremost is LANL's national security mission, which inherently has a need for science and technology beyond today's frontiers. T Division has a mission to respond to this need in a multifaceted way. We recruit the best scientific minds and capabilities to further our scientific understanding of the physical world and to establish a technical foundation for both current and future national defense and industrial and civilian needs. This foundation likewise fosters the exploration of interdisciplinary frontiers of scientific endeavor. In brief, T Division's three central mission elements are to:

1. provide the best science and scientists to LANL national security missions,
2. pursue frontier science to ensure excellence in science capabilities for LANL and the nation, and
3. create new scientific directions and attract scientific leaders to LANL.

1.3 Core Competencies, Business, and Future Directions

To accomplish its national security mission, LANL has assembled a core expertise in the *integration of theory, modeling, simulation, and visualization*. This is a bold strategy to provide new cutting-edge tools to interpret and guide experiments and to further our fundamental understanding of and predictive capabilities for complex phenomena. The Science-Based Stockpile Stewardship Program, the centerpiece of the DOE Weapons Complex, depends critically on the viability of this approach, **T Division plays a major role in this program.**

However, the applicability of this strategy extends well beyond the stewardship program. In fact, virtually every national security and scientific initiative at LANL relies heavily, if not critically, on this integrated capability. This reliance does, however, engender its own challenges. The coupling of computational simulations and experiments as a **cornerstone of technical programs in weapons, threat reduction, homeland security, energy security, biology, nanomaterials, infrastructure, and frontier science** requires a new generation of ideas and concepts to greatly improve the **fidelity, reliability, certainty, and usability of these tools.**

Addressing these challenges frames the core strategic directions for T Division

2.0 Technical Program Portfolio

2.1 Goals, Strategies, and Objectives

T Division's distinctive and enduring success derives from two central characteristics: the co-location of theory, modeling, and simulation excellence from a wide spectrum of disciplines and responsibilities, facilitating optimum excellence, relevance, and knowledge flow from and to partnering divisions and programs. Thus, the Division is notable for its very high rate of publications, honors, awards, and recognition in the worldwide science community.

Simultaneously, it has direct program delivery responsibilities in core LANL national security missions and has been responsible for incubating many new LANL programs. Of great importance is the multidisciplinary teaming within the Division and in partnership with other divisions. Exciting current teaming is in areas such as quantitative tools for complex networks, multiscale modeling methodologies, data science, biological physics, interfaces of particle-nuclear-astro physics and cosmology, techniques to address complexity in hard, soft, and biological matter, quantum information science, and so forth. T Division was the incubation home of the Center for Nonlinear Studies (CNLS), which continues to play a key Laboratory-wide role of nurturing interactions in new topics between divisions and acting as a vehicle for external collaborations with other major institutions *(see also Appendix G, Referenced Documents.)*

As the original division comprising the Laboratory at its 1943 founding (see *Theory in Action, Highlights in the Theoretical Division at Los Alamos 1943–2003*, LA-14000-H), T Division has long had a seminal role in the formulation and development of LANL's core integrated capabilities. Drawing from that rich history of service, the Division's current core strengths and directions emphasize the following areas.

2.1.1 Melding theory, modeling and simulation with experiment to provide new conceptual frameworks and predictive tools for systems whose complexity exceeds existing analytical capabilities. This framework is central to the Laboratory Goal of Science-Based Prediction and Uncertainty Quantification (UQ) for Complex Systems. (The present weapons UQ methodology at LANL originated with T Division staff.) Typically, the scientific method demands a careful balance of small- and large-scale experiments with theory, modeling, and simulation in deliberate, closed, iterative loops. Additionally, in the realm of complex systems, this intensive research process frequently involves applying techniques from one discipline to needs in another to create entirely new capabilities. The many examples where T Division has applied this approach include the following.

- Formulating models to describe matter under extreme conditions, devising numerical algorithms for hydrodynamic flow, and understanding exotic states of complex electronic materials. In all cases, successful conceptualization was followed by practical applications.

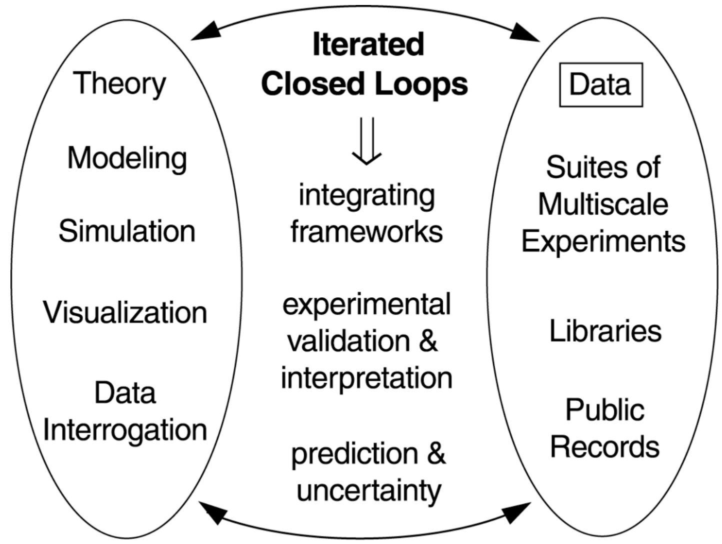
- Collecting the world's HIV sequence data into an annotated database and the development of a model to describe the evolution of the AIDS virus — one that could determine when it first appeared in humans. This is likely to be a critical issue in predicting the virus's future evolution, a model that could well spawn a therapeutic regimen that could save lives. These competencies now underpin our opportunities to support Homeland Security biothreat initiatives, such as the President's National Strategy for Pandemic Influenza.

- Surmounting uncharacterized obstacles at new science frontiers, such as the sciences of complex materials and systems biology. In a period of remarkable advances in experimental techniques available to probe complex matter on many scales, and with comparable advances in high-performance computing, a system approach is a compelling scientific frontier of this century.

The emerging strategic importance of our multiphysics, multidisciplinary approach, and the extreme demands that are placed on it to underpin our national security and other critical elements of the national enterprise, requires that its scientific and technical bases be continually reviewed and strengthened. T Division's response to this need is a set of new thrusts in innovative approaches to weapons science, threat reduction science, complex materials, quantum computing, biological systems, and fundamental processes *(see also Appendix A, Thrust Descriptions).*

2.1.2 Modeling complex systems via computational science. T Division is preeminent in formulating concepts and models for complex systems, translating them to optimized computational schemes, and carrying these through to robust and validated codes and computer platforms (clusters and mainframes). Just a few among many examples of this computational modeling capability include:

- the revolutionary use of Quantum Molecular Dynamics (QMD) to simulate shocked hydrocarbons for the nuclear weapons (NW) program,
- development of preconditioners for solvers in the new Advanced Simulation and Computing (ASC) codes,
- development of a disease-transmission methodology for use in epidemiological modeling of manmade and natural pathogen transmission, and
- development of physics models and algorithms for the national global climate modeling initiative.



THE SCIENTIFIC METHODOLOGY
Applied to Increasingly Complex Systems

The foundational nature of computational science in all facets of the Laboratory's national security, national infrastructure, and frontier science missions requires a vigorous and continual infusion of new talent, ideas, and tools. Irrespective of their disciplinary diversity, the commonality characterizing T Division's suite of thrusts is that they all contain at their core a robust effort to infuse new numerical methods, software design, algorithms, modeling techniques, and uncertainty quantification tools into the scientific problem under investigation.

2.2 Programs and Initiatives

As the largest multidisciplinary theory and modeling center in the world, T Division is uniquely equipped to provide novel approaches to large and complex national challenges. T Division's value to the Laboratory derives both from the potent collaborative capabilities of its internal network of key scientists and from their professional interactions with the larger scientific community. These associations facilitate solutions to complex problems and provide portals for the infusion of scientific advances and new scientific leadership from relevant fields of science. This outreach both inspires new approaches and provides a

critical test of LANL's scientific viability in broad and highly competitive venues.
T Division is *consistently* responsible for 25–30% of all external peer-reviewed publications from LANL, attesting to its role as a focus for scientific excellence and leadership. *(See Appendix G, Referenced Documents).*

2.2.1 National Security

2.2.1(i) Nuclear Weapons. T Division currently ensures that the best science is available to the Stockpile Stewardship Certification Program predominantly, but not solely, through its contributions to the ASC program. In turn, success for ASC demands that one includes the best possible science into the best new codes in a timely and evolutionary manner. For example, among the principal issues vigorously pursued by T Division is predictability and uncertainty quantification. This requires new mathematical and simulation strategies, as well as an extensive, deep knowledge of equations of state, material strength, nuclear cross sections, opacities, energetic materials, turbulence, and the chemistry and material properties of aging. T Division is a resource for the theoretical foundations and the modeling of these properties.

T Division has had lead management roles for the ASC Materials and Physics Program and remains its single largest contributor. This program element has responsibility for developing enhanced and validated physics modules and implementing them into simulation codes used for weapons assessment and certification. T Division has also managed the University Alliances program that provides links between the Laboratory and the nation's leading computer science and materials studies universities. T Division is increasingly partnering with NMT and ESA divisions to enhance the manufacturing science base at LANL.

Nuclear Weapons Programs Plan
(See also Appendix A)

- T Division has major responsibilities for integrating and applying to certification the Materials and Physics modules for the ASC program.
- T Division has major responsibilities in the University Alliances program.
- T Division works closely with other divisions in support of the Laboratory's NW goals, delivering program commitments on budget and schedule.

T Division will achieve its goals in the NW program by proactively participating in program management and execution and software quality management.

- T Division manages several projects within the ASC Materials and Physics program element.
- T Division staff provide the majority of the technical capability for the Materials and Physics program element.
- Staff provides leadership for new initiatives such as Uncertainty Quantification (UQ).
- T Division management and staff participate extensively in the planning of workshops and interactions with the CEA/DAM in basic research for the NW program and serve as points of contact (POC) for these interactions.

2.2.1(ii) Threat Reduction and Homeland Security. In support of the Laboratory's mission in Threat Reduction (TR) and Homeland Security (HS), there are several major projects underway, which, in order to address specific programmatic goals, draw upon the expertise of T Division in theory, modeling, and simulation. This expertise ranges from T Division's longstanding proficiency in nuclear nonproliferation to its more recent inroads into complex networks and data physics (extracting information from large data sets), biological systems (epidemiology, immunology, sensors), chemical systems (sensors, plume reactants), and infrastructure/social/economic systems modeling and simulation.

Nuclear nonproliferation capabilities include analysis of the nuclear fuel cycle, enrichment technologies, development of novel reactor-monitoring techniques, and novel materials for sensors. In data physics, research focuses on image segmentation, pattern recognition, data compression, and hyperspectral analysis, using established expertise in multiscale modeling, statistical physics, fast numerical algorithms, hierarchical decomposition of data, and nonlinear dynamical systems. These techniques are being expanded to address TR applications involving intelligence analysis, target camouflaging and recognition, early missile launch, and surveillance. The common thread among these activities is to provide the ability to systematically reduce massive input data sets to minimal, specific information data sets for decision making.

Research efforts in developing biological and chemical sensors for identifying specific pathological and toxic agents—with collaborations in the TR Directorate—are underway, and capabilities for chemical identification of plume reactants in early launch missile detection, as well as analysis and prediction of countermeasures for chemical toxins, are being investigated.

T Division staff provide key scientific underpinnings for several other nascent and ongoing programs in the TR program. Examples in which staff members have lead roles are quantum computing [advanced research and development activity/National Security Agency (ARDA/NSA)], computer vision and image recognition (DOE/NN-20), critical infrastructure modeling, biothreat reduction, and epidemiology [DOE/NN-20 and Defense Threat Reduction Agency (DTRA)], military space [Department of Defense (DoD)], and the joint DOE/DoD Munitions Technology Development Program.

Threat Reduction Plan
(See also Appendix A)

We will achieve our goals by serving on relevant boards and teams and by aggressively responding to new opportunities within the Laboratory and the nation, including those emerging with the creation of the U.S. Department of Homeland Security (DHS).

- T Division management serve on boards of directors for DoD/Defense Transformation/Intel, and partner with TR divisions on strategic Laboratory goals.
- T Division management serves on the LANL Center for Homeland Security Board of Directors.
- T Division staff and management participate in ongoing planning and serve on relevant thrust teams that plan and coordinate the Laboratory response to the bio-threat.
- T Division collaborates with Sandia National Laboratories (SNL), University of New Mexico (UNM), Santa Fe Institute (SFI), Monterey Institute, and others, in fostering new research and hosting high impact workshops and symposia.

2.2.1(iii) Emergent National Security Programs: Energy Security. T Division staff members have been strongly engaged in the framing of new Laboratory thrusts in Energy Security. Theory, modeling, and simulation capabilities are being applied to diverse areas in energy supply, energy transmission, and environmental impacts.

The Division leads a strong program in climate modeling (as a critical element of the national program) and the simulation of impacts of energy use. Infrastructure modeling is being applied to energy transmission networks, and advances in superconductivity may lead to more efficient electrical transmission and storage.

An increased focus on nuclear energy will require Division expertise in reactor safety and design, as well as actinide and accelerator research for an advanced nuclear fuel cycle and long-term waste issues. Fuel cell research will advance a new hydrogen economy.

Modeling and simulation of combustion engines and gas turbines will be important for more efficient fossil fuel use and to minimize emissions. Carbon management and water security need additional simulation capabilities and materials research.

Theoretical understanding of Tokomaks, through simulation and modeling of plasmas under extreme conditions, is essential to realizing the potential of fusion as an energy source.

Such diverse energy security issues require the broad theory, modeling, and simulation capabilities of T Division in effective partnerships with other divisions and laboratories.

Energy Security Plan
(See also Appendix A)

We will achieve our aims in the energy and environmental field by participating in the planning of future programs and by developing the necessary scientific underpinnings.

- T Division management serves on the Energy and Environmental Steering Council in LANL's Strategic Research (SR) Directorate.
- Staff serve on LANL's Science Advisory Board to provide subject area expertise.
- Staff serve as advisors to external bodies and build partnerships with other divisions and institutions.

2.2.2 Frontier Science

It is essential for the Division and the Laboratory that we strive to maintain distinction and world-class standards in all our science. The Division pursues its goals by establishing and maintaining a scientific environment that promotes creativity, innovation, and excellence. It undertakes research at the forefront of theoretical sciences, with emphasis on long-term goals, high risks, and multidisciplinary approaches, fostering communication—both within the Division and external communities—to fully realize the implications and benefits of our research. These values underlie our vitality, creativity, and recruitment on behalf of the Laboratory. T Division is prominent in the international scientific arena, providing a highly visible face of the Laboratory that the scientific community outside LANL acknowledges and respects. The Center for Nonlinear Studies (CNLS) provides a unique additional mechanism for sustaining the Division culture.

Frontier Science Plan
(See also Appendix A)

In addition to high quality, fundamental research, T Division staff will provide leadership by serving as Laboratory program managers in relevant areas. They will also:

- Provide an administrative base for the CNLS.
- Compete for external science funding [DOE Office of Science (DOE/SC)], National Institutes of Health (NIH), National Science Foundation (NSF), etc.] directly or in partnerships with academia.
- Serve on DOE/SC panels, NIH study groups, NSF review panels, national and international topical groups, and scientific advisory groups of other agencies.
- Serve on Laboratory Directed Research and Development (LDRD) review teams.
- Maintain high visibility by service on journal editorial boards and as editors to international scientific journals.
- Organize outreach educational programs for undergraduate and graduate students.
- Vigorously recruit the best and brightest postdoctoral fellows and early career/strategic hires.
- Be active at frontiers of science as part of the international infrastructure, including collaborating with academia and industry.

2.2.3 Strategic Thrusts. (See Appendix A for detailed thrust descriptions and associated business plans.) The Division identifies and evolves strategic thrusts with the aim of either a) building on existing strong foundations with qualitatively new approaches, or b) enabling new capabilities. The thrusts are chosen on the basis of scientific excitement, Laboratory goals and national needs, and growth and market potential. The aim of these thrusts is to build compelling core competencies that will provide attractive careers for present and future staff, as well as support critical Laboratory mission needs. The thrusts are reviewed periodically and progress is monitored regularly.

The current Division strategic thrusts are:

- Science-Based Prediction for Complex Systems
  - Innovative Science in Support of Stockpile Stewardship
  - Predictive Science and Technology for Threat Reduction and Homeland Security
  - Innovative Science and Technology for Energy Security
- Hard, Soft, and Biological Matter
  - Understanding and Design of Complex, Functional Materials
  - Modeling Biological Processes
- Fundamental Processes
  - Particle-Nuclear-Astro-Cosmology
  - Quantum Information
- High-End Computing Research

2.3 Innovation and Partnering

2.3.1 Individual Initiatives—The Entrepreneurial Spirit

Historically, there has been a strong tradition in T Division of placing a high value on individual entrepreneurship as a means of incubating new directions and programs and of developing the skills and realizing the potential of people. Thus, the Division nurtures smaller projects for their intrinsic scientific and technical interest to the Laboratory. Frequently, these smaller projects reach a level of development that attracts significant program funding and this process has led to the establishment of new groups and divisions, providing a flexibility that allows the Laboratory to more readily pursue new ideas.

2.3.2 Partnering for Success

Intergroup projects are uniquely positioned to respond to interdisciplinary opportunities and program needs. As such, these projects are actively supported by all Division management and promoted from the Division Office through the following.

- Formation of teams that transcend traditional disciplinary boundaries—including teams in nuclear weapons science, materials science, energy security, and complex systems.

- Utilization of program coordinators for the Division relevant to NW and TR programs and other program development.

- Investment in exploratory interdisciplinary fields—such as complex matter, quantum science and technology, and knowledge derivation from large data sets.

- Investment in numerous workshops and conferences, both internal and external.

Strategic partnerships *(see also Section 4.3, Collaborations, page 23)* between T and other divisions are essential to the LANL strengths of integrating science, programs, and performance. The Division not only shares responsibility for and supports the goals of the NW, TR, and SR directorates, but also promotes collaborative partnerships between these directorates. T Division supports the Stockpile Certification objective through strengthening the quality and integration of research in support of the ASC program, development of new techniques such as uncertainty quantification for use in certification, and support of Laboratory experimental programs within the framework of science-based prediction. The Division supports Laboratory Goals *(see also Section 2.4, page 9, and Appendix B, Laboratory Goals)* by providing scientific leadership and helping the Laboratory to nucleate new programs in energy and environment, critical infrastructure assurance, materials science (including nanoscience and technology), biological sciences allied with physical sciences, and by fostering and championing excellence in basic research.

Partnerships with the external scientific community are equally fundamental to T Division's vitality and mission. Our staff members are at the forefront of many frontier science areas and play central roles in national and international science and technology communities. These roles include serving on national committees, councils and boards; joint appointments and programs with academia; partnerships with major industrial sectors; organizing and lecturing at international conferences; publishing extensively in leading scientific journals; and serving on numerous editorial boards. Industrial partners have included Proctor and Gamble, British Petroleum, Motorola, Caterpillar, Kraft Foods, and Dow Chemical.

2.4 Alignment with Institutional Technical Goals

The core programs of the Division are derived from our primary sponsors and support the Laboratory strategic objectives. T Division's strategies, goals, and thrusts strongly engage and support all the current Laboratory Goals *(see also Appendix B, Laboratory Goals).* Approximately 35% of our business is from core NW funding, and elements of the Materials and Physics ASC program are managed by T Division project leaders for the Laboratory. This is reflected directly in our division thrusts *Science-Based Prediction for Complex Systems* and *Innovative Science in Support of Stockpile Stewardship* and are closely aligned with Lab Goals A and B. The Division also reports on its contributions to NW in our annual publication, *Nuclear Weapons Program Highlights (see Appendix G, Referenced Documents.)*

T Division staff have a long-standing role in nonproliferation activities in TR. In the last few years, these have deliberately been expanded into initiatives to provide underpinning science for the widening intelligence and HS portfolios at the Laboratory. T Division thrusts *Science-Based Prediction for Complex Systems*, *Predictive Science and Technology for Threat Reduction and Homeland Security*, and *Modeling Biological Processes* all closely align with Lab Goals C and D.

Materials science in its many manifestations represents the work of some 40% of T Division personnel. The Division embodies arguably the largest concentration of materials science theory, modeling, and simulation expertise in the world. This multidisciplinary capability, coordinated with the distinctive breadth of characterization and synthesis capabilities at LANL, provides the opportunity for Los Alamos to lead frontiers of materials science, such as complexity in hard, soft, and biological matter and increasingly predictive understanding of the "systems" aspects of modern organic and inorganic materials, composites, biological processes and biologically-inspired materials. Division expertise, goals and thrusts in *Science-Based Prediction for Complex Systems*, and *Hard, Soft, and Biological Matter* are central to Laboratory Goal E, as well as providing essential capabilities for Goals A, B, C, D.

The strategic partnership of T Division with the DOE/SC has been key to our success in theoretical research to further our scientific understanding of the physical world; in establishing the technical foundation for current and future defense, industrial, and civilian needs; and in exploring, jointly with international academic and scientific centers of excellence, new interdisciplinary areas of scientific endeavor. This partnership has led to the development of groundbreaking new approaches to discover, develop, and deploy the computational tools that enable scientific researchers to analyze, model, simulate, and predict complex physical, chemical, and biological phenomena important to the DOE. These tools are being applied to some of the most challenging problems in materials sciences, chemistry, plasma physics, applied mathematical sciences, global climate change, and bioscience that underpin the DOE missions in energy, environment, and national security. The Division shares and supports the DOE/SC Goal G, which continues to have far-reaching synergistic impacts in the NW, TR, and SR directorates of the Laboratory.

T Division is a major recruitment pipeline through its investment in summer programs and workshops for undergraduate and graduate students, the postdoctoral program (typically 70–80 in residence), and educational outreach, including many enduring partnerships, collaborations, and adjunct faculty appointments with many academic institutions, as well as extensive domestic and worldwide collaborations, thereby serving as a key resource for Lab Goals H and O.

2.5 Key Deliverables

2.5.1 Weapons Programs

T Division plays a central role in the NW program. T Division has significant involvement in approximately 16 Level 1 or 2 FY06 NW milestones. These key deliverables are reported on a quarterly basis through the NW Program Office. T Division plays a dominant role in a Level 1 milestone in FY06 for an updated pit lifetime estimate for predominant pit types. Drawing from the equation of state expertise, researchers are teaming with experimental colleagues throughout the Laboratory, and the design community, to revise the assessments of the useful lifetimes of weapons pits. In addition, the annual assessments of the weapons systems (also Level 1 milestones) now routinely use physics model improvements that T Division has developed and helped implement as prior year milestones. The following table shows the 16 Level 2 milestones for FY06 with very significant contributions from T Division staff. These milestones represent further improvements

Milestone Title	Level	NNSA Programs/ Subprograms	Completion Date	Adjusted Completion Date
Provide updated pit lifetime estimates for predominant pit types	1	Enhanced Surveillance	Oct-06	
Produce a report containing data for development of physical model of ejecta formation and transport	2	SC Primary Assess Technology	Sep-05	Sep-06
Verification Methodology	2	ASC Verification & Validation	Sep-06	
Primary Verification & Validation (V&V) Assessment Supporting Code Capabilities for Primary Burn	2	ASC Verification & Validation	Oct-06	
Secondary V&V Assessment Supporting W76-1 Life Extension Project (LEP) Certification (Intermediate)	2	ASC Verification & Validation	Jan-06	Nov-05
Validation assessment capability for simulation of engineering shock transmission through nonlinear materials	2	ASC Verification & Validation	Jun-06	
Plutonium Science for W88	2	ASC Physics Mat Models	Sep-06	
Multiphase EOS Capability	2	ASC Physics Mat Models	Oct-06	
Pilot Demonstration of UQ in 5 areas of physics and engineering	2	ASC Physics Mat Models	Sep-06	
Code B release to support Robust Replacement Warhead (RRW)	2	ASC Advanced Apps	Mar-06	
Code B release to support RRW and W76	2	ASC Advanced Apps	Sep-06	
Code A release to support RRW and W76	2	ASC Advanced Apps	Feb-06	
Code release A to support RRW and W76	2	ASC Advanced Apps	Aug-06	
Develop Quantification of Margins and Uncertainty (QMU) techniques for secondary assessment and demonstrate their applicability to a nuclear weapon system.	2	SC Secondary Assess Tech	Jun-06	
Complete an annual enhanced surveillance campaign (ESC) stockpile aging assessment report to support the annual assessment process	2	EC Enhanced Surveillance	Jul-06	
Utilize improved experimental and predictive modeling capabilities for pit aging to support lifetime assessments	2	EC Enhanced Surveillance	Jul-06	
Provide initial lifetime assessments for other pit types	2	EC Enhanced Surveillance	Sep-06	

in the predictive capabilities of the simulation tools that form the backbone of our stockpile assessment, arguably the primary current responsibility of the Laboratory.

2.5.2 Laboratory Directed Research and Development

T Division staff are currently Principal Investigator (PI) or involved in 81 active LDRD projects—35 Directed Research (DR) and 46 Exploratory Research (ER) projects. *Appendix C*, T Division FY06 Laboratory Directed Research and Development Portfolio, contains more detailed information on these projects, each with specific deliverables, which are monitored and coordinated by the Laboratory's Science and Technology Base (STB) Programs/LDRD Office. Program expenditures are reported to the DOE Albuquerque Operations Office quarterly by project. An annual progress report is required on each project and these are assembled into an LDRD annual report. This includes a technical and financial overview of the program and a list of publications emerging from the program. An individual final report is required for each completed project and these are submitted to the Office of Scientific and Technical Information of DOE during the fiscal year after the project ended. The LDRD Office also monitors operating and capital expenditures by each project.

2.5.3 Office of Science

The Division has a significant and diverse portfolio of projects supported by the DOE Office of Science (DOE/SC), amounting to approximately 12% of the Division's budget.

Office of Science — Materials Sciences

- *Predictive capabilities for strongly correlated electronic systems*. The metal-insulator transition in MnO has been studied using different many-body approaches. Our approach in T-12 (hybrid density functional theory) provides results in excellent agreement with experimental measurements. Collaborators at University of California (UC) Davis, UC Santa Barbara, LANL, and Oak Ridge National Laboratory (ORNL) are comparing various many-body approaches to unravel the details of the metal-insulator transition in MnO. The calculations will be completed in FY06 and the comparison published.
- *Novel Materials Theory Effort.* This project in T-11 studies the local electronic properties of strongly correlated materials and artificially created nanostructures, such as quantum dots, metal nanoparticles on DNA, impurity and vibronic states, Inelastic Electron Tunneling Spectroscopy (IETS), fast optical response of these materials, and electron-phonon coupled systems such as colossal magnetoresis-tance (CMR) manganites. We will further develop basic theoretical methods that will make possible detailed analysis and predictions about specific experimental properties.
- *Electronic Processes in Solid State Organic Electronic Materials (PI: D. Smith, T-11)*. Organic electronic materials are of great intrinsic scientific interest and technological importance because there is strong coupling of electron charge, spin, and lattice degrees of freedom and a rich spectrum of tunable ground states and excited states. We will attempt to determine which features of the electronic structure of the isolated molecules are maintained and which are modified in the condensed phase and use this to describe the behavior of the condensed phases, which have important intermolecular interactions. The goal is to understand the fundamental physical processes that are important in determining the properties of organic electronic materials.
- *Accelerated Molecular Dynamics Methods (PI: A. Voter, T-12).* We are developing accelerated molecular dynamics methods for reaching longer

time scales for simulations relevant to chemistry, physics, materials science, and biochemistry. Deliverables for FY06: 1) extend parallel-replica dynamics to biological systems, and 2) develop method and code for spatially parallelized temperature accelerated dynamics.

Office of Science — Nuclear Physics
The nuclear physics group, T-16, covers a wide range of nuclear theory relevant to LANL and national needs. Deliverables include studies of few- and many-body nuclear physics, dense matter in nuclear astrophysics, neutrino physics and properties of high energy-density quantum chromodynamics (QCD). The DOE/SC also funds work in nuclear data, including cross sections for astrophysics and energy research.

Office of Science — High Energy Physics
Cosmology, elementary particles and astrophysics using field theoretical and computational methods. T-8 staff aim to elucidate the mechanism for supersymmetry breaking, origin of masses of quarks and neutrinos, lattice QCD, precision tests of the standard model, neutrino interactions, large-scale structure of the universe and its evolution, gravity, alternatives to black holes, nonequilibrium field theory, phylogentics applied to HIV and Hepatitis C virus (HCV), statistical analysis of large data sets and automated image analysis.

Office of Science — Biological and Environmental Research
Metabolomic functional bacterial genome (PIs: B. Bruno and A. Perelson, T-10). FY06 deliverables: analysis of genome sequences.

Office of Science — Chemical Sciences
Heavy Element Chemistry Program (POC: R. Martin, T-12). T-12 supports experimental efforts in C and NMT divisions. FY06 deliverables: address the mechanism of C-H bond activation in organoactinide complexes and determine the properties of quasi-1D chains of actinide oxides using hybrid density functional theory.

Office of Science — Advanced Scientific Computing Research (ASCR)
ASCR Applied Mathematical Research Program (POC: M. Hyman, T-7). ASCR supports basic research in applied mathematics and computational techniques for problems critical to current Laboratory missions. The program serves as a bridge among university, industry, and Los Alamos researchers and encourages transfers to and from the Laboratory of state-of-the-art mathematical theory and advanced computational techniques.

2.5.4 Other DOE

- *Advanced Fuel Cycle Initiative (POC: J. Wills, T-1)*. We provide first-principles calculations in support of modeling new types of nuclear fuels. In FY06, we will provide 1) direct first-principles calculations of thermodynamic properties of actinide nitrides and actinide oxides, and 2) calculated material data in these materials for use in fitting modified embedded atomic method (MEAM) potentials for classical molecular dynamics (MD).
- The nuclear physics group (T-16) is also funded through the *Advanced Fuel Cycle Initiative* to produce cross sections and uncertainties for advanced fission reactor concepts.
- *Hydrogen research R&D (POC: N. Henson, T-12)*. In support of experimental research in C Division, we are simulating the structure and properties of novel materials with hydrogen storage capabilities as part of the DOE-EERE Center for Chemical Hydrogen Storage. We are currently investigating non-boron, main group element-based materials using first principles quantum chemical methods to calculate their catalytic activity.
- *Cationic Polyelectrolyte Membranes for Alkaline Fuel Cells (PI: B. Pivovar, MST-11).* Alkaline fuel cells should

permit replacement of the precious catalyst metal Pt with the nonprecious metal Ni. But new cationic polyelectrolyte membranes will have to be designed, synthesized, and characterized. An FY06 deliverable is to perform molecular modeling to address chemical stability and transport mechanisms for hydroxide conductivity of cationic polyelectrolyte membranes and modeling of carbonate formation in these membranes.

- *Material and Device Designs for Practical Organic Lighting (PI: D. Smith, T-11).* The objective is to establish high efficiency, low-voltage, stable materials for organic light emitting diode (OLED)-based general illumination. We have developed an extensive understanding of OLED device physics that has been incorporated into a predictive device model. We are using a tightly knit theory/fabrication/measurement approach to provide a detailed understanding of charge injection, transport and carrier recombination in OLEDs that is needed to guide new materials synthesis and device designs for these solid-state lighting applications.
- *Vehicle Technologies (PI: D. Torres, T-3). KIVA-4* is a computer code designed to simulate internal combustion engine performance with unstructured mesh capabilities. The goal is to improve KIVA-4 so that it can be used to improve engine efficiency and reduce vehicle emissions. FY06 deliverables include complementing the code with grid-generation capabilities, parallelizing the code so that it can run on multiple processors, and testing new turbulence models.
- *Threat Reduction* projects in the nuclear physics group (T-16) develop nuclear data for attribution applications.

2.5.5 Reimbursables/Work for Others

The Division's budget from reimbursables, which includes Work for Others for agencies such as the NIH, NSA, Defense Advanced Research Projects Agency (DARPA), National Aeronautics and Space Administration (NASA), and others, is approximately 20%. This portfolio includes many smaller projects with specific deliverables. The Division's NIH portfolio is significant, approximately 8% of the FY05 budget in T Division.

Reimbursables — Department of Health & Human Services:

- *HIV Database and Analysis (PIs: B. Korber and T. Leitner, T-10)*. FY06 deliverables: HIV Database and software tools.
- *Modeling Viral and T Lymphocyte Dynamics (PI: A. Perelson, T-10)*. FY06 deliverables: theoretical immunological models.
- *Multiscale Observation Molding of Ca Channels (PI: J. Pearson, T-10)*. FY06 deliverables: theoretical models of ion transport.
- *HIV-1 Diversity Optimized Vaccine (PIs: K. Yusim and B. Korber, T-10)*. FY06 deliverables: HIV vaccine design principles.
- *Large-Scale Simulations of Ribosome (PIs: K. Sanbonmatsu and C.-T. Tung, T-10)*. FY06 deliverables: molecular dynamics simulations of the ribosome.
- *Receptor Aggregation and Its Effects (PI: B. Goldstein, T-10)*. FY06 deliverables: theoretical models of cell signaling.
- *Immune System Modeling/HIV (PI: A. Perelson, T-10)*. FY06 deliverables: theoretical immunological models.
- *Hepatitis C Database (PI: C. Kuiken, T-10)*. FY06 deliverables: HCV database and software tools.
- *EPICAST: Epidemiological Forecast (PI: C. Macken, T-10)*. FY06 deliverables: agent-based models and software for epidemiology.

- *Influenza Viral Sequence (PI: C. Macken, T-10)*. FY06 deliverables: influenza virus database and software tools.
- *Analysis of HIV Drug Resistance Mutation (PI: B. Foley, T-10).* FY06 deliverables: models of mutation in HIV.
- *A Rational Vaccine Design (PI: A. Lapedes, T-13).* A new approach was developed based on mapping the antigenic and genetic evolution of influenza virus. This research was done in the frames of the World Health Organization programs in using new algorithms to choose the best annual influenza vaccine on a continuing basis. FY06 deliverables: develop the algorithm to analyze evolution of influenza.

Reimbursables — Other Federal Agencies—Defense-related activities:

- *Self-assembled quantum computation using electron spins in radicals as quantum bits of information (PI: G. Berman, T-13, for the NSA).* Calculated the region of parameters for performing quantum logic operations for concrete spin radicals with two quantum bits. FY06 deliverables: calculation of the dependence of g-factor for spin radicals on the electric field.
- *Design of a quantum microscope based on a single-spin resolution (PI: G. Berman, T-13, for DARPA).* Calculated the details on the frequency shift which is measured in experiments on spin resolution. This microscope, when in operation, will allow analysis of detailed structures in nanosystems and bio-molecules. FY06 deliverables: calculation of the cantilever frequency shift due to interaction with a single spin in high magnetic field gradient.

Reimbursables — Threat reduction and intelligence-related activities:

- *Classified research in support of the U.S. intelligence community (POC: R. Walker, T-12).* Projects utilize the Division's expertise in materials, chemistry, high-performance computing, and complex systems and are supported by several of the agencies of the U.S. government.
- *Distributed sensor networks (PI: D. Torney, T-10).* This project benefits the nation's threat reduction efforts. FY06 deliverables: mathematical modeling of biosensor networks.

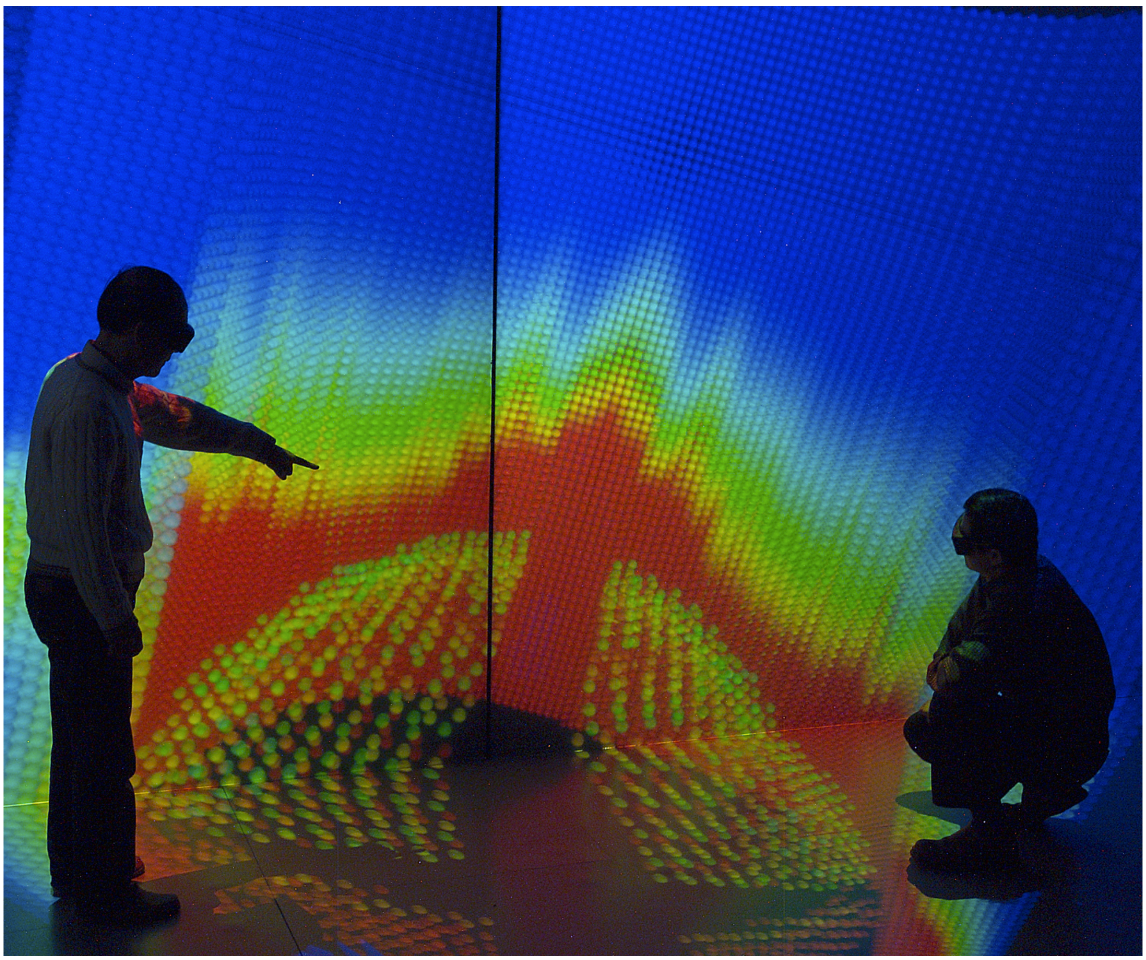
2.6 Honors, Awards, and International Participation

T Division is widely recognized throughout the international science community for its high rate of publications, honors, fellowships, and awards. Over the Division's more than 60-year history, its members have collected an impressive portfolio of international awards and honors, elections to international societies, and many internationally recognized fellowships.

The Division *Annual Self-Assessment* document contains the statistics of Division publications (both open literature and classified), invited presentations, awards, honors, memberships on editorial boards, staff serving as journal referees, and memberships of professional organizations, including election to the rank of Fellow within these organizations, for the preceding year *(see Appendix G, Referenced Documents.)*

Each year, the Division is responsible for approximately 25–30% of the Laboratory's annual total of peer-reviewed publications. Many of the Division's staff members also hold adjunct professorships with academic institutions, which relationships not only foster scientific exchanges and collaborations, but also serve as effective recruiting mechanisms.

T Division staff have received approximately 5 Ernest Orlando Lawrence Awards, 10 Humboldt Fellowships, 8 R&D 100 Awards, and currently 28 are APS Fellows, 3 are Fellows of the American Association for the Advancement of Science (AAAS), and 2 are members of the National Academy of Sciences. The quality of the senior Division staff is also reflected in the fact that a much larger fraction, relative to the number in other divisions, of T Division staff hold the rank of Laboratory Fellow and Senior Laboratory Fellow. As of 2005, T Division has 5 Senior Fellows and 31 Fellows (including retirees) on its active staff.



Theoretical Division staff in the Fluid Dynamics Group (T-3) won an R&D 100 Award for their work with the CartaBlanca simulation code. CartaBlanca is a pure Java, component-based systems simulation and prototyping tool for non-linear physics on unstructured grids and has applications in aerospace engineering, animation and special effects, computational fluid dynamics, fluid/solid interactions, automotive design, weapons / target interactions, pharmaceutical processing and homeland defense.

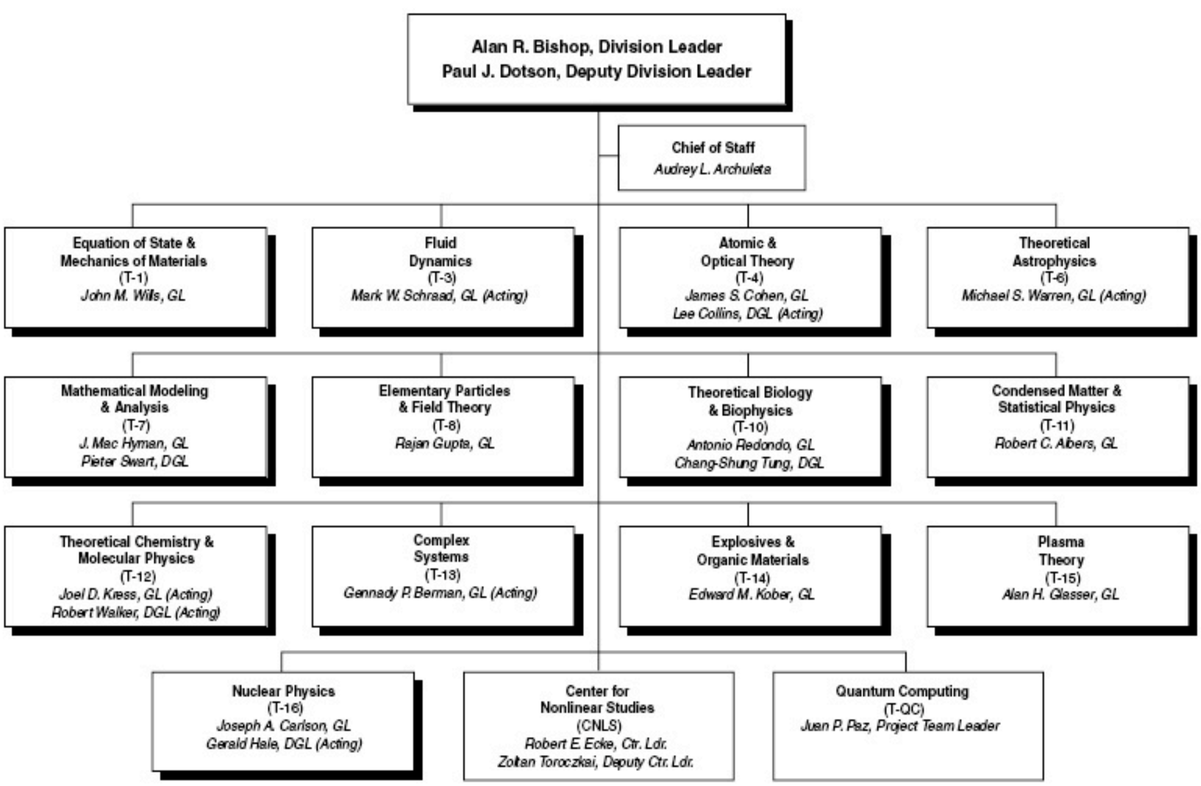
3.0 Organization, Workforce, and Operations

3.1 Organizational Structure

T Division is principally organized into discipline-based groups with a deliberate emphasis on intergroup collaborations and teaming with experimental partners (internal, external, and with members of our extensive visitor program). More detailed group descriptions can be found in *Appendix D, Group Technical Descriptions*, and detailed group profiles and business plans are available on request. The Center for Nonlinear Studies has a Laboratory-wide mandate, as described earlier *(see also Appendix G, Referenced Documents.)* This organizational structure has, as demonstrated over many decades, enabled leadership in interdisciplinary science based on discipline rigor and renewal, combined with maximum opportunities for dynamic teaming. Group structure and alignments were extensively reviewed during 2000–2002 by teams addressing crosswalks between disciplines and programs and intergroup alignments. The rotation of group leaders and succession planning is healthy, as documented in past Laboratory workforce reviews. *Group and division leader position descriptions are provided in Appendix E.*

The Division has capability in depth (approximately 400 staff, postdoctoral fellows, and students, and a robust visitor program of over 100 visiting researchers/collaborators per year) in core theoretical disciplines *(see also Section 2.0 page 2)*: fluid dynamics, materials chemistry and

THEORETICAL (T) DIVISION



Division UC and Contract Staff (Average): FY03–06					
	Sept. 2003	*Sept. 2004*	*Sept. 2005*	*FY06 est.*	*Change (FY03-06)*
UC staff (Regular/Long-term Visiting Staff)	**188**	**193**	**177**	**173**	**-15**
UC Staff (Limited term)	**47**	**47**	**55**	**62**	**+15**
Post-docs	**81**	**72**	**67**	**75**	**-6**
Students	**70**	**50**	**65**	**65**	**-5**
Contractors	**14**	**8**	**3**	**6**	**-8**
Total Division FTEs	**400**	**370**	**367**	**381**	**-19**

physics, atomic physics, nuclear physics, elementary particles and field theory, astrophysics, biophysics, condensed matter, statistical physics, plasma physics, and mathematical modeling and analysis. As noted, these disciplines are organized into groups (shown in organizational chart) for technical viability, but collaboration between groups is strongly encouraged, supported, and rewarded. This intergroup, multidisciplinary entrepreneurship is managed by a) program development points-of-contact in the Division Office for Laboratory and external customers, and b) through teams with representation from all relevant groups for key business areas.

3.2 People and Capabilities

T Division's main asset is its workforce. To accomplish its objectives and the Laboratory's expectations, T Division requires excellent scientific staff working with the most advanced hardware and software and interacting with colleagues in both theory and experiment. In pursuit of this objective, the Division supports extensive graduate student and postdoctoral training programs as a central component of its recruitment strategy. Recruiting the best and brightest also implies a robust foreign national population working on problems of national importance but with deliberate processes for protecting national security. In addition, the technical staff engage many colleagues from academia and other national and international scientific organizations to collaborate on a wide variety of programs and problems. This cross-fertilization of the Division's technical expertise provides numerous opportunities for solving important problems and is also an effective recruiting tool.

Pursuing frontier science is central to T Division's value to the Laboratory, because it poses complex, challenging problems that attract exceptional scientists. Each of these scientists brings with him/her a comprehensive tool kit of expertise, ranging from pure mathematics to numerical analysis to aggressive exploitation and development of state-of-the-art high-performance computers, to physics, chemistry, and biology.

Individuals are valued for their ability to think broadly and strategically about difficult problems. This diverse, sophisticated, and future-oriented capability, immersed in the multidisciplinary-mission environment of LANL, has stimulated these scientists to create new programs directly relevant to the core national security mission of the Laboratory (nuclear weapons and emerging threats), to undertake pioneering science, and provide leadership to multidisciplinary teams.

A full *capabilities list for T Division can be found in Appendix F*. The current technical workforce can be broadly categorized in the following subset of major capabilities.

Capabilities, Skills, Knowledge, and Experience	Current FTEs[1]		Estimated FY06 FTEs[1]	
	Theory, Modeling, and Analysis	*Simulation and High-Performance Computing*[2]	*Theory, Modeling, and Analysis*	*Simulation and High-Performance Computing*[2]
Astrophysics: including Supernovae and Compact Objects, Stellar Astrophysics, Cosmology, N-Body Simulations, and Magnetohydrodynamics, . . .	7	3	7	4
Atomic, Molecular, and Optical Physics: including Atomic Structure and Reactions, Opacities, Spectroscopy, Quantum Molecular Dynamics, Cold Atoms, and Quantum Optics	8	3.5	8	4
Biology: **i**ncluding Biophysics, Disease Progression & Transmission, DNA & RNA structure/dynamics/sequence, Molecular Physics, and Immune System	44[3]	5	44[3]	5
Chemistry: including Quantum Chemistry, Chemical Processes, Physical Chemistry, Actinide Chemistry, Organic Chemistry, Catalysis, and Biochemistry	6	1	6	1
Computational Mathematics/Computer Science: including Applied Mathematics, Software Engineering, Algorithms, Data Analysis, Image Analysis, and Uncertainty Quantification	31	6	30.5	6
Condensed Matter Physics: including Electronic Structure, Many-Body Theory, Quantum Computing, Device Physics, and Electronic & Magnetic Materials	13.5	3	13.5	3
Continuum Dynamics: including Fluid Dynamics, Solid Mechanical Engineering, Ocean Modeling, and other Fluid Modeling in nonplasma states	14	5	13	5
Elementary Particle Physics: including Physics Beyond the Standard Model, Quark-Gluon Plasma, Lattice QCD, Neutrino Physics, Gravity, . . .	7	1	7	1
Materials Science: including Equation of State, Constitutive Modeling, Materials Properties, Actinide Materials, Phase Transformations, and Explosives	21	4	23	6
Nuclear Physics: including Nuclear Structure and Reactions, QCD, Sensitivity Studies & Radchem Diagnostics, Data Evaluation, Processing, and Testing, . . .	17	5	14.5	5
Plasma Physics: including Magnetic Fusion Energy, and Kinetic and Continuum Plasma Models	13	3	11.5	3
Statistical Physics: including Complexity and Nonlinearity, Nonequilibrium Models, Large-Scale Data Analysis, Complex Networks, and Stochastic Systems	17	4	15.5	4
Totals	198.5	43.5	193.5	47

[1]FTEs include all TSMs and research/technical TECs, and Postdocs.
[2]Large-scale computing on high-end machines and platforms.
[3]Includes TECs building and maintaining databases for the biology community databases.

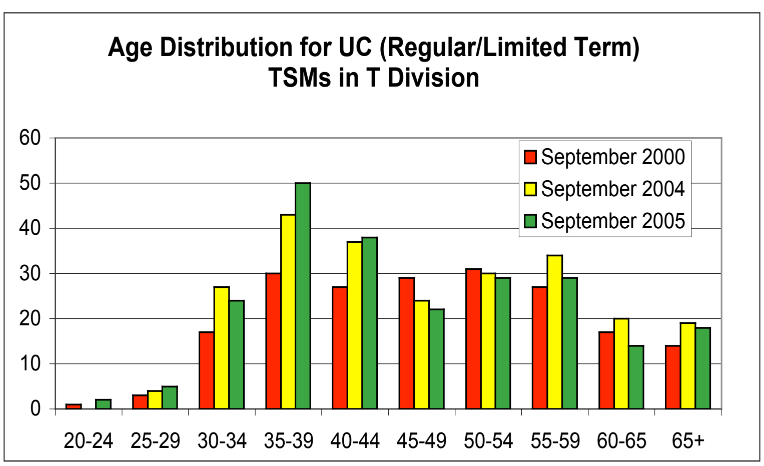
Every six months, the Division assesses the breadth and depth of the current staff and compares it against emerging areas of need and makes recruiting and development projections necessary to assure the continued vitality and orderly succession of our workforce (technical, management, and support tracks). With this information, the Division develops and implements a systematic approach for staff additions and workforce management. We examine those factors that lead to successful recruitment and retention of staff and develop a program that ensures hiring, retention, and professional development of high-quality individuals. We match results of this staff analysis with the programmatic requirements of T Division and the Weapons

Physics (WP), SR, and TR directorates to identify areas in which the Division does not have sufficient capability and those where capability exceeds requirements.

We thereby develop and implement 1) recruitment strategies with emphasis on addressing diversity issues and attracting the highest quality scientists available, including foreign nationals, and 2) division-level plans for employee development, succession planning, and training opportunities. The Division uses a mature **recruiting pipeline** that includes extensive utilization of summer schools, student and postdoc programs (including distinguished postdoctoral appointments), limited-term staff members, and senior or retired staff members as mentors and for knowledge transfer. Approximately 65% of our recruitment is accomplished via this highly effective, strategic pipeline.

The latest workforce review (Summer 2005) revealed a healthy demographic trend from the last five years of investing in a) early career recruiting, and b) systematic knowledge transfer and mentoring by senior staff. This demographic situation is illustrated here.

This healthy demographic situation has been challenged in 2005 by a significant number of retirements and some loss of mid-career talent, primarily driven by contract and benefits uncertainties. We are attempting to address this situation by a) careful recruitment to maintain the highly talented T Division capability base, b) engagement of retirees, as appropriate, for mentoring and specific skills, and c) continued emphasis on all stages of our well-established recruiting pipeline.



3.3 Culture

There are several cultural characteristics that the Division considers are integral to its success. The relationships between these important characteristics and the resulting benefits are described and demonstrated throughout the discussion of T Division's broad technical portfolio, innovations, and partnerships (see Section 2.0).

1. Technical excellence: maintaining the best science and providing it to fulfill the Laboratory mission.
2. Discipline-based excellence: integration of theory, modeling, and simulation, with a high degree of adaptability to respond rapidly to emerging challenges.
3. Intellectual diversity: the opportunity for interdisciplinary research and scientists that creates a creative environment for interactions.
4. Co-location and other minimal barriers to interdisciplinary teaming: provides for a high degree of internal collaboration and positively affects our ability to partner in order to deliver on major national security programs.
5. Extensive external collaborations and partnerships: a conduit to new ideas and a major recruiting pipeline for the Division and the Laboratory.
6. Recruiting and engaging the very best available talent: including a strong community of, and active engagement with, foreign national researchers.
7. Hiring pipeline: extensive utilization of the summer educational programs, student recruitment programs, postdoc program, and limited term

appointments to hire the best and brightest and provide career development opportunities; as well as effectively utilizing senior staff (Fellows and retirees) as mentors for the next generation of scientists and leaders.

8. External peer review: both being exposed to and contributing to the international science community through conference/workshop sponsorship/organization, robust publication and invited presentation records, participation in review boards/journals, and other international scientific organizations.
9. Equality of opportunity: a nonhierarchical TSM pool where each person has the opportunity to compete for funding and technical or programmatic impact and to establish his/her own place in the Laboratory.
10. A strong business model and opportunities for entrepreneurial program development.
11. Intellectual integrity and academic freedom (the managed freedom and flexibility for individuals to find their place with respect to individuality/teaming, basic/applied, etc.)

3.4 Facilities and Business Systems Infrastructure

Since reliable facilities and a modern infrastructure are prerequisites for world-class science, we work through the responsible Laboratory organizations to try to bring T Division's aging infrastructure up to current standards and requirements. Specific current goals in this area include working with the SR Directorate to develop plans for a modern Science Complex, maintaining and providing adequate electrical and cooling systems, developing and implementing a funding strategy to refurbish facilities, and effectively managing indirect resources to provide ergonomically correct furniture and equipment. The current facilities allow the Division to remain fairly co-located and in the TA-3 area, which is important to fostering collaborations with other technical Divisions *(see also Section 4.3, Collaborations, page 23)*. However, the current space is not adequate to meet the Division's large fluctuations in population, which occur because of our substantial student and visitor programs. During peak periods, staff must share space with students and visitors, students and visitors share small spaces, and not all groups can remain co-located. Safety considerations remain a high priority. More adequate space with flexibility for peak periods and a modernized communications and computer room (HVAC) infrastructure is important to sustain the high-profile research conducted in the Division.

T Division supports the Laboratory Strategic Plan objectives of best business practices, customer satisfaction, and stewardship of resources leading to cost-effective project delivery. We manage resources so as to ensure their effective use in a fashion that meets the needs of customers. We continue to examine the Division's business practices and promote continuous improvement and adoption of "best practice" systems throughout the Division. We work to identify new funding sources and facilitate the funding process. We also encourage and facilitate the patenting and licensing of Laboratory-generated intellectual property.

Occupied space by building (square footage)	***FY05***	***FY06 est.***
Permanent	47903	42977
Commercial	0	0
Transportainers (4)	640	888
Trailers	5431	4927
Transportables	16559	11427
Total	70533	60219
Occupied space by type (square footage)		
Office	65333	55019
Computer Rooms	5200	5200
Total	70533	60219
Data is from LANL's official space database, FATMAN, as of September 2005 (FY05) and November 2005 (FY06). Actual total occupied space is difficult to ascertain.		

Current goals include:

- utilizing and providing continuous process improvement feedback on new Laboratory-wide business systems to facilitate the development of truly effective systems for all,
- developing internal business processes and systems that are not redundant, are integrated with Laboratory systems, and that provide easier access to accurate data to identify trends and issues in a wide variety of business areas important to the Division; and
- identifying new funding sources and actively engaging in program development.

One of the Theoretical Division's office buildings, located in Technical Area (TA-3) within the 43 square miles of the Laboratory property.

3.5 Security, Environment, Safety, and Health

Our highest priorities are the health and safety of our workers and the public and Laboratory and national security. The Division employs the Laboratory's nested safety and security process and actively participates in the Management Walkaround and Environment Management systems. Our aims are to maintain a safe, secure, and well-trained workforce, to protect the environment, and manage our resources effectively. We work towards continually achieving measurable improvements in safety and ergonomics throughout the Division, and manage trends in security incidents and DRC/DART rates appropriately.

4.0 Customer and Sponsor, Funding, and Collaborations Profiles

4.1 Customers and Sponsors

T Division's customers align naturally with its funding profile–NW, LDRD, and non-NNSA. The Division manages relationships appropriate to each of these customers. For principal customers, points-of-contact operate from the Division Office, working closely with principal investigators and other appropriate Laboratory points-of-contact and program managers. NW Programs are reviewed through quarterly LANL and formal NNSA reviews.

T Division participates in many of the program components and has oversight responsibility for elements of the Materials and Physics component of ASC. The LDRD program is very competitive and is reviewed on a regular schedule internally and by the NNSA. DOE/SC, NIH, NASA, NSA and other Work for Others customers make awards on a rigorous, competitive basis and review our programs regularly using national review teams.

Another major customer for T Division is the international scientific community where peer review is the arbiter of success. Every year T Division staff publish approximately 650–700 peer-reviewed publications and over 20 classified publications, organize approximately 50 conferences and workshops, and organize and sponsor at least 4 summer programs for students. Our staff are also heavily involved in invited presentations at conferences and universities and serve on numerous international review and advisory committees. Detailed statistics are compiled annually and presented in the Division Self-assessment documents *(see Appendix G, Referenced Documents).*

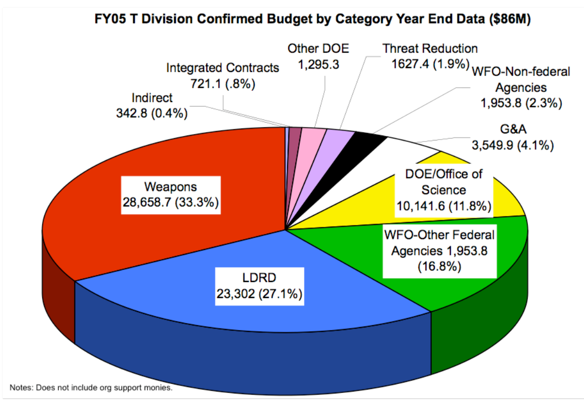
The Theoretical Division Review Committee (TDRC) reviews the balance and productivity of the Division annually. This input is an important peer review metric, and the TDRC's detailed reports are used in Division strategic planning. Copies of TDRC reports can be requested from the T Division Office.

Actual and Projected Division Funding ($M): FY03–06

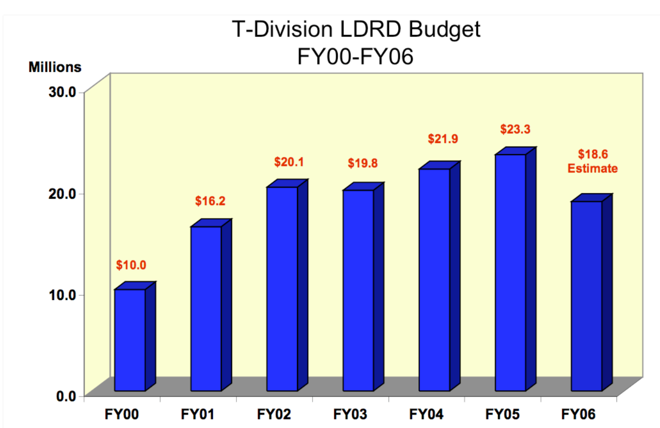
	FY03		*FY04*		*FY05*		*FY06 (est. as of Oct 31)*		*Change (FY03–06)*	
Program Area	*$(M)*	*% of funding*	*$(M)*	*% of funding*	*$(M)*	*% of funding*	*$(M)*	*% of funding*	*$(M)*	*% of funding*
Direct										
Defense Programs	**22.9**	**31.8**	**25.1**	**31.5**	**27.9**	**32.2**	**24.2**	**30.6**	**1.3**	**19.5**
Nonproliferation/ Intelligence Community	**2.8**	**3.9**	**3.1**	**3.9**	**2.8**	**3.3**	**2.0**	**2.5**	**-.8**	**-12.0**
Office of Science	**7.4**	**10.3**	**7.7**	**9.6**	**9.1**	**10.5**	**10.0**	**12.8**	**2.6**	**38.8**
Other DOE programs	**1.1**	**1.5**	**3.3**	**4.0**	**3.5**	**4.0**	**3.5**	**4.5**	**2.4**	**35.8**
Work-for-Others/ Reimbursables	**15.4**	**21.4**	**16.0**	**20.0**	**16.4**	**18.9**	**16.5**	**21.2**	**1.1**	**16.4**
Total Direct	**49.6**	**68.9**	**55.2**	**69.2**	**59.7**	**68.9**	**56.2**	**71.6**	**6.6**	**98.5**
Indirect										
LDRD	**20.0**	**27.9**	**21.9**	**27.5**	**23.3**	**26.9**	**18.6**	**23.6**	**-1.4**	**-20.9**
G&A	**2.3**	**3.2**	**2.6**	**3.3**	**3.6**	**4.2**	**3.8**	**4.8**	**1.5**	**22.4**
Total Indirect	**22.3**	**31.1**	**24.5**	**30.8**	**26.9**	**31.1**	**22.4**	**28.4**	**0.1**	**1.5**
Total Funding	**71.9**	**100**	**79.7**	**100**	**86.6**	**100**	**78.6**	**100**	**6.7**	**100**

4.2 Funding Portfolio

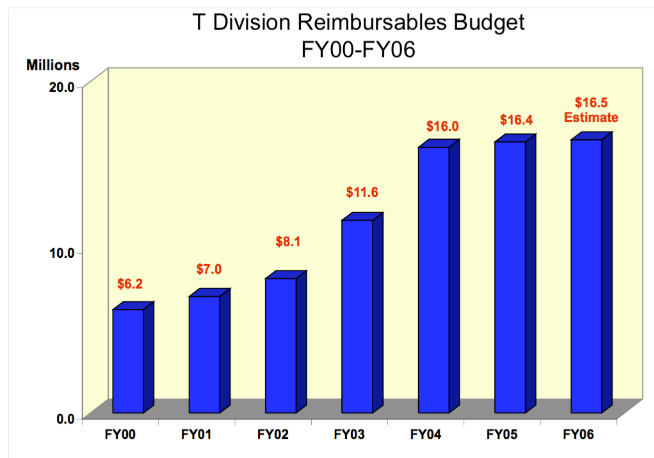
T Division pursues a balanced research portfolio that includes the NW, LDRD, TR programs, and other sponsors and agencies in the DOE, NIH, NSA, NASA, and industry, among others. This portfolio has allowed the Division to interact strongly with the academic community in areas of basic research, with designers in the weapons programs, and with customers in threat reduction and homeland security. This broad spectrum of research has provided a conduit that has facilitated transfer of new ideas and techniques from basic research into the applied programs throughout the Laboratory.



Researchers in T Division have successfully competed for the Laboratory's LDRD funding, which has allowed the Division to support and nurture a large number of innovative research directions. Many of these initiatives have expanded the capability for current programmatic efforts. These LDRD projects have also led to numerous publications *(see Appendix C, LDRD Portfolio)* and have been crucial in attracting and maintaining gifted and highly motivated researchers within the Division.



The Division's funding portfolio demonstrates successful diversification of its base, including pursuit of non-NNSA-sponsored research and development synergistic with current Laboratory missions. Staff have successfully pursued opportunities to work with industry or other agencies. New opportunities in HS and TR have also been vigorously pursued in addition to our continuously strong Work for Others/Reimbursable (DOE, NIH, NSA, NASA, etc.) portfolio.



4.3 Collaborations

All technical staff members in the Division are involved in collaborations with the scientific community (universities, industry, and other national laboratories) throughout the world (*see Appendix G, List of Referenced Documents, Self-assessment documents for detailed statistics*). In addition, several members of the Division serve as officers in the societies of which they are members. Division staff engage in personnel exchanges with industry and other federal laboratories and agencies as temporary staff on "Change of Station" assignments as program managers at NSF, NNSA, and Office of Science and Technology Policy (OSTP).

T Division staff are involved in a great number of external interdisciplinary programs, for example, the UC **Cooperative Agreement on Research and Education (CARE)** program, designed to identify and fund opportunities for promising students and faculty to participate in new and innovative research, enhance collaborations with universities in areas of strategic importance, and provide a research environment to encourage students to pursue technical careers. Division staff are closely involved in the **Santa Fe Institute's (SFI)** multidisciplinary programs and have played a seminal role in the Institute's foundation, along with continuing activity through collaborations and organization and participation in conferences. The newly founded NSF Center at the **UNM** for the **Consortium of the Americas for Interdisciplinary Research** was the result of a strong partnership between UNM and Los Alamos where T Division played the major role. Division staff serve on the **Governance Board** of the new **UC/LANL Memoranda of Understanding** with UC San Diego, UC Santa Barbara, UC Davis, UC Santa Cruz, and UC Riverside campuses.

T Division is a partner in the **NSF Nanoscale Science and Engineering Center** for Directed Assembly of Nanostructures at **Rensselaer Polytechnic Institute** and the **University of Illinois at Urbana-Champaign**, founded in September 2001. The mission of the center is to integrate research, education, and technology dissemination, and serve as a national resource for fundamental knowledge and applications in the directed assembly of nanostructures. The center research involves two major areas of emphasis: nanoparticle gels and polymer nanocomposites and nanostructured biomolecule composite architectures.

The Division hosts half of the members of the LANL **Climate, Ocean and Sea Ice Modeling (COSIM) project**. Ocean and sea ice models developed by COSIM are used in several of the world's leading global climate models. Predictions from these models are contributing to the Fourth Assessment Report of the Intergovernmental Panel on Climate Change, the most important confluence of international climate modeling expertise.

Important new projects started in T Division by the DOE/SC in FY05 include: 1) a theory, modeling, simulation element of Center for Integrated Nanotechnologies (CINT) (with **SNL**); 2) organic electronic materials; and 3) solid-state lighting (with SNL). New projects funded by NIH include world-leading all-atom simulations of biological machinery, and a joint project with the Harvard Medical School on transcription in DNA.

Despite the decline of CRADA initiatives nationally, staff throughout the Division remain actively engaged in responding to **collaborative opportunities with industry**. Division staff have made scientific contributions to U.S. industry, including partnering with Proctor & Gamble, petrochemical firms such as Exxon-Mobil and Dow Chemical, and automobile manufacturing giants such as Ford and Daimler-Chrysler on computer simulation of manufacturing processes and product performance. The Division current holds 13 active Non-Federal Work for Others Agreements, 2 active Nondisclosure Agreements, and 2 continuing CRADAs.

Several of the Division's projects involve the **design of software packages or computer algorithms**; some are packaged and made available for the general research community. Many of T Division's products are used in institutions around the world and are the benchmarks against which other codes or methods are compared. Some examples are:

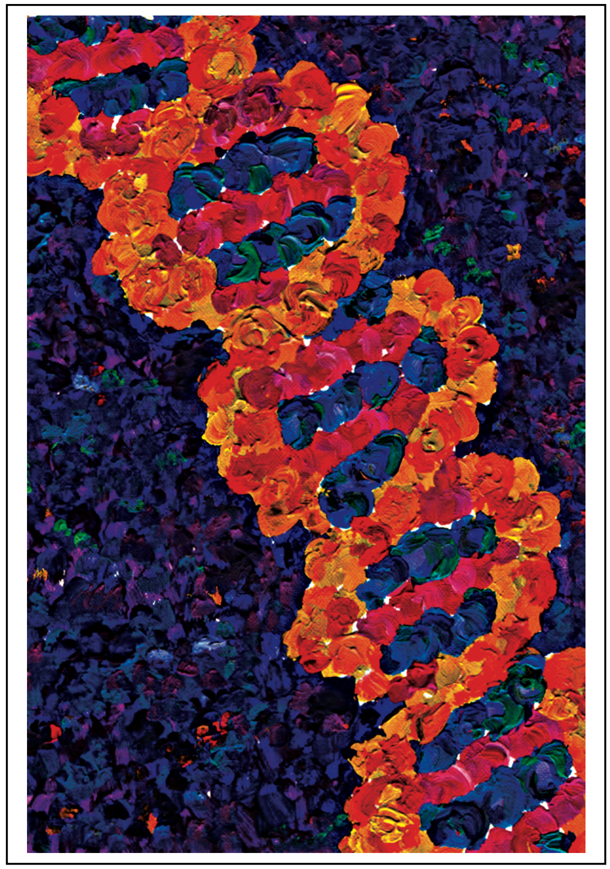
- CAVEAT, a 3-D hydro program used in many applications;
- NJOY, a data-processing package for nuclear reaction data;
- OpenSesame, a suite of equation-of-state tools and the accompanying

Sesame Library—a compendium of equation-of-state tables used by government, academic, and industrial institutions; and
- LAGriT (Los Alamos Grid Toolbox), a set of tools used by many academic institutions for creating and tracking unstructured grids in multimaterial applications.

In collaboration with the Physics Division, T Division hosts the **P/T Colloquium** series, which has been ongoing for over 10 years and has brought a wide variety of distinguished speakers to Los Alamos. In 2004, T Division hosted about half the speakers out of the total 33 talks given during the year. Another regular series hosted and organized by the Division is the **Quantum Lunch**, which features speakers from different organizations and academia with an interest in fostering continued collaborations and research and development in the quantum information science and technology field. These informal presentations and interactions occur approximately three times per month. In 2004, 32 talks were hosted.

Examples abound of the more **informal involvements** in interdisciplinary programs, including: 1) sponsorship of conferences and workshops (approximately 20 per year) to bring together experts from several disciplines around the world; 2) sponsoring/organizing approximately five educational programs per year for students in mathematics, physics, and biology, 3) fostering new collaborations in materials science involving materials modeling with accurate chemistry now deployed in the ASC and other programs; and 4) frequent interchange of information and ideas between Division staff and the rest of the Laboratory (including internal sabbaticals with X Division and several joint appointments).

Strategic **partnerships between T and other Laboratory divisions** are essential to the LANL strengths of integrating science, programs, and performance. T Division works closely to support Laboratory Goals *(see Appendix B, Laboratory Goals)* with other divisions for NW, TR, and the diverse energy security issues requiring the broad theory, modeling, and simulation capabilities of T Division. These close partnerships between T and other technical divisions include: B, C, CCS, D, DX, ESA, LANSCE, MST, NMT, P, and X divisions.

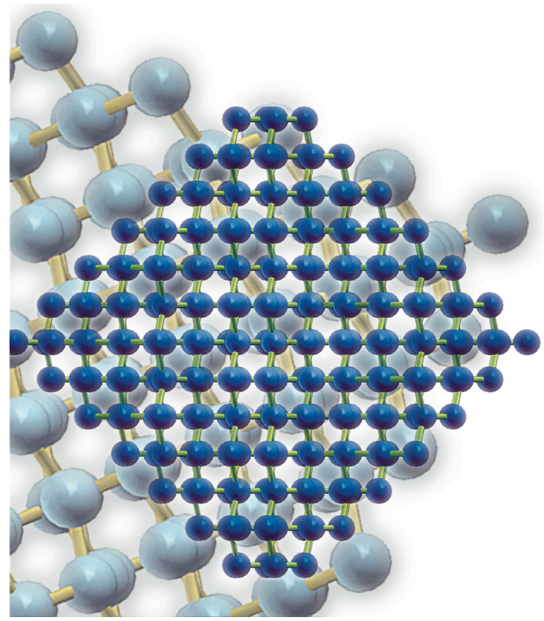


Biosciences is being performed in several groups in the Theoretical Division in collaboration with other parts of the Laboratory and researchers around the world. Current focuses are the frontiers of biological physics and computational biology.

5.0 Transition Issues

T Division views the future as history to be made with as much rich accomplishment on behalf of the nation as in its distinguished past. Immediate transitional issues to secure this future include the following key elements.

- Maintaining strengths of T Division culture, see Section 3.3, page 19.
- Attracting and maintaining strongest possible technical workforce (necessarily including a significant foreign national program and postdoctoral and student populations).
- Modernizing infrastructure for scientific productivity (flexible, modern computing, and access to large-scale machines; modern space/buildings; time-efficient administrative tools/ processes, etc.).
- Maintaining balance of capability development and program delivery.
- Minimizing barriers for interdivisional/directorate collaborations to maximize programmatic excellence and responsiveness to emerging national security missions.
- Maintaining strong collaborations with academia and external consortia (including industry); business case for entrepreneurial S&T; user facilities; non-NNSA programs.
- Maintaining the health of the Center for Nonlinear Studies



The graphic shows an example of materials science, in this case, the study of the stability of a material's crystal structures. The study of key materials is a vital part of the innovative science to support the Stockpile Stewardship program.

Experimental and observational advances over the last decade have led to unprecedented progress in our knowledge and understanding of the universe. Many of the most exciting science opportunities occur at the intersection of astrophysics, atomic, nuclear, and particle physics.

Appendix A – Science Thrusts for a Renewed Foundation

1. Science-Based Prediction for Complex Systems A2
a. Innovative Science in Support of Stockpile Stewardship A4
b. Predictive Science and Technology for Threat Reduction and Homeland Security A8
c. Innovative Science and Technology for Energy Security...A11

2. Hard, Soft, and Biological Matter A13
a. Understanding and Design of Complex Materials A13
b. Modeling Biological Processes A16

3. Fundamental Processes A19
a. Particle and Nuclear Astrophysics and Cosmology A21
b. T Division Support of the LANL Quantum Institute...A23

4. High-End Computing Research...A26

1. Science-Based Prediction for Complex Systems

Purpose: To coordinate and support T Division's response to Laboratory Strategic Goal A, Science-Based Prediction for Complex Systems (SBP/CS).

Rationale and Description: To accomplish its national security missions, LANL has assembled its core expertise in the *integration of experiment, theory, and computation* in a bold strategy to advance our scientific understanding of and predictive capabilities for complex phenomena. This strategy has been articulated in the Laboratory Strategic Goal SBP/CS. The Stockpile Stewardship Program depends critically on the viability of this approach. However, the need for SBP/CS extends well beyond the nuclear weapons program. Indeed, virtually every major initiative at LANL relies heavily on SBP/CS. This reliance does, of course, present a challenge and accomplishing the SBP/CS goals will require a new generation of major ideas and concepts to improve the fidelity, reliability, and usability of the tools for predictive science that are envisaged. Addressing this challenge frames the strategic direction for T Division, which can be summarized in a single phrase: ***Frontier Science for Laboratory Missions***. The examples listed below illustrate a few of the areas where we are taking steps to implement this basic objective in support of SBP/CS.

- **Nuclear Weapons —** T Division undertakes research in nuclear and atomic physics, materials science, hydrodynamics, and uncertainty quantification — all capabilities that are used in X Division design and certification activities. SBP/CS involves integrating theory advances, is motivated and validated by experiments, with measured data from all relevant experiments, including those undertaken at the NNSA's unique facilities. T Division co-led one of the five Goal A Pilot Projects (Detonation Science) and participated in another (Materials Science) during FY05. These contributed to the evolving implementation of SBP/CS within the weapons program.
- **Homeland Security –** Enhanced predictive capabilities will play a central role in meeting scientific challenges posed by TR and HS missions, and tie the SBP/CS and HS goals together. Established expertise in T Division in several disciplines and methodologies (nuclear physics, theoretical chemistry, biology, complex systems, data analysis, numerical algorithms) is being vigorously adapted and applied to HS problems.
- **Biology –** Following the heroic era of gene-sequencing, biology is beginning to enter the phase of quantitative predictive science. T Division is applying its expertise in theoretical biology and scientific computation to address national needs in health and security as part of its response to the SBP/CS goal. One focus of effort concerns the computation of protein structure and binding. This will support more rapid and efficient searches for new drugs. A second topic concerns development of vaccines against rapidly evolving viruses, like influenza, avian flu, and HIV.
- **Energy & Environment –** Predictive science is required to assess the cost and efficacy of strategies for energy production and environmental remediation. In supporting the SBP/CS goal, T Division will develop and apply predictive methods for multiscale modeling to selected problems for which experimental and observational data at many length scales are available, affording the opportunity to validate predictive scaling techniques.
- **Enabling Scientific Tools –** Progress on predictive science in the previously mentioned application areas will require vigorous development of supporting science in many areas, including: 1) uncertainty quantification for complex simulations; 2) advanced software design; 3) techniques for modeling multiscale and nonequilibrium processes; 4) effective methods for utilizing data; 5) new approaches for modeling complex stochastic processes; and 6) powerful methods for modeling complex networks, including agent-based models.

Partners: Scientific, organizational, and funding requirements for successful accomplishment of this thrust necessitate partnering with groups within and external to the Laboratory. Existing partnerships already include those with X, DX, CCS, EES, ESA, MST, and D divisions, as well as ones with DoD, NIH, numerous universities, and industrial organizations. Current partnerships will be strengthened and new ones established.

Customers: A new generation of predictive capabilities for complex mission-related problems will be available to a customer base that includes NNSA and other DOE programs, DoD, NIH, and private industry.

Business Plan: Science-Based Prediction for Complex Systems

Long-Term Goals: The overall goal of this thrust is to identify and support vigorous and constructive measures to align T Division with Laboratory Goal A. The goal encompasses strengthening our role in the Stockpile Stewardship program, and significant new starts in the TR area, including bio-chem threats and critical infrastructure modeling. A further goal is to develop an understanding of the functioning of complex organizations that could lead to more efficient operation of technical programs.

Program Measures: The number of new proposals that receive funding will measure the success of the program. This will include proposals in the NW area, as well as in biological and chemical threat reduction, critical infrastructure, energy, health, and environment, and organizational dynamics. Milestones for the application of SBP/CS and QMU within the weapons program have been prescribed with T Division involvement and will require support from the staff.

Actions over the next year to achieve the goal:
- Work to maintain a strong presence in Stockpile Stewardship by serving on boards that govern the planning process.
- Continue the series of summer programs for students and visitors in epidemiology.
- Support and ensure the success of SBP/CS and QMU milestones within the weapons program.
- Coordinate with other T Division thrusts on materials, biological and threat reduction modeling.
- Align LDRD-DR and pilot project proposals with Goal A and other Laboratory Goals.
- Carry out currently funded proposal for *Systems Modeling at LANL* using agent-based modeling and other appropriate tools.
- Play an active role on the Predictive Science Advisory Council.
- Continue T Division assistance on the *LA Science* publication.
- Plan joint LANL-SFI-EU workshop on science-based prediction.

Funding Sources: LDRD, DARPA, National Infrastructure Simulation and Analysis Center (NISAC), DOE/NN, DTRA

1a. Innovative Science in Support of Stockpile Stewardship

Purpose: To create more accurate fundamental physics models and data, *through integration of experiment, theory, and computation*, to enhance the science of certification in partnership with the goals of the NW directorates, and to exploit the large investment in basic science in T Division, which has created numerous opportunities to bring innovative ideas from many areas of science into weapons physics. This strategy has been articulated in the Laboratory Strategic Goal on Science-Based Prediction for Complex Systems and Nuclear Weapons.

Rationale and Description: A primary LANL mission is to certify the stockpile in the absence of nuclear testing. T Division undertakes research in nuclear and atomic physics, materials science, astrophysics, hydrodynamics, plasma physics, and uncertainty quantification—capabilities used in design codes. The thrust brings together, and provides enhanced visibility for, numerous innovative scientific concepts being pursued at LANL. The research will be conducted via collaborative teams that bring T Division scientists into workgroups with designers and code integrators in X and experimentalists in P, C, LANSCE, MST, DX, and ESA divisions. This will ensure that theoretical advances will be motivated and validated by experiments, assessed in a design context in an integrated way, and ultimately used in certification. The thrust will focus on:

1. nuclear and atomic physics and interactions of matter with radiation (nuclei far from stability, QMD simulations of density effects, novel diagnostics for mix, nonequilibrium processes for boost, opacities);
2. materials science (constitutive formulations developed from multiscale modeling for metals, high explosives, polymers, and other weapons materials; reaction laws; aging analysis and prediction; equations of state);
3. astrophysics of stars, supernovae, and compact objects (e.g., nucleosynthesis, high energy-density physics, and computing and computational science for multidimensional, time-dependent cosmic phenomena);
4. numerical methods and software for hydrodynamics (e.g., advanced hydrodynamics and solver algorithms, interface treatments, constitutive laws for particular mesh resolutions);
5. uncertainty quantification (metrics for stockpile certification and weapons physics in general, analysis of experimental data, both historical and modern);
6. Directed Stockpile Work (DSW), pit surveillance, enhanced surveillance, and manufacturing; and
7. strongly-coupled and/or high energy-density plasmas.

These efforts will be coordinated with one another and with parallel basic research initiatives for non-weapons materials and issues. From the weapons perspective, all possible sources of relevant data from experimental programs [e.g., enhanced surveillance, manufacturing, baselining of nuclear test data, above ground experiments (AGEX), Dual-axis Radiographic Hydrodynamic Test Facility (DARHT), Advanced Test Line for Actinide Separations (ATLAS), and National Ignition Facility (NIF)], and astrophysics will be considered and strong interaction with these programs encouraged. All of these issues are increasing in significance because of subtle variations in manufacturing and aging characteristics that need to be accounted for with enhanced fidelity in the maintenance of the stockpile. The demonstration of applications to problems outside the weapons arena will broaden the approach beyond weapons materials and issues and leverage investments in those areas.

Partners: Close collaborations with X, CCS, P, C, LANSCE, MST, DX, NMT, and ESA divisions, as well as with scientists from Livermore and Sandia laboratories, the United Kingdom's Atomic Weapons Establishment (AWE), and France's Comissariat á l'Énergie Atomique (CEA).

Customers: The primary customer, the nation's NW program, will be able to use more accurate and advanced science to certify the reliability and safety of the US stockpile. Many other customers throughout DOE science and technology programs will benefit from a new generation of simulation science, as well as TR, DHS, and DoD.

Business Plan: Innovative Science in Support of Stockpile Stewardship

<u>Thrust Leaders</u>: Edward Kober (T-14) and John Wills (T-1)

<u>Goals</u>: To create more accurate fundamental physics and materials models and data to enhance the science of certification, in partnership with the goals of the NW directorates, and to exploit the large investment in basic science in T Division, which has created numerous opportunities to bring innovative ideas from seemingly unrelated areas of science into weapons physics and materials applications.

<u>Program Measures</u>:
- Formation of collaborative teams
- Development of new physics modules for ASC codes
- Use of modules in certification process
- Successful execution of the ASC Materials and Physics Program element function

<u>Actions taken over FY05 to achieve the goal</u>:
- Ensured accomplishments were integrated as quickly as possible into weapons simulations, ASC milestone calculations, and certification baselines. Level 2 Milestones for implementation of a ductile failure model and an improved model for insensitive high explosives (HE) were accomplished.
- Weapon Supporting Research (WSR) proposals were developed targeting long-term research plans for the weapons program. Eleven proposals with T Division staff as PIs were funded.
- Provided X, MST, and NMT with science-based materials models and EOS to meet certification needs and to address aging issues.
- Started implementing UQ methods into materials, opacities, and equation-of-state (EOS) modeling efforts. Demonstrated first iteration and developed Level 2 Milestone goal for UQ methods implementation.
- Established collaborative teams involving researchers in X, CCS, P, C, LANSCE, MST, and DX divisions, as well as with Livermore and Sandia national laboratories, AWE, and CEA scientists.
- Used integral data and collaborations with LANSCE and X to determine important actinide cross-sections.
- Developed strong, collaborative LDRD-DR proposals supporting innovative science for Stockpile Stewardship.
- Funding for two "Predictive Science for Complex Systems" projects was successfully used for incubated projects in detonation theory and EOS theory (both relevant for RRW).

<u>Actions planned over FY06 to achieve the goal</u>:

- Supply leadership and technical expertise in accomplishing two Level 2 Milestones for ASC Materials & Physics program in QMU and Pu EOS.
- Support the scientific development of the WSR projects funded for this year and use that basis to evolve similar innovative proposals to support long-term research.
- Provide X, MST, and NMT with science-based materials models and EOS to meet certification needs, address aging issues, and to develop RRW concepts.
- Utilize UQ research and practices to determine impact of uncertainties on physical data and models on weapons performance, to establish priorities for modeling efforts, and to ensure customers are aware of critical scientific issues.
- Develop strong, collaborative LDRD-DR proposals supporting innovative science for Stockpile Stewardship.
- Be fully engaged with the RRW development teams and rapidly address scientific and design issues as they arise.

Funding Sources: DOE/DP, LDRD, DOE/SC

Thrust: Innovative Science in Stockpile Stewardship

Leaders: Kober, Wills Oct 2005

Goals
- T-div will bring high-quality *predictive science* into the weapons program
- Thrust encompasses many of the program and LDRD activities supporting NW, with a focus on new innovative science
- Thrust reflects the strategic importance of T-div successfully contributing to NW (>30% budget)

Participants
- High fraction of T-div groups
- Projects supported by ASC, DSW, ESC
- V&V projects
- LDRD-related projects
- WSR projects
- Collaborations with LLNL, SNL, AWE, CEA
- Technology supporting DHS programs…

Customers
- WP and WEM
- ASC, ESC, DSW
- Experiment (via theory-exp. collaborations)
- DOE/NNSA and DoD
- WP users implementing QMU methodology
- RRW will become big driver
- DHS efforts leveraged from this

Recent accomplishments
- Improved IHE L2 milestone with X-7
- TEPLA implementation L2 milestone
- 3 ASC M&P project leads in T Division
- ATOMIC opacity code validated for higher Z
- QMD calculation of benchmark opacities and HE EOS products
- Multi-phase Pu EOS on track for FY06
- Several weapons related LDRD-DR & ER proposals funded

Los Alamos NNSA

Innovative Science in Stockpile Stewardship

Leaders: Kober, Wills

Strengths
- High-quality science, subject to peer review, that directly impacts NW programs
- Versatility; our basic tools are supported by and applied to many program areas
- Diversity of expertise available within T, on theory, modeling, data & simulation
- Our approach to NW problems includes state of the art methods and expertise from outside the lab

Opportunities
- "Science Roadmap" and evolving management structure; better ASC, ESC, DSW coordination
- Reliable Replacement Warhead (RRW)
- Strong partnering with experimental programs to support NW deliverables(tight budget)
- Integrate new data & models into ASC codes & demonstrate impact
- Coordinate with CINT, MSEC, Materials Science and Predictive Science thrusts
- Increased capacity of open and classified computing; receptive support
- Demonstrated value of WSR

Weaknesses
- Our interactions with other divisions are improved, but continue encouragement
- Our partners need to perceive T-division as a long-term strong partner in achieving NW goals.
- Some important experimental work required for model improvement not being supported
- Retention & replacement
- NW, DHS, BES programs not as well-coordinated as could be (group by group)

Threats
- Gradual / abrupt decline in ASC, NW funding
- RRW, reduced NW footprint, new contractor
- Disagreements or lack of coordination between divisions
- Demise of critical experimental facilities
- Understaffing & retirement of critical staff
- Still recovering from stand-down,especially for experimental colleagues
- Evolving management structure
- New building & classified work

Los Alamos NNSA

1b. Predictive Science and Technology for Threat Reduction and Homeland Security

One of the greatest consequences of the events surrounding 911 is a collective understanding that the nation's vulnerabilities are closely tied to the complexity of our infrastructure, health system, government, economy and society, and that the lack of *understanding* of the workings of our "system" reduces our ability to respond to national and global needs. This thrust addresses the need to advance our knowledge on how these complex technical/social/economic/natural systems work at a fundamental level, particularly in response to our rapidly changing global system.

The strategic objectives are threefold: 1) develop core technologies that contribute across many application areas; 2) develop S&T projects and programs that address the needs of TR, intelligence, and HS programs; and 3) leverage the development of the technologies and resources derived from traditional mission areas in predictive science, built on the synergy of experiments, simulations and theory, to application areas within threat reduction, intelligence, and homeland security.

The thrust includes the following scientific grand challenges:
1. The interdependence of various components of a complex system — recognizing the essential parameters responsible for functionality and failure — and how system structures create "gaps" or vulnerabilities.
2. The role of extreme statistics (e.g., outliers, non-normal and long-tail probability distributions) on the robustness, sustainability, and intrinsic uncertainties of complex systems.
3. A dynamical understanding of *adaptive* and *co-adaptive* systems.
4. Quantified treatment of social and cognitive behavior to address complicated issues of individual behavior, societal influences, and response to threats.

These grand challenges apply to a wide variety of specific research areas, such as the properties and dynamics of infrastructure networks, agent-based modeling, information and knowledge technology, epidemiology, sensor networks, quantum technologies, modeling of nanodevices, etc.

The approach taken to develop the thrust is to create an integrated approach to address threat identification, prevention, response, and attribution-sharing resources; identify technological synergy across chemical-biological, radiological-nuclear, and critical infrastructure protection threats; reduce cost of threat protection by adding protection/response to existing or planned functions (e.g., combine detection and response to manmade biothreats to an improved day-to-day public health system); coordinate with the Laboratory Strategic Plan, other divisions, and outside resources to amplify T Division's unique strengths and create integrated programs where the Division does not contain essential resources (e.g., experimental facilities).

T Division has active programs that are beginning to develop core technologies related to this thrust. For example, the traditional expertise in fission cross-sections for the nuclear weapons programs has been applied to nonproliferation issues for the characterization and detection of special materials. T Division has taken the lead in the nation with "threat anticipation" modeling the formation of terrorist networks in the Middle East (Threat Anticipation Modeling Project). T Division leads the nation in the modeling of epidemics resolved at a national scale, for example, 280 million people (EpiCast Project). The Division has also shown leadership in developing new program areas by extending the Science-Based Prediction methodologies developed in the NW programs to TR programs, by championing the need for an understanding of social dynamics in many areas of national security, and by developing a national response to the need for simulations in crisis response in coordination with universities in the Norfolk-Hampton Roads region.

Business Plan: Predictive Science and Technology for Threat Reduction and Homeland Security

Thrust Leader: Gennady Berman (T-13)
Implementation Plans: Develop systems and technologies to identify across all threats.

- Precursors in threat preparation (chemical precursors, intel signatures, or accumulation of resources).
- Signatures of the threats (chemical activity, radioactivity, or changed cyber-information).
- Components combined with threats (explosives, cyber trail, or terrorist access to facilities).
- Attribution of threats after an event (epitopes or isotopes).
- Apply existing technologies and resources derived from traditional mission areas (NWT).
- Expand the predictive science methodology to address increased reliability and quantification.
- Identify technological synergy across threats.
- Reduce cost of threat protection by exploiting dual-use infrastructure.
- Add protection/response to other existing or planned functions (combine an improved day-to-day public health system with detection and response to manmade biothreats).
- Coordinate with Program Offices, other divisions, directorates, and outside resources.
- Amplify T Division's unique strengths.
- Create integrated programs where T Division does not have essential resources (experimental).
- Exploit recent advances in quantified treatment of cognitive and social behavior.

Program Measures: Number of successful/funded new proposals, number of staff whose primary focus is in TR, number of projects that include collaboration across the Laboratory and mission areas, and the hours spent by staff contributing to Laboratory and national TR planning.

Actions over the next year to achieve the goal: NNSA laboratories will play a key role in providing the S&T for the national homeland security solutions. T Division's goal is to use its expertise in a wide-range of technology foundations and its demonstrated academic outreach to support the rapidly growing needs of the Laboratory's HS programs, with the focal point being the Center for Homeland Security (CHS). Actions over the next year will include the following.

1. Actively engage in planning and program development activities within T Division, CHS, and national agencies to create the Laboratory-wide program.
2. Identify and grow technical thrust areas in TR for T Division. In particular, build on its successful programs such as the Threat Anticipation Modeling Project, EpiCast, Center for Theoretical and Computational Pathomics, and work with the U.S. Army Medical Research Institute for Infectious Diseases to study emerging and engineered pathogenic agents, computational immune and system biology, particularly in new growth areas of water, plant, and animal vulnerabilities.
3. Develop the scientific grand challenge of vulnerability, detection, mitigation, and control of infrastructure networks.
4. Coordinate with SR and CHS to develop hiring and resource plans to address growing needs, activating CNLS resources for academic and industrial engagement.
5. Algorithm development and models for passive remote sensors and hyperspectral imaging, signal recovery in chattered backgrounds, statistical detection and identification of anomalies, and large data set analysis.
6. Develop mathematical modeling of quantum technologies and nanoscale electro-optical devices.
7. Develop a new project for the Nuclear Emergency Search Team.
8. Develop dataphysics/image analysis/feature extraction (in collaboration with ISR Division).

Funding Sources: DHS, Department of Health and Human Services (HHS), and the intelligence community for chemical/biological areas, and DHS and DOE for radiation/nuclear areas. Industry is expected to play an increased role as technologies are deployed, particularly those already serving homeland security needs and nontraditional industries in homeland security. T Division has been an aggressive champion for this thrust via briefings and proposals to potential collaborators and sponsors: LDRD, DoD Defense Science Board, BioChem 2020, NIH RegionalCenters of Excellence for Homeland Security, CIA, Defense Intelligence Agency, DTRA, NSA, and the UK Ministry of Defense.

Mission: Predictive S&T for Threat Reduction, Intelligence, and Homeland Security

Strategic Objectives
- Develop core technologies and grand challenge science that contribute across many threat areas.
- Develop S&T projects and deliverables that address the current needs of national security.
- Specifically leverage the predictive science technologies and resources derived from NW.

Customers
- S&T Programs in DHS, DoD, NIH, USG/IC HHS, DOE – NA, NSA, Pentagon, CIA.

Principal actions and achievements
- T-Division teams with D, B, C, CCS, P, ISR, LANSCE, X, N-Divisions in:
  - Risk assessments (chem/bio/nuclear/terrorism).
  - New RN integrated technologies for risk reduction.
  - Behavioral modeling for counter-terrorism.
  - Network physics (vulnerability and control).
  - Large date set analysis (imaging, signal processing, ...)
  - Immunology, system biology, epidemiology.
- Funding increases in CHS (RN/CB, Critical. Infrastructure, and Homeland Security) and Intelligence Programs.
- Adapting our skill sets to meet the new demands of customers - DHS Fellows, training & education of new students and PostDocs, close coordination with customers.
- Driving the grand challenge on infrastructure networks.
- Advising WHO on choice of influenza vaccines.

Multi-Disciplinary Scientific Approaches
- T-Division coordinates expertise in Chemistry, Physics, Biology, Mathematics, Computer Science, Materials Science, Nuclear Physics, Socio-Behavioral Sciences, Statistics, and Network Physics towards customer demands.
- Cross disciplinary teams to leverage entire laboratory.
- Threat characterization and risk management.
- Modeling and simulation for scenario analysis and threat assessment
- Close working relationships with other (non-NNSA) agencies.
- Membership of planning groups for Intelligence, DoD, DHS, and NIH.

Future plans and opportunities
- Develop Lab wide capabilities for modeling complex systems and networks, adaptive and evolutionary systems, nano-devices and quantum technologies, dataphysics.
- Develop capabilities and proposals to meet the new demands of customers.
- Create Center for Theoretical and Computational Pathomics.
- Establish National Lab lead for Socio-Behavioral Modeling; Leverage our existing science advisor roles in the CIA and Pentagon, and build new connections with other intel agencies; Start of new DHS Terrorist Motivation & Intent Program.
- Nuclear physics integration with requirements of national security customers – detection, uncertainty reduction, attribution, NEST.
- Active collaboration with Industry in Homeland Security modeling.
- Develop dataphysics/image analysis/feature extraction (esp. with ISR).

SWOT for Predictive S&T for Threat Reduction, Intelligence, and Homeland Security
Theoretical Division Thrust

Strengths within T-Division
- Technical competencies in nuclear technology (cross sections, sensors, uncertainty reduction), immunology, epidemiology, pathogen databases, system biology, material sciences, nanotechnology, explosives research.
- Expertise in science-based prediction and systemmethodology for uncertainty quantification.
- Theory and modeling of dynamical systems, complex systems and networks.
- Competence in characterization and dynamics of non-equilibrium systems with extreme statistics.
- Socio-behavioral modeling and simulation.
- Drawing on/ integrity, unique interdisciplinary skill-base at LANL.

Opportunities
- Long-term demand in this area -- "this problem will be with us for a long time".
- T-Division can provide integrated solutions because it has capabilities in "all" the technologies and components – CB/RN/CIP, KDD, materials, complex system, intel, …
- T-Division is leading programs in this area now and expanding with new program development.
- We are engaged with many customers now and building long-term relationships (DHS, CIA, NSA, DOJ, DTRA, Secret Service, Pentagon Joint Staff, FBI, NGA, DIA, NIH, CDC, …)

Weaknesses and Challenges
- Most sponsors require immediate (1-2 years) capability and technologies, and are less inclined to support basic research.
- Customer's demands change rapidly.
- Because T-Division typically does not lead projects we are less involved in lab wide program development.
- Cross agency coordination difficulties.
- Protection of intellectual property.
- Short term projects, processing of funding, and staffing with optimal scientists to meet deliverables (hiring/re-training).

Threats to these Programs
- Competition from other labs and agencies.
- Lack of lab-wide coherence/coordination in those areas.
- Competition from more agile technology providers (cheaper, faster, better, …).
- Moving targets.
- LANL is less well represented at DOE and other agencies than LLNL/SNL.

1c. Innovative Science and Technology for Energy Security

To meet energy needs, the U.S. relies increasingly on sources of energy from unstable parts of the world and sources of energy with potential large-scale environmental impacts. In addition, the U.S. struggles with an aging infrastructure vulnerable to both natural disasters and human threats. The goal of energy security is to achieve energy independence with minimal environmental impact. Such a goal requires a broad research agenda to find abundant and reliable new sources, distribute existing resources more efficiently and securely, and reduce the environmental impacts of all energy use.

T Division has strong capabilities in both theory and modeling that can be applied to energy security research. In particular, the Division will focus on: 1) modeling the impacts of energy use on climate, building on existing climate modeling capabilities to address regional impacts, and further examine ocean carbon sequestration and the role of ocean ecosystems; 2) modeling of energy infrastructure to improve the efficiency, security, and reliability of the nation's energy infrastructure; 3) theory and modeling for new catalysts and mechanisms for more efficient and economical fuel cells; 4) basic actinide and accelerator research for advanced nuclear fuel cycle and other nuclear waste issues; 5) advanced technologies for more efficient lighting and photovoltaics; 6) modeling for reactor safety and reactor design for Gen IV nuclear power reactors; 7) combustion modeling for more efficient engines and turbines; 8) superconductor research for use in energy transmission and storage; and 9) continued long-term research and modeling for fusion energy.

Many areas of energy security are led by other divisions and federal agencies and will require T Division to build and maintain partnerships across the Laboratory and DOE complex. The Office of Energy and Environment Initiatives under SR coordinates strategic planning for the energy security goal at the Laboratory and sponsors the Energy and Environment Council in which T Division participates. The Nuclear Technology Office also plays an important role. Other Laboratory partners include CCS, EES, D, C, and MST divisions. The primary customers are the DOE Offices of: Science (SC), Fossil Energy (FE), Energy Efficiency and Renewable Energy (EERE), Electricity Delivery and Energy Reliability (EDER), and Nuclear Energy, Science and Technology. In addition, other agencies like NSF and the Department of Commerce play an important role. Working with other DOE and external agencies often requires partnerships with related laboratories such as National Renewable Energy Laboratory (NREL), National Energy Technology Laboratory (NETL), National Center for Atmospheric Research (NCAR), and National Oceanic and Atmospheric Administration (NOAA).

Business Plan: Innovative Science and Technology for Energy Security

Thrust Leaders: Phil Jones (T-3) and Rajan Gupta (T-8)

Goals: 1) continue to build and expand existing programs and capabilities, like climate modeling, infrastructure modeling, fuel cell research and others; 2) revive nascent capabilities for energy security applications, e.g., reactor safety and combustion modeling; and 3) partner with other divisions and laboratories to apply T Division expertise toward new program areas in energy security.

Program Measures: Success in energy security will be measured in two ways. For existing strengths and programs, success will be measured by publications and involvement in national and international programs. In other areas, success will be measured by the number of new initiatives or programs.

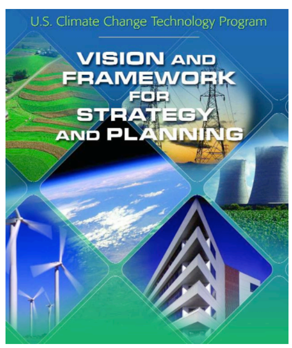
Actions: 1) continue building on existing strengths; 2) participate in the energy security roadmap and strategic planning, looking for new partnerships and new applications for T Division expertise; and 3) revive and market existing dormant capabilities for use in new areas.

Funding sources: DOE Offices (SC, FE, EERE, EDER, NEST) and LDRD or Institutional Program Development (IPD) funds.

Innovative Science and Technology for Energy Security
Thrust Leaders: Phil Jones (T-3) and Rajan Gupta (T-8)

Objectives

- Cheap, clean, copious supply
- Energy, independence with minimal environmental impact.



Relevant T activities/expertise

- Climate modeling
- CO2 sequestration
- Nuclear: actinides, reactor safety
- Fusion
- Infrastructure modeling
- Superconductivity
- Combustion, Combustion engines
- Surface water
- Reservoir Models/Groundwater
- Lighting

Components

- Production: fossil, nuclear, renewable
- Fusion: ultimate fuel
- Transmission: infrastructure, low-loss
- Efficiency: lighting, heating, materials
- Transportation: fuel and efficiency
- Storage: hydrogen, fuel cells, renew…
- CO2: sequestration, ZEC
- Impacts: climate change, water, SNF

Future directions (partners)

- Regional climate, water (EES)
- Infrastructure (D)
- Reactor safety/design (INL)
- Actinide science for fuel cycle
- Fusion: Tokomak simulations
- Superconductivity, CINT
- Fuel cells
- Energy/water initiative (EES/SNL)
- Next Generation Lighting (SNL)

2. Hard, Soft, and Biological Matter

2a. Understanding and Design of Complex Materials: Bridging Multiple Length and Time Scales

This thrust supports theory, modeling, and simulation in materials, an internationally recognized LANL strength that is at the cutting edge of current materials research. It involves new integrated multiscale (length and time) theoretical techniques that are experimentally validated wherever possible, but most importantly that can increasingly predict materials properties in regimes inaccessible to experiment (e.g., to accurately and reliably calculate the properties of matter under extreme conditions for the weapons program). In industrial and materials processing applications, the new advances will provide a way to guide the design of materials where a purely empirical trial-and-error approach is too costly or time consuming. In soft matter (biomaterials, polymers, organics, hybrid materials, etc.) and other complex materials (Pu, high explosives, foams, etc.), a theory, modeling, and simulation effort that is closely coupled with specific, well-designed experiments is essential to understand, design, and predict materials structure-property relations. A well-designed plan to capitalize on these strengths will help ensure that LANL is best positioned to foster critical technology for all of the technical goals (A–G) of the Laboratory and to become the premier materials science and technology laboratory in the world.

This thrust depends on aggressively pursuing new research efforts for the development of new mathematical, computational, physical models and techniques that span length and time scales from atoms to engineering. The range of techniques that must be integrated is thus quite large and incorporates many disciplines. New statistical models must be developed that capture the important scientific parameters and relevant variables at functional intermediate length and time scales. The importance of the breadth of T Division capabilities cannot be overstated – the development of new tools for modeling materials requires strongly interdisciplinary research.

In addition, to reach its leadership potential in materials research, LANL must optimize a program that integrates materials experiments with its modeling and simulation capabilities, since experimental guidance and validation of new theoretical and modeling techniques will be critical. A major test of the new theories will be how well they are able to guide the experimental program (e.g., suggesting new experiments and providing interpretive bases for the data). Although experimental and other collaborative ties are already strong with many joint programs already in progress, T Division is ready and eager to engage in constructive dialogue to even better integrate its capabilities with those of other divisions, recognizing that a more disciplined, focused, and planned approach will reap even greater benefits and drive the exciting science that will energize and integrate materials, chemical, and biological research at LANL for decades to come.

Important opportunities lie in our ability to take advantage of important LANL facilities such as the CINT, the Los Alamos Neutron Science Center (LANSCE), the National High Magnetic Field Laboratory (NHMFL), the DARHT facility, proton radiography, and, in particular, large-scale computing. Indeed, a principal competitive advantage for Los Alamos is our ability to apply high-end computer capabilities to important problems.

Our numerous collaborators in academia, industry, and other national laboratories are a significant resource. It will be important to consolidate current, somewhat scattered efforts into a coherent program with specific short- and long-term objectives and sustain the support of upper management for resources to establish and maintain an international reputation in this area. Integration of our efforts through LANL's Materials, Science, and Engineering Council (MSEC) will be critical.

Business Plan: Understanding and Design of Complex Materials: Bridging Multiple Length and Time Scales

Thrust Leaders: Robert Albers (T-11) and Joel Kress (T-12)

Research Goals:
- Provide an underpinning of theory, modeling, and simulation to guide the design and synthesis of new classes of complex materials and to help interpret and understand measurements at meso- and nanoscales and the physical processes controlling materials properties and device performance.
- Develop new, integrated multiscale (length and time) theoretical techniques to energize materials research at LANL to keep it at the cutting edge of international science as well as to foster critical technology for Stockpile Stewardship, TR, and the DOE.
- Push new frontiers such as the notion of *functional complexity*: a systems approach to emergent properties, and realizing/manipulating hard/multiferroic and soft/biological matter; and the role of interfaces in nanoscience (e.g., a broader understanding of active interfaces).
- Enhance connection between computational materials science and engineering models and synergy with high-performance computing initiative.

Management Goal: Consolidate current scattered efforts into a coherent program with specific short-term (e.g., active interfaces as a nanoscience frontier) and long-term objectives (e.g., enhanced predictive science) and generate the support of upper management for funding and staff to establish and maintain an international reputation in this area.

Program Measures:
- New, specific strategic thrust plans and proposals.
- Establishment of long-term mechanisms for maintaining coordination of thrust.
- Level of new funding and funding sources.
- Scientific excellence and international presence.
- Success of MSEC as a single voice for materials science at LANL.

Actions over the next year to achieve goal:
- Work with other divisions to push new materials initiatives and to take advantage of developing opportunities (e.g., CINT and nanotechnology and the Lighting Initiative) and integrate theory thrusts with corresponding experimental activity.
- Coordinate this activity with other Laboratory strategic goals, especially predictive science (uncertainty quantification), nuclear weapons (actinide science), threat reduction (sensors, mini-devices, communications), DOE/SC facilities (LANSCE, NHMFL, CINT), and industrial collaboration with business goals. Coordinate Laboratory-wide activities through MSEC.

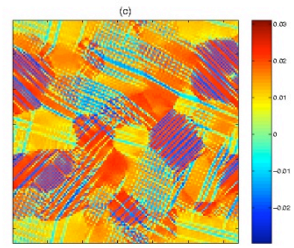
Funding Sources: DOE/SC, DOE/DP, DoD, DARPA, and LDRD

Thrust: Understanding and Design of Complex Materials: Bridging Multiple Length and Time Scales

Leaders: R. C. Albers (T-11) and J. D. Kress (T-12)

Goals:

- Provide an underpinning of theory, modeling, and simulation to guide the design of new classes of complex functional materials
- Interpret measurements at meso- and nano-scales and the processes controlling materials properties and device performance
- Develop new integrated multi-scale (length and time) theoretical and computational techniques that will cohere materials research at LANL



Accomplishments

- Worked with other divisions on new materials initiatives emphasizing theory-experiment integration (Joint LDRD with DX, MST, C, N, LANSCE, …)
- CINT opens its doors this year
- Lighting Initiative (organic electronics) underway
- Materials Science and Engineering Council reenergized
  - Science Roadmaps underway
  - Workshops being planned

Future Plans/Opportunities:

- Exploit and support CINT and Nanotechnology
- Grow opportunities in soft, organic, and biological materials
- Exploit opportunities created by Materials and Predictive Science Strategic Goals
- NW programs need more predictive materials models (demonstrated by Uncertainty Quant.)
- Forge closer ties with User facilities (LANSCE/NHMFL/CINT)
- Materials needs in Homeland Security & TR

NNSA Los Alamos

Thrust: Understanding and Design of Complex Materials: Bridging Multiple Length and Time Scales

Leaders: R. C. Albers (T-11) and J. D. Kress (T-12)

Strengths:

- Materials is a large fraction of the laboratory
- Extensive synthesis, characterization,and modeling facilities in one place
- LANL facilities (LANSCE, NHMFL, CINT, and computational)
- Long and successful history of experiment-theory teams
- Internationally recognized scientists and expertise in almost all relevant areas
- Strong University collaborations

Weaknesses:

- Not all relevant experimental facilities available on-site
- Relatively weak in nanoscience & fabrication?
- Difficulty in achieving sustainable balanced funding: short- vs. long-term
- No coherent Laboratory-wide plan for materials
- Duplication of similar capabilities in multiple divisions
- Need to forge stronger industrial ties

Opportunities:

- New national initiatives such as CINT and Nanotechnology and the National Lighting Initiative
- New technology needs in Homeland Security
- Need for predictive science (Uncertainty Quantification) in NW and TR programs
- A better coordinated effort in materials could greatly enhance effectiveness of existing programs
- Emergence of new areas; e.g., soft/biological matter: synergy with HE?

Threats:

- Current lack of coordination between diverse materials efforts at the Laboratory
- Basic science and applications not well integrated
- Many national competitors in nanoscience and soft matter

NNSA Los Alamos

2b. Modeling Biological Processes

Purpose: To develop mathematical and computational models of biological systems, bridging the multiple size and time scales relevant to the description of biological processes. These models will have applications in health, environment, and threat reduction problems and should help us establish and maintain a strong international reputation with applications in these areas. This thrust is aligned with Laboratory goals in science-based prediction (Goal A), homeland defense (Goal C), programs related to CINT and Genomes-to-Life (Goal G), and the Laboratory-wide bioscience and biotechnology goals.

Rationale and Description: Biological processes involve multiple size and time scales, from the molecular, to multicomponent molecular machines, to cells, organisms and populations. Phenomena from different scales are combined into the response of an organism interacting with other organisms (i.e., host-pathogen interactions in infectious and parasitic diseases). At the molecular level, proteins are the machines that perform most of the biological functions. In the performance of these functions, proteins interact with each other in a well-coordinated fashion, where an initial event can trigger a cascade of events that result in a large-scale response. The production and interaction of those proteins, and their role in helping replicate genetic materials, is often driven by interactions at the cell level, be it between different types of cells in tissue or between cells and pathogens (bacteria and viruses). The effects of these protein interactions are then felt at the tissue, organ, organism, and population levels. Consequently, the understanding of biological processes at various size and time scales will provide essential knowledge to prevent, modify and control biological processes, and will lead to the design of better treatment for disease and the development of defense tools against biological threats.

Applications in health and homeland defense: Integration of mathematical modeling, the study of the evolution of viruses with new informatics techniques, molecular modeling, and high-performance computing has been beneficial in the research against viral diseases like HIV, influenza, and Hepatitis C. Similar approaches are being used for dealing with other diseases, such as bacterial infections, and for forensics. Areas of development include the following.

- New statistical methods for the reliable determination of evolutionary trees from sequence data. These trees can be used to trace the origin of modified pathogens.
- The study of the cell-signaling pathways involved in immune response that can lead to the development of state-of-the-art sensors that mimic antigen recognition by the cell machinery.
- Molecular studies of protein-protein interactions that can help develop small protein or nuclei acid molecules that selectively recognize the proteins from pathogens that constitute a biological threat.
- The use of combinatorial chemistry to select biological molecules (peptides) with desired properties, and theoretical and computational models of protein-protein interactions that can establish the structural features that lead to specificity.
- Theory, modeling, and simulation of the anatomical, physiological, and biochemical progression of infectious diseases and their epidemiology.
- Mathematical and computational approaches leading neural information processing.

Business Plan: Modeling Biological Processes

Thrust Leader: Antonio Redondo (T-10)

Long-term Goals:
- Developing our capabilities and understanding of host-pathogen interactions and immune, regulatory, and transcription control networks will benefit the Genomes-to-Life program and TR. Research on health-related models will also benefit programs in NIH, DHS, HHS, DoD, and Centers for Disease Control and Prevention (CDC). This includes strong support of the Center for Theoretical and Computational Pathomics (CTCP).
- Consolidate current scattered efforts into a coherent program with specific short- and long-term objectives and generate upper management support for resources to establish and maintain an international reputation in this area.
- Develop partnerships with B, P, D, CCS, and ISR Divisions at LANL and with academia. Of great importance is coordinating the development of models with experimental efforts to validate these models. Use of high-performance computing in biological systems modeling may prove to be crucial for LANL competitiveness in a primarily academic research field.
- Planning and writing proposals to create a Biological Modeling Center at Los Alamos. This center will combine our expertise in systems and disease modeling, cell signaling, molecular modeling, bioinformatics, and computation to create a program that provides theoretical and computational support to experimental efforts at LANL and elsewhere.

Short-term Goals:
- Support and work toward creating the CTCP with congressional funding. This will include the exploration of the role of theoretical and computational modeling in assisting LANL efforts in HS. At the early stages, emphasis will be on the development of a research plan and supporting proposals. Later, funding may be available to study avian influenza and other pathogens.
- Planning and writing grant proposals in response to DOE's Genomes-to-Life program. At the early stages, major emphasis will be in the development of protein production facilities with T Division providing computational support for these facilities. At a later stage of development, funding may be available for the creation of advanced simulation facilities to model molecular machines.
- Participate in the Laboratory-wide bioscience and biotechnology goals.
- Participation in NIH Program grants for the development of novel biomimetic sensors.

Recent Accomplishments:
- Major participant in efforts to establish the CTCP at Los Alamos.
- Major participant in Biothreat Risk Assessment program.
- Accomplished first simulations of ribosome structure.
- Participation in new international NIH program in vaccine development (CHAVI).
- Continued development and maintenance of internationally known databases for HIV, HCV, and influenza.
- Maintenance of a leading international reputation in immunology, vaccine development, and structural biology.

Funding Sponsors: NIH, LDRD, CDC, DOE, DHS, and DoD.

<table>
<tr><th colspan="2">Modeling Biological Processes
SWOT Analysis</th></tr>
<tr><td>Strengths

1. World-class scientific staff in the areas of immunology, viral diseases, networks, complex systems modeling, quantum chemistry, molecular modeling, and high-performance computing.
2. State-of-the-art computational facilities at LANL and various groups in the division.</td><td>Weaknesses

1. Lack of diversified funding portfolio—currently 60% of funding is NIH.
2. Need to recruit new staff members to maintain group strength over next decade.
3. High cost of operations when compared to academia.</td></tr>
<tr><td>Opportunities

1. New funding in areas of homeland defense and pathomics.
2. Continuation of the Genomes-to-Life project in DOE—should prepare for strong competition in areas of computational modeling and molecular machines.
3. DoD call in biothreat countermeasure development.
4. NIH program calls in image analysis.</td><td>Threats

1. Academic competition in single investigator projects is not balanced (cost, access to students, cost of postdoctoral fellows.)
2. Other national laboratories are well prepared to compete for Homeland Security and Genomes-to-Life projects.</td></tr>
</table>

3. Fundamental Processes

Experimental and observational advances over the last decade have led to unprecedented progress in our knowledge and understanding of the universe from the smallest to the largest scales. Many of the most exciting science opportunities occur at the intersection of astrophysics, atomic, nuclear, and particle physics. An intriguing aspect of this enhanced understanding is the strong coupling between information obtained on large and small scales. Present cosmological observations (microwave background, large-scale structure) not only provide solid evidence for a new form of "dark" matter but also strongly constrain the relevant particle and nuclear physics (e.g., particle masses). Exciting advances have been made in understanding new states of matter in the laboratory and in astrophysical regimes. Novel states of matter such as Bose-Einstein and fermion condensates can be studied in the laboratory in cold atomic gases and their properties related to those of QCD at high baryon density. These new states of matter have recently been speculated to be near an absolute lower limit of viscosity, and relations to the quark-gluon plasma of high-temperature QCD are being explored.

There are many scientific tools and goals common to these exciting scientific challenges. We refer to this cross-disciplinary field encompassing key aspects of astrophysics, atomic physics, and nuclear and particle physics as *fundamental processes*. Fundamental processes include the basic building blocks of nature and their interactions. These range from the evolution of the universe and the formation of large-scale structure to the properties of atoms and nuclei and their role in extreme astrophysical environments, including neutron stars and supernovae; the properties and interactions of neutrinos with matter; the formation of the first stars in the universe, supernovae, the production of all the elements; and exotic new states of matter in atomic, nuclear, and particle physics regimes. To exploit opportunities arising from unique laboratory capabilities and strengths at the intersection of these fields, we have developed an initiative called PNAC, *Particle, Nuclear, Astrophysics and Cosmology*, to address the grand challenge of understanding fundamental processes at all scales—from quarks to the cosmos.

The strategic objectives are threefold:
1. to develop core competencies in advanced mathematics and simulation that contribute across many application areas,
2. to exploit recent empirical and conceptual progress in our understanding of fundamental processes to create a unified picture of processes applicable across scales from "quarks to the cosmos," and
3. to recruit and retain scientists of exceptional talent.

The thrust brings the uniquely powerful combined expertise of T Division to bear on problems at the cutting edge of present-day research, including the following:
- Exploring the standard model of elementary particles and its extensions. (T-8, T-16)
- Neutrino masses and mixing from terrestrial experiments and astrophysical observations. (T-6, T-8, T-16)
- Particle astrophysics and cosmology, focusing on the evolution of the universe, the origin and distribution of dark matter, and the generation of large-scale structures. (T-6, T-8, T-16)
- Formation of first stars, nucleosynthesis, and supernovae. (T-6, T-8, T-16)
- Nonequilibrium phenomena in nuclear (relativistic heavy ion collisions) and particle (baryogenesis) physics. (T-8, T-16)
- Equation of state for dense plasmas and neutrino propagation. (T-6, T-8, T-16)
- Exact calculations of nuclear bound states and reactions. (T-16)
- Generation and dynamics of Bose-Einstein, fermion and molecular condensates. (T-4, T-16)

- Super-short and super-intense pulse lasers. (T-4)
- Quantum information and computing. (T-4, T-8, T-11, T-QC)

The solution of these difficult and complex problems will require active collaboration of physicists possessing expertise in multiple areas of research. The integrated effort will make LANL the preferred laboratory for using high-performance computing and large data management for investigating fundamental processes and the structure of matter, and enhance science-based prediction by linking experiment, simulation, and theory. The work is aligned with the core efforts of the DOE/SC in these areas.

Business Plan – Fundamental Processes

Thrust Leaders: Rajan Gupta (T-8), Joseph Carlson (T-16), James Cohen (T-4), and Michael Warren
(T-6)

Implementation Plans:
- Recruit and retain scientists of exceptional talent and capabilities in theory, simulation, and modeling.
- Analyzing and mining large data sets to elucidate underlying principles and mechanisms.
- Work with experimental colleagues, internal and external, to interpret data and guide future experiments.
- Coordinate with program offices, other divisions, directorates, and outside resources to amplify T Division's unique strengths and to create integrated programs within T Division and develop external collaborations.
- Exploit recent advances in theory, mathematics, and high-performance computing.

Program Measures: Success of the program will be measured by publications in refereed journals, invited conference talks and seminars, participation in and organization of international conferences and schools, peer-reviewed grants and funding, new programs and research activities developed, and contributions to LANL programs, research, and outreach activities.

Actions over the next year to achieve the goal: Attract the very best scientists to LANL as postdoctoral fellows and to hire world-class scientists as staff members. Develop strong collaborations with experimentalists, both at LANL and internationally. Conduct outstanding research in the areas of:
1. standard model of elementary particle interactions and physics beyond;
2. neutrino masses, mixings, and interactions with matter;
3. large-scale structure of the universe and cosmology;
4. first stars, nucleosynthesis, and supernovae formation and evolution;
5. Bose-Einstein, fermion and molecular condensates and their relations to dense QCD, and
6. structure and reactions of nuclei relevant to fundamental symmetries and neutrino physics.

Funding Sources: DOE/NHEP, DOE Scientific Discovery through Advanced Computing (SciDAC) program, LDRD

Partners: The theoretical efforts in T Division partner with the experimental efforts in P, C, CCS, MST, and LANSCE divisions. These efforts provide valuable support to experimental programs at national facilities run by the DOE and NSF (RHIC/BNL, FERMILAB, SLAC, CESR, JLAB, LIGO, and international ground- and space-based astronomical and astrophysical observatories).

3a. Particle and Nuclear Astrophysics and Cosmology

It is widely recognized that some of the most exciting physics opportunities today lie at the intersection of nuclear, particle, astrophysics, and cosmology (PNAC). Los Alamos and T Division have both a rich tradition and a broad range of current exciting capabilities in these areas, and we have developed a multidisciplinary thrust at the intersection of these fields where LANL and the Division can play an important role.

The Division's effort in PNAC science are strong and diverse and include efforts in neutrinos and their interactions, dark energy and dark matter, cosmology and large-scale structure formation in the universe, supernovae, and the origin of the elements, the first stars in the universe, s- and r-process nucleosynthesis, neutron stars, and the phase diagram of QCD at high baryon densities. PNAC science is characterized by the requirement to understand physics at very different length scales in diverse astrophysical settings.

One intriguing example is the LANL investment in a project on the first stars in the universe, which ties together large-scale structure formation in the early universe with the evolution, collapse, and explosion of the first stars and the subatomic processes tied directly to present observations. Other important examples include cosmology and its close ties to particle physics through studies of dark matter and dark energy, and supernovae and the importance of neutrino physics in their evolution and the formation of the elements in the universe.

PNAC science in T Division is also characterized by the large-scale computations and data handling required at scales ranging from the nuclear through the astrophysical and cosmological scales. Los Alamos is unique in having important capabilities in all these regimes. The science involved is also closely tied to many of the Laboratory's most important missions, including computationally intensive magnetohydrodynamics simulations, N-body codes with long-range forces, and nuclear probes of physics in extreme environments. We also have close ties with observational and experimental groups in the Laboratory and beyond, including the neutrino physics experimental program in the Physics Division, and the Sloan Digital Sky Survey (SDSS-II).

We have worked to organize and form a coherent strategy for PNAC science at LANL during the past year. These include ongoing workshops in neutrino physics, supernovae and neutron stars, and cosmology. We also held a one-day workshop with renowned external scientists Jim Truran (University of Chicago), George Fuller (UCSD), and Josh Frieman (Fermilab). They have written a one-page report on PNAC activities in T-Division; highlights of their recommendations are shown to the right.

"It is clear that LANL Theoretical Division scientists are among the handful of world-leaders in several key areas of PNAC --"

"-- we are convinced that a coherent effort across disciplines could have a major scientific impact."

"Efforts should be made to exploit the large-scale simulation and data capabilities at LANL."

"We urge that LANL act quickly to explore ways to fully exploit the opportunities in particle and nuclear astrophysics and cosmology."

A white paper describing the PNAC efforts in T Division has also been written to give a more complete picture of the scientific activities in this area. We are presently pursuing plans to expand our initiative to more fully include scientists throughout the Laboratory and beyond. The collaboration of T-6, T-8, and T-16 with experimental, observational, and computational expertise throughout the Laboratory is crucial to moving this initiative forward.

Strengths	Opportunities
• Critical mass of theorists in nuclear, particle, and astrophysics • World-class computational expertise at all length scales • Ties to many lab and external observation and experiment	• Can develop excellent cross-disciplinary projects internally (1st stars DR, supernovae, X-ray bursters, ...) • Further develop ties to national projects (Sloan, RIA, DUSEL, ...)
Weaknesses	**Threats**
• Different projects with some overlap • Individual pieces well-recognized but overall effort not visible enough outside LANL • Need to further develop ties w/ experiment and observation; stronger ties to universities	• Other labs have already formed strong initiatives in these areas: LBL, FNAL, SLAC, etc. • Need to play world-leadership role in specific areas closely tied to LANL strengths

3b. T Division Support of the LANL Quantum Institute

Purpose: To expand our knowledge of quantum information processing devices and to design quantum simulators to study physics of materials as a milestone on the way to the quantum computer.

Rationale and Description: Several recent developments in quantum information science have motivated LANL to form the Quantum Institute. Reflecting LANL's acknowledged position as one of the world leaders in experimental and theoretical efforts on quantum computation, ARDA is currently funding five independent quantum computing research efforts at LANL, and there are currently seven LDRD-funded quantum-computing efforts in directed and exploratory research. Five groups in T Division play a major role in this field and strongly interact within the Quantum Institute and with four other divisions. Topics on which we are focusing include quantum simulators that efficiently model quantum processes, Bose Einstein condensate (BEC) physics, development of new ultrasensitive detection methods based on the use of exotic quantum states, and the self-assembly of large arrays of quantum bits.

The Quantum Institute has been established and is run by the Scientific Steering Committee with divisional representation. It is generating productive synergism that is benefiting many groups and sponsors. Staff expertise and experimental capabilities at LANL, combined with recent technical developments, are focusing on the following research topics.

- Quantum simulators, decoherence, quantum computation. (T-DO)
- Ultrasensitive quantum measurements. (T-4)
- Design of large quantum computers, qubit measurements, and decoherence. (T-13)
- Quantum cryptography and ion-trap quantum computation. (P-21, T-11, T-DO)
- Quantum interferometry based on BECs. (T-DO, T-4, T-13, P-21, C-INC)
- Solid-state quantum computation and spin measurements. (MST-8, T-13)
- Quantum microscope with single-spin resolution. (T-11, T-13)
- Quantum phase transitions, dynamics, and defect formation. (T-QC, T-11, T-4, T-16, P-21, C-INC)

Expected outcomes include operational quantum simulators and the creation of many new applications for quantum measurement and quantum control.

Partners: External collaborations exist with the Massachusetts Institute of Technology, Harvard University, Dartmouth College, Pennsylvania State University, Waterloo University, Rice University, Cornell University, University of New South Wales, Motorola, the U.S. Air Force, and IBM.

Customers: ARDA is continuing to coordinate the Inter-Agency Quantum Computing Program, which continues to invest about $100M/year in this field. DARPA has set up its own Quantum Computing Program, which it funds at about $30M/year.

Business Plan: T Division Support of the LANL Quantum Institute

Thrust Leaders: Juan P. Paz (T-DO) and Eddy Timmermans (T-4)

Research goals**:**
Short-term (major deliverables in the next 18 months):
- Demonstrate quantum simulators using cold atoms. (T- DO, T-4, T-11, P-21, C-INC)
- Demonstrate ultrasensitive quantum measurement strategies. (T-4)
- Optimize design of large quantum computers, qubit measurements, and decoherence. (T-13)
- Quantum cryptography and ion-trap quantum computation. (P-21, T-4, T-DO)

Longer-term:
- Quantum interferometry based on BECs. (T-DO, T-4, T-13, P-21, C-INC)
- Solid-state quantum computation and spin measurements. (MST-8, T-4, T-13)
- Quantum microscope with single-spin resolution. (T-11, T-13)
- Study dynamics and defect formation during quantum phase transitions. (T-DO, T-4, T-11, P-21, C-INC)

Management goals:
Short-term:
- Achieve Center status for the Quantum Institute.
- Recruit new staff working in frontier areas of quantum physics.

Longer-term:
- Develop support mechanisms in DOE, NSA, DARPA, and other agencies.
- Develop a network of partners in multiple LDRD-NNSA projects within the Laboratory.

Program Measures:
Research measures:
- Perform ion-trap, solid-state, nuclear magnetic resonance (NMR), and optical quantum operations and simulations.
- Develop new ultrasensitive detection schemes using quantum technologies.

Management measure:
- Continue development of the Quantum Institute.

Actions over the next year to achieve the goals:
- Coordinate LANL quantum groups to develop new proposals and actively participate in existing initiatives.
- Extend the involvement of the Quantum Institute to represent all quantum computing research efforts at LANL.

Funding Sources: ARDA, Army Resource Office (ARO), Air Force Office of Scientific Research (AFOSR), DARPA, DOE/DP, DOE/SC, NSA

Quantum Information and T Division

Quantum Information
- Demonstrate, engineer & exploit quantum mechanics
- Multidisciplinary, basic science
- T: tradition excellence + support/ collaborate P,C,CCS,MST,N,DX
- Quantum Institute lab focal point

Why?
- Important, high- profile, dynamic field
- Projected applications/lab mission: QKD, Q-comp, Q-metrology, high res. sensors
- Opportunities for multi-disciplinary/basic/ applied physics

Goals
- Provide expertise/push scientific boundaries
- Cross-division theory-experiment interactions
- Fully support/exploit Q.I.:
  - *Identify internal/external funding (+PD)
  - *visitor program, meetings, Q. lunch

Activities
- Partners in multiple LDRD-NNSA projects
- Informal workshops (Quantum simulators, quantum repeaters, Materials, Quest) -> new teams and projects
- Q.I. supported: PD, meetings (Squint, annual Q.I. workshop)

For more information on Q.I.: http://quantum.lanl.gov/

4. High-End Computing Research

Today's scientific world is experiencing a paradigm shift where the sophistication of mathematical models, the accuracy and efficiency of numerical algorithms, the robustness of computer software, and the power of computation have become so great that numerical simulations are now considered a third pillar, along with theory and experiment, in the triad of tools used for scientific discovery. The rate of advances in these fields, and our ability to simulate complex physical systems, will increasingly be the limiting factors in our ability to solve many of our most pressing scientific challenges.

Scientific discovery in many areas requires computational models that incorporate more complete and realistic descriptions of the phenomena being modeled than are possible today. More efficient algorithms, more accurate mathematical models, advanced software, and more powerful computers are essential to fueling the pace of scientific discovery and underpin the research and development that the Laboratory conducts to meet its energy and national security missions in Science-based Stockpile Stewardship, fusion science, biology, nanoscience, high energy and nuclear physics, fluid dynamics, applied mathematics, chemistry, climate, and related fields that provide high-fidelity descriptions of the underlying science. Because our computational capability is also so critical to scientific discovery in these core missions, T Division brings a renewed focus to this challenge.

We will renew our support for collaborations between computational scientists, application simulation developers, computer scientists, and applied mathematicians to create the complete set of necessary and sufficient advances in computer models, algorithms, software, and advanced hardware to meet the next generation of major scientific challenges facing the Laboratory. These challenges will be increasingly complex, progressively more multidisciplinary, and span a much larger range of spatial and temporal scales than in the past.

The thrust will increase our focus on creating the advanced scientific computing infrastructure and foundational base for synergistic multidisciplinary advances with the traditional theoretical and experimental sciences that will maximize the value derived from the Laboratory's facilities and research investments.

Work at the forefront of science can require the dedicated availability of the most advanced supercomputers for extended periods of time. To meet the need for effective computing, T Division will support the evaluation, installation, and application of new, very high-end computing architectures at the Laboratory. We will work with the Laboratory Institutional Computing Resources initiative to provide significant amounts of open computer resources to enable computations that could not be carried out on high-end workstations and conventional supercomputers.

Business Plan: High-End Computing Research

Long Term Goals: The overall goal of this thrust is to discover, develop, and deploy the computational tools that enable researchers in the scientific disciplines to analyze, model, simulate, and predict complex phenomena important to Laboratory missions. This is being achieved by fostering and supporting fundamental research in advanced scientific computing by developing fundamental mathematical methods and advanced scientific computing approaches to model complex physical systems on the highest performance computers available. The long-term goal is to create a strong scientific foundation for supporting high-performance computer simulations in support of the other goals of the strategic plan.

Program Measures: The high quality of the T Division research in advanced scientific computing is continuously evaluated through merit-based peer review, the impact on Laboratory programs, and support generated to sustain the effort from competitive funding agencies.

Actions over the next year to achieve the goal:

- Develop core technologies in algorithms, mathematical models, software, and advanced hardware that contribute across many application areas.
- Develop S&T projects and programs that address the needs of science-based predictive models.
- Leverage the development of the computing technologies and resources derived from programmatic areas in predictive science.
- Develop new and improved mathematical methods for addressing the challenges of multiscale problems.
- Incorporate the new models into scientific simulation software that achieves greater performance from supercomputers than we can achieve today.
- Progress toward developing the mathematics, algorithms, and software that enable effective, scientifically critical models of complex systems, including highly nonlinear or uncertain phenomena, or processes that interact on vastly different scales or contain both discrete and continuous elements.
- Collaborate closely with the science campaigns to ensure the vitality of the focused experimental programs upon which the credibility of new simulations depends.
- Provide the necessary computing capability to code users, in collaboration with industrial partners and government agencies.
- Evaluate mission-critical requirements to guide us in selecting particular architectures well suited to our workload.

Funding Sources: DOE/NN, LDRD, DOE/SC

High End Computing

Theoretical Division Contact: Mac Hyman

Strengths
- High-quality science with strong peer reviewed publication record
- Versatility; our basic tools are supported by and applied to many program areas
- Culture of strong multi-disciplinary teams with experts in theory, modeling, & simulation
- Strong collaborations with experts in academia and at other laboratories.

Opportunities
- Develop core technologies in algorithms, mathematical models, software and hardware that contribute across many application areas
- Develop programs that address the needs of science-based predictive models
- Leverage the development of the computing technologies and resources derived from programmatic areas in predictive science

Weaknesses
- Our interactions with other laboratories and divisions need strengthening to improve synergistic collaborations
- Need to strengthen our image as a long-term partner in achieving Laboratory goals based on science-based prediction
- Improve our collaborations with experimental scientists and our access to experimental data
- Our manpower is stretched too thin

Threats
- Anxiety created by the uncertainty in funding
- Under funding leading to understaffing for basic research in advanced models, algorithms, and software in critical programs
- Lack of coordination of T Division system managers with Science Complex Building designers
- Reduced computing access for foreign nationals

NNSA

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Ideas That Change the World

High End Computing

Theoretical Division Contact: Mac Hyman

Goals
-New and improved mathematical methods for multi-scale problems
-New models for scientific simulation software to achieve greater performance from supercomputers
-Closer collaboration to ensure the vitality of experimental programs

Participants
- All of the T-div groups + X, DX, CCS. EES, ESA, MST and D Divisions
- Collaborations with scientists in DOD, NIH, universities and industry
- ASC, LDRD, NIH, SC, ... teams
- DOE Laboratories: LLNL, SNL, ...

Customers
-A new generation of predictive capabilities for complex mission related programs in:
- DOE/NNSA
- DoD
- DOE Office of Science
- NIH and private industry.

Recent accomplishments
- Advances in scientific computing for nuclear and atomic physics, materials science, hydrodynamics, and uncertainty quantification in NW.
- Advances in multiscale modeling techniques applied to TR problems
- New algorithms and software of complex nonlinear systems

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Appendix B – List of LANL Strategic Goals

National Security Goals

A. Science-Based Prediction
Create an integrating core competency for Science-Based Prediction of complex systems linking experiment, simulation, and theory.
B. Nuclear Weapons
Design and engineer manufacturable and certifiable replacement nuclear weapons without new nuclear testing.
C. Nonproliferation
Be acknowledged as the premier laboratory for nonproliferation research and development.
D. Preferred Laboratory
Be the preferred laboratory for providing the defense, intelligence, and homeland security communities with revolutionary, success-enabling science and technology.
E. Materials Science
Be the best materials science and technology lab in the world in support of our mission.
F. Energy Security
Use LANL expertise and capability to solve national problems in energy security.
G. Office of Science
Be a strategic partner of the Office of Science to benefit their national missions and the science-base critical to our national security missions.

Enabling Goals

H. Workforce
Build the agile workforce for the future.
I. Business
Employ those business practices that best serve our trusted, competitive scientific solutions.
J. Corporate Approach
Institute an integrated corporate approach to plan, allocate, and manage Laboratory resources to maximize accomplishment of LANL mission.
K. Laboratory Management
Laboratory management leads a culture of trust in our people, mission, science, and business.
L. Communication
Communicate accurately and consistently in a timely, open, and interactive way.
M. Facilities
Modernize and consolidate facilities/infrastructure to support safe, secure, and efficient Laboratory operations.
N. Compliance
Improve efficiency with which we achieve regulatory compliance and manage risk to support operational excellence.
O. Creativity
Enhance science & technology creativity and productivity.
P. Knowledge Management
Adopt the best knowledge management solution for LANL.

Source: http://int.lanl.gov/goals/ (November 7, 2005)

Appendix C – Theoretical Division FY06 Laboratory Directed Research and Development Portfolio

Principal Investigator (PI)	PI's Group	Project Number	Project Title	T Division Group(s) Involvement
Directed Research Projects with a T Division Principal Investigator				
Eddy Timmermans	T-4	20040134DR	Bose-Einstein Condensate Physics: Dynamics and Applications	T-DO/QC, T-4, T-8, T-11, T-13,
Alexander Heger	T-6	20050031DR	Coming Out of the Cosmic Dark Ages - The First Stars in the Universe	T-6, T-7, T-8, T-16
Byron Goldstein	T-10	20040087DR	Understanding the Molecular Mechanisms of Pathogen Recognition by the Immune System: Biothreat Reduction through Predictive Science	T-10, T-12, T-13
Bette Korber	T-10	20050155DR	Rational Vaccine Design: Theory and Experimental Validation	T-8, T-10, T-13
Alexander Balatsky	T-11	20051164DR	Nanoscale Fluctuations in Multifunctional Materials	T-11
Darryl Smith	T-11	20060136DR	New Classes of Materials For Gamma-Ray and Neutron Detection	T-11
Joel Kress	T-12	20040842DR	Fission Fragment Physics in Extreme Environments (U)	T-4, T-12, T-16
A. Hayes-Sterbenz	T-16	20051149DR	Cross sections for the Isomer of 235U	T-6, T-16
A. Hayes-Sterbenz	T-16	20060081DR	Mix Processes in Inertial Confinement Fusion	T-6, T-16
Juan Paz	T-DO/QC	20050076DR	Cold Atom Quantum Simulators	T-DO/QC, T-4, T-11
Zoltan Toroczkai	CNLS	20040141DR	Statistical Physics of Infrastructure Networks	CNLS, T-7, T-10, T-12, T-13
Robert Ecke	CNLS	20041010DR	Dynamics of Complex Networks: Biology, Information, and Security	CNLS, T-7, T-12, T-13
Robert Ecke	CNLS	20050631DR	Nonlinear Behavior in Complex Systems	CNLS, T-7, T-8, T-11, T-12, T-13
Robert Ecke	CNLS	20050632DR	Cooperative Phenomena in Soft Matter	CNLS, T-10, T-11, T-12, T-13
Directed Research Projects with a Non-T Division Principal Investigator				
Pat Unkefer	B-3	20050123DR	Metabolome Scale Characterization of the Biothreat Agent, Bacillus anthracis	T-10
Jaqueline Kiplinger	C-SIC	20040093DR	Understanding Electronic and Magnetic Communication Between f-Electrons in Actinide and Lanthanide Materials	T-11, T-12
Thomas McCleskey	C-SIC	20050127DR	Be-Specific Human Immune Response and Development of CBD	T-10, T-12
James Carey	EES-6	20040042DR	Science of Geological Carbon Sequestration: Integration of Experimentation and Simulation	T-13
Manvendra Dubey	EES-6	20050014DR	Resolving the Aerosol-Climate-Water Puzzle: Predictive Science for Global Stability and Security	T-7

Principal Investigator (PI)	PI's Group	Project Number	Project Title	T Division Group(s) Involvement
Steen Rasmussen	EES-6	20050064DR	Protocell Assembly	T-6, T-7
Tom Vestrand	ISR-1	20050161DR	Thinking Telescopes: Pursuing a New Paradigm for Discovery in Observational Science	T-6
Geoff Reeves	ISR-1	20060060DR	DREAM: a Dynamic Radiation Environment Assimilation Model to understand acceleration, transport, and losses in natural and HANE-produced radiation belts	T-8
W. Priedhorsky	ISR-DO	20040072DR	Radiography with Background Radiation	T-7
John Sarrao	MST-10	20040014DR	Localization and Itinerancy in Plutonium	T-1, T-11
Robert Ecke	MST-10	20050066DR	Lagrangian Measurements of Fluid Mixing	CNLS, T-7, T-11, T-12, T-13, T-14
Marilyn Hawley	MST-8	20040049DR	Solid-State Quantum Information Processing : A New Approach to Demonstrate Quantum Entanglement	T-4, T-13
James Glownia	MST-CINT	20050107DR	Material Response During Dynamic Loading at Subpicosecond Time and Nanometer Length Scales	T-4, T-11
Jeremy Mitchell	NMT-16	20040844DR	Phase Transitions and Strong Anharmonicities in Plutonium	T-DO, T-1, T-11
David Moore	NMT-16	20050043DR	Pu-H Interactions: Studies of Plutonium Hydride Phenomena (U)	T-DO, T-1, T-12
David L. Clark	NMT-DO	20060019DR	Structure and Bonding in Actinide Oxides	T-12
Gordon Jarvinen	NMT-DO	20060088DR	Advanced Actinide Separations in Alkaline Media for Spent Nuclear Fuel and Defense Materials Processing	T-12
Andrew Hime	P-23	20030030DR	Neutrino Physics and Fundamental Symmetries	T-6, T-8, T-16
Juan Fernandez	P-24	20040064DR	Energetic-Particle Interactions with Dense Plasmas: A Study Relevant to Boost and to Fast Ignition Using Laser-Driven High-Current Charge-Neutralized, Mev/Nucleon Ion Beams	T-4, T-12, T-15
Patrick McGaughey	P-25	20060049DR	Heavy Quarks as a Probe of a New State of Matter	T-8, T-16
Mark Chadwick	PADNWP	20050184DR	New Americium Delta-A Metric for Primary Certification (U)	T-16
Exploratory Research Projects with a T Division Principal Investigator				
Anders Niklasson	T-1	20060551ER	Simulation and Modeling of the Quantum Response	T-1, T-12, T-14
Dana Knoll	T-3	20050271ER	A System-Scale Theory for Fast Magnetic Reconnection	T-3, T-15
Duan Zhang	T-3	20060693ER	Next Generation Data Structure for Carta Blanca	T-3
Eddy Timmermans	T-4	20040461ER	Secure Communications in Fiber Links Using Randomness and Nonlinearity of Optical Fibers	T-4, T-7, T-11, T-13
Michael S. Warren	T-6	20040195ER	Precision Cosmology: A First Principles Approach to Galaxy Clustering	T-DO, T-6, T-8
Michael S. Warren	T-6	20060350ER	A Faster Multipole Method	T-6, T-10, T-11
Kevin Vixie	T-7	20040379ER	Modeling Invariance in Data Space	T-7
Daniel Tartakovsky	T-7	20040481ER	Efficient Modeling of Systems with Uncertainty on Multiple Scales	T-7
Salman Habib	T-8	20050379ER	Taming and Accelerating Particle-In-Cell	T-8

Principal Investigator (PI)	PI's Group	Project Number	Project Title	T Division Group(s) Involvement
Rajan Gupta	T-8	20060340ER	Multigene Correlations and Their Implications for Cardiovascular Disease	T-8
Yuri Shirman	T-8	20060694ER	Supersymmetry Breaking in Various Dimensions	T-8
Hans Frauenfelder	T-10	20030839ER	Proteins in Protein Networks	T-10
K. Sanbonmatsu	T-10	20060230ER	Nascent Protein Folding Inside the Tunnel of the Ribosome: Cotranslational Folding	T-10
Kim Rasmussen	T-11	20040262ER	Understanding and Predicting the Initiation of DNA Transcription	T-10, T-11, T-13
Ivar Martin	T-11	20040391ER	Quantum Devices for Electronic Circuitry and Advanced Detection	T-4, T-11, T-13
James Gubernatis	T-11	20060272ER	Monte Carlo Estimation of Eigenvalues of Ultradimensional Matrices and Continuous Operators	T-11
Darryl Smith	T-11	20060589ER	Manipulation and Control of Electron Spins in Semiconductors with Strain Engineering	T-11
Richard Martin	T-12	20040256ER	Hybrid Density Functional Theory Investigations in Condensed Matter	T-12
David Hanson	T-12	20060226ER	Development of an Engineering Model for Rubber Elasticity	T-12
Gennady Berman	T-13	20040237ER	New Mathematical Tools for the Quantum Dynamics of a Bose-Einstein Condensate	T-13, T-QC
Eli Ben-Naim	T-13	20060305ER	Energy Distributions in Granular Flows	CNLS, T-13
Michael Chertkov	T-13	20060473ER	Novel Physics Inspired Approach to Error-Correction	T-7, T-13
Alejandro Strachan	T-14	20050343ER	Atomistic Studies of Fast Chemical Processes in Nano-structured Metastable Composites	T-14
Giovanni Lapenta	T-15	20030129ER	Collisionless Magnetic Reconnection in 3D Geometries	T-15
Luis Chacon	T-15	20040218ER	Error-Minimizing, Implicit Adaptive-Grid Solutions of Time Dependent Problems	T-15
Giovanni Lapenta	T-15	20060399ER	Role of a New Attractive Force on the Genesis of Solar Systems	T-15
Joseph Carlson	T-16	20040415ER	Supernovae Neutrinos	T-6, T-16
A. Hayes-Sterbenz	T-16	20051087ER	Antineutrino Monitoring of Reactors	T-6, T-8, T-16
Robert Ecke	CNLS	20040284ER	The Dynamics of Two-Dimensional Turbulence	CNLS
Exploratory Research Projects with a Non-T Division Principal Investigator				
John Dunbar	B-1	20040393ER	Genetic Programs Underlying Key Physiological States in Burkholderia Pseudomallei	CNLS
Reginaldo Rocha	B-4	20060518ER	Improved Molecular Catalysts for Water Splitting	T-12
Christian Forst	B-5	20040184ER	Response Networks of M. Tuberculosis and Bio-Threat Agents	CNLS
Michael Wall	CCS-3	20040295ER	Design Principles of Genetic Regulatory Networks	T-10
Michael Pernice	CCS-3	20050315ER	Implicit Adaptive Mesh Refinement: a Magnetohydrodynamics Application	T-15
Xinxin Zhao	C-INC	20040171ER	Fermion Quantum Phase Transitions	T-4

Principal Investigator (PI)	PI's Group	Project Number	Project Title	T Division Group(s) Involvement
Shawn McGrane	DX-2	20040358ER	Measurement of Vibrational Anharmonicities for Chemical Dynamics	T-12
Manvendra Dubey	EES-6	20060686ER	Complex Dynamical Climate Systems at IGPP	T-3, T-7
Claudia Lewis	EES-9	20060688ER	Solid Earth Geoscience at IGPP: Transient & Steady-State Earth Processes	T-7
Katrin Heitmann	ISR-1	20060495ER	Exploring the Darkness: Cosmic Voids	T-6, T-8
Reiner Friedel	ISR-1	20060687ER	Space Weather at IGPP	T-15
Rene Reifarth	LANSCE-3	20060357ER	The s-Process in the Sm-Eu-Gd Region - A Probe for Stellar Mixing	T-6
R. Movshovich	MST-10	20050430ER	Fulde-Ferrell-Larkin-Ovchinnikov Inhomogeneous Superconducting State	T-11
Marcelo Jaime	MST-NHMFL	20040294ER	Study of Phases with Hidden Order Parameter in the Actinides and other Strongly Correlated Electron Systems	T-11
Quanxi Jia	MST-STC	20060497ER	Use of Strain Engineering to Tune the Physical Properties of Nanoscale Metal-oxide Films	T-11
Todd Haines	P-23	20040923ER	Development of Technology for Particle Astrophysics and Other Applications	T-6
Hui Li	X-1	20051169ER	Physics of Astrophysical Jets	T-6, T-15

Appendix D – Technical Descriptions of Groups

Theoretical Division Office/Special Projects Office—Quantum Computing (T-DO)

Division technical staff are engaged in special projects that do not organizationally fit into an established group in the Division. A major effort is the study of the transition from quantum to classical ("decoherence") physics, and the study of quantum-based information and computing and their associated technology, closely coordinated with the Los Alamos Quantum Institute. In addition, technical staff members carry out research in relativistic heavy ions, high-spin states in nuclei, neutron physics, electronic and structural materials, and nonlinear science. **Technical staff includes approximately 7 Technical Staff Members (including 2 Senior Fellows and 4 Fellows), 2 Limited-term Technical Staff Members, 1 Postdoctoral Associate, and 2 Graduate Research Assistants.**

Equation of State and Mechanics of Materials (T-1)

T-1 develops theory and computational models to describe the Equation of State and Mechanics of Materials (EOS/MOM), including, but not limited to, materials of interest to nuclear weapons, and implements these models in computer codes that contribute in particular to the SESAME Equation-of-State and Materials Properties Library, which is maintained by T-1. The group has an active research program outside the EOS/MOM program developing theory, methodology, and calculation to support and enhance that program, funded by sources both internal (LDRD) and external (DoD), Advanced Fuel Cycle Initiative, and others) to the Laboratory. Relevant areas of research include strong electron correlation; actinide electronic structure; first-principles prediction of mechanical and thermodynamic properties of multicomponent materials; multiphase EOS theory; microscopic, mesoscopic, and continuum-level mechanical behavior of materials; direct numerical simulation of materials properties; energetic materials; grain growth phenomena; and order-N numerical techniques for electronic structure calculation. Capability developed in support of EOS/MOM is used to support related programs such as Pu aging studies and other projects in the nuclear and conventional defense communities, civilian research communities, commercial applications, and threat reduction. **Technical staff includes approximately 13 Technical Staff Members (including 1 Fellow), 4 Limited-term Technical Staff Members, 4 Postdoctoral Associates, and 1 Graduate Research Assistant.**

Fluid Dynamics (T-3)

T-3 staff members are involved in modern hydrodynamic theory, materials modeling, and computational simulations. There is an emphasis on coupling advanced numerical methods for fluid dynamics at all flow velocities with models for other processes, including chemical reactions, phase change, heat and mass transfer, plasma behavior, constitutive properties of structural materials, and combustion. Advanced models and methods are incorporated in fully functional 2- and 3-D computer simulation codes and implemented on the full spectrum of computing hardware from high-performance workstations to massively parallel supercomputers. Current application areas include nuclear and conventional weapons, internal combustion engines, structural materials, process chemistry for the oil and gas industries, ferrous metals and chemical industries, models for casting, and circulation models for the global ocean. **Technical staff includes approximately 27 Technical Staff Members, 1 Limited-term Technical Staff Member, 2 Postdoctoral Associates, and 2 Graduate Research Assistants.**

Atomic and Optical Theory (T-4)

T-4 staff members develop methods for and perform calculations of atomic structure, scattering cross sections, opacities, exotic atoms, and quantum and nonlinear optics, including effects of high energy-density environments and interaction with external electromagnetic fields. Current efforts include the evaluation of opacities for a wide range of physical conditions, nonequilibrium kinetics, quantum molecular dynamics simulations of dense plasmas and shocked hydrocarbons, hohlraum spectroscopy, plasma sources of x-ray ultraviolet radiation, strong-field ionization and scattering, decoherence and chaos, quantum computing, and Bose-Einstein and Fermion condensates of cold atoms. The group provides interactive web sites for user calculations of opacities of mixtures and for calculations of atomic structure and cross sections. It also organizes and partially sponsors the annual Los Alamos Summer School for undergraduate students in physics. **Technical staff includes approximately 7 Technical Staff Members (including 1 Fellow), 4 Limited-term Technical Staff Members, and 8 Postdoctoral Associates.**

Theoretical Astrophysics (T-6)

T-6 staff members are involved in 1) studies of stellar evolution including supernovae, intermediate mass stars, nucleosynthesis, and oscillations; 2) nuclear physics and its applications; 3) large-scale structures in the universe; 4) relativistic astrophysics involving compact objects such as white dwarfs, neutron stars, and black holes; 5) comets and asteroids in the solar system; and 6) planetary interiors and evolution. The group has considerable strength in computer and computational science issues underlying multidimensional simulations and the analysis of massive data sets. T-6 is exceptional among theoretical astrophysics organizations across the nation in its explicit emphasis on connecting fundamental science to national needs and Laboratory missions. **Technical staff includes approximately 8 Technical Staff Members (including 1 Fellow), 3 Limited-term Technical Staff Members, 5 Postdoctoral Associates, 3 Graduate Research Assistants, and 4 Undergraduate Students.**

Mathematical Modeling and Analysis (T-7)

T-7 combines the strengths of applied mathematicians, mathematical physicists, and numerical analysts to derive, analyze, and solve mathematical models of complex problems. Its mission is to conduct forefront basic and applied research in mathematical modeling and analysis, provide theoretical leadership and support for the Laboratory and other programs of national interest, and to furnish an effective interface with academic science. In accordance with this mission, T-7 maintains its multidisciplinary, but highly mathematically oriented character, by supporting a strong applied research effort that is grounded in basic research. The applied mathematicians in T-7 have made substantial contributions in solving large systems of linear and nonlinear equations, the theoretical and numerical solutions of nonlinear partial differential equations, modeling the long-time predictability of ocean dynamics, nonlinear optical transmission lines, the applications of wavelets, applied stochastic modeling and deriving effective parameters for homogenizing multiscale problems, and the mathematical modeling of disease transmission and pattern formation in biological systems. **Technical staff includes approximately 8 Technical Staff Members, 11 Limited-term Technical Staff Members, 6 Postdoctoral Associates, 6 Graduate Research Assistants, and 1 Undergraduate Student.**

Elementary Particles and Field Theory (T-8)

T-8 conducts research in particle physics, both on the standard model of electromagnetic, weak and strong interactions, and on theories that extend it. This includes a strong program in computational quantum chromodynamics to calculate the hadron spectrum, quark masses, and weak matrix elements, especially those that are required to quantitatively understand the experimentally observed CP violation. There is a significant effort to elucidate the structure of theories that invoke supersymmetry and extra dimensions. Cosmology, particle-astrophysics, gravity, and formation and evolution of large-scale structure in the universe are growing activities in the group. Fundamental issues of quantum field theory forms another key focus of research, especially in the arena of systems far from equilibrium and the study of long-distance structure of quantized gravity. Multidisciplinary efforts include studies at the interface of elementary particle physics, nuclear physics, and astrophysics; application of scaling ideas to biological and ecological systems; and the study of viral evolution with an eye to understanding and controlling the AIDS epidemic. Efforts in quantum science and technology include understanding the emergence of classical behavior from underlying quantum dynamics and designing feedback control for quantum dynamical systems. Computational science is a major thrust area, with applications to scaling theory to stochastic equations for nonequilibrium dynamics, modern dynamical systems theory for accelerator design, and the study of biological systems. This group maintains close ties with experimental efforts in neutrino physics and astrophysics, satellite tracking, cosmological surveys, and has made a major contribution to the production and trapping of anti-hydrogen. **Technical staff includes approximately 7 Technical Staff Members (including 1 Fellow), 5 Postdoctoral Associates, 2 Graduate Research Assistants, and 1 Undergraduate Student.**

Theoretical Biology and Biophysics (T-10)
T-10 focuses on the modeling of biological systems, molecular modeling, and the analysis and informatics of molecular and cellular biological data. Its activities reflect the needs both to further our understanding of living systems at the cellular and molecular levels and to improve the nation's health and economic welfare. T-10 is one of the few research groups in the world devoted to mathematical modeling and computational analysis of problems in cellular and molecular biology. T-10 has created and is responsible for the maintenance of the HIV, HCV, and Influenza Sequence databases, as well as the HIV Immunology Database and the HIV Resistance Database. Research efforts span a number of topics including understanding dynamics and treatment of viral diseases such as HIV, influenza, and hepatitis; immune system modeling; receptor-ligand interactions and cell signaling; computational aspects of the human genome initiative; pattern recognition in DNA sequences; high-performance computational studies of macromolecular structure and dynamics; RNA structure; membranes and membrane proteins; protein function and dynamics; and protein folding. **Technical staff includes approximately 13 Technical Staff Members (including 2 Senior Fellows and 1 Fellow), 6 Limited-term Technical Staff Members, 7 Postdoctoral Associates, 8 Technicians, 3 Graduate Research Assistants, and 2 Undergraduate Students.**

Condensed Matter and Statistical Physics (T-11)
T-11 conducts research in condensed matter theory including electronic, structural, and transport properties of metals, semiconductors, compounds and alloys; microscopic modeling of materials properties and textures; fundamental studies of nonlinear and nonequilibrium systems; quantum field theory and algebraic approaches to statistical mechanics and materials physics; investigations of the properties of heavy fermions, high-temperature and organic superconductors and other strongly correlated electronic systems; phenomenology and other aspects of layered anisotropic superconductors; development of advanced algorithms for scientific computing (e.g., quantum Monte Carlo, molecular and Langevin dynamics involving multiple time and length scales) and the development of visualization tools for large data sets; magnetoresistance in perovskites; Ginzburg-Landau models of elastic, martensitic, and displacive phase-transformation materials; microscopic aspects of shock waves in materials; aspects of quantum information related to condensed matter systems; device physics; nanophysics and nanotechnology; and applications of condensed matter physics to soft matter (polymers, organics, and biomaterials). **Technical staff includes approximately 11 Technical Staff Members (including 2 Fellows), 5 Limited-term Technical Staff Members, 9 Postdoctoral Associates, 3 Graduate Research Assistants, and 1 Undergraduate Student.**

Theoretical Chemistry and Molecular Physics (T-12)

This group is staffed by theoretical chemists and physicists who work on projects aimed towards an improved understanding of the behavior of matter. Generally, projects seek to describe how basic forces operating at the atomic, molecular, and mesoscopic level manifest themselves in the properties of matter at more macroscopic scales. Current activities include research both in gas-phase and condensed-phase phenomena and projects apply state-of-the-art computational approaches in fundamental and applied studies of the physics and chemistry of molecules and materials. Research projects include the development and application of techniques for calculating the electronic properties of molecules, the dynamics and kinetics of chemical reactions, atomistic simulations of materials, molecular modeling of catalysts, the study of solute-solvent interactions, and chemical and biological process modeling. **Technical staff includes approximately 13 Technical Staff Members (including 2 Fellows), 3 Limited-term Technical Staff Members, 9 Postdoctoral Associates, and 2 Graduate Research Assistants.**

Complex Systems (T-13)

T-13 creates new methods for solving complex problems and applies them to problems at the forefront of technology. This group also initiates and coordinates work on complex systems throughout the Division. Incomplete knowledge of the factors that govern the behavior of complex systems leads to the need for a probabilistic description. In keeping with this fact, T-13 has a strong program in several branches of statistical physics. This work includes complex networks, statistical fluid dynamics, with application to turbulent and multiphase fluid mixing, granular flow, and modeling of fluid flow in petroleum reservoirs. Each of these efforts has a theoretical and computational component, which is also closely tied to experiment. Another strong effort involves the modeling of laser-matter interactions for inertial confinement fusion studies. A vigorous program on uncertainty quantification addresses the problem of assigning error bars or confidence levels to predictions based on large-scale simulations. Computational and theoretical work on complex biological systems is represented by research on the spread of influenza, recognition mechanisms for protein-DNA binding, control of transcription, and regulation of gene expression. Modeling and simulation of nanodevices and large quantum computers is also an active area of research that has attracted wide interest. **Technical staff includes approximately 11 Technical Staff Members, 1 Long-term Visiting Staff Member, 2 Limited-term Technical Staff Members, and 6 Postdoctoral Associates.**

Explosives and Organic Materials (T-14)

The group is involved with the modeling and prediction of the properties and response characteristics of explosives and other organic materials, particularly polymers. A majority of the work is funded by the nuclear weapons program and has direct impact on both stockpile certification calculations and the design and analysis of experiments for validation purposes. Within that context, T-14 strives to obtain fundamental understanding of the various processes involved and connect them together with appropriate multiscale modeling programs. This group interacts strongly with other groups within the Division, Laboratory, and universities to accomplish this goal. Topics of general interest are the mechanical and reactive behavior of organic crystals and polymeric materials, ignition and detonation characteristics of explosive formulations, and how detonation and explosion waves interact with other materials. Included within the group is expertise in hydrodynamics and shock interactions, reactive flow simulations, equations of state for organic materials, molecular modeling with classical and quantum mechanical methods, micromechanical simulations, and material response characterization. Current projects include studies of the initiation and burn processes in damaged and intact explosive materials, advanced energetic equations of state, response characteristics of composite polymeric materials, and the prediction of materials and chemical reaction properties with molecular modeling. These efforts support advanced defense applications, including nuclear and counterterrorism programs. **Technical staff includes approximately 8 Technical Staff Members, 2 Limited-term Technical Staff Members, 3 Postdoctoral Associates, and 3 Graduate Research Assistants.**

Plasma Theory (T-15)

T-15 studies the theory of the fourth state of matter (after solid, liquid, and gas), plasma, or ionized gas. Most of the matter in the universe is in the plasma state: flames, fluorescent lights, the earth's magnetosphere, the sun, the stars, nebulae, thermonuclear explosions, plasmas confined in magnetic fields for magnetic fusion energy, and plasmas used for industrial processing. Because plasmas are ionized and carry electric currents, they interact strongly with electromagnetic fields. This group studies the basic properties and collective motions of plasmas and electromagnetic fields. A major activity is development of efficient, parallel computer codes for the modeling and simulation of plasmas, using both fluid and kinetic descriptions. Numerical simulation of magnetized plasmas is particularly challenging because of the high degree of anisotropy and large range of length and time scales. Some codes developed by T-15 are in wide use throughout the U.S. magnetic fusion community, including the NIMROD toroidal simulation code, the DCON code for rapid determination of the stability of axisymmetric toroidal plasmas, and the CHIP code for modeling helicity injection into tokamaks. Other more powerful codes are under development using advanced numerical methods. Another topic of interest is astrophysical plasmas, particularly the behavior of plasmas undergoing magnetic reconnection, and their role in the evolution of active galactic nuclei. A relatively new and rapidly growing area of emphasis is the study of strongly coupled plasmas of interest in high energy-density physics. **Technical staff includes approximately 7 Technical Staff Members, 1 Limited-term Technical Staff Member, 4 Postdoctoral Associates, and 6 Graduate Research Assistants.**

Nuclear Physics (T-16)

T-16 covers a wide range of basic and applied nuclear physics relevant to the Laboratory, NNSA, and the DOE. Basic nuclear physics research in T-16 includes few- to many-body nuclear physics including nuclear structure and reactions; QCD at high density in astrophysics and at high energy-density addressing RHIC physics; nuclear astrophysics; neutrino physics; and fundamental symmetries. Current projects include high-density QCD and neutrino physics relevant to astrophysical phenomenon and high-energy density QCD as revealed in relativistic heavy ion collider (RHIC) experiments. The theory effort is closely tied to the Laboratory and national DOE experimental nuclear physics program. Applied nuclear physics encompasses nuclear physics relevant to TR and Stockpile Stewardship, including fission theory, reaction theory, sensitivity studies, and analyzing and testing nuclear data and providing it to the Laboratory and the nation. Current efforts include modeling of nuclear cross-sections and spectra, improvement of fission theories, developing codes and libraries for transmutation and radioactivity calculations, and nuclear data processing and testing for use in radiation transport codes. T-16 maintains close ties with leading university and national laboratory groups in both basic and applied theory. **Technical staff includes approximately 12 Technical Staff Members (including 2 Fellows), 1 Limited-term Technical Staff Member, 4 Postdoctoral Associates, and 1 Graduate Research Assistant.**

Center for Nonlinear Studies (CNLS)

CNLS identifies and studies fundamental nonlinear and complex problems and promotes the use of the results in applied research. It stimulates interdisciplinary research and information exchanges inside and outside the Laboratory and provides a Laboratory focal point for collaboration with academic and other centers of excellence in nonlinear science. CNLS disseminates recent developments in nonlinear science and introduces students and postdoctoral researchers to this subject. The Center achieves these goals by hosting and co-hosting conferences and workshops; through extensive visitor, postdoctoral, and student programs; and through interactions with Laboratory staff. The major research areas include networks research with applications to biology, information science and agent-based systems, biological physics, statistical physics and nonequilibrium statistical mechanics, turbulence, condensed matter physics (both soft materials and electronic properties), and computer science. **Technical staff includes approximately 2 Technical Staff Members (including 1 Fellow), 19 Postdoctoral Associates, and 2 Graduate Research Assistants.**

Appendix E – Management Position Descriptions

Name: John M. Wills	**Organization:** T-1, Equation of State and Mechanics of Materials Group		
Job Title: Group Leader	**Series/Level:** TSM	**Pay Basis:** Exempt	**Clearance Level:** Q
Reports to: Alan Bishop, Theoretical Division Leader			
Summary: As a member of the Theoretical Division management team, the group leader provides leadership, project management, capability development, and line management for the Equation of State and Mechanics of Materials Group (T-1). The group develops theory and computational models to describe the Equation of State and Mechanics of Materials (EOS/MOM), including, but not limited to, materials of interest to nuclear weapons, and implements these models in computer codes that contribute in particular to the SESAME Equation-of-State and Materials Properties Library, which is maintained by T-1. The group also has an active research program developing theory, methodology, and calculation to support and enhance that program. Other relevant areas of research include strong electron correlation; actinide electronic structure; first-principles prediction of mechanical and thermodynamic properties of multicomponent materials; linear scaling electronic structure theory; multiphase EOS theory; microscopic, mesoscopic, and continuum-level mechanical behavior of materials; direct numerical simulation of materials properties; energetic materials; grain growth phenomena; and order-N numerical techniques for electronic structure calculation. Capability developed in support of EOS/MOM is used to support related programs such as Pu aging studies and other projects in the nuclear and conventional defense communities, civilian research communities, commercial applications, and threat reduction.			
Primary Functions and Responsibilities (may not include all duties assigned): The group leader will develop and manage the group's human, financial, computing, and other resources; will develop new programs and funding on behalf of the group and Division; will assist staff in pursuing new and innovative research ideas; and will develop staff members and postdoctoral appointees in all key capability areas within the group. The group leader will be proactive and decisive in handling all personnel issues. The group leader will also maintain an active research effort, at the half to three-fourths level. The group leader is responsible for nurturing a safe and secure working environment through the proper implementation of ISM, ISSM, IWM, and AA/EEO objectives. The group leader ensures that group operations are consistent with applicable Division, Laboratory, and DOE policies. In addition to ensuring that the group delivers on program deliverables as agreed to with customers, the group leader is responsible for maintaining close working relationships with other groups within the Division, with relevant program managers, and with other organizations outside the Division and Laboratory.			
Technical Expertise and Responsibilities: Research experience in electronic structure theory and computational methodology, particularly applied to the electronic, magnetic, and structural properties of *f*-electron elements and compounds and strongly-correlated *f*-electron materials. Research experience in first-principles EOS theory and computation. Dr. Wills participates in LDRD-funded projects on plutonium and plutonium-compound electronic structure, structural phase stability, structural parameters, thermodynamics, magnetic structure, and superconducting properties. He is also a researcher for Advanced Fuel Cycle Initiative (AFCI)-funded projects on first-principles modeling of advanced nuclear fuels, and is the PI for EOS theory and modeling of aging effects in plutonium for the ESC.			
Required Knowledge, Skills and Abilities: Demonstrated knowledge and research experience in one or more of the group's technical focus areas listed above, as well as demonstrated impact in the community through refereed publications, invited talks at national and international conferences, and service to the scientific community. Performance in previous work assignments that demonstrate good business practices, scientific leadership, and effective project leadership skills is necessary. This includes, in particular, project planning and implementation; motivation, consensus building and conflict resolution involving personnel at diverse levels; and the ability to satisfy customer requirements in a timely manner by making sound programmatic and technical decisions. Demonstrated excellent verbal and written communication skills. Demonstrated ability to formulate research programs that should attract support from both internal (LDRD) and external (DOE, DoD, AFCI, and others) agencies and programs is required. This position requires a Q access authorization, which normally requires U.S. citizenship.			
Desired Knowledge, Skills, and Abilities: Experience in line management. Experience in program development, including NNSA and DoD programs. Familiarity with LANL management policies on employment, affirmative action, and salary management.			
Management/Supervisory Responsibilities: As group line manager, responsibilities include all business, operations, HR management actions/issues.			
Working Conditions: Office and computational work and frequent domestic and foreign travel.			

<table>
<tr><td colspan="2">Name: Mark Schraad</td><td colspan="2">Organization: T-3, Fluid Dynamics Group</td></tr>
<tr><td>Job Title: Acting Group Leader</td><td>Series/Level: TSM</td><td>Pay Basis: Exempt</td><td>Clearance Level: Q</td></tr>
<tr><td colspan="4">Reports to: Alan Bishop, Theoretical Division Leader</td></tr>
<tr><td colspan="4">Summary: As a member of the Theoretical Division management team, the group leader provides leadership, project management, capability development and line management for the Fluid Dynamics Group (T-3). The group performs basic research in the area of computational continuum mechanics. Members of the group develop basic numerical algorithms for low/high-speed fluid dynamics, including multiphase/field, reacting flows with turbulence. A continuum mechanics component of the group pursues models for high-rate plasticity, brittle and ductile failure, and solid-solid phase transformations for metallic, ceramic, and composite materials. The group also develops numerical methods for global climate modeling, including ocean and sea ice models and is engaged in the coupling of these models with atmospheric components. In addition to ensuring that the group delivers on program deliverables as agreed to with customers, the group leader will be responsible for maintaining close working relationships with other groups within the Division, with relevant program managers, and with other organizations outside the Division and Laboratory.</td></tr>
<tr><td colspan="4">Primary Functions and Responsibilities (may not include all duties assigned): The group leader will develop and manage the group's human, financial, computing, and other resources; will develop new programs and funding on behalf of the group and Division; will assist staff in pursuing new and innovative research ideas; and will develop staff members and postdoctoral appointees in all key capability areas within the group. The group leader will be proactive and decisive in handling all personnel issues. The group leader will also maintain an active research effort, at the half to three-fourths level. The group leader is responsible for nurturing a safe and secure working environment through the proper implementation of ISM, ISSM, IWM, and AA/EEO objectives. The group leader ensures that group operations are consistent with applicable Division, Laboratory, and DOE policies.</td></tr>
<tr><td colspan="4">Technical Expertise and Responsibilities: The T-3 group leader maintains technical expertise in the general areas of computational solid mechanics, materials modeling, multifield flow, and fluid-solid interaction. General research interests include multiscale constitutive modeling of composite, cellular, micro-, and nano-structured materials; micromechanics, homogenization techniques, and nonlocal continuum theories; and scale-dependent behavior, instabilities, and localization phenomena in structured media. Dr. Schraad is the PIfor the Cellular Materials Modeling component of the Engineering Analysis Project under the ASC Materials & Physics program element. Specific research efforts are directed toward modeling the dynamic behavior of soft cellular material systems and the development of numerical algorithms for the simulation of such behavior.</td></tr>
<tr><td colspan="4">Required Knowledge, Skills and Abilities: Demonstrated knowledge and research experience in one or more of the group's technical focus areas listed above. Demonstrated impact in the computational physics community through refereed publications, invited talks at national and international conferences, and service to the scientific community. Performance in previous work assignments that demonstrate good business practices, scientific leadership, and effective project leadership skills is necessary. This includes, in particular, project planning and implementation; motivation, consensus building and conflict resolution involving personnel at diverse levels; and the ability to satisfy customer requirements in a timely manner by making sound programmatic and technical decisions. Demonstrated excellent verbal and written communication skills. Demonstrated ability to formulate research programs that should attract support from the DOE, DoD, LDRD, and/or NW programs is required. This position requires a Q access authorization, which normally requires U.S. citizenship.</td></tr>
<tr><td colspan="4">Desired Knowledge, Skills, and Abilities: Experience in line management. Experience in program development, including NNSA and DoD programs. Familiarity with LANL management policies on employment, affirmative action, and salary management.</td></tr>
<tr><td colspan="4">Management/Supervisory Responsibilities: As group line manager, responsibilities include all business, operations, and human resource management actions/issues.</td></tr>
<tr><td colspan="4">Working Conditions: Office and computational work and frequent domestic and foreign travel.</td></tr>
</table>

Name: James Cohen	**Organization:** T-4, Atomic and Optical Theory Group		
Job Title: Group Leader	**Series/Level:** TSM	**Pay Basis:** Exempt	**Clearance Level:** Q
Reports to: Alan Bishop, Theoretical Division Leader			

Summary:
As a member of the Theoretical Division management team, the group leader provides leadership, project management, capability development and line management for the Atomic and Optical Theory Group (T-4). Group T-4 develops methods for and performs calculations of atomic structure, scattering cross sections, atomic kinetics, opacities, quantum molecular dynamics, exotic atoms, quantum and nonlinear optics, and cold atom physics. Current applications include a new opacity code, high energy-density environments, warm dense matter, nonequilibrium kinetics, radiative properties of hot dense matter, quantum simulations of dense plasmas and shock dynamics, strong-field ionization and scattering, electromagnetic wave propagation, adaptive optics, coherence and chaos in ion traps, quantum computing, and Bose-Einstein and Fermion condensates. The group provides interactive web sites for user calculations of opacities of mixtures and for calculations of atomic structure and cross sections. It also organizes and partially sponsors the annual Los Alamos Summer School for undergraduate students in physics.

Primary Functions and Responsibilities (may not include all duties assigned):
The group leader will develop and manage the group's human, financial, computing, and other resources; will develop new programs and funding on behalf of the group and Division; will assist staff in pursuing new and innovative research ideas; and will develop staff members and postdoctoral appointees in all key capability areas within the group. The group leader will be proactive and decisive in handling all personnel issues. The group leader will also maintain an active research effort, at the half to three-fourths level. The group leader is responsible for nurturing a safe and secure working environment through the proper implementation of ISM, ISSM, IWM, and AA/EEO objectives. The group leader ensures that group operations are consistent with applicable Division, Laboratory, and DOE policies. In addition to ensuring that the group delivers on program deliverables as agreed to with customers, the group leader will be responsible for maintaining close working relationships with other groups within the Division, with relevant program managers, and with other organizations outside the Division and Laboratory.

Technical Expertise and Responsibilities:
Dr. Cohen has general expertise in atomic, molecular, and optical physics. He is responsible for overseeing and evaluating research in this discipline. Cohen's personal research is mainly in the areas of developing methods for and calculating cross sections for atomic collisions. This expertise includes the interface of atomic and nuclear physics.

Required Knowledge, Skills and Abilities:
Demonstrated knowledge and research experience in one or more of the group's technical focus areas listed above. Demonstrated impact in the technical community through refereed publications, invited talks at national and international conferences, and service to the scientific community. Performance in previous work assignments that demonstrate good business practices, scientific leadership, and effective project leadership skills is necessary. This includes, in particular, project planning and implementation; motivation, consensus building and conflict resolution involving personnel at diverse levels; and the ability to satisfy customer requirements in a timely manner by making sound programmatic and technical decisions. Demonstrated excellent verbal and written communication skills. Demonstrated ability to formulate research programs that should attract support from the DOE, LDRD, and/or nuclear weapons programs is required. This position requires a Q access authorization, which normally requires U.S. citizenship.

Desired Knowledge, Skills, and Abilities:
Experience in line management. Experience in program development. Familiarity with LANL management policies on employment, affirmative action, and salary management.

Management/Supervisory Responsibilities:
As group line manager, responsibilities include all business, operations, and human resource management actions/issues.

Working Conditions:
Office and computational work and frequent domestic and foreign travel.

Name: Michael Warren	**Organization:** T-6, Theoretical Astrophysics Group		
Job Title: Acting Group Leader	**Series/Level:** TSM	**Pay Basis:** Exempt	**Clearance Level:** Q
Reports to: Alan Bishop, Theoretical Division Leader			

Summary: As a member of the Theoretical Division management team, the Theoretical Astrophysics (T-6) Group Leader will lead the theoretical astrophysics effort in the Division, provide scientific leadership and line management of the group, as well as carry out his/her own research. Researchers in T-6 work in a broad range of areas in stellar, nuclear, and high-energy astrophysics including the formation and evolution of stars, planets, supernovae, compact objects, active galactic nuclei (AGN), x-ray bursts, gamma-ray bursts, large scale structures and cosmology. The position offers the opportunity to grow programs in theoretical and computational astrophysics and build or expand collaborations with other groups at Los Alamos and beyond in areas such as gamma-ray observations, high-energy-astrophysics and space-science satellites, thinking telescopes, nuclear and particle theory and experiments, radiation and particle transport and hydrodynamics, and high-density equation of state. LANL is part of a number of scientific collaborations [e.g., Supernova Science Center (SSC), Joint Institute for Nuclear Astrophysics (JINA)] and observational initiatives (e.g., SDSS, Swift, DESTINY). T-6 is also responsible for the important task of developing and exploiting the synergy between theoretical astrophysics and national defense programs (e.g., analysis of data from complex, multiscale events) and for the recruitment of outstanding new talent.

Primary Functions and Responsibilities (may not include all duties assigned): The group leader will develop and manage the group's human, financial, computing, and other resources; will develop new programs and funding on behalf of the group and Division; will assist staff in pursuing new and innovative research ideas; and will develop staff members and postdoctoral appointees in all key capability areas within the group. The group leader will be proactive and decisive in handling all personnel issues. The group leader will also maintain an active research effort, at the half to three-fourths level. The group leader is responsible for nurturing a safe and secure working environment through the proper implementation of ISM, ISSM, IWM, and AA/EEO objectives. The group leader ensures that group operations are consistent with applicable Division, Laboratory, and DOE policies.

Technical Expertise and Responsibilities: Lead software development and manage output of multibillion particle simulations of large-scale structure in the universe. Demonstrated world-class expertise in programming of state-of-the-art parallel supercomputers. Design of cost-effective clustered computing systems. Development of "A Faster Multipole Method," which will be the world's first memory-efficient scalable biomolecular simulation algorithm. Develop the hardware and basic software infrastructure for "Thinking Telescopes" in order to manage hundreds of terabytes of time-domain sky imagery. Develop cosmological hydrodynamics methods for the simulation of primordial stars. Maintain and further develop parallel code for 3-D simulations of core-collapse supernovae. Software development, architecture evaluation, and management of the NASA project "Software Tools for Reliable High-Performance Distributed Disk Arrays."

Required Knowledge, Skills and Abilities: Demonstrated impact in the astrophysics community. Demonstrated ability to provide scientific and project leadership, project management skills, and fiscally responsible business practices. These include planning and implementation, motivation, consensus building and conflict resolution, and the ability to satisfy sponsor requirements in a timely manner by making sound programmatic and technical decisions. Demonstrated ability to function effectively in an environment of rapidly changing priorities. Demonstrated effective communication skills, both oral and written. Demonstrated ability to attract and establish research programs from sponsors comparable to those that support activities within the group, such as the DOE, LDRD, industrial partners, and other agencies. Demonstrated commitment to safe and secure working practices that are comparable to Laboratory ISM, ISSM, and IWM policies. Demonstrated commitment to workforce diversity objectives. Ability to obtain a DOE Q clearance, which normally requires U.S. citizenship.

Desired Knowledge, Skills, and Abilities: Experience in line management. Experience in program development, including NNSA programs. Familiarity with LANL management policies on employment, affirmative action, and salary management.

Management/Supervisory Responsibilities: As group line manager, responsibilities include all business, operations, and human resource management actions/issues.

Working Conditions: Office and computational work and frequent domestic and foreign travel.

Name: James (Mac) Hyman		**Organization:** T-7, Mathematical Modeling and Analysis Group	
Job Title: Group Leader	**Series/Level:** TSM	**Pay Basis:** Exempt	**Clearance Level:** Q
Reports to: Alan Bishop, Theoretical Division Leader			

Summary: As a member of the Theoretical Division management team, the group leader provides leadership, project management, capability development, and line management for the Mathematical Modeling and Analysis Group (T-7). This group combines the strengths of applied mathematicians, mathematical physicists, and numerical analysts to derive, analyze, and solve mathematical models of complex problems. T-7 maintains its multidisciplinary, but highly mathematically oriented character, by supporting a strong applied research effort that is grounded in basic research. The applied mathematicians in T-7 have made substantial contributions in solving large systems of linear and nonlinear equations, the theoretical and numerical solutions of nonlinear partial differential equations, modeling the long-time predictability of ocean dynamics, nonlinear optical transmission lines, the applications of wavelets, in applied stochastic modeling and deriving effective parameters for homogenizing multiscale problems, and the mathematical modeling of disease transmission and pattern formation in biological systems. The group also organizes and co-sponsors (with Arizona State University) the annual Mathematical and Theoretical Biology Institute, an intensive summer workshop designed to give undergraduate minority students hands-on experience with mathematical, statistical, and scientific research.

Primary Functions and Responsibilities (may not include all duties assigned): The group leader will develop and manage the group's human, financial, computing, and other resources; will develop new programs and funding on behalf of the group and Division; will assist staff in pursuing new and innovative research ideas; and will develop staff members and postdoctoral appointees in all key capability areas within the group. The group leader will be proactive and decisive in handling all personnel issues. The group leader will also maintain an active research effort, at the half to three-fourths level. The group leader is responsible for nurturing a safe and secure working environment through the proper implementation of ISM, ISSM, IWM, and AA/EEO objectives. The group leader ensures that group operations are consistent with applicable Division, Laboratory, and DOE policies. In addition to ensuring that the group delivers on program deliverables as agreed to with customers, the group leader will be responsible for maintaining close working relationships with other groups in the Division, relevant program managers, and other organizations outside the Division and Laboratory.

Technical Expertise and Responsibilities: The group leader has a strong publication record in numerical methods for partial differential equations and the mathematical analysis of nonlinear models with applications to weapons physics and national security simulations, such as modeling the spread of epidemics. Dr. Hyman has demonstrated ability to build, fund, and lead programs in computational science and engineering. The group leader is also responsible for technical leadership in the analysis of mathematical models, theoretical biology, numerical algorithms, and software design.

Required Knowledge, Skills and Abilities: Demonstrated knowledge and research experience in one or more of the group's technical focus areas listed above. Demonstrated impact in the technical community through refereed publications, invited talks at national and international conferences, and service to the scientific community. Performance in previous work assignments that demonstrate good business practices, scientific leadership, and effective project leadership skills is necessary. This includes, in particular, project planning and implementation; motivation, consensus building and conflict resolution involving personnel at diverse levels; and the ability to satisfy customer requirements in a timely manner by making sound programmatic and technical decisions. Demonstrated excellent verbal and written communication skills. Demonstrated ability to formulate research programs that should attract support from the DOE, LDRD, and/or nuclear weapons programs is required. This position requires a Q access authorization, which normally requires U.S. citizenship.

Desired Knowledge, Skills, and Abilities: Experience in line management. Experience in program development. Familiarity with LANL management policies on employment, affirmative action, and salary management.

Management/Supervisory Responsibilities: As group line manager, responsibilities include all business, operations, and human resource management actions/issues.

Working Conditions: Office and computational work and frequent domestic and foreign travel.

Name: Rajan Gupta		**Organization:** T-8, Elementary Particles and Field Theory Group	
Job Title: Group Leader	**Series/Level:** TSM	**Pay Basis:** Exempt	**Clearance Level:** Q

Reports to: Alan Bishop, Theoretical Division Leader

Summary: As a member of the Theoretical Division management team, the group leader provides leadership, capability development, and line management for the Elementary Particles and Field Theory Group (T-8). This group conducts research in particle physics, including a strong program in computational quantum chromodynamics to calculate the hadron spectrum, quark masses, and weak matrix elements, especially those required to quantitatively understand the experimentally observed CP violation. There is an effort to elucidate the structure of theories that invoke supersymmetry and extra dimensions and understand neutrino interactions and masses. Cosmology, particle-astrophysics, gravity, and studies of the formation and evolution of the large-scale structure of the universe are growing activities. Fundamental issues of quantum field theory is another key focus of research, especially in systems far from equilibrium and the study of long-distance structure of quantized gravity. Multidisciplinary efforts include studies at the interface of elementary particle physics, nuclear physics, and astrophysics; application of scaling ideas to biological and ecological systems; and the study of viral evolution with an eye to understanding and controlling the AIDS epidemic. Efforts in quantum science and technology include understanding the emergence of classical behavior from underlying quantum dynamics and designing feedback control for quantum dynamical systems. Computational science is a major area, with applications to scaling theory to stochastic equations for nonequilibrium dynamics, modern dynamical systems theory for accelerator design, to the study of biological systems. The group maintains ties with experimental efforts in neutrino- and astrophysics, satellite tracking, cosmological surveys, and contributed to the production and trapping of anti-hydrogen efforts.

Primary Functions and Responsibilities (may not include all duties assigned): Develop and manage the group's human, financial, computing, and other resources; develop new programs and funding on behalf of the group and Division; assist staff in pursuing new and innovative research ideas; and develop staff members and postdoctoral appointees in all key capability areas within the group. The group leader will be proactive and decisive in handling all personnel issues. The group leader will also maintain an active research effort, at the half to three-fourths level. The group leader is responsible for nurturing a safe and secure working environment through the proper implementation of ISM, ISSM, IWM, and AA/EEO objectives. The group leader ensures that group operations are consistent with applicable Division, Laboratory, and DOE policies. In addition to ensuring that the group delivers on program deliverables as agreed to with customers, the group leader will be responsible for maintaining close working relationships with other groups in the Division, relevant program managers, and other organizations outside the Division and Laboratory.

Technical Expertise and Responsibilities: Dr. Gupta has a 25-year record of distinguished research and leadership at the national and international level in Lattice QCD and high-performance computing. He provides scientific leadership within the Lab, nationally and internationally. Dr. Gupta helps group members obtain funding, provides an environment supportive of research, and recruits outstanding staff members, post-doctoral fellows, and students. Dr Gupta developed and is leading multidisciplinary efforts in national security, computational biology, and automated image processing.

Required Knowledge, Skills and Abilities: Demonstrated knowledge and research experience in one or more of the group's technical focus areas listed above. Demonstrated impact in the technical community through refereed publications, invited talks at national and international conferences, and service to the scientific community. Performance in previous work assignments that demonstrate good business practices, scientific leadership, and effective project leadership skills is necessary. This includes, in particular, project planning and implementation; motivation, consensus building and conflict resolution involving personnel at diverse levels; and the ability to satisfy customer requirements in a timely manner by making sound programmatic and technical decisions. Demonstrated excellent verbal and written communication skills. Demonstrated ability to formulate research programs that should attract support from the DOE, LDRD, and other agencies is required. This position requires a Q access authorization, which normally requires U.S. citizenship.

Desired Knowledge, Skills, and Abilities: Experience in line management and program development. Familiarity with LANL management policies on employment, affirmative action, and salary management.

Management/Supervisory Responsibilities: As line manager, responsibilities include all business, operations, and human resource management actions.

Working Conditions: Office and computational work and frequent domestic and foreign travel.

Name: Antonio Redondo	**Organization:** T-10, Theoretical Biology and Biophysics Group		
Job Title: Group Leader	**Series/Level:** TSM	**Pay Basis:** Exempt	**Clearance Level:** Q
Reports to: Alan Bishop, Theoretical Division Leader			
Summary: As a member of the Theoretical Division management team, the group leader provides leadership, project management, capability development, and line management for the Theoretical Biology and Biophysics Group (T-10). This group focuses on the modeling of biological systems, molecular modeling, and the analysis and informatics of molecular and cellular biological data. Its activities reflect the needs both to further our understanding of living systems at the cellular and molecular levels and to improve the nation's health and economic welfare. T-10 is one of the few research groups in the world devoted to mathematical modeling and computational analysis of problems in cellular and molecular biology. The group has created and is responsible for the maintenance of the HIV, HCV, and Influenza Sequence databases, as well as the HIV Immunology Database, and the HIV Resistance Database. Research efforts span a number of topics including understanding dynamics and treatment of infectious diseases such as HIV, influenza, and hepatitis; host-pathogen interactions; immune system modeling; cell signaling; computational aspects of the human genome initiative; pattern recognition in DNA sequences; high-performance computational studies of macromolecular structure and dynamics; RNA structure; membranes and membrane proteins; protein function and dynamics; and protein folding.			
Primary Functions and Responsibilities (may not include all duties assigned): The group leader will develop and manage the group's human, financial, computing, and other resources; will develop new programs and funding on behalf of the group and Division; will assist staff in pursuing new and innovative research ideas; and will develop staff members and postdoctoral appointees in all key capability areas within the group. The group leader will be proactive and decisive in handling all personnel issues. The group leader will also maintain an active research effort, at the half to three-fourths level. The group leader is responsible for nurturing a safe and secure working environment through the proper implementation of ISM, ISSM, IWM, and AA/EEO objectives. The group leader ensures that group operations are consistent with applicable Division, Laboratory, and DOE policies. In addition to ensuring that the group delivers on program deliverables as agreed to with customers, the group leader will be responsible for maintaining close working relationships with other groups in the Division, relevant program managers, and other organizations outside the Division and Laboratory.			
Technical Expertise and Responsibilities: Dr. Redondo has a Ph.D. in Applied Physics from the California Institute of Technology. Dr. Redondo has active research efforts in immunology/cell signaling and in modeling infectious diseases. He has been a major organizer, with Gary Resnick of the CHS, of the CTCP. He has been a group leader in T Division for 11.5 years, 11 in the Theoretical Chemistry and Molecular Physics Group, and currently for the Theoretical Biology and Biophysics Group. He has an extensive publication record and has been PI for a multitude of research projects involving internal and external collaborations.			
Required Knowledge, Skills and Abilities: Demonstrated knowledge and research experience in one or more of the group's technical focus areas listed above. Demonstrated impact in the technical community through refereed publications, invited talks at national and international conferences, and service to the scientific community. Performance in previous work assignments that demonstrate good business practices, scientific leadership, and effective project leadership skills is necessary. This includes project planning and implementation; motivation, consensus building and conflict resolution involving personnel at diverse levels; and the ability to satisfy customer requirements in a timely manner by making sound programmatic and technical decisions. Demonstrated excellent verbal and written communication skills. Demonstrated ability to formulate research programs that should attract support from the DOE, NIH, DoD, LDRD, and other external agencies is required. This position requires a Q access authorization, which normally requires U.S. citizenship.			
Desired Knowledge, Skills, and Abilities: Experience in line management and program development. Familiarity with LANL management policies on employment, affirmative action, and salary management.			
Management/Supervisory Responsibilities: As group line manager, responsibilities include all business, operations, and human resource management actions/issues.			
Working Conditions: Office and computational work and frequent domestic and foreign travel.			

Name: Robert C. Albers | **Organization:** T-11, Condensed Matter and Statistical Physics Group

Job Title: Group Leader | **Series/Level:** TSM | **Pay Basis:** Exempt | **Clearance Level:** Q

Reports to: Alan Bishop, Theoretical Division Leader

Summary: As a member of the Theoretical Division management team, the group leader provides leadership, project management, capability development, and line management for the Condensed Matter and Statistical Physics Group (T-11). This group conducts research in condensed matter theory including electronic, structural, and transport properties of metals, semiconductors, compounds and alloys; microscopic modeling of materials properties and textures; fundamental studies of nonlinear and nonequilibrium systems; quantum field theory and algebraic approaches to statistical mechanics and materials physics; investigations of the properties of heavy fermions, high-temperature and organic superconductors and other strongly correlated electronic systems; phenomenology and other aspects of layered anisotropic superconductors; development of advanced algorithms for scientific computing and the development of visualization tools for large data sets; magnetoresistance in perovskites; Ginzburg-Landau models of elastic, martensitic, and displacive phase-transformation materials; microscopic aspects of shock waves in materials; aspects of quantum information related to condensed matter systems; device physics; nanophysics and nanotechnology; and applications of condensed matter physics to soft matter (polymers, organics, and biomaterials).

Primary Functions and Responsibilities (list may not include all duties assigned):
The group leader will develop and manage the group's human, financial, computing, and other resources; will develop new programs and funding on behalf of the group and Division; will assist staff in pursuing new and innovative research ideas; and will develop staff members and postdoctoral appointees in all key capability areas within the group. The group leader will be proactive and decisive in handling all personnel issues. The group leader will also maintain an active research effort, at the half to three-fourths level. The group leader is responsible for nurturing a safe and secure working environment through the proper implementation of ISM, ISSM, IWM, and AA/EEO objectives. The group leader ensures that group operations are consistent with applicable Division, Laboratory, and DOE policies. In addition to ensuring that the group delivers on program deliverables as agreed to with customers, the group leader will be responsible for maintaining close working relationships with other groups in the Division, relevant program managers, and other organizations outside the Division and Laboratory.

Technical Expertise and Responsibilities:
The T-11 Group Leader, Dr. Albers, has technical expertise in electronic structure of materials, including simple-metal, transition-metal, rare-earth, actinide, and heavy-electron materials, with a particular emphasis on systems with strong electron-electron correlations; tight-binding approaches to materials modeling; mechanical and structural properties of transition-metal and actinide materials; modeling of solid-solid phase transitions including martensitic and complex materials; and multiple-scattering theories of x-ray absorption structure (in both the XANES and EXAFS regimes), some knowledge of photoemission and related electronic spectroscopies.

Required Knowledge, Skills and Abilities (minimum KSAs required for job performance):
Demonstrated knowledge and research experience in one or more of the group's technical focus areas listed above. Demonstrated impact in the technical community through refereed publications, invited talks at national and international conferences, and service to the scientific community. Performance in previous work assignments that demonstrate good business practices, scientific leadership, and effective project leadership skills is necessary. This includes project planning and implementation; motivation, consensus building and conflict resolution involving personnel at diverse levels; and the ability to satisfy customer requirements in a timely manner by making sound programmatic and technical decisions. Demonstrated excellent verbal and written communication skills. Demonstrated ability to formulate research programs that should attract support from LDRD, the DOE, and other external agencies is required. This position requires a Q access authorization, which normally requires U.S. citizenship.

Desired Knowledge, Skills, and Abilities:
Experience in line management. Experience in program development. Familiarity with LANL management policies on employment, affirmative action, and salary management.

Management/Supervisory Responsibilities:
As group line manager, responsibilities include all business, operations, and human resource management actions/issues.

Working Conditions: Office and computational work and frequent domestic and foreign travel.

Name: Joel D. Kress	**Organization:** T-12, Theoretical Chemistry and Molecular Physics Group		
Job Title: Acting Group Leader	**Series/Level:** TSM	**Pay Basis:** Exempt	**Clearance Level:** Q
Reports to: Alan Bishop, Theoretical Division Leader			
Summary: As a member of the Theoretical Division management team, the group leader provides scientific leadership, project management, capability development, and line management for the group. The members of T-12 seek to understand the behavior of materials by describing how basic forces operating at the atomic and molecular level manifest themselves in the properties of matter at more macroscopic levels. Current activities in T-12 include research both in gas phase and condensed phase phenomena. These projects apply state-of-the-art computational approaches for fundamental and applied studies of the physics and chemistry of molecules and materials. Research projects include the development and application of techniques for calculating the electronic properties of molecules and solids, atomistic simulations of materials, the dynamics and kinetics of chemical reactions, molecular modeling of catalysts, and the study of solute-solvent interactions. Particular applications of this research are to the properties of actinide materials and transition metals, to the properties of polymers, biological solvation processes, and fuel cell technologies. Work in the group supports applied missions of the Laboratory, including the ASC program, threat reduction programs, and the DOE Basic Energy Sciences programs. The group also obtains significant support from the LDRD program in both its exploratory research and developmental research missions.			
Primary Functions and Responsibilities (may not include all duties assigned): The group leader will develop and manage the group's human, financial, computing, and other resources; will develop new programs and funding on behalf of the group and Division; will assist staff in pursuing new and innovative research ideas; and will develop staff members and postdoctoral appointees in all key capability areas within the group. The group leader will be proactive and decisive in handling all personnel issues. The group leader will also maintain an active research effort, at the half to three-fourths level. The group leader is responsible for nurturing a safe and secure working environment through the proper implementation of ISM, ISSM, IWM, and AA/EEO objectives. The group leader ensures that group operations are consistent with applicable Division, Laboratory, and DOE policies.			
Technical Expertise and Responsibilities: Dr. Kress is the PI for the *Theory and Simulation of Polymer Aging* task supported by the ESC, where results from this work are presented quarterly at the PBX 9501 Working Group meetings and annually at the LANL Energetic Materials Review. He is also PI for the LDRD-DR project *Fission Fragment Physics in Extreme Environments (U)* and participates in the LDRD-DR project *Energetic-Particle Interactions With Dense Plasmas*. He participates in an Office of Science funded project on developing metal catalysts for hydrogen fuel cells. Dr. Kress' research experience includes coupling molecular dynamics simulations with electronic structure theory, with applications to the equation-of-state and optical properties of shock-compressed molecular fluids and materials, aqueous chemical processes, and nanotechnology.			
Required Knowledge, Skills and Abilities: Demonstrated knowledge and research accomplishments in one or more of the group's technical research focus areas. Demonstrated ability to provide scientific and project leadership, project management skills, and fiscally responsible business practices. These include planning and implementation, motivation, consensus building and conflict resolution, and the ability to satisfy sponsor requirements in a timely manner by making sound programmatic and technical decisions. Demonstrated ability to function effectively in an environment of rapidly changing priorities. Demonstrated effective communication skills, both oral and written. Demonstrated ability to attract and establish research programs from sponsors that support activities within the group, such as DOE, LDRD, industrial partners, and other agencies. Demonstrated commitment to safe and secure work practices comparable to Laboratory ISM, ISSM, and IWM policies. Demonstrated commitment to workforce diversity objectives. Ability to obtain a DOE Q clearance, which normally requires U.S. citizenship.			
Desired Knowledge, Skills, and Abilities: Experience working with DOE or other federal program office personnel. Familiarity with LANL policies on employment, affirmative action, and salary management. Formal training in technical management.			
Management/Supervisory Responsibilities: As group line manager, responsibilities include all business, operations, and human resource management actions/issues.			
Working Conditions: Office and computational work and frequent domestic and foreign travel.			

<table>
<tr><td>Name: Gennady P. Berman</td><td colspan="3">Organization: T-13, Theoretical Complex Systems Group</td></tr>
<tr><td>Job Title: Acting Group Leader</td><td>Series/Level: TSM</td><td>Pay Basis: Exempt</td><td>Clearance Level: Q</td></tr>
<tr><td colspan="4">Reports to: Alan Bishop, Theoretical Division Leader</td></tr>
<tr><td colspan="4">Summary: As a member of the Theoretical Division management team, the group leader provides scientific leadership, project management, capability development, and line management for the Theoretical Complex Systems Group (T-13). The complex systems group is strongly interdisciplinary, conducting research under the umbrella of statistical and nonlinear physics with applications in physical, information, and biological sciences. Specific core competencies include computational fluid dynamics, granular flow, colloidal systems, coding theory, complex networks, uncertainty quantification, quantum-computing technologies, algorithm development, agent-based systems modeling, and theoretical and computational biology in the areas of genomics, proteomics, and epidemiology. T-13 is a vanguard research group at the Laboratory focusing on developing fundamentally novel solutions and technologies that are later put in practice by its customers. The basic research is supported by NIH, DOE, and LDRD funds, and applied research and technology development is supported by DARPA, NSA, DTRA, DHS, and USG/IC. In addition to ensuring that the group delivers on program objectives as agreed to with customers, the group leader will be responsible for maintaining close working relationships with other groups in the Division, with relevant program managers, and with other organizations outside the Division (especially C, B, and D divisions) and outside the Laboratory.</td></tr>
<tr><td colspan="4">Primary Functions and Responsibilities (may not include all duties assigned): The group leader will work with the deputy group leader and T-13 project leaders/PIs to develop and manage the group's human, financial, computing, and other resources; will develop new programs and funding on behalf of the group and Division; will assist staff in pursuing new and innovative research ideas; and will develop staff members and postdoctoral appointees in all key capability areas within the group. The group leader will be proactive and decisive in handling all personnel issues. The group leader will also maintain an active research effort, at the half to three-fourths level. The group leader is responsible for nurturing a safe and secure working environment through the proper implementation of ISM, ISSM, IWM, and AA/EEO objectives. The group leader ensures that group operations are consistent with applicable Division, Laboratory, and DOE policies.</td></tr>
<tr><td colspan="4">Technical Expertise and Responsibilities: Dr. Berman’s expertise is in quantum and classical nonlinear dynamical systems; scalable quantum computation (PI on ARDA/NSA, LDRD projects); novel algorithms for detecting fraudulent activities (with CITIgroup, PI on IPD project); quantum measurement (PI on DARPA project); quantum technologies and nanodevices (LDRD project); Bose-Einstein condensates (PI on LDRD project); chemical and biosensors; negative refraction index materials—applications to novel antennas; compound resonances in heavy nuclei; and neutron dynamics in the trap (with P-23, LANSCE). Established collaborations with ARO, NSA, ARDA, DARPA, U.S. Air Force, and other agencies.</td></tr>
<tr><td colspan="4">Required Knowledge, Skills and Abilities: Demonstrated knowledge and research excellence in one or more of the group's technical focus areas listed above. Performance in previous work assignments that demonstrate scientific leadership, effective project leadership skills, and good business practices; these include project planning and implementation, motivation, consensus building, and conflict resolution, and the ability to satisfy customer requirements in a timely manner by making sound programmatic and technical decisions. Demonstrated effective communication skills, oral and written. Good interpersonal skills. Ability to build effective research teams. Demonstrated strong impact in complex-systems-related research, as evidenced by publications, level of citations, talks, and service to the scientific and DOE community. Demonstrated ability to formulate research programs that attract support from external funding agencies. Demonstrated commitment to Laboratory ISM, ISSM, and IWM policies; responsible fiscal management; and workforce diversity.</td></tr>
<tr><td colspan="4">Desired Knowledge, Skills, and Abilities: Successful record of mentoring and motivating workers. Demonstrated engagement with customers and sponsors, and experience in building and ensuring funding for new projects. Experience in interacting effectively with DOE and other federal program managers.</td></tr>
<tr><td colspan="4">Management/Supervisory Responsibilities: As group line manager, responsibilities include all business, operations, and human resource management actions/issues.</td></tr>
<tr><td colspan="4">Working Conditions: Office and computational work and frequent domestic and foreign travel.</td></tr>
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Name: Edward M. Kober	**Organization:** T-14, Explosives and Organic Materials Group		
Job Title: Group Leader	**Series/Level:** TSM	**Pay Basis:** Exempt	**Clearance Level:** Q
Reports to: Alan Bishop, Theoretical Division Leader			
Summary: As a member of the Theoretical Division management team, the group leader provides leadership, project management, capability development, and line management for the Explosives and Organic Materials Group (T-14). This group is involved with the modeling and prediction of the properties and response characteristics of explosives and other organic materials, particularly polymers. A majority of the work has direct impact on both stockpile certification calculations and the design and analysis of experiments for validation purposes, therefore, the group strives to obtain fundamental understanding of the various processes involved and connect them with appropriate multiscale modeling programs. Topics of general interest are the mechanical and reactive behavior of organic crystals and polymeric materials, ignition and detonation characteristics of explosive formulations, and how detonation and explosion waves interact with other materials. Included within the group is expertise in hydrodynamics and shock interactions, reactive flow simulations, equations of state for organic materials, molecular modeling with classical and quantum mechanical methods, micromechanical simulations, and material response characterization. Current projects include studies of the initiation and burn processes in damaged and intact explosive materials, advanced energetic equations of state, response characteristics of composite polymeric materials, and the prediction of materials and chemical reaction properties with molecular modeling. These efforts support advanced defense applications, including nuclear and counterterrorism programs.			
Primary Functions and Responsibilities (may not include all duties assigned): The group leader will develop and manage the group's human, financial, computing, and other resources; will develop new programs and funding on behalf of the group and Division; will assist staff in pursuing new and innovative research ideas; and will develop staff members and postdoctoral appointees in all key capability areas within the group. The group leader will be proactive and decisive in handling all personnel issues. The group leader will also maintain an active research effort, at the half to three-fourths level. The group leader is responsible for nurturing a safe and secure working environment through the proper implementation of ISM, ISSM, IWM, and AA/EEO objectives. The group leader ensures that group operations are consistent with applicable Division, Laboratory, and DOE policies. In addition to ensuring that the group delivers on program deliverables as agreed to with customers, the group leader will be responsible for maintaining close working relationships with other groups in the Division, relevant program managers, and other organizations outside the Division and Laboratory.			
Technical Expertise and Responsibilities: The T-14 Group Leader currently contributes to several projects requiring expertise in quantum chemical and molecular dynamics simulations, including: 1) modeling the physical properties of polymeric materials and relating the simulations to experimental results and higher length-scale models, 2) modeling the reaction properties of energetic materials at high temperatures and pressures, and 3) modeling the aging properties of a weapons material. Dr. Kober also assists in the development and evaluation of continuum level reactive burn models.			
Required Knowledge, Skills and Abilities: Demonstrated knowledge and research experience in one or more of the group's technical focus areas listed above. Demonstrated impact in the technical community through refereed publications, invited talks at national and international conferences, and service to the scientific community. Performance in previous work assignments that demonstrate good business practices, scientific leadership, and effective project leadership skills is necessary. This includes project planning and implementation; motivation, consensus building and conflict resolution involving personnel at diverse levels; and the ability to satisfy customer requirements in a timely manner by making sound programmatic and technical decisions. Demonstrated excellent verbal and written communication skills. Demonstrated ability to formulate research programs that attract support from LDRD, NNSA, and other external agencies is required. This position requires a Q access authorization, which normally requires U.S. citizenship.			
Desired Knowledge, Skills, and Abilities: Experience in line management and program development. Familiarity with LANL management policies on employment, affirmative action, and salary management.			
Management/Supervisory Responsibilities: As group line manager, responsibilities include all business, operations, and human resource management actions/issues.			
Working Conditions: Office and computational work and frequent domestic and foreign travel.			

Name: Alan H. Glasser	**Organization:** T-15, Plasma Theory Group		
Job Title: Group Leader	**Series/Level:** TSM	**Pay Basis:** Exempt	**Clearance Level:** Q
Reports to: Alan Bishop, Theoretical Division Leader			

Summary: As a member of the T Division management team, the group leader provides leadership, project management, capability development, and line management for the Plasma Theory Group (T-15). This group studies the theory of the fourth state of matter, plasma, or ionized gas. This group studies the basic properties and collective motions of plasmas and electromagnetic fields. A major activity is development of efficient, parallel computer codes for the modeling and simulation of plasmas, using both fluid and kinetic descriptions. Numerical simulation of magnetized plasmas is particularly challenging because of the high degree of anisotropy and large range of length and time scales. Codes developed by T-15 are in wide use throughout the U.S. magnetic fusion community, including the NIMROD toroidal simulation code, the DCON code for rapid determination of the stability of axisymmetric toroidal plasmas, and the CHIP code for modeling helicity injection into tokamaks. Other codes are under development using advanced numerical methods. Another topic of interest is astrophysical plasmas, particularly the behavior of plasmas undergoing magnetic reconnection, and their role in the evolution of active galactic nuclei. A relatively new and rapidly growing area of emphasis is the study of strongly coupled plasmas of interest in high energy-density physics.

Primary Functions and Responsibilities (may not include all duties assigned):
The group leader will develop and manage the group's human, financial, computing, and other resources; will develop new programs and funding on behalf of the group and Division; will assist staff in pursuing new and innovative research ideas; and will develop staff members and postdoctoral appointees in all key capability areas within the group. The group leader will be proactive and decisive in handling all personnel issues. The group leader will also maintain an active research effort, at the half to three-fourths level. The group leader is responsible for nurturing a safe and secure working environment through the proper implementation of ISM, ISSM, IWM, and AA/EEO objectives. The group leader ensures that group operations are consistent with applicable Division, Laboratory, and DOE policies. In addition to ensuring that the group delivers on program deliverables as agreed to with customers, the group leader will be responsible for maintaining close working relationships with other groups in the Division, relevant program managers, and other organizations outside the Division and Laboratory.

Technical Expertise and Responsibilities:
The T-15 Group Leader has expertise in theoretical and computational plasma physics, magnetic fusion energy, astrophysical plasmas, strongly coupled plasmas, high energy-density physics, advanced computational methods, and applied mathematics. Dr. Glasser is familiar with funding agencies such as the DOE Office of Fusion Energy Sciences, LDRD, and the nuclear weapons program.

Required Knowledge, Skills and Abilities:
Demonstrated knowledge and research experience in one or more of the group's technical focus areas listed above. Demonstrated impact in the technical community through refereed publications, invited talks at national and international conferences, and service to the scientific community. Performance in previous work assignments that demonstrate good business practices, scientific leadership, and effective project leadership skills is necessary. This includes project planning and implementation; motivation, consensus building and conflict resolution involving personnel at diverse levels; and the ability to satisfy customer requirements in a timely manner by making sound programmatic and technical decisions. Demonstrated excellent verbal and written communication skills. Demonstrated ability to formulate research programs that attract support from LDRD, the DOE, and other external agencies is required. This position requires a Q access authorization, which normally requires U.S. citizenship.

Desired Knowledge, Skills, and Abilities:
Experience in line management. Experience in program development. Familiarity with LANL management policies on employment, affirmative action, and salary management.

Management/Supervisory Responsibilities:
As group line manager, responsibilities include all business, operations, and human resource management actions/issues.

Working Conditions:
Office and computational work and frequent domestic and foreign travel.

<table>
<tr><td>Name: Joseph A. Carlson</td><td colspan="3">Organization: T-16, Nuclear Physics Group</td></tr>
<tr><td>Job Title: Group Leader</td><td>Series/Level: TSM</td><td>Pay Basis: Exempt</td><td>Clearance Level: Q</td></tr>
<tr><td colspan="4">Reports to: Alan Bishop, Theoretical Division Leader</td></tr>
<tr><td colspan="4">Summary: As a member of the T Division management team, the group leader provides leadership, project management, capability development, and line management for the Nuclear Physics Group (T-16). This group studies fundamental nuclear theory, nuclear reaction mechanisms, nuclear structure, and provides nuclear data to the nation. The applied theory team studies nuclear reaction and structure theory for light, medium, and heavy nuclei, including fission theory. Areas of application include stockpile stewardship, nonproliferation applications, advanced nuclear reactor and accelerator systems for energy production and nuclear waste transmutation, radiochemical diagnostics used in critical assemblies, criticality safety, light-element fusion, standard cross sections, and nuclear astrophysics. The basic theory team studies physics relevant to the Laboratory and the national DOE nuclear physics program, including neutrino physics, few- and many-body physics, fundamental symmetries and extensions of the standard model, effective field theory, hadronic physics and high density and high energy-density QCD related, respectively, to astrophysics and to RHIC experiments. T-16 maintains close ties with leading university and national laboratory groups.</td></tr>
<tr><td colspan="4">Primary Functions and Responsibilities (may not include all duties assigned): The group leader will develop and manage the group's human, financial, computing, and other resources; will develop new programs and funding on behalf of the group and Division; will assist staff in pursuing new and innovative research ideas; and will develop staff members and postdoctoral appointees in all key capability areas within the group. The group leader will be proactive and decisive in handling all personnel issues. The group leader will also maintain an active research effort, at the half to three-fourths level. The group leader is responsible for nurturing a safe and secure working environment through the proper implementation of ISM, ISSM, IWM, and AA/EEO objectives. The group leader ensures that group operations are consistent with applicable Division, Laboratory, and DOE policies. In addition to ensuring that the group delivers on program deliverables as agreed to with customers, the group leader will be responsible for maintaining close working relationships with other groups in the Division, relevant program managers, and other organizations outside the Division and Laboratory.</td></tr>
<tr><td colspan="4">Technical Expertise and Responsibilities: The T-16 Group Leader conducts forefront research in areas relevant to the Laboratory and the national nuclear physics program. Dr. Carlson's research role encompasses few- and many-body nuclear physics, including nuclear structure and low energy reactions, and connections to many-body quantum physics in other areas. He also conducts research in neutrino and nuclear astrophysics, and fundamental symmetries, in areas directly related to the Laboratory's experimental nuclear physics program. Research in these areas includes studies of neutrino physics in astrophysical and experimental environments and studies of hadronic physics through parity violation in hadronic systems.</td></tr>
<tr><td colspan="4">Required Knowledge, Skills and Abilities: Demonstrated knowledge and research experience in one or more of the group's technical focus areas listed above. Demonstrated impact in the technical community through refereed publications, invited talks at national and international conferences, and service to the scientific community. Performance in previous work assignments that demonstrate good business practices, scientific leadership, and effective project leadership skills is necessary. This includes project planning and implementation; motivation, consensus building and conflict resolution involving personnel at diverse levels; and the ability to satisfy customer requirements in a timely manner by making sound programmatic and technical decisions. Demonstrated excellent verbal and written communication skills. Demonstrated ability to formulate research programs that attract support from LDRD, DOE, and other external agencies is required. This position requires a Q access authorization, which normally requires U.S. citizenship.</td></tr>
<tr><td colspan="4">Desired Knowledge, Skills, and Abilities: Experience in line management. Experience in program development. Familiarity with LANL management policies on employment, affirmative action, and salary management.</td></tr>
<tr><td colspan="4">Management/Supervisory Responsibilities: As group line manager, responsibilities include all business, operations, and human resource management actions/issues.</td></tr>
<tr><td colspan="4">Working Conditions: Office and computational work and frequent domestic and foreign travel.</td></tr>
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<table>
<tr><td>Name: Robert E. Ecke</td><td colspan="3">Organization: T-CNLS, Center for Nonlinear Studies</td></tr>
<tr><td>Job Title: Center Leader</td><td>Series/Level: TSM</td><td>Pay Basis: Exempt</td><td>Clearance Level: Q</td></tr>
<tr><td colspan="4">Reports to: Alan Bishop, Theoretical Division Leader</td></tr>
<tr><td colspan="4">Summary:
As a member of the T Division management team, the center leader provides leadership and line management for the Laboratory’s Center for Nonlinear Studies (CNLS). The center identifies and studies nonlinear and complex problems arising in both basic and applied research, coordinates the study of these problems into interdisciplinary themes, and fosters research collaborations among researchers. The CNLS provides a link for effective interactions with academic and industrial centers of excellence in nonlinear research. The CNLS hosts numerous visiting scholars, postdoctoral fellows, and graduate students; organizes lectures, workshops, and conferences on topics of current scientific interest; and conducts a research program in the theoretical physical, biological, and mathematical sciences, with strong ties to experimental activities. The center leader provides scientific leadership and line management of CNLS and plays an institutional role in collaboration with scientists throughout the Laboratory.</td></tr>
<tr><td colspan="4">Primary Functions and Responsibilities (list may not include all duties assigned):
The center leader is expected to develop and lead a program to target and create cooperative long-term research programs consistent with the Laboratory's strategic research objectives; to develop a strong working relationship with the CNLS External Advisory Committee; and maintain effective working relationships throughout all levels of the Laboratory, government entities, academia, and industry. The center leader is expected to maintain an active research program while providing technical vision to nurture and support existing programs of others at the center. The center leader should be energetic, results-oriented, a catalyst for change, and an outstanding relationship builder. Line management responsibilities includes accountability for quality of research; management of financial and human resources; proactive support of Laboratory and Division ES&H, security, and AA/EEO/Diversity objectives; the communications/marketing strategy for the center; and collaboration with the Theoretical Division to provide strategic direction for the organization.</td></tr>
<tr><td colspan="4">Technical Expertise and Responsibilities:
The CNLS center leader has technical expertise in nonlinear dynamical systems, hard and soft condensed matter physics, statistical physics, pattern formation, hydrodynamic stability, granular materials, and fluid turbulence. Although Dr. Ecke’s primary experience is in experimental physics, he also has secondary expertise in numerical simulation and in theory. He is currently the PI on five LDRD projects with main supervisory responsibility for four: a DR project on Fluid Mixing, an ER project on 2-D turbulence, and two CNLS projects on soft matter physics and nonlinear/complex phenomena. Ecke’s current research consists of dense granular flow, dynamics of 2-D turbulence, and Lagrangian mixing in inhomogeneous fluid turbulence.</td></tr>
<tr><td colspan="4">Required Knowledge, Skills and Abilities (minimum KSA’s required for job performance):
Record of scientific accomplishment in an area of research relevant to the center as evidenced by an outstanding publication record and/or demonstrable national or international reputation. Demonstrated success in management of a scientific organization, including effective resource management. Demonstrated ability to foster an environment of teamwork, quality, technical excellence, innovation, and creativity. Demonstrated experience in building collaborative relationships across boundaries (group, division, directorate, Laboratory, and external.) Ability to balance competing interests with available resources and establish clear priorities and focus. Exceptional skills in leading and engaging staff; and possess the ability to build rapport within the Laboratory. Demonstrated excellence in effective written and oral communications skills. Demonstrated knowledge of and commitment to Laboratory goals in assuring a healthy, safe, and secure working environment.</td></tr>
<tr><td colspan="4">Desired Knowledge, Skills, and Abilities:
Knowledge of national and international programs of relevance to the center's activities. Experience in effective decision-making and comfort with measuring, defining and taking prudent risks. Proven track record using collaboration with subject matter experts to solve problems and implement solutions. Q access authorization, which normally requires U.S. citizenship.</td></tr>
<tr><td colspan="4">Management/Supervisory Responsibilities:
As a line manager, responsibilities include all business, operations, and human resource management actions/issues.</td></tr>
<tr><td colspan="4">Working Conditions: Office and computational work and frequent domestic and foreign travel.</td></tr>
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Name: Paul J. Dotson	**Organization:** T-DO, Theoretical Division Office		
Job Title: Deputy Division Leader	**Series/Level:** TSM	**Pay Basis:** Exempt	**Clearance Level:** Q
Reports to: Alan Bishop, Theoretical Division Leader			

Summary: The Theoretical Division strives to recruit the best scientific minds and capabilities to further our scientific understanding of the physical world and to establish a technical foundation for both current and future national defense, industrial and civilian needs. This foundation fosters the exploration of interdisciplinary frontiers of scientific endeavor. In brief, the Division's three central mission elements are to provide the best science and scientists to LANL national security missions; pursue frontier science to ensure excellence in science capabilities for LANL and the nation; and to create new scientific directions and attract scientific leaders to LANL. As a member of the Division management team, the deputy division leader works in conjunction with the division leader to provide external visibility for the Division, leadership for collaborations for solving challenging and complex scientific problems, is responsible for promoting operational and scientific excellence, and provides scientific, technical and operational leadership to a workforce of approximately 400 in 13 groups and a Laboratory center with an annual budget of approximately $85M. The deputy division leader leads by example and nurtures a safe, secure, stimulating, productive, and cost-effective work environment, providing direction and priorities to groups and programs, and addresses Laboratory goals in recruiting, diversity, ISM, ISSM, maintains positive, effective working relationships within the Division, with other managers and researchers at the Laboratory, and with external customers, sponsors, and stakeholders.

Primary Functions and Responsibilities (may not include all duties assigned): Together with the division leader, the deputy division leader provides leadership and management of T Division, including overall effectiveness of research and operations. Effective establishment and maintenance of an active recruiting pipeline, including nurturing and succession planning of the next generation of the Division's leaders (technical, team, project, group, and division). Responsible for ISM, ISSM, resource management, and other priorities/goals of the Laboratory. Provide top-level support for program execution/development. Responsible for strategic planning, productivity and quality assessment, organization and sizing, allocation of space and facilities, and effective use of institutional resources allocated to the Division. Responsible for the safety of Division employees, ensuring all relevant security requirements are adhered to, minimizing the environmental impact of the Division, and adherence to all applicable Laboratory and DOE policies. The deputy division leader is expected to maintain active research interests while providing technical vision to nurture and support existing programs of others throughout the Division.

Required Knowledge, Skills and Abilities: Demonstrated knowledge and research experience in one or more of the Division's technical focus areas. Demonstrated high impact in the technical community through an extensive history of refereed publications, invited talks at national and international conferences, participation in professional societies, service to the scientific community, and other professional accomplishments. A strong record of significant expertise and distinguished scientific and managerial accomplishment demonstrating the following scientific leadership characteristics/skills: ability to effectively lead change; ability to develop people, including future leaders; experience building and maintaining effective leadership teams; demonstrated drive for excellence and results; ability to build and sustain effective sponsor relationships; and exemplary personal accountability, integrity, and trust building skills. Demonstrated interpersonal and communication skills, including proactive and decisive handling of all personnel issues. Demonstrated commitment to high-quality operations and execution of defense and basic research activities, including scientific excellence, safety, security, environment, diversity, recruiting, retention, employee development, conflict resolution, fiscal responsibility, encouragement of innovation and risk-taking, program development, and project management.

Desired Knowledge, Skills, and Abilities: Knowledge of national defense science and technology related to weapons of mass destruction, energy security, homeland defense, conventional munitions, and the international intelligence community. Ability to obtain intelligence compartmented clearances. Demonstrated program development success.

Management/Supervisory Responsibilities: As a Division line manager, responsibilities include all business, operations, and human resource management actions/issues across the Division. Function as division leader in the leader's absence.

Working Conditions: Office work and frequent domestic and foreign travel.

Name: Alan R. Bishop	**Organization:** T-DO, Theoretical Division Office		
Job Title: Division Leader	**Series/Level:** TSM	**Pay Basis:** Exempt	**Clearance Level:** Q
Reports to: Associate Director for Strategic Research			
Summary: The Theoretical Division strives to recruit the best scientific minds and capabilities to further our scientific understanding of the physical world and to establish a technical foundation for both current and future national defense, industrial, and civilian needs. This foundation fosters the exploration of interdisciplinary frontiers of scientific endeavor. In brief, the Division's three central mission elements are to provide the best science and scientists to LANL national security missions; pursue frontier science to ensure excellence in science capabilities for LANL and the nation; and to create new scientific directions and attract scientific leaders to LANL. The division leader provides external visibility for the Division and leadership for collaborations for solving challenging and complex scientific problems, is responsible for promoting operational and scientific excellence, and provides scientific, technical, and operational leadership to a workforce of approximately 400 in 13 groups and a Laboratory center with an annual budget of approximately $85M. The division leader leads by example and nurtures a safe, secure, stimulating, productive, and cost-effective work environment, providing direction and priorities to groups and programs. The division leader effectively addresses Laboratory goals in recruiting, diversity, ISM, ISSM, and maintains positive, effective working relationships within the Division, with other managers and researchers at the Laboratory, and with external customers, sponsors, and stakeholders. The division leader is an active member of the SR Directorate management team, supports Laboratory mission planning and goals, and is also expected to team with other division and program directors to be a major contributor to the strategic planning, policy definition, and decision-making for the Laboratory.			
Primary Functions and Responsibilities (may not include all duties assigned): Leadership and management of T Division, including overall effectiveness of research and operations. Effective establishment and maintenance of an active recruiting pipeline, including nurturing and succession planning of the next generation of the Division's leaders (technical, team, project, group, and division). Responsible for ISM, ISSM, resource management, and other priorities/goals of the Laboratory. Provide top-level support for program execution/development. Responsible for strategic planning, productivity and quality assessment, organization and sizing, allocation of space and facilities, and effective use of institutional resources allocated to the Division. Responsible for the safety of Division employees, ensuring all relevant security requirements are adhered to, minimizing the environmental impact of the Division, and adherence to all applicable Laboratory and DOE policies. The T Division Leader is expected to maintain active research interests while providing technical vision to nurture and support existing programs of others throughout the Division.			
Required Knowledge, Skills and Abilities: Demonstrated knowledge and research experience in one or more of the Division's technical focus areas. Demonstrated high impact in the technical community through an extensive history of refereed publications, invited talks at national and international conferences, participation in professional societies, service to the scientific community, and other professional accomplishments. A strong record of significant expertise and distinguished scientific and managerial accomplishment demonstrating the following scientific leadership characteristics/skills: ability to effectively lead change; ability to develop people, including future leaders; experience building and maintaining effective leadership teams; demonstrated drive for excellence and results; ability to build and sustain effective sponsor relationships; and exemplary personal accountability, integrity, and trust building skills. Demonstrated interpersonal and communication skills, including proactive and decisive handling of all personnel issues. Demonstrated commitment to high-quality operations and execution of defense and basic research activities, including scientific excellence, safety, security, environment, diversity, recruiting, retention, employee development, conflict resolution, fiscal responsibility, encouragement of innovation and risk-taking, program development, and project management.			
Desired Knowledge, Skills, and Abilities: Knowledge of DOE, NNSA, DoD, and DHS, as well as other national and international programs of relevance to the Division's activities. Practical knowledge of Laboratory operations and administration practices and procedures.			
Management/Supervisory Responsibilities: As a line manager, responsibilities include all business, operations, and human resource management actions/issues. The deputy division leader, group leaders, CNLS Center Leader, and division office support staff all report directly to the division leader.			
Working Conditions: Office work and frequent domestic and foreign travel.			

Appendix F – Division Capabilities Quick Reference Guide

A posteriori error estimates: T-7
Ab initio molecules & solids: T-1, -11, -12
Accelerator design: T-8
Adaptive mesh methods: T-1, -3, -6, -7
Adaptive optics: T-4
Agent-based modeling: T-7, -13, T-DO
Aqueous solutions/solvation: T-10, -12
AIDS virus mechanics, applications, & research: T-7, -8, -10
Algorithms for scientific computing: T-6, -7, -8, -11, -12, -13, CNLS
Analysis of frequent patterns: T-13
Anomalous fluctuations in nuclear reactions: T-13
Antihydrogen formation: T-4
Applied mathematics: T-7, -13, CNLS
Approximation theory: T-7
Astrophysics: T-4, -6, -8, -15, -16
Atomic struct., collisions, kinetics, & spectroscopy: T-1, -4, CNLS

Beams: T-15; (nuclear astrophysics & radioactive): T-6, -16
Biocatalysts: T-10
Bioinformatics: T-7, -10, -13
Biomaterials & biomechanics: T-3
Biological systems: T-7, -10, -12, -13, CNLS
Biophysics: T-7, -8, -10, -11, -12, -13, CNLS
Biothreat risk analysis: T-10
Black holes: T-6
Bose-Einstein condensation: T-4, -12 , -13, CNLS

Casting: T-3
Cell receptors: T-10, -12
Cell signaling: T-10, -12
Cellular biology analysis: T-7, -10, -13
Cellular materials: T-3
Ceramic research: T-1
Chemical industries: T-3, -12
Chemical reactions/processes: T-3, -12, -14, CNLS
Chiral perturbation theory: T-8, -16
Coding theory: CNLS
Cold atoms: T-4
Combustion systems: T-3, -6, -12
Comets & asteroids: T-6
Compact stellar remnants: T-6
Complex fluids: T-3, -7, -12. -13, CNLS
Complex networks: T-7, -10, -13, CNLS
Complex systems and biological networks: T-10
Composite research: T-1, -3, -12
Computational electromagnetics: T-7
Computational fluid dynamics: T-3, -6, -7, -12, -13, CNLS
Computational geometry: T-7
Computer-aided manufacturing: T-3
Computers (large quantum): T-13, CNLS
Condensed matter statistical physics: T-11, -12, CNLS
Condensed matter theory: T-7, -11, -12, CNLS
Conformal field theory: T-8
Continuum mechanics: T-3, -13
Cosmic large-scale structure: T-6, -8
Cosmic magnetic field phenomena: T-3, -6
C-P violations: T-6, -8, -16

Degenerate fermionic gases: T-4
Dense plasmas: T-4, -6, -12, -15
Design of solid state quantum computers: T-13
Developmental genetics: T-13
DNA sequences (pattern recognition): T-7, -10, -13
DNA & RNA structure & dynamics: T-10, CNLS
Dynamical systems (mathematics): T-7, -13, CNLS
Dynamics & kinetics of chemical reactions: T-12

Early universe: T-6, -8, T-DO
Electrodynamics: T-15
Electromagnetic interactions: T-6, -8, -16
Electromagnetic propagation: T-4
Electronic & structural principles: T-1, -11, -12, T-DO
Electronic structure calculations: T-1, -10, -11, -12
Electroweak interactions: T-6, -16
Elementary particle interactions: T-8
Epidemiology: T-6, -7, -8, -10, -13, CNLS
Equation of state: T-1, -4, -6, -12, -14
Environmental systems: T-7, -12
Exhaust studies: T-3
Exotic atoms & molecules: T-4
Exotic nuclei: T-6, -16
Explosives: T-3, -12, -14

Ferrous metals: T-3
Few-body (exact calculations): T-16
Fission & fusion reactor analysis: T-16
Fluid structure interactions: T-3
Forces at atomic, molecular, & solid level: T-11, -12, -14, CNLS
Frequency conversion: T-4
Fusion energy: T-15

Gas phase & condensed phenomena: T-12

Gas process chemistry: T-3
Gene expression analysis: T-10, -13
General relativity: T-6, -8
Geometrical mechanics: T-7
Geosciences: T-3, -7
Global climate studies: T-3, -7
Grid generation/optimization: T-1, -3, -7

Hadron spectrum calculations: T-8
Hadronic scattering: T-6, -16
Hadrons: T-8, -16
HCV sequence database: T-10
Hearing processes: T-DO
Heat transfer: T-3
Heavy ions: T-8, -16, T-DO
High explosives: T-3, -12, -14
High-spin states in nuclei: T-DO
High-temperature superconductors: T-11, CNLS
HIV studies: T-7, -8, -10
HIV sequence database: T-10
Hohlraum spectroscopy: T-4
Homology and comparative modeling: T-10
Host-pathogen interactions: T-10
Hydrodynamics & shock interactions: T-3, -6, -7, -12, -13, -14
Hydrophobic effects: T-10, -12

Image analysis development: T-1, -7, -12, CNLS
Immune response: T-10
Influenza sequence database: T-10
Information scanning & gathering: T-13
Information sciences: CNLS
Integratable systems: T-7, -13, CNLS
Interface between nuclear & particle physics: T-6, -16
Intermetallic research: T-1, -11
Ion traps: T-4
Isomer physics: T-6, -16

Large data set analysis: T-6, -7, CNLS
Large-scale simulation of biomolecular complexes: T-10
Laser-matter interactions: T-4, -13
Lasers: T-4
Linear & nonlinear solvers: T-3, -7, CNLS
Liquids: T-3, -10, -12

Many body condensed matter theory: T-11, CNLS
Martensites & shape-memory alloys: T-11
Mass transfer: T-3

Materials:
  Atomistic simul. of: T-11, -12, CNLS
  Behavior: T-11, -12
  Burn process in: T-14
  Composites & casting: T-3
  Mathematical probl. in mat. sci.: T-3, -7, -13. CNLS
  Memory (shape-alloy): T-3, -7, -11
  Microscopic modeling of: T-11, -12, CNLS
  Organic materials: T-11, -12, -14
  Properties library: T-1
  Static & dynamic properties of: T-1, -11, -12
  Study of physics & chemistry of: T-11, -12
  Thermodynam. & mech. behav. of: T-1, -3, -11, -12, 13
Mathematical biology: T-10
Mesh generation modeling: T-3, -7
  Membrane: T-10
  Membrane proteins: T-10
Micromechanics: T-3
Mimetic discretization methods: T-7
Modeling: all groups
Molecules:
  Biology: T-10, -12, CNLS
  Calculating electronic properties: T-12
  Catalysts: T-12
    Biocatalysts: T-10
  Determining shapes: T-13
  Large-scale molecular dynamics: T-10, -11, -12, CNLS
  Ligand binding: T-10, -12
  Properties: T-12, -14, CNLS
  Protein folding: T-10, -12
  Transcriptional control: T-11, -13, CNLS
Molecular genetics: T-13
Multigrid methods: T-3, -6, -7
Multiphase flow: T-3, -13
Multiscale physics modeling: T-3, -6, -7, -11, CNLS
Multiscale materials: T-1, -3, -11, -12, -14, CNLS
Muonic & antiprotonic atoms: T-4

Nanotechnology: T-8, -11, -12, -13, CNLS
Nebulae & interstellar matter: T-4, -6
Neural network pattern recognition: T-10, -13, -16
Neurophysics: T-11, CNLS
Neutron sources: T-15
Neutrino properties: T-6, -8, -16
Nonequilibrium kinetics: T-4, -12
Nonequilibrium statistical mechanics: T-1, -8, -12, -13, CNLS
Nonlinear physics: T-7, -8, -11, -13, CNLS
Nonlinear systems analysis: T-3, -7, -12, -13, CNLS
Nuclear & conventional defense: T-1, -3, -13
Nuclear applications: T-6, -16
Nuclear astrophysics: T-6, -16

Nuclear data libraries: T-16
Nuclear physics: T-6, -16
Nuclear reaction mechanisms: T-6, -16
Nuclear structure studies: T-6, -16, T-DO
Numerical analysis: T-3, -7

Object-oriented scientific computing: T-3
Ocean circulation models: T-3
Ocean dynamics (long-term): T-3, -7
Oil process chemistry: T-3, -12
Opacities & interactive website: T-4, -6
Optical properties of materials: T-11, -12, CNLS
Optics: T-4
Organic device physics: T-11, -12

Parallel algorithms : T-3, -6, -7, -8, -10, -11, -12, CNLS
Partial differential equations: T-7, -13, CNLS
Pattern recognition: T-1, -10, -12
Petroleum recovery: T-7, -13
Phase transformations in materials: T-3, -11, -12
Phylogenetics and evolution: T-10
Photonics: T-7, -12, -13, CNLS
Plasma behavior: T-3, -12
Plasma physics theory: T-13, -15
Polymer chemistry & physics: T-11, -12, -14, CNLS
Proliferation issues: T-6, -14, -16
Properties: transcriptional control: CNLS
Protein-ligand interactions: T-10
Protein structure & folding: T-10, -12, -13, CNLS

Quantum chemistry: T-12
Quantum chromodynamics: T-8
Quantum computing: T-4, -8, -11, -13, T-DO, CNLS
Quantum field theory: T-8, -11
Quantum measurement: T-8, -13
Quantum Monte Carlo: T-11, -16
Quantum neural technologies: T-13
Quark-gluon plasma: T-8, -16
Quasars & galaxy formation: T-6

Rare isotope accelerators: T-6, -16
Radiative/collisional processes in plasmas: T-4, -12
Radiochemistry: T-6
Reactor safety: T-3, -16
Reaction theory: T-6, -12, -16
Reactive flow: T-3, -6, -12, -14
Receptor-ligand interactions: T-10, -12

Scaling laws: T-8
Semiconductors: T-1, -11, -12
Sequence analysis: T-10
Signal processing: T-1, -7, -12, T-DO
Simulations: all groups
Soft matter: T-11, -12, -13, CNLS
Software engineering: T-7
Solar & stellar physics: T-3, -4, -6
Solitons in transmission lines: T-7, CNLS
Statistical physics: T-1, -7, -8, -10, -11, -12, -13, CNLS
Stochastic equations: T-7, -8, -11, -13, CNLS
Stochastic processes T-7, -11, -12, -13
Stockpile safety: T-DO
Structural pathomics
Structural modeling of biomolecular complexes
Superconductivity theory: T-11
Supernovae: T-6, -16
Systems, accelerator-driven (reactions & scattering in): T-16

Theoretical physics: all groups
Theoretical biology: T-10
Theoretical biophysics: T-10
Tokomak disruptions: T-15
Transition from quantum to classical physics: T-8, -13
Turbulence studies: T-3, -7, -13, CNLS

Ultracold plasmas: T-4
Uncertainty quantification: T-6, -7, -13, -16
Upscaling: T-7, -13

Vaccine design: T-10
Viral diseases & dynamics: T-6, -7, -8, -10, CNLS

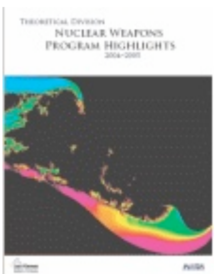
Warm Dense Matter: T-15
Wavelet theory: T-1, -7, -12, -14, -DO, CNLS
Weapons suppport: most groups to varying degrees
- Certification methodology: T-13
- Conventional: T-3
- Equation of state: T-1, -12
- Explosives: T-12, -14
- Fluid dynamics: T-3, -7, -13
- High-energy density physics: T-4, -6
- Materials: T-11, -12
- Nuclear: T-3, -6, -16
- Opacities: T-4
- Sensitivity Studies: T-6

Wildfire studies: T-3

Appendix G – List of Referenced Documents

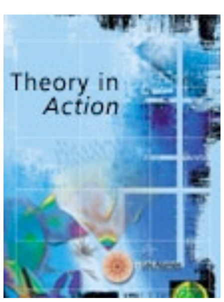
Publications are available on the Theoretical Division web site at
http://www.lanl.gov/orgs/t/publications.
Hard copies may be obtained by contacting the Division Office at 505-667-4401.

The *Annual Self-Assessment*, an institutional document, includes an organizational summary, details about the Division's current thrust areas, its contributions to Appendix F measures, and data on publications, invited presentations, honors, awards, professional memberships, and other statistics about the Division and its technical staff. The most current version, *Self-Assessment 2004-2005* (LA-UR-05-2732) is available at www.lanl.gov/orgs/t/publications/self_assessment_2005.shtml. Versions from previous years are available in hard copy.



Theoretical Division's *Nuclear Weapons Program Highlights* is published annually, usually in late spring. This publication contains two-page unclassified technical highlights of research and projects in support of the Laboratory's Nuclear Weapons Program. *Nuclear Weapons Program Highlights 2004-2005* (LA-UR-05-3853) is at www.lanl.gov/orgs/t/publications/research_highlights_2005.shtml. Versions from previous years are available in hard copy.

Theoretical Division Research Highlights document complements the annual Self-Assessment document. Organized by group/discipline, this publication contains two-page technical highlights of research conducted by the Division staff over the previous year and reflects the broad spectrum of problems and projects addressed by T Division. (This publication was previously titled "Special Feature.") *Research Highlights 2005* (LA-UR-05-1500) can be found on the web at www.lanl.gov/orgs/t/publications/research_highlights_2005.shtml. The previous year's version, *Special Feature 2004*, is at www.lanl.gov/orgs/t/publications/docs/special_feature2004.pdf. Versions from previous years are available in hard copy.



Composed of contributions from more than 90 distinguished Theoretical Division staff and alumni, this two-volume book—*Theory in Action, Highlights in the Theoretical Division at Los Alamos 1943–2003* (LA-14000-H)—is an archival window into six decades of creativity, major discipline and mission challenges, and successes. The book addresses 19 areas of research that extend to virtually every major technical initiative at Los Alamos. It is on the web as a PDF at www.lanl.gov/orgs/t/publications/docs/theory_action2004.pdf.

Formed in October 1980, the Center for Nonlinear Studies (CNLS) organizes research related to nonlinear and complex systems phenomena. More information, publications, and details on current activities can be found at http://cnls.lanl.gov/External/.

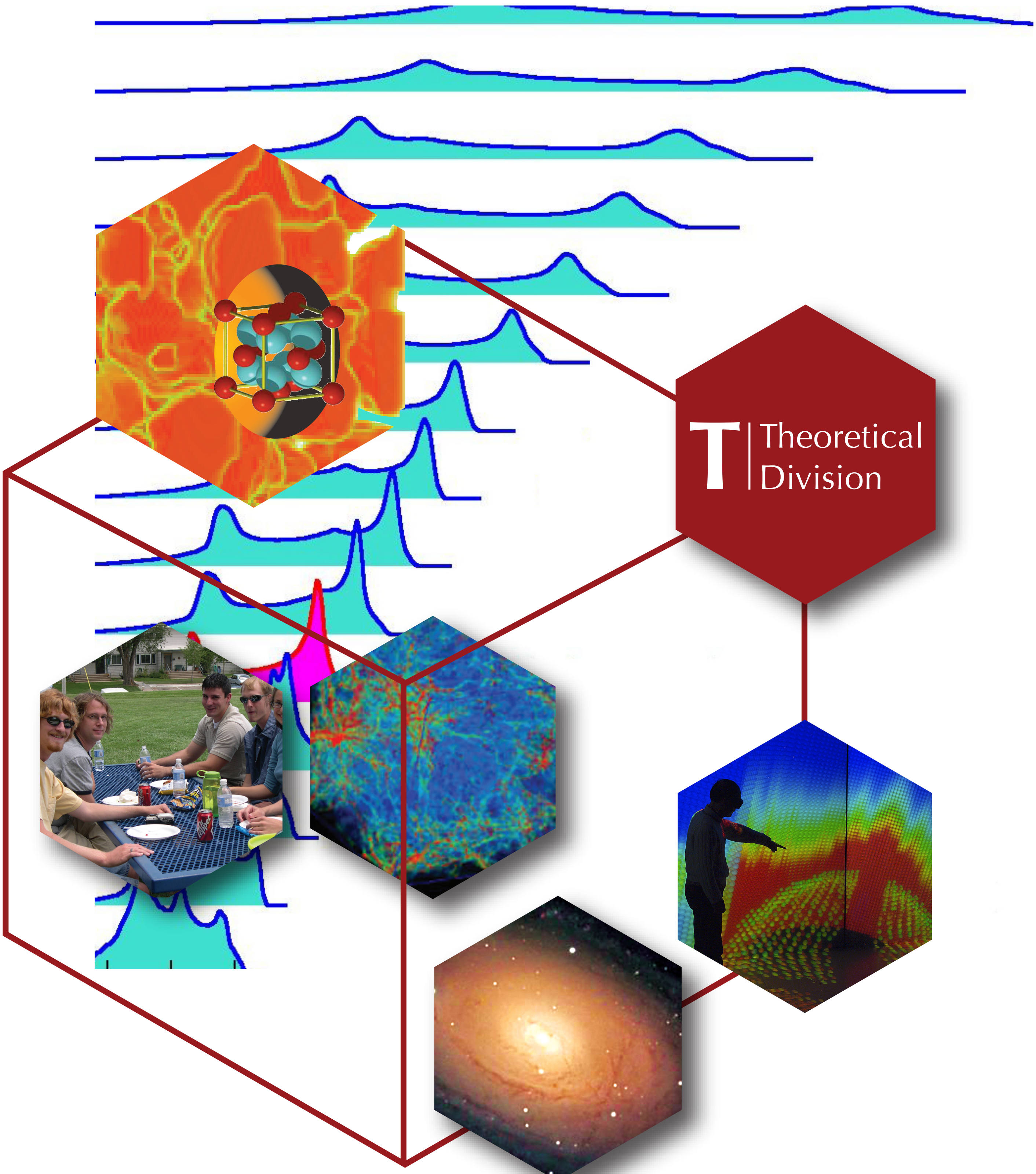
- Theoretical Division Review Committee reports are available on a limited distribution basis. Requests should be made to the Theoretical Division Office, 505-667-4401.

- Detailed descriptions of each group in the Theoretical Division are available upon request; contact the Theoretical Division Office, 505-667-4401.

Appendix H – Acronym List

Acronym	Definition
AAAS	American Association for the Advancement of Science
AFCI	Advanced fuel cycle initiative
AFOSR	Air Force Office of Scientific Research
AGEX	above ground experiments
AGN	active galactic nuclei
ARDA	advanced research and development activity
ARO	Army Resource Office
ASC	Advanced Simulation and Computing
ASCR	Advanced Scientific Computing Research
ATLAS	Advanced test line for actinide separations
AWE	UK Atomic Weapons Establishment
BEC	Bose Einstein condensate
C Division	Chemistry Division
CARE	Cooperative Agreement on Research and Education
CDC	Centers for Disease Control and Prevention
CEA	Comissariat á l'Énergie Atomique (France)
CHS	Center for Homeland Security
CINT	LANL Center for Integrated Nanotechnologies
CMR	colossal magnetoresistance
CNLS	Center for Nonlinear Studies
COSIM	LANL Climate, Ocean and Sea Ice Modeling project
CRADA	Cooperative Research & Development agreement
CTCP	Center for Theoretical and Computational Pathomics
DARHT	Dual-Axis Radiographic Hydrodynamic Test
DARPA	Defense Advanced Research Projects Agency
DHS	Department of Homeland Security
DoD	Department of Defense
DOE	Department of Energy
DOE/DP	DOE/Defense Programs
DOE/EERE	Energy Efficiency and Renewable Energy
DOE/NN-20	DOE/Nuclear Nonproliferation
DOE/SC	DOE Office of Science
TRC/DART	Total Recordable Cases/Days Away From Work, Restricted Work Activity, or Transfers to Another Job
DSW	Directed Stockpile Work
DTRA	U.S. Defense Threat Reduction Agency
EOS	equation of state
EOS-MOM	Equation of State and Mechanics of Materials
ESC	enhanced surveillance campaign
HCV	Hepatitis C virus
HE	High Explosives
HHS	US Department of Health and Human Services
HS	Homeland Security
IETS	Inelastic Electron Tunneling Spectroscopy
ISM	Integrated Safety Management
ISSM	Integrated Safeguards & Security Management
IWM	Integrated Work Management
JINA	Joint Institute for Nuclear Astrophysics
LANL	Los Alamos National Laboratory
LANSCE	Los Alamos Neutron Science Center

Acronym	Definition
LDRD	Laboratory Directed Research and Development
LDRD DR	LDRD Directed Research
LDRD ER	LDRD Exploratory Research
LEP	Life Extension Project
LLNL	Lawrence Livermore National Laboratory
MD	Molecular Dynamics
MEAM	Modified embedded atomic method
MSEC	Materials, Science, and Engineering Council
NASA	National Aeronautics and Space Administration
NCAR	National Center for Atmospheric Research
NETL	National Energy Technology Laboratory
NHMFL	National High Magnetic Field Laboratory
NIF	National Ignition Facility
NIH	National Institutes of Health
NISAC	National Infrastructure Simulation and Analysis Center
NMR	nuclear magnetic resonance
NMT Division	Nuclear Materials Technology Division
NNSA	National Oceanic and Atmospheric Administration
NOAA	National Renewable Energy Laboratory
NREL	
NSA	National Security Administration
NSF	National Science Foundation
NW	Nuclear Weapons
OLED	organic light emitting diode
ORNL	Oak Ridge National Laboratory
OSTP	U.S. Office of Science and Technology Policy
PI	Principal Investigator
PNAC	Particle and Nuclear Astrophysics and Cosmology
POC	point of contact
QCD	Quantum Chromodynamics
QMD	Quantum Molecular Dynamics
QMU	Quantification of Margins and Uncertainty
RHIC	relativistic heavy ion collider
RRW	Robust Replacement Warhead
SBP/CS	Science-based Prediction for Complex Systems
SciDAC	DOE Scientific Discovery through Advanced Computing
SDSS-II	Sloan Digital Sky Survey
SFI	Santa Fe Institute
SNL	Sandia National Laboratories
SR	Strategic Research Directorate
SSC	Supernova Science Center
STB	Science and Technology Base Programs
TDRC	Theoretical Division Review Committee
TR	Threat Reduction
UC	University of California
UNM	University of New Mexico
UQ	Uncertainty Quantification
V&V	Verification & Validation
WP	Weapons Physics Directorate
WSR	Weapon Supporting Research



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