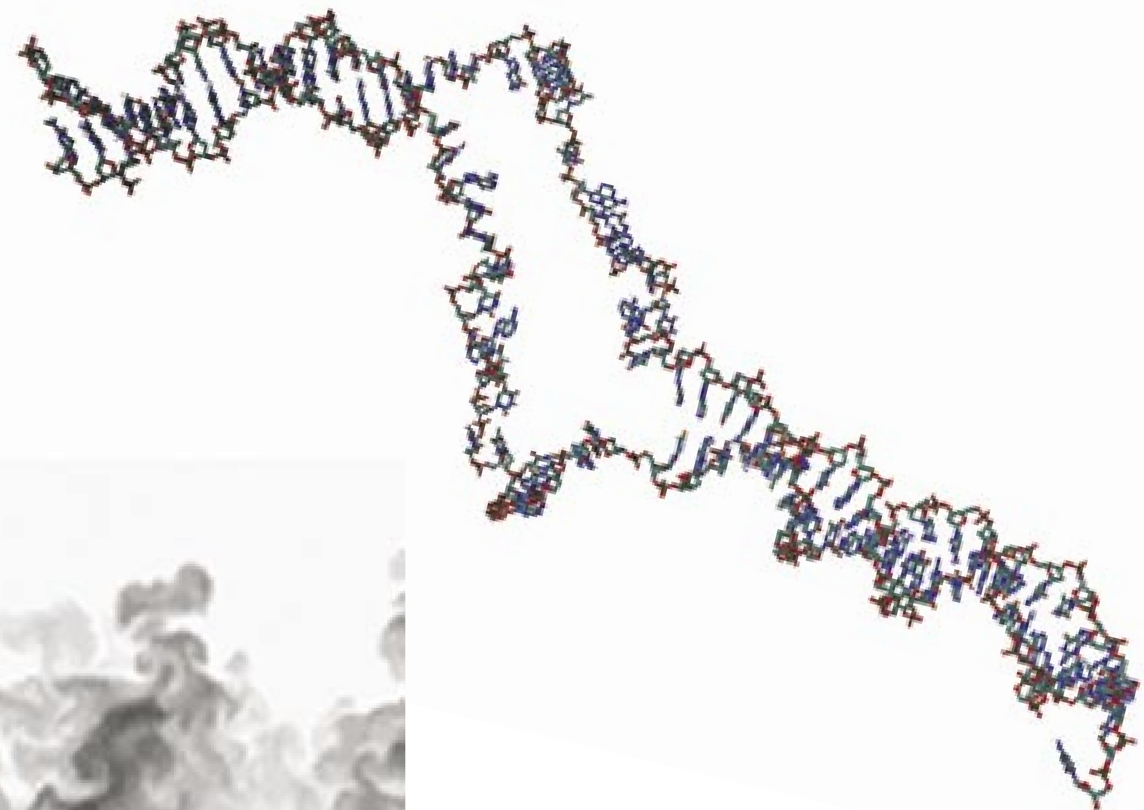
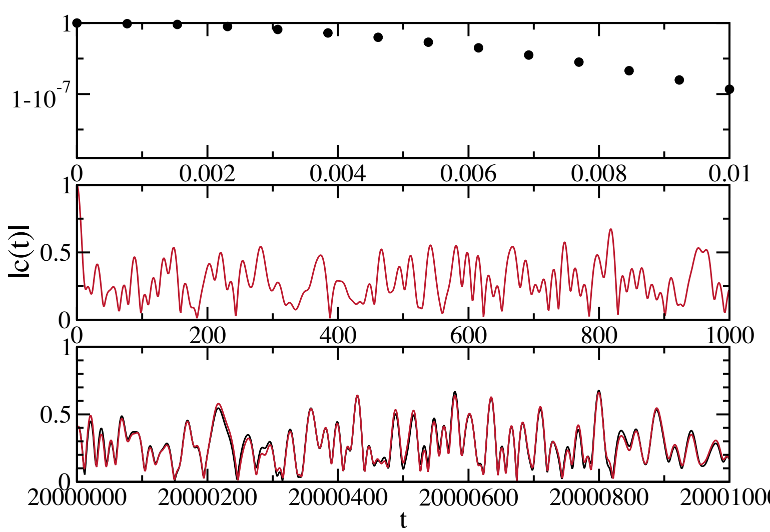
Division Scientific Thrusts





DIVISION SCIENTIFIC THRUSTS

Scientific thrust areas are an integral component of the T Division Strategic Plan. They identify areas where the Division can make significant scientific and technical contributions to the Laboratory mission, and are used to focus scientific and managerial resources on areas that will provide a significant return on investment in new science, programs, and recruitment. The current thrust areas are:

- Science-Based Prediction for Complex Systems, including:
  —Innovative Science in Support of Stockpile Stewardship (including a developing thrust in High Energy-Density Physics) and
  —Predictive Science and Technology for Threat Reduction and Homeland Security.
- Modeling Biological Processes
- Fundamental Processes (including a developing thrust in Astro-Nuclear-Particle Physics)
- Advanced Scientific Computing Research

Science-Based Prediction for Complex Systems

Coordinating and supporting T Division's response to Laboratory Strategic Goal A, Science-Based Prediction for Complex Systems, is critical given that virtually every major initiative at the Laboratory—from stockpile stewardship to the network analysis of living organisms—relies heavily on Goal A elements. To accomplish its National Security missions, the Laboratory has assembled its core expertise in the integration of experiment, theory, and computation to advance scientific understanding of and predictive capabilities for complex phenomena. This strategy will require a new generation of major ideas and concepts to improve the fidelity, reliability, and usability of the tools for predictive science. The following examples are illustrative of implementation goals.

Nuclear Weapons. T Division research in nuclear and atomic physics, materials science, hydrodynamics, and uncertainty quantification is used in the Laboratory's Applied Physics (X) Division design and certification programs. Science-Based Prediction for Complex Systems will integrate experimentally validated theoretical advances with measured data from all relevant experiments (including from NNSA's unique facilities).

Homeland Security. To meet scientific challenges posed by threat reduction and to tie together Science-Based Prediction for Complex Systems and homeland security goals, T Division's broad range of enhanced predictive capabilities (nuclear physics, theoretical chemistry, biology, complex systems, data analysis, numerical algorithms) is being adapted and applied to homeland security problems such as securing and improving infrastructure integrity, developing detection and attribution tools, and biothreats.

Biology. Entering a phase of quantitative predictive science, biology is evolving from its gene-sequencing focus toward a dependence on scientific computation for modeling genetic and other cellular complexity. One biology focus is computation of protein structure and binding, which will support more efficient new drug discovery. Development of vaccines against rapidly evolving viruses (e.g., influenza and HIV) is another theoretical focus relevant to public health and national security.

Energy and Environment. Assessment of the cost and efficacy of strategies for energy production and environmental remediation requires developing and applying predictive methods for multiscale modeling to problems for which experimental and observational data at many length scales are available, in order to validate predictive scaling techniques.

Enabling Scientific Tools. Progress in the predictive science of complexity will require vigorous development of supporting science in, for example, uncertainty quantification, advanced software design, modeling multiscale and nonequilibrium processes and complex stochastic processes, effective data-utilization methods, and agent-based models, and other methods for modeling complex and adaptive networks.

Successful accomplishment of this thrust necessitates strengthening existing partnerships and developing new partnerships with both internal and extramural groups. Existing partners include X, DX, CCS, EES, ESA, MST, and D Divisions at the Laboratory, and the Department of Defense (DoD), the National Institute of Health (NIH), numerous universities, and industrial organizations such as Procter & Gamble and Motorola. Through this thrust, a new generation of predictive capabilities will be available to a customer base that includes the National Nuclear Security Administration (NNSA) and other Department of Energy (DOE) programs, DoD, NIH, and private industry.

Goals/Activities for 2004–2005:

- Maintain a strong presence in stockpile stewardship by serving on boards that govern the planning process.
- Continue summer programs in epidemiology for students and visitors.
- Respond to invitations for pilot projects in science-based prediction.
- Align LDRD-DR and pilot project proposals with Division thrusts and other Laboratory Goals.
- Execute the Director's funded *Systems Modeling at LANL* proposal using agent-based modeling and other tools.
- Play an active role on the Predictive Science Advisory Council at Los Alamos.
- Continue T Division participation in *LA Science* publications on science-based prediction.
- Plan a joint LANL-Santa Fe Institute-European Union workshop on science-based prediction.

Funding Sources: Laboratory Directed Research and Development (LDRD), DOE/Nuclear Nonproliferation, Defense Threat Reduction Agency (DTRA), Defense Advanced Research Projects Agency (DARPA), National Infrastructure Simulation and Analysis Center (NISAC)

Innovative Science in Support of Stockpile Stewardship

The purpose of this thrust is to create more accurate fundamental physics models and data through integration of experiment, theory, and computation; enhance the science of certification in partnership with the goals of the Nuclear Weapons Directorates; and exploit the large investment in T Division's basic science, which creates numerous opportunities to bring innovative ideas from other areas of science into weapons physics.

In support of the mission to certify the stockpile in the absence of nuclear testing, T Division research brings together numerous innovative scientific concepts conducted via collaborative workgroups comprised of T Division scientists, X Division designers and code integrators, and experimentalists in P, C, LANSCE, MST, DX, and ESA Divisions at the Laboratory, as well as from Lawrence Livermore National Laboratory (LLNL) and Bruyères-le-Châtel (CEA) in France. Such collaborations ensure that theoretical advances will be motivated and validated by experiments, assessed in an integrated design context, and ultimately used in certification for the nuclear weapons program, the primary customer for this research. Other customers are found throughout DOE Science and Technology programs, particularly those benefiting from a new generation of simulation science or those involved in threat reduction and homeland security initiatives.

Efforts are also coordinated with non-weapons basic research initiatives. Subtle variations in stockpile manufacturing and aging characteristics must be accounted for with enhanced fidelity in the maintenance of the stockpile. The demonstration of applications to problems outside the weapons arena broadens the approach and leverages investments in those non-weapons areas.

Goals/Activities for 2004–2005:

- Nuclear and atomic physics and interactions of matter with radiation—nuclei far from stability, quantum molecular dynamics simulations of density effects, novel diagnostics for mix, nonequilibrium processes for Boost, and opacities.
- Materials science—constitutive formulations developed from multiscale modeling for metals, high explosives, polymers and other weapons materials; reaction laws; aging analysis and prediction; and equations of state.
- Numerical methods and software for hydrodynamics (e.g., advanced hydrodynamics and solver algorithms, interface treatments, constitutive laws for particular mesh resolutions).
- Uncertainty quantification—metrics for stockpile certification and weapons physics, analysis of experimental data (both historical and modern).
- Directed Stockpile Workload, pit surveillance, and enhanced surveillance and manufacturing.
- Strongly coupled plasmas.
- 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).

Funding Sources: NNSA, LDRD

Division Scientific Thrusts

High Energy-Density Physics

High Energy-Density Physics (HEDP) is the study of matter under conditions that exceed one megabar in pressure, which includes environments such as giant planet interiors, white dwarf interiors, inertial confinement fusion implosions, and laser-matter interaction experiments. There are numerous Los Alamos opportunities in HEDP, with established and new collaborations in place, as well as mechanisms to help increase interactions. The Laboratory's Science Roadmaps are great opportunities to expand HEDP science.

An enhanced HEDP program contributes to other National and Laboratory goals such as science-based prediction of complex systems, materials science, and energy security (fusion). HEDP is also a highly visible science area and extremely valuable for external collaborations and recruitment opportunities. The research areas of several T Division groups, particularly T-1, -3, -4, -6, and -15, fall naturally under the HEDP umbrella, with smaller efforts in other groups (e.g., T-12 and T-13) falling within HEDP. The thrust area has three focus topics: nonequilibrium phenomena, radiation hydrodynamics, and quantum simulation methods.

Goals/Activities for 2004–2005:

- Enhance HEDP programs with a more dedicated funding base and research themes at Los Alamos, including promoting coordination across groups/divisions and program boundaries.
- Coordinate closely with experimental activities being carried out at the Laboratory, in particular with P Division, and other international efforts, including CEA (Paris).
- Conduct innovative HEDP science important to the weapons program.
- Develop predictive models of matter under HEDP conditions.
- Develop long-range hiring strategy with line and program input, and hire new staff and post-docs in key areas.

Funding Sources: NNSA, LDRD

Predictive Science and Technology for Threat Reduction and Homeland Security

One of the greatest consequences of the events surrounding September 11, 2001, 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 systems work at a fundamental level, particularly in response to our rapidly changing global system.

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

This thrust includes the development of an understanding of the following scientific grand challenge areas: (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, and (4) quantified treatments of social and cognitive behavior to address complicating issues of individual behavior, societal influences, and response to threats. These grand challenge areas 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, etc.

The approach taken to develop this thrust is to: (1) address threat identification, prevention, response and attribution—sharing resources and creating an integrated approach; (2) identify technological synergy across chemistry-biological, radiological-nuclear, and critical infrastructure protection threats; (3) reduce the cost of threat protection by adding protection/response to existing or planned functions (e.g., combine detection and response to man-made biothreats to an improved day-to-day public health system); (4) coordinate with Laboratory Strategic Plan, other divisions and outside resources to amplify the T Division's distinguishing 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 of the formation of terrorist networks in the Middle-East (T-13 Threat Anticipation Modeling Project). Again, T Division leads the Nation in the modeling of epidemics resolved at the National scale—280 million people (T-10, T-11, and T-3 EpiCast Project). T Division has also shown leadership in developing new program areas, for example, by extending the Science-Based Prediction methodologies developed in the Nuclear Weapons (NW) programs to Threat Reduction 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.

Goals/Activities for 2004-2005:

- Actively engage in planning and program development activities within T Division, the Center for Homeland Security (CHS), and national agencies to contribute to the Laboratory-wide program creation.
- Identify and grow technical thrust areas in Threat Reduction within T Division. In particular, build upon successful programs such as the Threat Anticipation Modeling Project, EpiCast, pathogen databases, and computational immune and system biology, particularly in new growth areas of water, plant, and animal vulnerabilities.
- Coordinate within the Associate Directorate for Strategic Research (ADSR) and with the Center for Homeland Security to develop hiring and resource plans to address growing needs, including activating CNLS resources for academic and industrial engagement.

Funding Sources: Department of Homeland Security (DHS), Health and Human Services (HHS), U.S. Intelligence Agencies, DOE, industrial partners

Understanding and Design of Complex Materials

This thrust supports theory, modeling, and simulation in materials, an internationally recognized Laboratory strength 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 important, that can increasingly predict material properties in regimes inaccessible to experiment (e.g., accurately and reliably calculating properties of matter under extreme conditions for the weapons program).

In industrial and materials processing applications, new advances will 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) and other complex materials (Pu, high explosives, foams), 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 the Laboratory is best positioned to foster critical technology for all of its technical goals (Laboratory Goals A through G) and to become the premier materials science and technology laboratory in the world.

This thrust depends on aggressively pursuing 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, Los Alamos must optimize a program that integrates experiment with its modeling and simulation capabilities, since experimental guidance and validation of new theoretical 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 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 for decades to come.

Key opportunities lie in our ability to take advantage of important facilities such as the Center for Integrated Nanotechnology (CINT), Los Alamos Neutron Science Center (LANSCE), National High Magnetic Field Laboratory (NHMFL), Dual Axis Radiographic Hydrodynamics Test Facility (DARHT), the proton radiography facility at LANSCE and, in particular, large-scale computing. Indeed, a principal competitive advantage for Los Alamos is its ability to apply high-end computer capabilities to important problems. Our numerous collaborators in universities, industry, and other national laboratories are a significant resource. It will be important to consolidate efforts into a coherent program with specific short-term and long-term objectives and to sustain the support for funding and staff to establish and maintain an international reputation in this area.

Goals/Activities for 2004–2005:
- Work with the Laboratory's Materials Science and Engineering Council to better coordinate theory with experiment in Laboratory programs.
- Work with CINT leadership to establish an outstanding program in theoretical nanoscience and as a way to exploit growing opportunities in soft/organic/biological materials.
- Continue to forge close ties with user facilities (LANSCE, NHFML, etc.).
- Take advantage of the new Weapons Supporting Research program as a possible new funding source for complex materials and as a way to integrate these capabilities for nuclear weapons applications.
- Seek new opportunities for applications of complex materials to Threat Reduction programs (e.g., sensors).

Funding Sources: DOE Office of Basic Energy Science, DOE/Defense Programs, DoD, Defense Advanced Research Projects Agency (DARPA), LDRD

Modeling Biological Processes

This thrust area aligns with several of the Laboratory's seven national security goals, especially in strengthening the science base and science prediction capability at Los Alamos. It is directly related to key DOE, DHS, and DoD programs and has wide applications in Threat Reduction and improving human health in general. This thrust area is positioned to take advantage of the Laboratory's world-class scientists and capabilities in the areas of immunology, epidemiology, viral dynamics, networks, complex system modeling, quantum chemistry, molecular modeling/simulation, and high-performance computing. Additionally, it will benefit from access to state-of-the-art computational facilities and facilities such as the neutron source at LANSCE, electron microscopies, and CINT facilities at Los Alamos.

Goals/Activities for 2004–2005:
- Work towards establishing a Biological Modeling/Pathomics Center at Los Alamos. (See also PO 4.0 on page 20)
- Participate in the Genomes to Life program at DOE.
- Develop a program in vaccine design.
- Developing novel biomimetic sensors.
- Provide and enhance the science base for the Laboratory's efforts in Threat Reduction (see above).
- Integration of different expertise at the Laboratory into coherent programs to support research in system biology.
- Develop capabilities and strengths in areas of immune, regulatory, and transcription control networks to support programs in Genomes to Life, Threat Reduction, and Homeland Defense.
- Enhance partnerships with other divisions (B, CCS, D, MST, P) on structural biology, mass spectroscopy, microchip arrays, informatics, and databases.

Funding Sources: DHS, NIH, DOE Office of Science (DOE/SC), LDRD

Fundamental Processes

This thrust area aims to cover those aspects of science that provide the basic understanding of microscopic and macroscopic processes. The two primary objectives are to coordinate and support the Division's response to Laboratory

Strategic Goal G (DOE/SC) and to integrate theory, modeling, simulations, and experiment to elucidate the basic microscopic and macroscopic theories that describe natural phenomena.

There are several large national and international projects, facilities, and capabilities that are driving theoretical investigations in areas covered under this thrust. For example, the Large Hadron Collider at CERN (2007+) will study electroweak symmetry breaking, the Higgs phenomena, and whether fundamental interactions at very high energies respect supersymmetry. Use of the Relativistic Heavy Ion Collider at Brookhaven National Laboratory will probe Quantum Chromodynamics (QCD) at high temperature and density, with implications for early universe. Precision experiments at SLAC, Fermilab, and KEK, which when combined with nonperturbative calculations of matrix elements within hadronic states using Lattice QCD, will look for possible deviations from the standard model. Accelerator and nonaccelerator neutrino experiments will tell us about neutrino masses and mixing; resolution of the anomalous acceleration of Pioneer will test gravity; and high precision data on cosmic microwave background (CMB) will help elucidate the evolution and large-scale structure of the universe.

The Division has, through a new LDRD/DR, initiated a study of the structure and formation of First Stars (T-6, -8, and -16). This adds to the already significant effort in the study of nuclear structure and rates, nuclear astrophysics, high-density nuclear matter, fundamental symmetries, and QCD.

The thrust also has major efforts in cold atoms and in quantum dynamics of correlated electron systems, including coupled electron-phonon systems, electron-spin systems, photoemission, and inelastic tunneling. In addition, there are significant efforts to develop new technology with the capability to engineer microscopic physics of quantum degenerate many-body systems. Current efforts include: BEC-BCS-crossover, fermion pairing mismatched fermi-surfaces, quantum → classical transition, ultra-cold plasmas, strongly coupled fermion superfluid, fermion-boson mixtures, BEC-coherence and dynamics, ion traps, and solid-state devices to realize quantum information protocols and quantum simulators, optical lattices, many-body quantum entanglement, effective Hamiltonians (strongly correlated fermions), exotic states of matter, and quantum phase transitions.

Goals/Activities for 2004–2005:

- Investigate opportunities for enhanced research at common frontiers of astro, nuclear, and particle physics.
- Coordinate efforts in quantum information research with the LANL Quantum Institute.
- Carry out cutting edge research that helps maintain LANL's position as a premier scientific laboratory.
- Develop a broad-based core capability in mathematical and physical sciences that provides the underpinnings of the science and technology mission of the Laboratory.
- Develop modeling, simulation, and analysis capability to study complex systems and elucidate the basic principles underlying observed phenomena.
- Recruit and retain excellent scientists.

Funding Sources: DOE/SC, NRO, DARPA, Air Force, ARDA/NSA, IBM, NRL, CITIgroup, LDRD, SciDAC

Advanced Scientific Computing Research

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. The paradigm shift in today's scientific world is such that 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 and prediction. The rate of advance in these fields and the ability to simulate complex physical systems will increasingly be the limiting factors in our ability to effectively confront many pressing scientific challenges.

Therefore, it is essential to foster and support 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 Division Strategic Plan.

Division Scientific Thrusts

Many research areas require computational models incorporating more complete and realistic descriptions of phenomena than are currently possible. More efficient algorithms, more accurate mathematical models, advanced software, and more powerful computers are essential to fueling the pace of scientific discovery underpinning the Laboratory's research and development for its energy and national security missions in stockpile stewardship, fusion science, biology, nanoscience, high-energy and nuclear physics, fluid dynamics, applied mathematics, chemistry, climatology, and related fields. Because computational capability is also so critical to scientific discovery in these core missions, T Division aims to bring a renewed focus to this challenge.

This focus includes a renewed 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 Laboratory's next generation of major scientific challenges. These challenges will be increasingly complex, progressively more multidisciplinary, and span a much larger range of spatial and temporal scales.

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. We will work with the Laboratory's 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.

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

Goals/Activities for 2004–2005:

- 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 is currently achievable.
- Progress toward developing the mathematics, algorithms, and software enabling 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 Nuclear Weapons (NW) 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: NNSA, LDRD, DOE/SC