ADVANCED PHOTON SOURCE (APS)

The Advanced Photon Source (APS) is a national synchrotron x-ray research facility funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences. The APS provides this hemisphere's most powerful x-ray beams for research by thousands of scientists, engineers, students, and technicians from universities, industries, medical schools, and research labs (federal and private). The APS electron beam acceleration and storage system comprises of a 450-MeV electron linac; a 7-GeV booster synchrotron, and an 1104-m-circumference electron storage ring with a nominal energy of 7 GeV. The storage ring provides synchrotron radiation-based, high-brilliance x-ray beams to users via 68 beamlines (34 orginating at insertion devices, the other 34 originating at a bending magnets).

400 ACCELERATOR RESEARCH AND DEVELOPMENT

Current research activities include accelerator physics research, charged-particle beam dynamics calculations, particle-beam transport design, measurement of accelerator magnets, fabrication and testing of vacuum system chambers, radio-frequency acceleration system measurements, accelerator diagnostic system research and development, and computer-based accelerator control system.

401 ADVANCED NUCLEAR REACTOR SYSTEMS FOR HYDROGEN PRODUCTION

To facilitate a transition to a hydrogen-based economy, the laboratory is working on a number of projects centered around an advanced nuclear reactor. Such a reactor would operate at a temperature well in excess of the reactors that are currently in commercial operation and would be used to either pyrolyze natural gas or crack water in order to make hydrogen. It is predicted that this hydrogen will be needed to fuel both automobiles and homes in the near future. Specific projects in this area include development of processes for separating plutonium and fission products from molten salt, development of a process for reducing oxide fuels to metallic form, design of high temperature nuclear reactors, and development of chemical processes for efficiently converting hydrocarbons or water into hydrogen. This is a wide-ranging, multi-disciplinary project that requires the skills of nuclear, chemical, and mechanical engineers as well as physicists, chemists, applied mathematicians, and computer scientists.

402 X-RAY SCIENCE DIVISION

These activities include research in many areas of Chemistry, Materials Science, Magnetic Materials and Condensed Matter Physics as well as the development of instrumentation needed for a broad range of x-ray microscopy, scattering, spectroscopy, imaging, and time-resolved experiments in these fields to be performed at the Advanced Photon Source. In addition to research in many scientific areas, current activities are related to development of electronics for state of the art X-ray detectors, X-ray optics that allow focusing at the nanometer scale, novel synchrotron radiation instrumentation, and experimental equipment useful for various research applications.

403 FACILITIES CONSTRUCTION AND PROJECT MANAGEMENT

These activities include construction-related field engineering, safety and environmental engineering, quality assurance, and project management; civil, structural, mechanical, and electrical engineering; site improvements, and construction or modification of several buildings and utility systems.

404 BIOPHYSICS (BIO-CAT)

Primary foci are on the structure of partically ordered biological molecules, complexes of biomolecules, and cellular structures under conditions similar to those present in living cells. Research goals include the determination of detailed mechanisms of action of biological systems at the molecular level. Techniques used include x-ray fiber diffraction, x-ray scattering, x-ray absorption/emissions spectroscopy, and diffraction enhanced imaging. Consortium includes Illinois Institute of Technology.

405 CONSORTIUM FOR ADVANCED RADIATION SOURCES (CARS-CAT)

The consortium includes The University of Chicago, Northern Illinois University, Southern Illinois University, and Australian Nuclear Science and Technology Organization, and represents four national user groups: BioCARS for structural biology, GeoCARS for geophysical sciences, SoilEnvironCARS for soil/environmental sciences, and ChemMatCARS for chemistry and materials science. Techniques used include high pressure diffraction, microspectroscopy, microtomography, x-ray scattering, and crystallography.

406 DU PONT-NORTHWESTERN UNIVERSITY-DOW (DND-CAT)

This facility is dedicated to advancing x-ray study on new materials. Foci include the study of the atomic structures of bulk materials, the study of two-dimensional atomic structures, and polymer science and technology. Techniques include imaging, crystallography, scattering, and tomography.

407 INDUSTRIAL MACROMOLECULAR CRYSTALLOGRAPHY ASSOCIATION (IMCA-CAT)

This consortium involves crystallographic groups from 12 companies in the United States with major pharmaceutical research labs, in association with the Center for Synchrotron Radiation Research at the Illinois Institute of Technology. A large fraction of the research is proprietary. Techniques include multiwavelength anomalous diffraction.

408 MATERIALS RESEARCH (MR-CAT)

Illinois Institute of Technology is among four universities and one major corporation (BP-Amoco) involved with this collaboration. Foci includes studies of advanced materials in situ as a means of characterizing their structure and electronic properties, as well as understanding their preparation. Primary techniques include wide- and small-angle scattering, single-crystal and powder diffraction, absorption spectroscopy, reflectivity, standing waves, diffraction anomalous fine structure, and time-dependent and microfocus techniques.

BIOSCIENCES DIVISION (BIO)

The principal mission of the Biosciences Division is to conduct multidisciplinary, basic research that further increases the understanding of fundamental molecular mechanisms of life, enabling valuable advances in environmental protection and remediation, energy production and sustainability, and human health and welfare. Research projects in the Division range from fundamental studies of DNA sequences using molecular biology and computational strategies to practical use of genomic information, including selection of targets for protein function and structure determinations and protein engineering to elucidate natural biological processes. Management of two structural biology user facilities at the Advanced Photon Source, the Structural Biology Center funded by the Department of Energy and the GM/CA CAT funded by the National Institutes of Health, also falls within the Biosciences Division. The Sections are:

STRUCTURAL BIOLOGY

409 MIDWEST CENTER FOR STRUCTURAL GENOMICS

The Midwest Center for Structural Genomics (MCSG) is a consortium of the Argonne National Laboratory, European Bioinformatics Institute, Northwestern University, University of Toronto, Washington University, University College London, University of Virginia and the University of Texas and a part of the NIH-funded the Protein Structure Initiative. The primary objective of the MCSG is to rapidly determine the structures of strategically selected and bio-medically important targets including proteins from pathogens and higher eukaryotes. The MCSG goal is to elucidate protein folding space and ultimately provide structural coverage of major protein families with sufficient granularity to allow 3D homology modeling of all proteins using only computational methods. This will provide the foundation for 21st century structural biology when structures of virtually all proteins will be found in the Protein Data Bank (PDB) or derived by computational methods.

410 CENTER FOR STRUCTURAL GENOMICS OF INFECTIOUS DISEASES

CSGID applies state-of-the-art high-throughput (HTP) structural biology technologies to experimentally characterize the three dimensional atomic structure of targeted proteins from pathogens in the NIAID Category A-C priority lists and organisms causing emerging and re-emerging infectious diseases

411 STRUCTURAL CORRELATES OF PROTEIN FUNCTION

We focus on the characterization and structure determination of proteins. Our ultimate goal is to understand how the structures and functions of proteins are related. The samples that we work with include proteins that are important in (1) bioremediation (multiheme cytochromes, heme based sensors), (2) biofuels (hydrolytic enzymes), (3) human health (immunoglobulin light chains), and (4) photosynthesis (reaction center)

412 MEMBRANE PROTEIN ENGINEERING

Membrane-bound proteins pose particular challenges for biochemical and biophysical studies. Our development of novel expression systems and stabilizing reagents for membrane proteins advances the potential for study of these highly specialized molecular systems.

413 WIDE-ANGLE X-RAY SCATTERING

The high-resolution, three-dimensional structure of a protein provides an important basis for evaluating protein function. Unfortunately, high resolution structural imaging via macromolecular crystallography and NMR spectroscopy is applicable only to a relatively small proportion of the proteome and published success rates for high-throughput (HTP) structural genomics centers are currently less than 2%

414 GREAT LAKES REGIONAL CENTER OF EXCELLENCE FOR BIODEFENSE AND EMERGING INFECTIOUS DISEASES

Research Projects in the Great Lakes RCE are multi-year, multi-disciplinary studies aimed at the development of new vaccines or therapies against diseases caused by agents that can be used as biological weapons.

COMPUTATIONAL BIOLOGY

415 HOMOLOGY ANALYSIS FOR STRUCTURE, FUNCTION, AND MALFUNCTION

A major challenge for structural biology is to maximize the information content in the amino acid sequence of a protein. The information relevant to functional genomics includes function(s), stability, and interaction partners.

416 MOLECULAR DYNAMICS

Molecular dynamics (MD) consists of constructing detailed atomic models of the macromolecular system and, having described the microscopic forces with a potential function, using Newton's classical equation, *F=MA*, to literally "simulate" the dynamical motions of all the atoms as a function of time

417 BIOINFORMATICS

Several bioinformatics tools have been developed at the Biosciences division to support structural genomics and proteomics research, ranging from target design, surface survey of protein structures, to interpretation of mass spectrometry data

ENVIRONMENTAL BIOLOGY

418 SUBSURFACE SCIENCE

MESG is part of Biosciences Division at Argonne National Laboratory. One of the main foci during the creation and growth of the Molecular Environmental Science Group has been the development of an internationally recognized integrated multidisciplinary scientific team focused on the investigation of fundamental biogeochemical questions. Presently, expertise that is represented by members of the MES Group includes high-energy x-ray Physics, Environmental Chemistry, Environmental Microbiology, and radiolimnology.

419 TERRESTRIAL ECOLOGY

Terrestrial ecology research includes studies of plant-soil-atmosphere interactions and biogeochemistry at molecular to landscape scales, with specific emphasis on the belowground ecosystem. Research projects focus on belowground responses to environmental change, improving knowledge of terrestrial components of the global carbon cycle, and methods for enhancing carbon sequestration by terrestrial ecosystems

MOLECULAR AND SYSTEMS BIOLOGY

420 PRODUCTION AND FUNCTIONAL CHARACTERIZATION OF PROTEINS

The objective of this project is to use high throughput proteomics, protein expression and enzyme assays to rapidly generate meaningful functional annotation of proteins.

421 INTERVENTIONAL BIOLOGY

Research in the Interventional Biology Group takes an interdisciplinary approach to intervene in biological events in order to redirect their course, enable new functions and prevent undesired consequences. While intervention may also be achieved through conventional molecular biology methods, we are promoting novel interventional routes via a combination of molecular biology methods with materials and phenomena adapted from the physical sciences for both molecular and kinetic interventions.

422 METALLOPROTEIN RESEARCH

An estimated one third of all proteins bind metal ions, and many of these proteins have regulatory or catalytic functions. This project takes a simple, comprehensive approach for identifying and quantifying metalloproteins in complex samples using native-PAGE and synchrotron x-ray fluorescence imaging. By pairing the development of specialized, non-coordinating, non-denaturing 2D gel electrophoresis techniques with the development of dedicated, rapid wide-area XRM imaging capabilities, we aim to identify the entire complement of metalloproteins in a given biological sample.

423 PROTEOMICS

Proteomics is an area of research that seeks to identify the proteins in a biological system at a specific point in time and to understand variations in the abundance of those proteins as a function of cell growth environments. Proteomics researchers isolate, separate, identify, and characterize the proteins from biological systems to better understand what factors influence the relative abundance of those proteins, what functions/metabolic processes are represented by those proteins, and how those functions/metabolic processes are regulated.

424 CLINICAL PROTEOMICS AND BIOMARKER DISCOVERY IN CANCER RESEARCH

The goal of Argonne National Laboratory's NCI protein production program is the production, characterization, and distribution of peptides and proteins for use in the development and validation of clinical cancer proteomic technology platforms.

CENTER FOR NANOSCALE MATERIALS (CNM)

The Center for Nanoscale Materials (CNM) at Argonne National Laboratory is a national user facility that provides capabilities explicitly tailored to the creation and characterization of new functional materials on the nanoscale. The CNM mission includes supporting basic research and advanced instrumentation development. The facility supports a user program that is open to the academic, industrial, government, and international communities. It has core capabilities in materials synthesis, nanofabrication research, proximal probes, a dedicated hard x-ray nanoprobe beamline at the APS, and computational nanoscience – including a state-of-the art Beowulf-class supercomputer accommodating highly parallel compute-intensive applications has a compute capacity of approximately 10 Tflops. The six main scientific research themes are Electronic & Magnetic Materials & Devices, Nanobio Interfaces, Nanofabrication, Nanophotonics, Theory & Modeling, and X-ray Microscopy. Please see http://nano.anl.gov for many more details.

425 SELF-ASSEMBLY OF SOFT MATTER NANOMATERIALS

Traditional methods for creating nanostructures based on “top-down” techniques are rapidly approaching intrinsic limitations. Furthermore, the majority of advanced lithographic techniques are serial and therefore expensive and slow. Advancing nanoscience and nanotechnology will necessitate innovations that allow parallel synthesis of hierarchical structures in the 1–100 nm size range. “Bottom-up” self-assembly approaches, predicated on chemical or biological processes, offer a promising route to overcome the shortcomings of lithography. This project involves investigations of novel polymeric nanomaterials, hybrid organic-inorganic nanocomposites, and biomaterial arrays. Potential applications range from solar cells to magnetic recording. A broad spectrum of characterization tools are utilized including, but not limited to, atomic force microscopy, spectroscopy, and thermal analysis.

CHEMICAL SCIENCES AND ENGINEERING DIVISION (CSE)

The Chemical Sciences and Engineering Division is one of the largest Divisions at Argonne National Laboratory, a leading R&D center with the mission to advance scientific knowledge, sustainable energy, national security, and environmental management. The Division is a science-based research, development, and early-stage engineering organization that conducts both fundamental and applied research using experimental, theoretical, and computational approaches. Our R&D is distinguished by the development and application of fundamental understanding to yield transformational solutions that address issues of scientific and technological importance to the U.S. Department of Energy (DOE) and the nation.

The Division is multidisciplinary. Its people have formal training in chemistry; physics; materials science; and electrical, mechanical, chemical, and nuclear engineering. They are specialists in catalysis; electrochemical systems; nuclear fuel cycle; combustion chemistry; and time-resolved, multiscale, and ultrafast chemistry. Our researchers have experience working in and collaborating with university, industry, and government research and development laboratories throughout the world.

The Division's R&D is focused around five theme areas:

- *<u>Fundamental Interactions</u> — programs in atomic, molecular, and optical physics; chemical dynamics in the gas phase; and photosynthesis.*
- *<u>Catalysis and Energy Conversion</u> — programs in heterogeneous and homogeneous catalysis, hydrogen production and storage, and fuel cell materials development and systems analysis.*
- *<u>Electrochemical Energy Storage</u> — programs in advanced cell chemistry and materials development of lithium-ion batteries for transportation and other applications and independent battery testing.*
- *<u>Nuclear and Environmental Processes</u> — programs in heavy element chemistry, separation science, nuclear fuel separations, repository performance, and radioactive waste management.*
- *<u>National Security</u> — programs in forensics and attribution of radiological dispersal devices, radiological decontamination technologies, sensors/detectors, and analytical chemistry.*

The Division hosts several facilities, including the Actinide Facility, Analytical Chemistry Laboratory, Electrochemical Analysis and Diagnostics Laboratory, Glassblowing Shop, and Premium Coal Sample Facility, providing technical support of research within and outside Argonne.

FUNDAMENTAL INTERACTIONS

Since its inception, Argonne has been involved in long-term fundamental research that addresses problems in the chemical sciences that are related to the mission-oriented activities of the Department of Energy. Our programs in this area are directed to basic research in atomic, molecular, and optical science; chemical physics; photochemistry; and physical chemistry. Our research seeks to understand chemical reactivity through studies of the interactions of atoms, molecules, and ions with photons and electrons; the making and breaking of chemical bonds in the gas phase; and energy transfer processes within and between molecules.

Ultimately, this research leads to the development of such advances as efficient combustion systems with reduced emissions of pollutants, new solar photoconversion processes, and improved development and application of novel x-ray light sources at current and planned DOE user facilities.

426 ATOMIC, MOLECULAR, AND OPTICAL PHYSICS

This program combines experiment and theory in developing a quantitative understanding of x-ray interactions with atoms and molecules from the weak-field limit to the strong-field regime. Research thrusts are in x-ray probes of optical strong-field processes, inner-shell processes with intense ultrafast x-rays, theory and the development of synchrotron-based 1 ps x-ray source at the Advanced Photon Source. Experimental results are used to challenge and calibrate some of the most detailed theoretical models in atomic physics.

427 CHEMICAL DYNAMICS

This program merges theoretical and experimental work on the energetics, kinetics, and dynamics of chemical reactions in the gas phase with particular emphasis on combustion reactions. Shock tube, flow tube, and photo-ionization techniques provide fundamental measurements on the high- and low-temperature kinetics of radical-radical and radical-molecule reactions, on the thermochemistry of radicals, and on vibrational/rotational selected photodissociation of small molecules. A comparable theoretical effort maps out potential energy surfaces by electronic structure techniques; follows the dynamics and kinetics on surfaces with trajectories, wave packets, and statistical models; and couples multiple processes together in kinetics simulations. The synergism between comparable experimental and theoretical efforts is a hallmark of this effort.

428 PHOTOSYNTHESIS

Researchers are defining the basic principles in solar energy conversion that govern charge separation in molecules via the study of electron transfer reactions within natural and biomimetic photosynthetic structures. Work on the mechanism of charge separation in natural photosystems is being extended to construct novel artificial systems to mimic the natural process. The program approach features the resolution of structural dynamics linked to ET reactions by the application of a suite of advanced, multifrequency, pulsed magnetic resonance, transient optical, and x-ray techniques to follow light-activated structural dynamics across multiple time (10^{-13} s to 1 s) and length (1 Å to 500 Å) scales. The research develops a fundamental understanding of structure-function relationships in biological photosynthesis and establishes principles for the design of biomimetic systems for solar energy conversion.

CATALYSIS AND ENERGY CONVERSION

The development of new energy technologies is essential to our nation to promote economic prosperity, to enhance energy security, and to provide for environmental preservation. The Catalysis and Energy Conversion Department conducts basic and applied research in two critical energy-related technologies: catalysis (homogeneous and heterogeneous) and fuel cells and hydrogen (fuel cell engineering, hydrogen and fuel cell materials, and ceramic electrochemistry).

Researchers are developing new catalytic materials and processes for converting resources such as biomass and coal to transportation fuels and chemical commodities, reducing NOx emissions, and fundamental research aimed at improving our understanding of how catalysts promote chemical reactions. In Fuel Cells and Hydrogen, researchers are developing technologies for the production, storage, and utilization of hydrogen necessary to realize the potential of fuel cells as clean, efficient power sources for automotive, stationary, and portable power applications.

429 CATALYSIS

Research in heterogeneous catalysis focuses on developing new catalyst and processes for decomposing and converting cellulosic materials into liquid fuels and chemical commodities, for use in selective oxidation and dehydrogenation reactions, for reducing nitrogen oxide emissions, hydrogen production, and the conversion of synthesis gas, a mixture of $CO + H_2$, that can be derived from carbonaceous materials such as biomass and coal into liquid fuels. We also explore fundamental issues in catalysis such advancing our understanding of the structure/composition/ function relationships in nanoscale catalytic materials. We are also working to advance the use of x-ray spectroscopy techniques for studying catalytic reactions under “real world” operating conditions.

Research in homogeneous catalysis explores fuel-related catalysis mechanisms, new catalytic species, and new catalytic reaction chemistry using an array of powerful *in-situ* spectroscopic and kinetic techniques at the high pressures and temperatures that are frequently used in industrial processes.

We are also working at the forefront of fundamental catalysis as partners with Northwestern University in the Institute for Catalysis in Energy Processes. Catalysis research at the Institute integrates theory, modeling, synthesis, characterization, and testing with the ultimate goal of achieving selective chemical transformations through new catalyst designs that position multiple catalytic functionalities and control structure and composition with subnanometer precision.

430 FUEL CELLS AND HYDROGEN

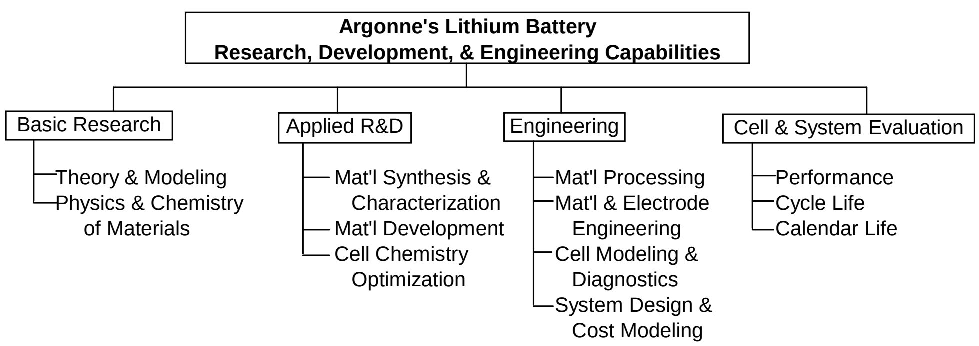
Our researchers are developing technologies for the production, storage, and utilization of hydrogen necessary to realize the potential of fuel cells as clean, efficient power sources for automotive, stationary, and portable power applications. R&D in hydrogen production spans fuel reforming (catalytic conversion of natural gas, gasoline, diesel, ethanol to ethanol), high-temperature electrolysis, and thermochemical cycles. For fuel cells, we are developing advanced materials and electrocatalysts to reduce the cost and improve the durability of both solid-oxide and polymer-electrolyte membrane technologies. A distinguishing strength of our research is in the analysis of the complex systems associated with hydrogen production, storage, and fuel cell applications.

ELECTROCHEMICAL ENERGY STORAGE

431 LITHIUM BATTERY RESEARCH, DEVELOPMENT, AND ENGINEERING

Argonne National Laboratory has been actively involved in the development of advanced batteries since the late 1960s when it initiated R&D on high-temperature lithium-sulfur batteries. In the early 1970s, the Department of Energy established its first independent battery test facility at Argonne and named it the National Battery Test Laboratory (NBTL), for the purpose of conducting independent evaluations on advanced battery technologies that were potential candidates for use in battery-powered electric vehicles. The NBTL incorporated a well-equipped post-test analysis laboratory that was instrumental in helping to identify life-limiting mechanisms with several candidate battery technologies. Even in these early days of the battery program, Argonne was internationally respected for its advanced battery work. Over the last 40 years, Argonne's battery program has evolved and expanded, becoming internationally recognized as a world-class center for lithium battery R&D.

Integrating Basic Research, Applied R&D, and Engineering: The current organization of Argonne's Electrochemical Energy Storage Department includes a battery test group and three battery R&D groups. The battery test laboratory changed its name to the Electrochemical Analysis and Diagnostics Laboratory (EADL), but it continues to provide DOE's transportation program and U.S. auto companies with the same type of independent evaluations, using standardized test protocols that the EADL helped to develop for DOE. The Department's three R&D groups cover the lithium battery landscape from the basic science perspective to the engineering design of batteries for specific applications. This integration of basic research, applied R&D, and engineering (as shown below) has played a key role in Argonne's success.



The integrated capabilities of the Department can be described using an example of the process it employs to develop more optimal materials and cell chemistries for a specific application. When existing cell chemistries suffer from life, inherent safety, or performance limitations, detailed diagnostic and electrochemical cell modeling studies are used to identify the limiting factors and new materials are developed to overcome these limitations. These can be new electrode materials with enhanced structural, chemical, electrochemical, and thermal stability that are designed (with the aid of *ab initio* modeling) to increase specific capacity, extend life, and/or enhance inherent safety. Additionally, with the aid of quantum mechanical modeling, electrolyte additives with the proper redox potentials and physicochemical properties are developed to help stabilize the electrode/electrolyte interfaces. These new materials are thoroughly characterized and compared with existing materials to provide assurance that they will help stabilize cell chemistry. Once the characterization work and preliminary aging studies verify enhanced stability, the materials are produced in sufficient quantity to allow thorough evaluations in hermetically sealed cells, which are obtained from industrial battery manufacturers. Argonne employs its detailed battery design model to develop the electrode design specifications, and the battery manufacturer coats electrodes and produces cells to Argonne's specifications. These hermetically sealed cells are then subjected to extensive accelerated aging and abuse tests to quantify the improvements relative to a baseline cell chemistry. Results from detailed diagnostic and modeling studies on these cells are then used to further refine and optimize the materials, if needed. Using this process, Argonne has developed a large portfolio of intellectual property on advanced materials that is available for licensing by the battery industry and its material suppliers.

Leading Major DOE Initiatives: Argonne is DOE's lead laboratory for its applied battery R&D program for hybrid electric vehicle (HEV) applications, the Advanced Technology Development (ATD) program. This program is a multi-Laboratory program that involves support from four other DOE national laboratories: Brookhaven, Idaho, Lawrence Berkeley, and Sandia. The objective of this program is to help the industrial developers of Li-Ion batteries to overcome the key barriers of calendar life, abuse tolerance, low-temperature performance, and cost for Li-Ion batteries in HEV applications. Also, Argonne is a major participant in DOE's longer-range R&D program, the Batteries for Advanced Transportation Technologies (BATT) program. Here, Argonne's role is in the development of novel anode and cathode materials that can help advance Li-Ion battery technology for transportation applications. DOE also is looking to Argonne's Electrochemical Energy Storage Department to make significant contributions to its new initiative on plug-in hybrid electric vehicles (PHEVs). Argonne is: (1) testing prototype PHEV cells to establish baseline performance characteristics and to aid in the development of standardized PHEV testing protocols, (2) developing PHEV battery performance models that are used in PHEV vehicle simulation studies, and (3) conducting R&D on new advanced electrode materials, with the goal of significantly increasing the energy density of lithium-ion batteries for this application.

Working with Others: In addition to projects funded directly by DOE projects, Argonne conducts R&D for industrial firms under Work for Others contracts. Some of these contracts involve R&D support to industrial battery companies that are funded by DOE via its collaborative R&D agreement with the U.S. auto companies [the U.S. Advanced Battery Consortium (USABC)]. Other contracts are with industrial firms that seek Argonne's help to develop and optimize cell materials, components, and/or cell chemistries for a variety of applications.

To further support advanced battery research, Argonne's Electrochemical Analysis and Diagnostics Laboratory is available to assist Argonne and non-Argonne battery researchers by conducting evaluations that can be used to identify potential design or material changes that may improve battery performance. The EADL conducts independent performance and life studies on DOE/USABC contract deliverables and similar benchmark studies on advanced battery technologies developed without DOE support. Services of this type also are available to the private sector.

NUCLEAR AND ENVIRONMENTAL PROCESSES

For more than sixty years, Argonne National Laboratory has been a world leader in the development of nuclear technologies. The Chemical Sciences and Engineering Division and its predecessors have had an important role in these developments, advancing the science of actinide chemistry and innovating solutions for the "back end" of the nuclear fuel cycle. Today, our researchers are at the forefront in the development of technologies for nuclear separations, waste management, and nonproliferation to achieve sustainable nuclear energy.

Programs in our nuclear and environmental processes thrust are organized into four areas.

432 HEAVY ELEMENT AND SEPARATIONS SCIENCE

Basic science research of heavy element and fission product atomic and molecular-scale chemistry with focus on actinide aggregation in solution and precipitates, metal-ligand interactions, and electronic properties. Researchers are using novel instruments at the Advanced Photon Source to elucidate the electronic structure and magnetic properties of actinide nanoclusters, providing new insights into their behavior in separations processes and their migration in the environment. In related studies, they are designing, synthesizing, and characterizing chelating agents for metals separations and recovery.

433 INTERFACIAL PROCESSES

Basic science research of mineral/water interactions to advance the fundamental understanding of geochemical processes important to predicting the performance of geological repositories. Researchers are deploying advanced *in-situ* spectroscopy and imaging techniques to explore mineral surface hydration, ion adsorption structures, and mineral growth and dissolution processes.

434 PROCESS CHEMISTRY AND ENGINEERING

Application of integrated expertise in chemical engineering and actinide chemistry to develop, model, design, and demonstrate solvent extraction processes for spent fuel and radioactive waste treatment, and nuclear nonproliferation. For the Department of Energy's Advanced Fuel Cycle Initiative, researchers invented, demonstrated, and continue to develop the UREX+ suite of multistage solvent extraction process for selective recovery of fission products in spent fuel. For the DOE's Reduced Enrichment for Research and Test Reactors program, researchers are developing the separation technologies required to produce the medical isotope molybdenum-99 from low-enriched uranium targets.

435 NUCLEAR TECHNOLOGY

Application of multidisciplinary expertise to innovate, develop, and engineer commercially viable electrochemical processes for nuclear separations. Researchers are developing novel processes for the recovery of actinides and stabilization of fission products from metal, oxide, carbide, nitride, and other advanced nuclear reactor fuels. Recent inventions include high-throughput uranium electrorefining and electrolytic oxide reduction.

NATIONAL SECURITY

436 ANALYTICAL CHEMISTRY LABORATORY

The Analytical Chemistry Laboratory (ACL) provides a broad range of analytical chemistry support services to the scientific and engineering programs at Argonne National Laboratory and specialized analysis for government, academic, and industrial organizations. Our analytical services and research comprise inorganic, radiochemical, organic, microstructural characterization, and environmental analyses and studies.

437 NANOSCALE ENGINEERING FOR BIOMEDICINE AND NATIONAL SECURITY

Previous work on the use of magnetic microparticles to recover metals, fission products, and high-level radionuclides from liquid waste streams has led to research that uses magnetic nanospheres for biomedical and national security applications.

We are leading a team of scientists, engineers, and medical researchers in the development of technology that uses magnetic nanospheres for human detoxification of blood-borne toxins (radiological, biological, and chemical). Originally developed for in-field use by military personnel, the work also will have application in the early diagnosis and treatment of certain medical conditions.

In other nanoscale engineering work, our researchers are completing development of a system to quickly and nondestructively decontaminate structures such as buildings and monuments using a spray-on, super-absorbent gel and engineered microparticles. The technology will help the nation be more prepared in the event of a terrorist attack with a “dirty bomb” or other radioactive dispersal device.

COMMUNICATIONS AND PUBLIC AFFAIRS DIVISION (C&PA)

438 JOURNALISM AND PUBLIC RELATIONS OPPORTUNITIES

The Communications and Public Affairs Division has internship opportunities for students interested in science-related journalism and public relations. The student would do "hands-on" activities in many areas of the Communications and Public Affairs, including: preparing news releases reporting on scientific and technical advances at Argonne; assisting in the publication of the Argonne News, employee publications, and Argonne Now, a bi-annual scientific feature magazine. This internship requires a strong background in journalism and an interest in science. Articles generated during the internship are printed in Argonne publications with author credit and used in news-release form to scientific and general media.

COMPUTING AND INFORMATION SYSTEMS DIVISION (CIS)

The Computing and Information Systems Division is committed to the introduction and provision of the computing, instrumentation, electronics and communications infrastructure to enhance the productivity of and provide new capabilities for the Laboratory's, scientific, engineering and administrative programs. The primary goal of CIS is to establish and promote a seamless environment where individual researchers and workers can easily access and use all elements of the ANL information resources hierarchy, independent of the diverse computer, electronics, and telecommunications technologies they choose to use.

439 SYSTEMS MANAGEMENT

Systems administrators manage the architecture, implementation, and ongoing maintenance of Windows, Solaris, and Linux-based servers. Other facets of systems management including filesystems, storage area networks, backup technologies, and core Internet protocols including mail, DNS, web, and other services. Systems administrators provide the backbone for key applications to function in a highly available environment for Laboratory users. Internship opportunities exist to work with professional staff on evaluating new technologies, analyzing and upgrading existing systems, and developing management tools.

440 AUTHENTICATION TECHNOLOGIES

The ability to identify network users confidently is a fundamental requirement for distributed applications. Strong authentication enables sharing sensitive data across unsecured networks. Technologies such as LDAP, Kerberos, and public/private keys are used to provide alternate authentication strategies. Argonne actively works to incorporate technologies into UNIX and Microsoft environments. Internship opportunities exist to evaluate, develop, and test new and/or expanded authentication technologies.

441 HIGH-SPEED NETWORKING

High performance computing systems being planned currently have the potential to achieve a petaflop of computing power. If petascale systems can fulfill their promise and if software can scale to take advantage of these more complex systems, they will definitately change the nature of scientific questions that can be pursued via simulation in every scientific field. To support these initiatives effective high-speed networking will be an essential component. Argonne is active in the testing, monitoring, and tuning of high-performance networks.

442 LOCAL-AREA NETWORKING

Argonne has been striving to achieve an effective balance of both science and security within our campus network infrastructure. Networking projects include the deployment of a 10 Gigabit Ethernet backbone, high-performance data center infrastructure, wide spread wireless deployments, with a complimentary mix of cyber security measures – firewalls, vpn’s, and intrusion detection systems. With these efforts we are striving to provide in breed infrastructure for supporting scientific research.

443 CYBERSECURITY

The Argonne Cyber Security Program plays an integral part in maintaining the integrity and cyber wellbeing of the users and data on Argonne's computer systems and networks. The office is responsible for the technical implementation and policy governance of the systems in place that protect the Laboratory. Activities of the office include Vulnerability Scanning and Tracking, Firewall configuration review, Intrusion Detection System (IDS) development, Scripting and Automation and administration of a lab wide detection infrastructure.

444 APPLICATION DEVELOPMENT

Programmer/analysts interact with clients, design and develop or maintain computer programs, and conduct tests on the Laboratory's business information systems. These systems may be stand-alone, multi-tiered client/server, and/or web-based applications. The Division is migrating to a Service Oriented Architecture using modern Web 2.0 technologies. Internship opportunities exist for students to work with professional staff on developing and upgrading real-world applications in the new paradignm.

445 TECHNOLOGY EVALUATION

As part of its mission in operation support for the laboratory, CIS maintains a program of technology evaluation with potential for increased operation efficiency or new capability creation in support of the laboratory's mission. Internship opportunities exist to work with CIS staff evaluating application of IT to a wide variety of operational needs (energy efficiency, automation, sensor and control systems, etc.

446 OPERATIONS COMPUTING SUPPORT

Supporting the computing end users is an essential role to maintaining administrative operations at the lab. The operations computing environment consists of Microsoft Windows and Apple Mac OS platforms that are managed through Active Directory. Ongoing activities include telephone and remote computer maintenance and troubleshooting support, account administration, software and hardware installations, hardware repairs and desktop and server maintenance and administration. Other activities include infrastructural and service planning and upgrades, client and server backups, patching and virus protection. Internship opportunities exist in operations as well as new technology evaluation/deployment.

DECISION AND INFORMATION SCIENCES DIVISION (DIS)

The Decision and Information Sciences Division is composed of several sections that focus their research activities in distinct but related technical areas. The mission of the Division is to develop innovative decision support tools, models, and information systems and apply them to the analysis and resolution of problems of regional, national, and global significance.

447 ADVANCED MULTIDISCIPLINARY SIMULATION

The Division develops, promotes, and utilizes advanced computer modeling and simulation tools and technologies for both research and operational applications. These tools facilitate the construction of complex, heterogeneous simulations that integrate modeling representations of many diverse dynamic processes across time and space to address difficult problems that require multidisciplinary solutions. Representative recent and ongoing projects include:

- Simulation frameworks for the study of the stability and sustainability of societies under stress due to such factors as climatic, economic, energy and technological change and political turmoil. A pilot study involves constructing detailed socioecological simulations of representative villages and sub-regions in rural Southeast Asia.
- An agent-based simulation system to help inform debate on national healthcare policy reform. The system models the relevant characteristics and dynamic behaviors of the major actors in the U.S. healthcare scene: Federal and state governments; insurers; healthcare providers; employers; and individual persons and households embedded in social networks relating to family, employment, insurance, finance, etc.
- Agent-based socioecological simulations of ancient Mesopotamian settlement systems, addressing interactions among natural processes (hydrology, crop growth, weather, etc.) and social processes (kin-based behaviors, agricultural practices, social stratification, etc.) on a daily basis across multi-generational time spans.
- Diverse applications in computational linguistics, multinational law enforcement, ocean physics, health and welfare of disadvantaged children, and many others.

These projects tend to have an inherently synergistic, integrative focus that provides research opportunities for computer-literate investigators with interests and expertise in a wide variety academic disciplines.

448 INFRASTRUCTURE ASSURANCE

The Division has worked to develop Argonne as the lead lab for infrastructure protection with the Department of Homeland Security. The Division's infrastructure expertise is supported by a large suite of models, simulation tools and extensive databases that include:

- GIS-based gas supply system database
- Gas and electricity energy supply systems modeling and simulation
- Toolset to analyze the condition of gas supply systems
- Comprehensive U.S. electric supply system database
- Infrastructure analysis in gas, oil, electricity, and infrastructure interdependencies

449 PACKAGING CERTIFICATIN AND LIFE CYCLE MANAGMENET

The Division supports Department of Energy's (DOE's) Environmental Management (EM), Office of Safety Management & Operations Packaging Certification Program, and Nuclear Regulatory Commission's (NRC's) programs on operating reactor licensing actions, regulatory improvement activities, and new reactor design guidance documents. The Division's expertise in these areas include:

- Materials and structural analysis
- Thermal and containment analysis
- Radiation shielding and criticality analysis
- Quality assurance and the ASME Code and Standards

Federal regulations for certification of fissile and radioactive material packagings in storage, transportation and disposal. The Division is also developing advanced technology, such as radiofrequency identification system for nuclear material management.

450 INFORMATION SCIENCES

The Division develops architectures and systems that organize and integrate large-scale, complex, and heterogeneous information. The systems include:

- Data warehousing tools, such as intelligent query visualization to provide context for information retrieval
- Develop and enhance the information network for the Atmospheric Radiation Measurement (ARM) Climate Research Facility
- Develop petabyte-scale scientific data access and storage solutions for the Large Hadron Collider at CERN

451 MODELING, SIMULATION, AND VISUALIZATION

The Division develops expert systems and artificial intelligence. These include:

- Develops the logistics planning tools used by the Department of Defense to plan military operations
- Develops complex adaptive systems modeling and simulation software and applications
- Develop technologies to study environmental impacts of military operations, endangered species, health care systems, command and control strategies, and ancient civilizations.

ENERGY SYSTEM ASSESSMENT

The nation is again focused on the need to address issues of energy supply and demand, to choose appropriate energy technologies, and to develop new and existing energy supplies.

452 ENERGY, ENVIRONMENTAL, AND ECONOMIC SYSTEMS ANALYSIS

The Division develops energy demand projections, evaluates alternative energy supply systems, and evaluates energy and environmental policies bearing on energy development. The Division's work includes:

- Models used to make energy market decisions
- Suite of energy/environmental/economic models, now used in more than 60 countries
- Models to analyze the deregulated electricity marketplace
- Database with information on all electricity generating stations in the U.S.

453 EMERGENCY PREPAREDNESS

The Division has considerable expertise in emergency preparedness and planning for technology-related accidents, terrorist attacks, and other emergencies. Current topics include:

- Provide emergency preparedness expertise to FEMA, DOE , DOT and the U.S. Army
- Develop emergency preparedness system for use in subways to detect chemical agent attacks and provide first responders with crisis management information
- Develop GIS-based Special Population Planner to identify and locate populations and facilities needing special assistance in emergency situations
- Develop Emergency Response Synchronization Matrix (ERSM) to assist in creating an integrated response plan involving multiple (federal, state, local) jurisdictions

ENERGY SYSTEMS DIVISION (ES)

The Energy Systems Division (ES) of Argonne National Laboratory conducts research and development efforts in energy production, efficient energy conversion and use, mitigation of the environmental effects associated with producing and using energy, and methods of restoring contaminated and degraded lands to a usable, productive state. The Division concentrates on laboratory research needed to enable a cleaner and more efficient use of energy resources and on field studies pertaining to the wise use and maintenance of environmental and natural resources

The ES Division is organized into three areas: (1) The Process Engineering Section and the Chemical and Biological Group are committed to developing and transferring clean, efficient energy and industry-related environmental technologies into the marketplace to benefit U.S. companies, the federal government, customers, and the general public, (2) The Center for Environmental Restoration Systems develops and performs research, development and demonstration programs to support the complete environmental restoration process, from start to finish, addressing each of the three stages of the process, and to transfer the knowledge and technologies obtained to sponsors and other potential users of that information, and (3) The Center for Transportation Research conducts research to evaluate and develop transportation technologies, with emphasis on reducing petroleum-fuel requirements, costs and the environmental consequences of transportation systems.

INDUSTRIAL TECHNOLOGIES

454 ENVIRONMENTALLY FRIENDLY SOLVENTS

Widely used chemical solvents, such as chlorofluorocarbons, damage the earth's ozone layer, while chloroform and trichloroethylene remain the most common groundwater pollutants. Ethyl lactate, a non-toxic and biodegradable solvent, occurs naturally in beer, wine, and soy products and is approved as an additive by the U.S. Food and Drug Administration. Argonne has developed a technology that can sufficiently reduce the cost of the environmentally benign solvent, ethyl lactate, to make it competitive in the marketplace against toxic solvents. A novel membrane-based process to produce lactate esters is being developed through an industry/government initiative.

455 BIOCATALYTIC SYSTEMS FOR THE PRODUCTION OF CHEMICALS FROM RENEWABLE RESOURCES

Through industry/government partnerships, Argonne is part of a consortium to develop a new, integrated process approach for synthesizing industrial chemical intermediates and derivatives from renewable biomass. Argonne's role is to apply its technical expertise in genetic engineering, bioprocess engineering, and polymer development to targeted products and processes. For example, Argonne is improving fermentation efficiency by using conventional and genetic techniques to develop superior succinic-acid-producing organisms. Its purification process uses advanced desalting and water-splitting electrodialysis technologies.

456 CHEMICAL AND BIOLOGICAL TECHNOLOGY

This area is focused on integrating chemical engineering with biological processes. A major objective is the development of new methods to produce chemicals utilizing both fermentation and biocatalytic systems, which are integrated with separation and purification technologies utilizing new membrane technologies. Methods to produce a "green" solvent from corn, ethyl lactate, have led to a licensed joint venture and three national awards. Another objective is the development of detection and treatment methods for controlling and understanding sustained localized pitting corrosion influenced by microbes. Other projects include phytoremediation, examining the use of plants for environmental remediation, sonication or advanced oxidation to remediate groundwater and soil, the development and use of new biomodified catalysts, and the use of paleoclimate changes to model hydrocarbon exploration and global warning.

457 CARBON MANAGEMENT

This effort seeks to develop cost-effective, high efficiency, low-greenhouse-gas, and low environmental impact technologies. Ultimately, these technologies will be used in the Utility, Industrial, and Transportation sectors. In cooperation with industry, studies will use full-energy cycle analysis of advanced utility and industrial fossil fuel-based systems to establish base-line greenhouse gas inventories for several current technologies. We are developing a capability to understand and coordinate with groups studying terrestrial and ocean response to natural and anthropogenic induced changes in atmospheric concentrations of greenhouse gases.

458 PROCESS EVALUATION

Our focus is on the development of advanced waste minimization/pollution prevention technology, with an emphasis on materials recycling. We have three core activities: (1) physical/chemical separation process development, (2) hydro/pyrometallurgical process development, and (3) process simulation and cost analysis. Representative projects where student help is anticipated include: (1) recovery of materials from auto shredder residue (thermoplastics, polyurethane foams, oxides of iron and silicon for cement-making), (2) recovery and separation of thermoplastics from obsolete appliances and electronics, and (3) evaluation of non-consumable anodes for molten salt electrowinning of metals.

ENVIRONMENTAL RESTORATION

This area performs research, development and demonstration programs to attain all aspects of environmental restoration from start to finish, including site characterization, selection and implementation of remediation technologies for site cleanup, and final restoration of a site to usefulness.

459 PHYTOREMEDIATION

Phytoremediation, the engineered use of green plants to remove, contain, or render harmless such environmental contaminants as heavy metals, trace elements, organic compounds, and radioactive compounds, is an emerging cleanup technology for contaminated soils, groundwater, and wastewater that is both low-tech and low-cost. In 1995, greenhouse experiments on zinc uptake in hybrid poplar were conducted to confirm and extend field data from Applied Natural Sciences, Inc. in a collaborative research and development effort. Analyses indicate that part-per-million levels of zinc are totally sequestered by the plants through the root system in several hours in a single pass. Similar experiments with a grass show similar patterns partitioning and sequestration as the poplar experiments but with the growth and transpiration more suppressed. Current studies include groundwater remediation and field demonstrations for the uptake of halogenated organics in hybrid poplar.

460 GEOLOGIC AND HYDROLOGIC ENGINEERING

Studies of interaction between energy operations and systems and the environment often involve investigations related to geologic or hydrologic engineering. Current studies deal with development of methods for measuring the effectiveness of site-characterization methods, groundwater modeling, and field measurements associated with environmental compliance at facilities located in diverse settings and locations.

461 RESEARCH AND DEVELOPMENT PROGRAMS TO REMEDIATE CONTAMINATED SITES

Studies of sites contaminated with hazardous and toxic materials require data acquisition, analyses, and interpretation on many site conditions that determine migration and fate of contaminants. Site properties related to hydrology, soils, geology, geochemistry, and related conditions must be understood to evaluate environmental risks and site cleanup alternatives. Current studies involve environmental geophysics in a range of geologic settings; field investigations of subsurface geology related to contaminant migration; evaluation of the fate of contaminants in soils and uptake of these materials by plants, phytoremediation of soil and plumes, development of standardized analytical chemistry techniques for contaminants; and evaluation of treatment technologies to remediate contaminated soils and groundwater.

CENTER FOR TRANSPORTATION RESEARCH

The Center for Transportation Research (CTR) conducts applied research for the U.S. Department of Energy on advanced transportation technologies and their energy, economic, and environmental impacts. A broad spectrum of technologies are being researched; some examples include alternative-fueled vehicles, studies of energy use and transportation demand under different future scenarios, environmental assessments and modeling of existing and new technologies, and issues and strategies for a transition to alternative fuels. Due to the breadth of current research topics, CTR is interested in attracting both students and faculty from a diverse set of disciplines to contribute to our research efforts.

462 ALTERNATIVE FUELS FOR TRANSPORTATION

CTR is conducting technical, economic, policy, and environmental analyses for a transition to non-petroleum fuels for the transportation system. Projects span light- and heavy-duty vehicles and buses, and include fleet demonstrations. Analysis of alternative transportation fuels in CTR includes: (1) assessment of engine, vehicle, and fuel supply technologies; (2) assessment of the properties of fuels, their combustion products, and atmospheric side effects; (3) econometric analysis of consumer response to the cost changes of fuels and vehicles when adopting alternative fuels; and (4) economic assessment of policies designed to promote the introduction of alternative fuels. Two specified examples of ongoing projects are listed below.

463 ALTERNATIVE TRANSPORTATION FUELS - VEHICLE AND FUELS CHARACTERIZATION

This project involves the study of the attributes of engines and fuel systems for various fuels and technologies and develops comparisons of advantages and disadvantages of each. Emissions, energy consumption, power density, and other measures are used as a basis of comparison. Participants in this program may also study fuel-processing and transportation systems such as refineries, pipelines, and ships and may estimate costs of technologies, working with economists.

464 ALTERNATIVE TRANSPORTATION FUELS - ECONOMIC ASSESSMENTS

Work in this area involves the study of consumer responses to vehicle and fuel characteristics, including price changes and factors such as performance and safety. Policy questions, including issues of short-run costs vs. long-run savings induced by inter-fuel competition are also under investigation Participants in this program will work with engineers to develop cost estimates for new technologies.

465 ENGINE AND EMISSIONS RESEARCH

A Mechanical Engineering Assistant is needed for acquiring engine test data using high-speed data acquisition system and analyzing the data. The Advanced Powertrain Test Facility (APTF) is an integrated test facility capable of testing vehicles and powertrain components by means of state-of-the-art measurement equipment and control hardware. The APTF has conducted vehicle-and component-level testing of commercially available and OAAT-developed hybrid electric vehicles to characterize and enhance these technologies. The test data have also helped to evolve and validate the DOE vehicle simulation models. A mechanical or electrical engineer is needed to assist in the design and implementation of experiments, gather and analyze data collected from complex testing of engines, battery packs, motors and vehicles, and assist in the publication of reports and technical papers. The student or faculty will work test engines to make performance and emissions measurements. Additional projects involve characterization of diesel and gasoline fuel sprays using lasers and x-rays. Data collection, analysis and consolidation will be part of the student/faculty function.

466 ANALYTICAL ENGINEER

A Mechanical Engineering or computer systems engineer is needed to conduct simulation studies of engines and vehicle systems. Work in this area involves assisting with PSAT (modeling software) model refinement, validation, integration, and documentation. The engineer may also use PSAT-PRO (control software) at the Advanced Powertrain Testing Facility for technology validation using hardware-in-the-loop testing process. Tasks may include refinement of powertrain controllers to evaluate component technology potential.

BIODETECTION TECHNOLOGIES

Biotechnology research at Argonne National Laboratory deals with applying biology and biochemistry principles and breakthroughs to problems of national interest. In health-related studies, researchers advance the development and use of biological microchips, or biochips, to speed DNA sequencing of human genes and to identify organisms and toxins of bacteria, viruses, and other microorganisms. In collaborative efforts, Laboratory staff study the effects of biochemicals to control leukemia and other cellular malignancies, target enzymes to screen for new drugs, and study cellular replication, differentiation, apoptosis in tumors.

467 BIOCHIP TECHNOLOGY

Argonne National Laboratory works toward commercializing and marketing advanced biological microchips, or biochips, and related analytical technologies to permit faster and more efficient detection of mutations in genetic information encoded in DNA, the macromolecule of human genes which is packaged in the chromosomes in cells. Polyacrylamide micro-gel pads – thousands of them on a single one-square-inch glass slide – act as microscopic laboratory test tubes in which biological targets can be tested against chemical compounds. With known strands fixed in place, robots and other automated equipment allow researchers to use the slides as templates to test and decode unknown DNA samples. Primary applications include medical diagnostics, drug discovery and medical treatment, environmental restoration, and agricultural-product testing.

468 BIOCHIP TECHNOLOGY – ADVANCED APPLICATIONS

Argonne National Laboratory is exploring and expanding the biochip's wide range of applications in:

- DNA sequence analysis and proofreading.
- Analysis of changes in genetic makeup (mutations),
- Analysis of population differences in genetic coding (polymorphism),
- Identification of bacteria, viruses, and other microorganisms,
- Advanced medical diagnostic and monitoring of treatment, and
- Development of Polymerase Chain Reaction (PCR) on **M**icro **A**rrays of **G**el-**I**mmobilized **C**ompounds on a **Chip** (MAGIChip™).

469 CELL GROWTH AND DIFFERENTIATION

This research seeks to examine the molecular events that govern cellular replication, differentiation, and programmed cell death (apoptosis) in normal and tumor cells.

- Chemicals are being studied for their roles in signal transduction events (such as activation of protein kinases, production and interaction of adhesion molecules, and transcription factors) that alter cellular replication, differentiation, or apoptosis.
- Laboratory staff are characterizing human genes that code for proteins that modulate cellular replication, differentiation, and or apoptosis in normal and tumor cells.
- Research on inosine 5'-monophosphate dehydrogenase (IMPDH), a target for immunosuppressive antimicrobial and anticancer drugs, focuses on its regulation and structure.

Results could provide the foundation for the development of agents that could be used as targets for the development of pharmaceuticals.

[Also, see related listing under the Biosciences Division.]

470 CERAMICS

Ceramic processing development and new ceramic-materials synthesis for a wide variety of applications are carried out in this section. Much of the work is done on a collaborative basis with other groups both within and outside of Argonne. An example is the dielectric materials for capacitors. The Ceramics Section staff have fabricated ceramic dielectrics with high permittivity by conventional solid-state and chemical solution deposition techniques. Other areas include mixed-conductors for batteries, fuel cells, sensors, and gas-separation; and low-temperature, chemically bonded phosphate ceramics for the containment of nuclear waste. High strength, better-performing cements are being developed for some applications. Generally, the Ceramics Section work includes microstructural characterization by optical and electron microscopy, phase identification by X-ray diffraction and thermal analysis, mechanical properties measurements, and electrical characterization. Those interested in hands-on ceramics laboratory work should apply for a position in this section.

471 TRIBOLOGY

The Tribology section is concerned with developing and improving materials and surfaces that have low friction and high wear resistance for engineering application. The goal of this research is to make advancements in applications as diverse as spacecraft, fuel-cell vehicles, trucks, sensors, manufacturing, micromachines, and human artificial joints. A participant would typically be involved in one or more of the following activities: (1) Deposition of coatings with improved tribological properties. The group has state-of-the art equipment (plasma, sputtering, ion beam) that is used to deposit many different kinds of thin coatings which are then characterized and tested. Materials include amorphous carbon, diamond, nitride, and carbide coatings. (2) Friction and wear testing. The group has a variety of testing machines that measure friction and wear of rolling and sliding components. The testing may be done in air, in controlled environments (vacuum, inert gas, liquid), at various speeds and motions. (3) Characterization and analysis of the surfaces and coatings, either as they are produced, or after they have been tested. Available methods include scanning- and transmission-electron microscopy, Raman spectroscopy, optical microscopy and optical profilometry, X-ray analysis (using the Advanced Photon Source), hardness, adhesion, and Rutherford backscattering. Surface morphology, composition, microstructure, and properties are determined and related to performance. A participant would typically learn to operate one or more of the machines, deposit coatings, test coatings, or characterize them, and analyze the data which is obtained.

ENVIRONMENT, SAFETY AND HEALTH/QUALITY ASSURANCE OVERSIGHT DIVISION (EQO)

The Environment, Safety and Health/Quality Assurance Oversight Division ensures a safe work environment for Argonne employees. Division personnel are engaged in the wide scope of activities required to make recommendations for, and maintain safe work practices and conditions throughout the Laboratory. Activities include, industrial hygiene and safety services, personnel monitoring, training, safety analyses, and environmental monitoring and surveillance.

472 INDUSTRIAL HYGIENE

Industrial Hygiene provides sitewide guidance and technical support for assessment and control of workplace exposures to chemicals and physical agents, excluding ionizing radiation. Exposures to solvents, gases, vapors, dusts, and mists are measured using a variety of direct-reading instruments and personal sampling devices which collect samples from workplace air for laboratory analysis. Other activities involve exposure surveys for indoor air quality, noise, ultraviolet light and microwaves, selection, fit testing and user training of respiratory protective devices, and particle collection efficiency measurements of high-performance air-cleaning systems. A wide variety of instrumentation is used, including infrared, electrochemical cell and photoionization type gas and vapor monitors, aerosol photometers, data loggers, noise and microwave meters, and instruments for collecting and measuring airborne nanoparticles.

Projects are available concentrating on a specific aspect of industrial hygiene.

473 ES&H TRAINING

This section designs, develops, and presents training on environment, safety, and health (ESH) issues throughout the Laboratory. Training classes, courses, and programs respond to various DOE, EPA, OSHA, federal, and state regulations, as well as identified environment, safety, and health training needs. Design, development, and implementation of training may involve work lab-wide with subject matter experts. Varied training needs provide multiple opportunities to undertake creative approaches to instructional design and performance technology as well as technology-based training solutions. Curriculum design, course design, and the associated front end work that incorporates needs analysis, determination of entry characteristics and behaviors, development of performance objectives, and creation of instructionally sound testing mechanisms are used. Evaluation of training programs, courses, means of instruction, and instructor competence are facets of ES&H Training. As a research and development facility, Argonne provides a setting that encourages innovative technology-assisted training approaches. These include the design, development, testing for efficacy, and application of Computer-Based Training (CBT) and Web-Based Training (WBT) strategies involving creative software applications as well as participation in the design and development of Argonne specific software programs. Projects include significant concentration on utilization of the Web, and effective optimization between databases.

474 RADIOLOGICAL SAFETY

Radiological Safety group supports nuclear research and accelerator operations to ensure protection of workers, the public, and the environment from the hazards of ionizing radiation. Students with interests in the physical sciences, electronics, and mathematics may find career-enhancing opportunities in the field of radiological safety, also known as health physics. [Further information on the growing field of health physics is also available at http://www.hps.org/]. Student opportunities available in the Argonne Radiological Safety Group include work with radiation detection and monitoring equipment as well as direct involvement in radiation safety support of work in nuclear and radiological laboratories and accelerators.

ENVIRONMENTAL SCIENCE DIVISION (EVS)

The Environmental Science Division has developed a broad program of interdisciplinary, applied research and development, undertaken from a system's perspective. Research activities in this division include a broad spectrum of fundamental and applied investigations into the functioning of the environmental systems, particularly in response to anthropogenic stresses. Consequently, the information derived from the various research projects addresses critical environmental issues that face society. The staff addresses a wide range of issues associated with risk and waste management; natural resource system and integrated assessments; restoration, compliance and pollution prevention. Environmental and resource assessments are conducted by professionals with expertise in the hydrogeological, physical, social, and ecological sciences and in radiological and health risk assessment. Our policy staff consists of environmental lawyers, sociologists, land-use planners, and archaeologists, and provides sophisticated analyses of government policy and strategy options. Special areas of interest include environmental data management and communication, risk assessments including ecological and human health, technology assessments, and environmental restoration. We are experienced in building interdisciplinary technical teams for specific environmental projects, since many of our programs require integration of a wide range of skills. Additional information can be found at www.evs.anl.gov.

475 CLIMATE CHANGE RESEARCH

Field studies and modeling are emphasized. GLOBAL CHANGE studies use observational facilities in the Southern Great Plains to study processes that are important in climate modeling. Improved subgrid-scale parameterizations are developed for the structure of the planetary boundary layer and the air-surface exchange of heat, moisture, and solar and infrared radiation. REMOTE SENSING from the ground uses Doppler acoustic, radar, and laser systems along with *in situ* observational systems to study the structure of the planetary boundary layer and to evaluate the transport and dispersive properties of the lower atmosphere above complete terrain. Satellite data on optical radiance reflectances from land surfaces are used to study energy balances and the corresponding biological properties that affect energy flows. For WATER and BIOCHEMICAL CYCLE studies, heat, water vapor, and carbon dioxide fluxes, nitrogen deposition and fluxes as well as soil moisture content are evaluated over large terrestrial areas with models and results are compared to local observations made in the field sites located at Southern Great Plains and Fermi Lab. NUMERICAL MODELS are developed and applied to study the structure of planetary boundary layer as it affects energy flows, meteorological conditions, and the transport and dispersion of trace chemicals.

476 ATMOSPHERIC SCIENCES

The Division evaluates construction and operation of energy technology systems and other industrial activities to assess their potential impacts on ambient air quality, climate, meteorology, and the acoustic environment. The effectiveness of control technologies and related government regulations in mitigating these impacts are also evaluated. Air-quality databases and new and improved methods of modeling air pollutant emissions, environmental transport and transformation processes, and noise propagation are developed as part of this work. Models are developed and performance evaluations are conducted to address emerging health and safety issues and to give environmental managers additional information on uncertainty in model predictions for consideration in formulating national and international energy and environmental policies. In addition, hazard analyses and risk and consequence assessments are performed to determine the impacts from possible releases of nuclear, chemical and biological agents. Recent projects have provided guidance to government agencies in hazard analysis, risk management, emergency response, and pollution prevention and control.

477 ATMOSPHERIC CHEMISTRY

We are studying the chemical transformations and fates of energy-related air pollutants released into the atmosphere over urban and regional areas for the Department of Energy's Atmospheric Science Program. This program focuses on determining the regional and global climatic effects that result from radiative forcing of the atmosphere by aerosols. Our limited comprehension of aerosol effects prevents us from understanding how energy use will affect future climate. Some topics of investigation include:

- Measurement of aerosol profiles using remote sensing instruments, such as Micropulse LiDAR in conjunction with measurement of vertifical profiles of relevant atmospheric dynamic variables such as wind temperature and stability of the planetary boundary layer.
- Use of numerical models of atmospheric chemistry and transport to interpret and generalize the findings from the observational studies.
- Use of numerical models to evaluate the uncertainty in calculating the radiative forcing from aerosols.
- Develop better constrained models for evaluating the uncertainty in calculating the aerosol radiative forcing using data assimilation methods and models.

478 ENVIRONMENTAL RESTORATION AND WASTE MANAGEMENT

The assessment of contamination problems at federal facilities and the evaluation and implementation of tailored cleanup methods and technologies play an important role in the Division's activities. Extensive environmental analyses and remediation studies are conducted to support cleanup and environmental restoration work at contaminated sites. The Division analyzes health and environmental risks and management alternatives designed to address different site wastes and contaminants in air, soil, surface water, groundwater, biota, and structures/equipment. Innovative technologies and regulatory impacts on waste management and environmental remediation options are also analyzed. These analyses, which are used for remedial investigations, baseline risk assessments, and feasibility studies, often extend to the development of sampling and remedial design strategies; these combined evaluations rely on integrated data analyses and atmospheric, hydrogeologic, ecological, and health modeling and analyses. Also pollution prevention and material disposition studies emphasize improved waste

479 ENVIRONMENTAL DATA MANAGEMENT AND COMMUNICATIONS

In keeping with the Division's mission to advance informed environmental decision making, this technical area emphasizes the use and development of information technology tools relevant to environmental problems. Most environmental data have a spatial, or geographic, component as well as other attributes, and the Division employs geographic information system (GIS) technologies to analyze and communicate these spatial data. Also, advanced visualization approaches, including virtual reality systems, are used to communicate both these data and the results of environmental modeling to technical and non-technical audiences. In addition, World Wide Web technologies are applied to a large number of environmental studies within the Division. The applications range from public information dissemination to secure working Web sites where data integration and analyses support distributed decision making. The Division continues to explore new means of delivering spatial information to users across various environmental projects and programs, with tools ranging from hand-held devices to large-scale collaborative systems such as the Access Grid. (See other technical areas.)

480 HYDROGEOLOGY/HYDROLOGY

Analytical and numerical models of surface flow, groundwater flow and solute transport are developed, assessed, and applied by the Division to evaluate environmental contamination problems in various settings. These models are used to support the evaluation of impacts to human health and environmental resources, including endangered species. Geostatistics, advanced scientific visualization, graphical database, multi-media, and virtual reality techniques are used to prepare, analyze, and communicate the results of these studies. This area is multi-disciplinary and taps a wide range of skills and knowledge available within the Division. Evaluating the interaction among water, geologic materials, and contaminants is a common component of many environmental projects and programs.

481 NUCLEAR MATERIAL TRANSPORT

This area involves assessing impacts that could result from the release of radioactive materials during the transportation of nuclear waste materials, including both radiological and chemical impacts. The Division models the fate of materials via various environmental pathways and exposure routes to assess potential radiation and chemical exposures to humans. This modeling includes computer simulation of accident probabilities, atmospheric dispersion and other transport pathways, with links to demographic data, to support the evaluation of radiation and other health effects.

482 ENVIRONMENTAL SYSTEMS PLANNING, AND COMPLIANCE

Multi-media and medium-specific approaches are employed to assess and solve existing environmental problems and to manage environmental systems at federal facilities. The Division's activities in this area cover both analytical studies and field work, including development of planning and guidance materials; audits of environmental compliance at federal facilities and associated corrective action plans; presentation of workshops on environmental laws, regulations, and compliance; preparation of baseline surveys and emission inventories; and development of database management expert computer systems, web-based systems for environmental compliance information, and preparation of National Environmental Policy Act (NEPA) documents and management of the NEPA process for specific projects. Planning may include entire environmental management systems including natural and cultural resources.

483 APPLIED GEOSCIENCE AND ENVIRONMENTAL MANAGEMENT AND FIELD RESEARCH

Argonne's research program in applied geosciences and environmental management is improving the characterization and remediation of contamination in complex geologic and hydroglic media through innovations in (1) sampling and analysis; (2) technologies for restoration of natural systems; (3) monitoring and evaluation of the performance of in-situ remediation systems; and (4) watershed-based methods for simulating large-scale hydrologic systems. Argonne's environmental site characterization process integrates targeted sampling, geologic a hydrologic systems analyses, and numerical modeling of flow and contaminant transport to improve delineation of contaminant migration and reduce remediation costs. Several advances in direct-push sampling technologies and chemical analysis have been awarded patents. Two innovative remediation technologies for groundwater that are now in field application in Nebraska, under sponsorship of the U.S. Department of Agriculture, are (1) evaporation of carbon tetrachloride by spray irrigation equipment, with beneficial reuse of the treated water (http://www.cooperative/conservationamerica.org/viewproject). Development of both remediation technologies required innovative approaches to performance monitoring and geologic and hydrologic systems analysis. An improved approach for simulation of large-scale hydrologic systems being applied to Egypt's deserts couples groundwater and surface water systems combining satellite remote sensing data on climate, land use, and land cover with ground measurements.

484 LONG-TERM ENVIRONMENTAL STEWARDSHIP

The terms "environmental stewardship" and "long-term stewardship" have been used to represent the mechanisms (processes and tools) necessary to ensure both short- and long-term protection of the public and the environment from wastes and residual environmental contamination that will remain at sites after active cleanups are completed. These mechanisms and tools extend from physical and institutional controls and information management to environmental monitoring and risk assessment. The Division is evaluating these interrelated technical issues to support sustainable decision making at these sites, including: understanding and monitoring material deterioration in barriers and closure systems; managing and maintaining critical information systems with access for future generations; and sensing and assessing changes in site risks from contaminants that will persist from decades to generations. The Division places emphasis on the optimization of long-term monitoring systems.

485 ECOLOGICAL AND GEOGRAPHICAL SCIENCES

The Division analyzes the effects of both natural processes and human activities on aquatic, terrestrial, and wetland ecosystems, ecological communities, plant and animal populations, threatened and endangered species, and cultural resources. Impacts examined include hydrologic alteration, habitat effects, land disturbance, ecological effects of radiological and chemical contamination, and related cumulative impacts. Ecological risk assessments are performed for contaminated sites to support the development of ecological cleanup criteria and the evaluation of remediation alternatives. Mitigation or management strategies such as ecological restoration are developed to reduce impacts and enhance ecosystem function. Information is gathered through field and laboratory studies, remote sensing, and literature searches, and is analyzed using statistical techniques, modeling, and geographic information system (GIS) approaches. Recent projects have examined the effects of dam operations on aquatic and terrestrial ecosystems, have evaluated biodiversity and habitat, have assessed ecological risks at contaminated sites, and have assessed wetland and prairie restorations.

486 ENVIRONMENTAL POLICY ANALYSIS (Washington, DC location)

The Division assesses environmental, technological, and economic implications associated with developing and implementing national environmental laws, regulations, and policies to identify areas for improvement. Both multidisciplinary and focused assessments are conducted on environmental topics ranging from management practices for controlling air and water pollutants to managing wastes. The environmental, energy, and economic effects of these practices and the impacts of different strategies to minimize these effects are also assessed. Policy makers use these assessments in their decision making on issues of national importance and for specific regional or sector-specific planning.

487 NATURAL RESOURCES

Natural resource management plans are prepared for federal facilities to identify goals and objectives, commonly over five-year periods, to guide planning and implementation of various federal programs. The Division takes an integrated approach in developing these plans for specific federal agencies, by examining planned facility missions and programs, the current baseline physical and natural environment, and potential impacts associated with the given program. Program activities are considered together with objectives within such natural resource areas as fish and wildlife management, forestry resources, federal and state protected species, recreational programs, wetland resources, waste management and cleanup, and adjacent land use. Integrated natural resource management plans are then used to develop detailed operational plans that typically describe specific tasks, associated labor effort, cost, and final products anticipated by implementing the tasks to meet overall plan objectives. Other focus areas include evaluations of transportation risks, risks to the ecosystem, probabilistic environmental risk assessments, cumulative risks to natural resources from combined impacts of multiple contaminants, and natural resource risk communication.

488 ENVIRONMENTAL IMPACT ASSESSMENT

The Division assesses potential impacts of proposed federal actions in accordance with the National Environmental Policy Act (NEPA) and related environmental requirements. These NEPA analyses evaluate the baseline (no-action) situation as well as the environmental consequences of a given proposed action (which can be project-specific or programmatic) and its alternatives. This assessment of potential impacts to the human environment extends across natural and ecological resources to social and cultural resources and health effects. Potential impacts are analyzed and presented in environmental impact statements, environmental assessments, and other documents prepared by the Division. Activities include conducting public involvement activities and responding to issues of public concern, examining regulatory issues, gathering and evaluating information and data, developing databases and multi-media tools, retrieving and archiving information, and developing management tools. These activities are performed by closely integrated multi-disciplinary teams tapping expertise across the Division. (See the other technical areas.)

489 RISK ASSESSMENT

Risk assessment is a key element of many Division projects and is used to guide a broad variety of environmental decisions that extend from managing contaminated sites to planning and preparedness for homeland security. The scope covers a wide range of technical, environmental, and human health issues in various settings, from urban areas to remote facilities. These assessments are conducted by teams that integrate across all of the Divisions' technical areas, and they address both radionuclides and chemicals under different types of controls and release events. The assessments support multiple decisions over time, from short-term consequence management to intermediate cleanup actions and long-term control and sustainability. For these assessments, the Division has developed an extensive set of analytical tools and approaches to assess the sources of risk and specific hazards involved, evaluate the potential incidents (e.g., releases) and related exposures that could harm people or the environment, and assess the nature of the risks that could be incurred. These analyses consider the mechanisms and pathways by which humans or ecological/ environmental receptors could be exposed to hazards from the facilities, areas, or activities being assessed, as well as the outcome of those exposures, considering acute to chronic effects. These risk tools and approaches include the RESRAD computer code, which is used to identify site-specific cleanup levels for radioactively contaminated sites and includes a probabilistic risk component, as well as models to assess transportation risks, ecological risks, and human health risks, including risks from exposures to mixtures and cumulative risk analyses. The Division also promotes risk communication and educational outreach, including through risk assessment training and health-related fact sheets for chemicals and radionuclides found at many DOE sites, many of which are also important to homeland security.

490 RADIOLOGICAL ANALYSIS SOFTWARE DEVELOPMENT

Using analytical methods formulated within the Division, radiological analysis software is being developed by the Division for use nationally and internationally. An example of software developed is the RESRAD Family of Codes (web.ead.anl.gov/resrad/home2/). Most of the software also includes probabilistic analysis capability for studying parameter uncertainty. Input data sets needed to use the software are also compiled and default parameter distributions are included for typical applications. The software tools are coded in Fortran, Visual Basic, and C languages with user-friendly interfaces and follow stringent quality assurance standards.

491 BIOTA DOSE ASSESSMENT

Impact to animals and plants from exposure to radionuclides in the environment is an emerging research area, and the assumption that "if humans are protected then animals and plants are also protected" is being challenged in many applications. The Division is developing Dose Conversion Coefficients for assessing radiological doses to nonhuman biota (animals and plants). Transfer coefficients from environmental media (soil, water, sediment) to biota are also being collected. A software tool named RESRAD- BIOTA developed by the Division is the first of its kind available for radiological biota dose assessment.

FACILITIES MANAGEMENT AND SERVICES DIVISION (FMS)

492 FACILITIES ENGINEERING SERVICES

This activity consists of performing functions as an engineering assistant in the Engineering Department. These activities include working with one or more engineers from various Engineering disciplines, i.e. mechanical, electrical, structural, civil, pressure vessel and/or architectural. Work will include engineering support of buildings and site systems as related to construction, modifications and/or maintenance. Tasks may include engineering surveys, studies, field work, design assistance, database management, review and preparation of specifications / drawings, quality assurance, safety reviews, and investigation into engineering problems.

HIGH ENERGY PHYSICS DIVISION (HEP)

The Division conducts research into the nature and properties of elementary particles -- the building blocks of matter. The program includes colliding beam and neutrino experiments at nearby Fermi National Accelerator Laboratory and at CERN, the European Organization for Nuclear Physics. The effects of spin in elementary particle scattering are being studied over a wide range of energies. Research not requiring particle accelerators or detectors includes the use of superspeed multinode processors for lattice gauge theory. The Division's theoretical group is active in several areas of elementary particle theory. Accelerator physics research includes development of new acceleration techniques and designs for new accelerator facilities.

493 DETECTOR DEVELOPMENT OF THE INTERNATIONAL LINEAR COLLIDER

A Lepton Collider (LC) will be the next big accelerator project of High Energy Physics. The LC with a center-of-mass energy of 500 to 3000 GeV will make crucial contributions to the understanding of the Higgs sector, of Supersymmetry and of other phenomena beyond the current Standard Model of particle physics. In order to fully exploit the physics potential of the LC, detectors with unprecedented precision are needed. In this context, our group is developing a highly segmented hadron calorimeter as part of a new concept of imaging calorimeters. We develop Resistive Plate Chambers (RPCs) as active media of the calorimeter and the corresponding electronic readout system capable of handling large numbers of channels (of the order of tens of millions). We currently construct a major prototype section of such a hadron calorimeter to validate our new approach to calorimetry. The prototype section will undergo detailed testing in the Fermilab test beam.

494 MINOS LONG BASELINE NEUTRINO EXPERIMENT

Underground cosmic-ray experiments give convincing evidence that the phenomenon of neutrino oscillations occurs in Nature. This implies that a neutrino which is created in one of the three flavors might interact as a different flavor neutrino. In particular, it is believed that muon neutrinos oscillate into tau neutrinos. This implies that neutrinos have a small but finite mass.

An international collaboration of physicists and engineers from Argonne and thirty other laboratories and universities has built a neutrino beam and two massive particle detectors for the MINOS experiment. These are being used to measure changes in neutrinos along a 735 km flight path between Fermilab and northern Minnesota. There are opportunities for students and faculty to be involved in the simulation and analysis of data for the new experiment, and to work on electronics and scintillator components for the MINOS detectors. Other topics for visiting faculty and students include working with HEP Division physicists on design studies for the next generation of neutrino experiments.

495 EXPERIMENTS USING POLARIZED BEAMS

The Argonne group is working at the Relativistic Heavy Ion Collider (RHIC) on spin experiments at Brookhaven National Laboratory. In the past, we were involved in the design and construction of an electromagnetic calorimeter for one of the large RHIC detectors (STAR). Present tasks include analysis of data collected with STAR and the electromagnetic calorimeter, studies of systematic effects in various RHIC polarimeters, and the design and construction of a data acquisition system for a new prototype tracking detector for STAR. The primary physics issues that will be studied at center of mass collision energies from 200 to 500 GeV are: 1) the spin content of the proton, including measurements of the gluon and sea quark helicity distributions; 2) checking of the electroweak couplings including parity violation in $W^{\pm}$ and Z^{0} production; and 3) measurements with transversely polarized beams. To achieve these physics goals, there will be detection of jets, direct photons, and electrons from $W^{\pm}$ and Z^{0} decays; the electromagnetic calorimeter and new tracking detectors will play crucial roles in these measurements.

496 PROTON-ANTIPROTON COLLIDER

This activity is part of an international collaborative effort to study proton-antiproton collisions using the Collider Detector (CDF II) at the Fermilab Tevatron. The 2 TeV center-of-mass energy will remain the highest available in particle physics until the startup of the Large Hadron Collider at CERN in 2008. The CDF II detector includes charged-particle tracking chambers with microvertex detectors, embedded in a large solenoidal magnet. The solenoid is surrounded by calorimeters and muon detectors. The Argonne group led the design and construction of the central electromagnetic calorimeter, including fine grained shower-maximum and preshower detectors and the associated front-end electronics readout. Between 2001 and 2008 CDF II accumulated over 4 fb^{-1} of integrated luminosity. With current Tevatron peak luminosities in excess of 2 10^{32}, it is anticipated that the total accumulated luminosity will increase to 6-7 fb^{-1} by the end of the Tevatron running in 2010.

CDF II data taking is based on a sophisticated trigger system that can identify combinations of charged particle tracks, electrons, muons, photons, and jets. The tracking triggers provide precision measurements of particle momenta and impact parameters, which allow for identification of long-lived bottom and charm quarks at the trigger level. As a result, CDF II has a rich and diverse physics program that includes precision measurements of the properties of top, bottom, and charm heavy quarks, precision measurements of the gauge-boson masses, searches for a wide range of new physics phenomena (supersymmetry, extra dimensions, Higgs bosons), and a variety of QCD studies ranging from high energy jet and photon production to rare diffractive processes at the few GeV scale. Recent accomplishments include the measurement of the mixing frequency of the neutral bottom-strange meson and 1% measurements of the top-quark mass. As the already huge amount of data increases, there are opportunities for students and faculty to get involved in novel physics analyses of their choice.

497 ATLAS EXEPERIMENT AT CERN

The ATLAS experiment will be investigating the behavior of matter, energy, space and time and the smallest distance scales ever probed. Located at the Large Hadron Collider at CERN, the European Organization for Nuclear Physics, near Geneva, Switzerland, ATLAS will observe the highest energy proton-proton collisions ever achieved: 14 TeV. ATLAS is a large general-purpose detector with several major subsystems: inner (tracking) detector, superconducting solenoid, electromagnetic calorimeter, hadronic calorimeter and muon spectrometer. Argonne has played major roles in the hadronic calorimeter, elements of the trigger, and the data handling for the unprecedented data volumes that will be produced in the course of the experiment - and distributed worldwide. We have continued these construction responsibilities into detector operations and maintenance for the corresponding detector systems. In the last two years we have expanded our roles to include establishing a regional center for Atlas physics analysis, which hosts workshops and visitors, and have installed a remote monitoring station to allow detector monitoring shifts to be taken from Argonne.

The detector is complete and has been commissioned using cosmic rays to be ready for the observation of the first LHC collisions, expected in the fall of 2008. Argonne physicists' lines of investigation include studying quantum chromodynamics - the behavior of quarks and gluons - at the energy frontier, electroweak symmetry breaking and the question of why some particles have mass and others do not, whether or not large extra dimensions exist, and whether or not supersymmetric particles exist or not. More details on these activities and the contributions of Argonne to the detectors systems can be found at the following website:
http://www.uslhc.us/The_US_and_the_LHC/Collaborating_Institutions/Argonne_National_Laboratory
There are opportunities for students and faculty to get involved with detector operations and monitoring, data analysis and computer simulation.

LEADERSHIP COMPUTING FACILITY (LCF)

The Leadership Computing Facility Division operates the Argonne Leadership Computing Facility – the ALCF – as part of the U.S. Department of Energy's (DOE) effort to provide leadership-class computing resources to the scientific community. The mission of the ALCF, established in 2006, is to provide the computational science community with a leading computing capability dedicated to breakthrough science and engineering. The ALCF provides resources that make computationally intensive projects of the largest scale possible. ALCF staff members operate this facility for the U.S. Department of Energy's Office of Science and also provide in-depth expertise and assistance in using ALCF systems and optimizing their applications. DOE selects major ALCF projects through the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program. This program seeks computationally intensive research projects of large scale that can make high-impact scientific advances through the use of a large allocation of computer time, resources, and data storage.

498 COMPUTING FACILITIES

The Argonne Leadership Computing Facility currently operates the IBM Blue Gene/P Intrepid and Surveyor systems. These supercomputers are dedicated to a mix of DOE INCITE (Innovative and Novel Computational Impact on Theory and Experiment) projects, discretionary projects, and scalable software evaluation and development projects. In June 2008, Intrepid was ranked as the world's fastest open science supercomputer, with a peak speed of 557 teraflops and Linpack speed of 450 teraflops. Intrepid features 40,960 nodes, each with four processors or cores for a total of 163,840 cores and 80 terabytes of memory. The world's largest installation of NVIDIA Quadro Plex S4 external graphics processing units will boost Intrepid's capabilities in 2009. This new supercomputer installation, nicknamed Eureka, will deliver a major advance in visual compute density, enabling breakthrough levels of productivity and capability in visualization and data analysis.

Surveyor has 4,096 processors and 2 terabytes of memory. It is used primarily for tool and application porting, software testing and optimization, and systems software development. For more information, see the ALCF website (http://www.alcf.anl.gov).

499 APPLICATIONS ANALYSIS FOR PETAFLOPS ARCHITECTURES

This project is developing the detailed understanding of computationally intensive applications required to make the best possible use of the upcoming petaflops systems. We are working with a suite of applications that cover many strategic efforts for the Laboratory and DOE. Specific efforts include evaluation of each applicant's computation and I/O scalability properties, creation of appropriate methods for porting these codes to systems like IBM's Blue Gene, and development of system-level benchmarks based on these codes. Participants in this project can expect to learn a great deal about scalable applications and their use on petaflops systems. *http://www.alcf.anl.gov/*

MATERIALS SCIENCE DIVISION (MSD)

This Division conducts basic research on metals, alloys, ceramics -- including high-T_C superconductors -- and glasses that could have applications in advanced energy systems. The research programs are focused on the structure and properties of materials under extreme conditions of temperature, pressure, radiation flux, and chemical environment. The Division operates the high-voltage electron-microscope Tandem-Accelerator System as a national user facility.

500 EMERGING MATERIALS

The Emerging Materials group explores the fundamental science of complex materials that exhibit collective electronic, magnetic and structural behaviors, with an emphasis on low-dimensional oxide systems. Current and planned research plans concentrate on phase competition and short-range order, new geometrically frustrated magnets, exotic magnets, superconductors and quantum critical materials. Synergy between properties measurement and materials synthesis stands as the cornerstone of our activity. We employ both exploratory and strategic synthesis to expose new science in both unknown and previously-discovered materials. Our high-quality crystals grown by zone, flux and vapor transport methods drive our local research and are in high demand worldwide. Characterization techniques include magnetism, transport, tunneling and diffraction studies both locally and at DOE user facilities. Looking forward, we plan to expand the scope of our materials synthesis activities by growing our own program, through strategic connections with local universities, and through DOE system-wide initiatives in materials design, discovery, and growth.

501 MAGNETIC NANOSTRUCTURES

This group prepares and characterizes ultrathin films and related magnetic nanostructures with novel properties. The goals are to explore ultra-strong permanent magnets made possible via nanotechnology, and spintronic device concepts and prototypes that could become important as the semiconductor electronics roadmap for miniaturization reaches its limits in the foreseeable future. The materials are prepared as surfaces, interfaces, heterostructures, superlattices, and patterned array structures using molecular-beam epitaxy, sputtering, lithography and self-assembly techniques. Characterization techniques include ultrahigh-vacuum electron spectroscopies and diffraction, magneto-optic Kerr effect, magnetometry, magnetotransport, scanning probes, and x-ray diffraction. Participants aid in the preparation of the nanostructures, and analysis and modeling of physical properties. Data handling via computer is usually part of the assignment.

502 APPLIED SUPERCONDUCTIVITY

This research concentrates on high-temperature oxide superconductors. It addresses materials fabrication and fundamental scientific issues that affect the end uses of these materials. As an example, characterizations of these materials by transmission electron microscopy help to bridge the connection between current carrying capability and fabrication conditions so that better materials can be made. Thus an important properties characterization involves low temperature electrical conduction measurements (made down to a temperature of 2K) using superconducting magnets to provide fields of up to 9T. We study the magnetic flux lines which penetrate the superconductor in a field with aim of better understanding their dynamics. This is of great interest from the point of view of fundamental physics, but is also very important for high current applications since flux motion leads to voltages within the superconductor and thereby the loss of perfect conduction.

503 BASIC SUPERCONDUCTIVITY

Our research includes both experimental and theoretical investigations into the physics of a wide class of magnetic and superconducting materials. Current activities are concerned with characterizing the electronic properties of high temperature and two band superconductors, hybrid magnetic and superconducting heterostructures, synthesis and characterization of magnetic and superconducting nanowires and wire networks, and exploration of vortex physics in mesoscopic superconductors. Experimental techniques include high field/low temperature magneto-transport measurements, UHV/low-temperature/high-field scanning tunneling microscopy, low temperature atomic force microscopy, magnetization measurements with Hall probes and superconducting quantum interference devices (SQUID), nanocalorimetry and high resolution magneto-optics to visualize magnetic flux motion in real time. Participants will be involved with a variety of measuring techniques and instrumentation, and learn through hands-on experience, the fundamentals of experimentation including computer interfaces.

504 NEUTRON AND X-RAY SCATTERING

Members of the Neutron and X-ray Scattering Group pursue diverse multidisciplinary research programs that combine MSD's strengths in materials synthesis, characterization, and theory with state-of-the-art probes of the structure and dynamics of materials at major neutron and x-ray scattering facilities. A strong theme that permeates much of the group's research is the effect of phase competition on material properties, whether arising from the delicate balance of competing interactions within bulk complex oxides, proximity effects in artificial heterostructures, or phase segregation in multicomponent biomembranes. When scientific goals are hindered by limitations in existing instrumentation, the group has a strong tradition of developing new techniques that extend the capabilities of the field, and members play a lead role in the development of novel instrumentation and techniques at the Advanced Photon Source and the Spallation Neutron Source at Oak Ridge National Laboratory.

505 SYNCHROTRON RADIATION STUDIES

The synchrotron radiation studies group utilizes a variety of synchrotron techniques ranging from surface X-ray diffraction for in-situ studies of interfaces, to angle-resolved UV photoemission measurements for studies of electronic structure of materials. These studies are carried out at the Advanced Photon Source at Argonne and the Synchrotron Radiation Center in Stoughton, Wisconsin. Of particular interest are real-time studies of MOCVD growth of ferroelectrics and solid-state lighting materials, electrocatalysis, and electronic structure of high-temperature superconductors. Participants are invited to join with a group member in research of mutual interest or to contribute to on-going research efforts.

506 CONDENSED MATTER THEORY

Projects are available in a variety of areas involving analytical and numerical simulations of condensed matter systems. Past participant projects included studies of various properties of superconductors (microscopic and phenomenological theories, high temperature superconductors, vortices, etc.), electronic structure and properties of strongly correlated metals (including analysis of spectroscopic data), quantum critical and heavy fermion physics, and mesoscopic science (properties of quantum wires and quantum dots). Participant responsibilities include analytical solution of models, programming and running simulations, data analysis, and participation in discussions of their scientific implications. Participants will have the opportunity to use supercomputers and parallel processors.

507 CERAMIC EPITAXIAL FILMS AND COMPOSITES

Thin-film ceramic materials are widely used in a variety of device applications with significant economic impact. The physical properties of such films differ from bulk properties because of epitaxial strains and growth defects resulting from lattice mismatch and other interfacial effects. This program focuses on the processing, characterization, and property determination of single-crystal and polycrystalline epitaxial ceramic films and layered composites prepared by metal-organic chemical vapor deposition (MOCVD) techniques and by means of atomistic computer simulations (the latter involving lattice statics, lattice dynamics, molecular dynamics and Monte Carlo techniques). The main objectives are twofold, namely (a) to enhance our fundamental understanding of the processing-structure-property relationship of thin ceramic films and multilayers and (b) to measure and/or simulate tensor properties of single-crystalline films, thus elucidating the physical basis for the performance of these materials. In the past, devices using these materials have been made almost exclusively in polycrystalline form. Our main emphasis is on electro-ceramic materials, involving their dielectric, piezoelectric, electro-optic, acousto-optic and elastic behavior, with particular emphasis on the role of interfaces, such as grain and phase boundaries.

508 INTERFACES IN THIN FILM OXIDE HETEROSTRUCTURES

This program addresses interface-related properties of advanced thin film oxide heterostructures, with particular emphasis on atomic-level investigations of the structure and chemistry of the interfaces. Thin film oxide heterostructures are used, for example, in nanoscale ferroelectric devices and in magnetic tunnel junction structures, both of which have applications in information storage and memory. In this program we are combining advanced methods for the synthesis of these materials in nanophase, multilayer and/or thin-film form with atomic-level experimental characterization techniques and first-principles simulations of novel materials. Among the issues that we are addressing are the influence of the surface environment of ferroelectric films on domain formation, and the way in which integration into heterostructures affects the behavior of thin magnetic and ferroelectric films. The program draws heavily on three major Argonne facilities: the Electron Microscopy Center (HREM, AEM), the Advanced Photon Source, and the Center for Nanoscale Materials. Advanced facilities for synthesis and in-situ characterization, together with ex-situ transport measurement and computation facilities exist within the group.

509 ELECTRON MICROSCOPY CENTER FOR MATERIALS RESEARCH

Research in the Electron Microscopy Center is directed toward the experimental determination of the morphology, crystallography, elemental and chemical composition, and electronic structure of phases, interfaces, surfaces, and defects present in pure elements, alloys, ceramics, and other technologically important materials. State-of-the-art transmission and scanning-transmission electron microscopes (TEM/STEM's) are employed to characterize the microstructure of solids using conventional diffraction contrast techniques. Quantitative analytical information is obtained through the use of X-ray energy dispersive and electron energy-loss spectrometers for elemental, chemical, and electronic structure studies interfaced to the above instruments. This analytical information is obtainable from regions that can be as small as 10 nanometers in diameter. Investigators can choose to concentrate on applications of transmission electron-microscopy-based techniques to characterize materials, or research on fundamental (experimental or theoretical) studies of electron/solid interactions to advance state-of-the-art understanding and techniques for characterization. When appropriate, joint appointments between the Electron Microscopy Center and various MSD research groups will be suggested.

510 MOLECULAR MATERIALS: CONDUCTIVE ORGANIC THIN FILMS

This project is centered around the fabrication and characterization of thin conducting films composed of organic molecules. Thin films of these unusual materials are especially suitable for their eventual application, e.g., in chemical sensors or electronic devices. Electrochemical and chemical techniques are employed to prepare the charge transfer organic thin films. Infrared, Raman, and UV-Vis spectroscopies, x-ray diffraction, scanning probe microscopy, conductivity measurements, etc., will be used to characterize the structural and physical properties of these thin films.

511 SURFACE AND INTERFACIAL CHEMISTRY

Exemplified by the increasingly stringent demands of the electronic industry for unambiguous quantitative identification of trace impurities in semiconductor materials at high lateral resolution and by the environmental need for isotopic and elemental analysis of micron sized grains, trace analysis on samples of atomic dimensions has become an important analytical problem. Resonance Ionization Mass Spectrometers (RIMS) have been developed that combine both high sensitivity and high discrimination allowing for the first time trace analysis of samples with impurity atom counts of only a few hundred - even when the impurity concentration is below 1 ppt. Additional benefits of the instrumentation are discrimination from isobaric impurities and an ability to make measurements in regions of changing chemical compositions.

These RIMS instruments are being applied to a wide range of fundamental and applied surface science problems. Presently under investigation are (1) the fundamentals of energetic ion and laser - solid interactions, (2) ultra-trace semiconductor impurity analysis, (3) ways of improving plastics by understanding additive surface diffusion, and (4) isotopic analysis of nanopatterned samples.

512 MOLECULAR MATERIALS: NANOSTRUCTURED BLOCK COPOLYMERS

Block copolymer is a unique class of material that undergoes microphase separation into the submicron region. One-, two-, and three-dimensional nanostructured materials in 10 to 100 nm domain have been reported. These materials may lead to nonlithographic techniques for surface patterning. The aim of this project is to study the self-assembly processes in these block copolymers, to characterize the microphase separation and physical properties of the resulting materials, and to utilize the copolymers as structure-directing templates in order to prepare nanostructured materials with desirable optical, magnetic, or electrical properties.

513 MOLECULAR MATERIALS: BIOMIMETIC NANOSTRUCTURES

The level of control of supramolecular architecture found in nature far exceeds that currently achievable in synthetic materials chemistry. Our work involves studying and applying the concepts of supramolecular organization to produce hierarchically ordered self-assembled systems. Chemical systems and materials derived from these efforts include biomimetic complex fluids, liquid crystals, and polymers. These spatially organized structures exhibit functional behavior on multiple-length scales and may provide the basis for the development of a wide range of molecular devices of possible utility in such diverse areas as catalysis, bioprocessing, energy storage and transduction, chemical and biological sensors, and nanolithography. This research involves the synthesis of novel materials and their characterization using small angle neutron, X-ray, and light scattering, thermal analysis, and magnetic resonance, and vibrational, and optical spectroscopies.

514 PROXIMITY EFFECTS IN CONDUCTING OXIDE HETEROSTRUCTURES

This program seeks to create, characterize, and understand thin film oxide heterostructures that exhibit novel ionic, electronic, or mixed conduction properties. By exploiting proximity effects induced by heterointerfaces through space charge, elastic strain, and interfacial atomic structure, new materials are created with controllable properties that are unattainable in bulk materials. These proximity effects are amplified in heterostructures when layer spacings are reduced below distances where electronic charges strongly interact or strain-fields overlap. The program focuses on epitaxially-strained two-phase nanocomposite heterostructures that phase-separate during growth to form single crystal nanolamellae, nanopillars, or nanodots embedded in single crystal thin film matrices. The unique capabilities of in situ synchrotron x-ray techniques at the Advanced Photon Source are exploited to determine depth-resolved atomic-level structure and film composition in real-time, in the near-atmospheric pressure, elevated temperature environments that are integral to growth and transport behavior. Complementary multi-scale simulations provide understanding of the factors that control strain, composition, and structure during growth, and play a key role in identifying and elucidating charge transport mechanisms.

515 DOMAIN BEHAVIOR IN FERROIC MATERIALS

The behavior and properties of ferroelectric and magnetic heterostructures are dependent on the behavior of their domains, i.e. on the way in which domains form and move as a function of an applied field. In turn the domains and their dynamics are controlled by the microstructure and composition of the films through interactions with features such as grain boundaries, defects, the presence of interfaces, and of confinement between bounding layers of the heterostructure. Further control of domain structure and dynamics can be achieved by lateral confinement, for example via patterning to produce 3-D nanostructures. The aim of this program is to develop a clear understanding of how the structural/defect properties of such materials affect their magnetic and electric response. This is being done through in-situ studies of local domain structure and dynamics combined with microstructural and elemental analysis, and with in-situ TEM studies of local tunneling characteristics. The program makes use of in-situ transmission electron microscopy and X-ray scattering techniques at two of Argonne’s user facilities to explore the domain behavior in magnetic and ferroelectric thin films and heterostructures. Examples of problems that are being addressed are the interactions between magnetic nanostructures patterned into arrays, the role of surface environment on domain formation in ferroelectric films and the interaction of ferroelectric domain walls with defects in thin films.

516 SCIENCE OF DISSIMILAR MATERIALS INTEGRATION

This program addresses the science of film growth and interface processes between dissimilar materials, and resulting properties. Studies focus on oxide/diamond heterostructure film interfaces and polarizable and biocompatible oxide/biomolecules interaction. Emphasis is on atomic-level investigations of the structure and chemistry of these interfaces. In this program we are combining advanced methods for the synthesis of dissimilar materials in nanophase, multilayer and/or thin-film form with atomic-level experimental characterization techniques and first-principles simulations. Critical scientific issues being addressed include discovery of diffusion barriers to integrate oxides with diamond, for example, and investigation of biomolecule/oxide interfaces. The program draws heavily on three major Argonne facilities: the Electron Microscopy Center (HREM, AEM), the Advanced Photon Source, and the Center for Nanoscale Materials. This program also includes the development of microelectromechanical and nanoelectromechanical system (MEMS/NEMS) devices to study micro and nanotribological and mechanical phenomena at the micro and nanoscales and use the understanding to develop novel multifunctional devices.

517 COSMO CHEMISTRY

We are using unique analytical tools to measure how stars work. We have four sources of materials to study which come from other stars. Two of these samples were returned by the Genesis and the Stardust space craft. The Genesis samples tell us about the isotopic and elemental composition of our own star – the sun. These samples like a third collection rare isotopes found in deap sea sediments tell us about how the average star in our universe behaves. The Stardust samples include materials which condensed around other stars and have been collected in our solar system but are unchanged since condensation. Similarly a fourth sample type meteoritic grains are presolar in origin. The isotopic and elemental composition of these grains allows us to measure for the first time the nucleosynthetic conditions of individual stars.

518 PHYSICS OF GRANULAR AND BIOLOGICAL MATERIALS

Our research includes innovative experimental and theoretical investigations of the wide range of phenomena at the frontier of condensed matter and biological physics: flows of granular materials, dynamic self-assembly of micro and nano particles, and more recently, organization collective behavior of various biological objects, such as molecular motors, microtubules, bacteria. Experimental techniques include a variety of high-speed, fluorescent, phase contrast, dark field video microscopy, and the state-of-the art image processing of experimental video data. Theoretical studies include computer modeling of dynamic processes of self-organization, and molecular dynamics simulations. Participants will be involved with a variety of microscopy and experimental image processing techniques, bio sample preparations, and learn through first hand experience, the fundamentals of experimentation and computer modeling.

MATHEMATICS AND COMPUTER SCIENCE DIVISION (MCS)

The Mathematics and Computer Science Division is a basic research division, where applied mathematicians and computer scientists collaborate with computational scientists to advance the state of the art of scientific computing. Our goals are to discover, adapt, and apply computational techniques that promise to be useful in solving scientific and engineering problems. In keeping with our goals, we choose selected applications to evaluate the methods, algorithms, and tools that we develop in our research activities. These applications may come from fluid mechanics, atmospheric science, materials science, molecular biology, or any other area of scientific interest where we believe that mathematics and computer science can advance the state of the art. Because parallel computers are playing an increasingly significant role in scientific computing, most of our research is directed toward parallel architectures.

ALGORITHMS AND SOFTWARE

An essential part of the MCS Division research program involves designing algorithms for the numerical solution of problems common to many scientific and engineering applications and implementing these algorithms on high-performance computers.

519 INTEROPERABLE MESH AND GEOMETRY TOOLS

This project investigates algorithms and tools for the generation, representation and processing of meshes for PDE-based simulation. These tools are used for mesh pre- and postprocessing but also link directly to parallel simulations to provide mesh I/O and other services.
http://trac.mcs.anl.gov/projects/ITAPS/wiki

520 HARDWARE AND SOFTWARE SUPPORT FOR RUN-TIME REORDERING TRANSFORMATIONS

Reordering data and iterations at run time dramatically improves the performance of applications with irregular memory access patterns. This project is investigating the use of hardware features to support run-time reordering transformations and the development of new algorithms and software for run-time reordering. The reference platform is the IBM Blue Gene/P system, and the target applications are mesh-based scientific applications. Applicants should have a working knowledge of C/C++/Java. Experience with parallel programming is highly desirable.

521 NUMERICAL LINEAR ALGEBRA

Efforts in numerical linear algebra focus on both theory and application. We are interested in the design and analysis of algorithms for solving large-scale problems on parallel architectures, with emphasis on the development of reusable software tools. Our current focus is on the solution of nonlinear algebraic equations arising in the solution of partial differential equations. These equations are used to model a variety of physical phenomena, including fluid flow and structural mechanics. *http://www.mcs.anl.gov/petsc/*

522 SENSITIVITY ANALYSIS AND DESIGN OPTIMIZATION

Sensitivity analysis determines the change in responses of a computational model with respect to perturbations in certain key parameters. Given a way to assess the sensitivity of model parameters to key parameters, one can then embed the model code in a numerical optimization procedure to find the values of input parameters that result in the desired model behavior. In this context, we are applying computational differentiation, optimization, and parallel programming techniques to problems as diverse as climate modeling, automotive manufacturing, aeronautics design, biomechanical engineering, disease modeling, and environmental assessment and remediation. *http://www.mcs.anl.gov/autodiff*

523 COMBINATORIAL PROBLEMS IN SCIENTIFIC COMPUTING

The Computational Differentiation group develops compiler-based software engineering tools, primarily automatic differentiation (AD) tools that generate source code for computing mathematical derivatives, given arbitrarily complex source code for computing mathematical functions. We invite students and faculty to participate in the following projects: integration of automatic differentiation tools with optimization software and with toolkits for numerical solution of differential equations; development of Web-based application services for numerical software; performance optimization of AD-generated code; investigation of novel algorithms that can benefit from higher-order cheaper derivatives; development and implementation of techniques for uncertainty quantification and sensitivity analysis; development of compiler-based tools for source-to-source transformations; implementation of program analysis and optimization algorithms; and development of a test suite for AD tools. *http://www.mcs.anl.gov/autodiff*

524 PERFORMANCE ANALYSIS AND TUNING TOOLS

We are developing tools for analysis and user-guided tuning of Fortran and C/C++ codes. Source-based analysis tools are used to predict the maximum achievable performance for a particular architecture. Such performance-bounding tools enable application programmers to design more effective code and to evaluate an implementation, for example, by identifying sections of code where performance is limited by memory bandwidth or instruction scheduling. In our performance tuning research, we provide a high-level annotations language, which expresses the semantics of the computation, along with low-level performance tuning hints, such as variable alignment, loop unrolling, and various platform-specific optimizations. Based on these annotations, we generate multiple tuned versions of critical code kernels and experimentally select the best performing one for use in production application runs. We invite students and faculty to help develop source-based performance-bounding analysis tools, as well as tools for generating tuned code based on high-level user annotations. *http://www.mcs.anl.gov/performance/*

525 OPTIMIZATION

Optimization research centers on the development of algorithms and software for solving large-scale optimization problems on high-performance architectures. An important research project is the Toolkit for Advanced Optimization (TAO). The object-oriented design of TAO is motivated by the scattered support for parallel computations and lack of reuse of linear algebra software in currently available optimization software. Students will participate in the development of TAO and its use in interesting applications. Other research activities involve interior-point methods, trust-region methods, nonlinear complementarity, optimal control, and PDE-constrained optimization. Applications include reaction pathways, support vector machines, and macromolecular modeling.
http://www.mcs.anl.gov/optimization or http://www.mcs.anl.gov/tao

526 OPTIMIZATION TECHNOLOGY CENTER

The Optimization Technology Center, operated jointly by Argonne and Northwestern University, is devoted to the development of optimization solutions to scientific computing problems. Research focuses on optimization algorithms and software, Internet and distributed computing, and problem-solving environments. A major project, funded by the National Science Foundation under the Information Technology Research initiative, is exploring advanced application service provider technology for large-scale optimization. *http://www.mcs.anl.gov/otc/*

527 THE NETWORK-ENABLED OPTIMIZATION SYSTEM - NEOS

The NEOS Server is a novel environment for solving optimization problems over the Internet. There is no need to download an optimization solver, write code to call the optimization solver, or compute derivatives for nonlinear problems. The NEOS Server uses state-of-the-art optimization software, modeling language interfaces, software tools for remote usage and job processing, and automatic differentiation tools. This research project has attracted considerable attention from the user community, and as a result we are currently processing more than 5,000 submissions per month. Students will expand the capabilities of the NEOS Server by developing new solvers, interfaces, and scheduling algorithms. *http://neos.mcs.anl.gov/*

528 EXPLOITING PERFORMANCE-POWER TRADEOFFS IN SCIENTIFIC COMPUTING

Current high-end platforms are ensembles of multiple fast CPUs with deep memory hierarchies and high-speed interconnects. Geometric scaling of raw power (Moore's law) arises from more and faster transistors on a chip. However, chips are approaching their packaging thermal limits, and the power-related costs for high-end systems, both electrical power consumed (in megawatts) and machine room cooling loads, continue to grow as a quadratic function of peak execution rates and clock frequencies. We study the tradeoffs between reducing power consumption and achieving good performance on current and future high-performance architectures with a focus on scientific applications. The project's goal is twofold: we develop explicitly power-aware scientific computing tools for current platforms and provide insights that can be used by the designers of systems software and microprocessors to develop future extreme-scale systems. A significant component of this work is an outreach and education effort, particularly targeted at women and minority students from the middle school through graduate levels, with the goal of broadening the participation of these groups in computer science, engineering, and computational science.
http://www.cse.psu.edu/~raghavan/PxP.html

529 COMMON COMPONENT ARCHITECTURE (CCA)

As computational science progresses toward ever more realistic multiphysics and multiscale applications, the complexity is becoming such that no single research group can effectively develop, select, or tune all of the components in a given application, and no single tool, solver, or solution strategy can seamlessly span the entire spectrum efficiently. A goal of the multi-institutional Common Component Architecture (CCA) project is to help manage this complexity in high-performance scientific computing by facilitating the interoperability of different software libraries developed by different groups. Work at Argonne includes the development of scalable component-based libraries of linear, nonlinear, and optimization solvers as well as parallel coupling tools. We are also developing infrastructure for computational quality of service, which facilitates making sound choices from among available implementations and parameters, with suitable tradeoffs among performance, accuracy, mathematical consistency, and reliability. Such choices are important both for the initial composition and configuration of applications and for adaptive control during runtime. http://www.mcs.anl.gov/cca

COMPUTER SCIENCE

Computer science research addresses ways in which researchers can reduce the time required to write programs, increase program adaptability to high-performance computers, transform existing programs to derive sensitivity information, and enhance program clarity and correctness. For example, we are developing parallel-programming tools for transporting programs to new computer architectures. In addition, we continue to work with applications-oriented groups on projects such as computational biology.

530 DERIVATIVE CODE FOR MULTICORE ARCHITECTURES

Automatic differentiation tools (www.mcs.anl.gov/autodiff) generate source code for computing derivatives from source code for computing a function. In many cases, the generated code contains inherent parallelism that should be exploited in order to fully realize the potential of modern multicore architectures. This project will examine the generation of derivative code that includes Open-MP pragmas for parallelism, as well as alternative parallelization strategies for homogeneous and heterogeneous multicore architectures (including the Cell BE and general purpose GPUs).

531 COORDINATED INFRASTRUCTURE FOR FAULT TOLERANT SYSTEMS (CIFTS)

In the next few years SciDAC applications will use petascale systems with tens of thousands to hundreds of thousands of processors, hundreds of I/O nodes, and thousands of disks. This leap of two orders of magnitude in scale from today's typical systems is causing a critical gap in fault management of these systems. Currently, systems software components for large-scale machines remain largely independent in their fault awareness and notification strategies. The goal of the CIFTS (Coordinated Infrastructure for Fault Tolerant Systems) project is to provide a coordinated infrastructure that will enable fault-tolerant systems to adapt to faults occurring in the operating environment in a holistic manner. We are currently designing the API and a reference implementation of a fault awareness and notification backplane to provide common uniform event handling and notification mechanisms for fault-aware libraries and middleware. We also plan to extend key software components belonging to areas of middleware, operating systems, job schedulers, file systems, math libraries, and applications with the fault tolerance backplane API to form the critical mass necessary for adoption in the community. *http://www.mcs.anl.gov/research/cifts/*

532 OPERATING SYSTEMS FOR MASSIVELY PARALLEL ARCHITECTURES

ZeptoOS is a research project studying operating systems for petascale architectures with 10,000 to 1 million CPUs. Operating system and run-time software is strained by ultra-scale machines, and a variety of fascinating research topics are revealed at such amazing scale. Our current activities focus on IBM's Blue Gene/P architecture. We are working on replacing proprietary elements of the software stack with open source ones, to facilitate better usability, more advanced optimizations, etc. In particular, we are working on a Linux-based compute node kernel, file and socket I/O forwarding infrastructure, and communication libraries. *http://www.zeptoos.org/*

533 URGENT COMPUTING

There is an increasingly growing domain of problems that are guided by scientific computation, such as global warming and city planning. Within this domain is a set of problems that are constrained by strict deadlines where results produced after that deadline may have very little use. Examples of such problems include severe weather modeling. In such a scenario, the results of a simulation may help guide the evacuation of residents in the target area. Clearly, if the results are produced after the severe weather event, they have little practical use. The Special PRiority and Urgent Computing Environment (SPRUCE) seeks to enable urgent computing through elevated batch priority, elevated network bandwidth and resource reservations. The primary focus is to decrease the amount (and the variability) of time it takes to produce results. Research areas include: resource selection, data movement, data storage, and many more. *http://spruce.uchicago.edu*

534 COMPILER-SUPPORT FOR DOMAIN-SPECIFIC TRANSFORMATIONS

Domain-specific transformations, such as automatic differentiation, require both traditional and domain-specific compiler analyses. This research includes implementation of advanced analysis algorithms in the OpenAnalysis framework and the investigation of ways to incorporate domain-specific concepts into data dependence analysis. The design and implementation of techniques for array data flow analysis also are considered. Applicants should have completed at least one compiler course (multiple semesters preferred) and have a working knowledge of C/C++. Experience with XML or numerical computing is also desirable. *http://www.mcs.anl.gov/autodiff/*

535 COMPUTATIONAL DIFFERENTIATION

The Computational Differentiation group develops compiler-based software engineering tools, primarily automatic differentiation (AD) tools that generate source code for computing mathematical derivatives, given arbitrarily complex source code for computing mathematical functions. We invite students and faculty to participate in the following projects: integration of automatic differentiation tools with optimization software and with toolkits for numerical solution of differential equations; development of Web-based application services for numerical software; performance optimization of AD-generated code; investigation of novel algorithms that can benefit from higher-order and/or cheaper derivatives; and development and implementation of techniques for uncertainty quantification and sensitivity analysis. *http://www.mcs.anl.gov/autodiff/*

536 PARALLEL-PROGRAMMING LIBRARIES

We develop libraries and tools that enable users to write portable parallel programs and also achieve high performance. Central to this effort is our MPICH2 implementation of MPI, which won the 2005 R&D 100 award. MPICH2 runs on many parallel architectures and modern networks and is used by many computer system vendors as the basis of their own MPI implementations. We are also interested in the design and implementation of high-level parallel programming languages and advanced programming models and tools for improving programmer productivity.
http://www.mcs.anl.gov/research/projects/mpich2

537 COMPUTATIONAL BIOLOGY

The objective of this research is to develop, implement, and use logic-based tools for the solution of scientific problems in molecular biology and genetics on high-performance computers. Current emphasis is on genetic sequence analysis and reconstruction of the metabolic network for sequenced genomes, tool development for automated analysis of metabolic models, and design of user-friendly querying tools to support research in biology and medicine. *http://compbio.mcs.anl.gov.*

538 MATHEMATICS OF PHYSICAL SYSTEMS

We are interested in nonlinear differential equations arising from the modeling of physical systems. Those currently studied come from condensed-matter physics and fluid mechanics and include the Landau-Lifshitz-Gilbert equations of micromagnetism, the Ginzburg-Landau equations of superconductivity, and the Navier-Stokes equations of fluid dynamics. We explore the solutions of these equations through large-scale numerical simulations, apply scientific visualization techniques and postprocessing software to obtain qualitative and quantitative information, and use analytical methods where possible to interpret the results.
http://www-unix.mcs.anl.gov/appliedmath/Flow/cfd.html

539 HIGH-PERFORMANCE I/O

A key component of any high-performance computing system is the I/O system. In order to provide the I/O bandwidth necessary for today's scientific applications, hundreds of individual disks are combined through software into a single, logical storage device. We develop software solutions for providing very high performance I/O while at the same time allowing application scientists to describe I/O accesses in terms of structures more familiar to them, such as arrays of data. Current projects include the PVFS parallel file system, the ROMIO MPI-IO implementation, the Parallel netCDF application I/O interface, and the DOE SciDAC project on Scientific Data Management.
http://www.mcs.anl.gov/hpio

540 GRID TECHNOLOGIES FOR DATA-INTENSIVE SCIENTIFIC COLLABORATION

Distributed scientific and engineering applications often require access to large amounts of data (terabytes or petabytes). Future applications envisioned by our team also require widely distributed access to data (for example, access in many places by many people or through virtual collaborative environments). Our work seeks to identify, prototype, and evaluate the key technologies required to support data grids for scientific and engineering collaborations. This work includes the following major activities: defining data grid architecture, implementing key software for data grids, constructing data grids for real scientific projects, and evaluating our software solutions. *http://www.globus.org/*toolkit/docs/2.4/datagrid

541 GRID INFORMATION SERVICES FOR SCIENTIFIC COLLABORATION

High-performance execution in distributed computing environments often requires careful selection and configuration, not only of computers, networks, and other resources, but also of the protocols and algorithms used by applications. Selection and configuration in turn require access to accurate, up-to-date information on the structure and state of available resources. We are working on requirements, designs, and prototypes of a Grid information service that satisfies these infrastructure-level requirements. *http://www.globus.org/toolkit/mds*

542 SECURITY SERVICES FOR SCIENTIFIC COLLABORATION

Security in computational Grids is complicated by the need to establish secure relationships between a large number of dynamically created subjects and across a range of administrative domains, each with its own local security policy. Our work in this area ranges from developing basic security algorithms for secure group communications and techniques based on delegation of trust for managing trust relationships to developing new mechanisms for fine-grained access control.
*http://www.globus.org/*toolkitdocs/4.0/security/

543 TERAGRID SCIENCE GATEWAYS

The complexity of distributed computing, or Grid, environments demands significant investment in the development of applications. Science Gateway activities focus on simplifying access to the TeraGrid, a large-scale Grid infrastructure involving resources at eleven laboratories and universities nationwide, for a given community. This simplification could come in a variety of forms, including simplified access to job activation and data movement; integration of workflow tools; and data-streaming protocols to provide easy client-side access to instrument data, sensors, visualization services, and databases. We are currently working with a number of science partners in disciplines ranging from biology to meteorology, integrating tools via Portal technology. *http://www.teragrid.org*

NUCLEAR ENGINEERING DIVISION (NE)

The Nuclear Engineering (NE) Division conducts both theoretical and experimental research & development, engineering, and computation, with emphasis in nuclear technology and related sciences. Major areas include advanced reactor design and analysis, advanced materials studies, nuclear safety, reactor fuel cycle analysis, reactor physics, criticality safety, and environmental management. The Division also has significant capability in advanced simulation of multi-physics phenomena in support of advanced reactor development using leadership-class computers.

A major mission of the Division is in Arms Control, National Security, and Nonproliferation. The Reduced Enrichment for Research and Test Reactors (RERTR) program is an important area that has made significant contributions to global threat reduction. A primary objective of RERTR is the development of high density, low enrichment fuel that can be used to replace the current high-enrichment fuels in research and test reactors worldwide, thereby reducing the threat that these reactors could be subverted for a weapons program. Other program areas include export control, nuclear material control and accounting, nuclear and radiological material security, and information technology and security.

The Dismantlement, Deactivation, Decontamination, Decommissioning and Disposal (generally abbreviated as D&D) of aging nuclear facilities is a key area that addresses a large problem for the DOE, US nuclear utilities and international organizations. The development of new technologies and their demonstrations on surplus ANL nuclear facilities and elsewhere form a key part of the work. In addition, there are a number of other areas in which technology development is being undertaken. These include sensor and detector technology, robotics, rad-waste technology and security, and laser applications.

544 COMPUTATIONAL MECHANICS

Development of parallel finite element based software that would be used to resolve structural integrity issues arising in the design of next generation reactor plants. The work would include the extension of current software to include additional nonlinear mechanics, contact-impact phenomena and heat conduction.

Knowledge of engineering mechanics and/or heat conduction, numerical methods, Fortran 90/95, MPI, parallel programming and Linux would be desirable.

545 COMPUTER STUDIES OF NUCLEAR REACTORS

Analyses are performed to predict the behavior of nuclear reactor systems in steady state or in operational and accidental transients. Large-scale computer codes containing models of heat transfer, single and two-phase flow, reactor physics (cross section data processing, reactor statics, fuel depletion, and reactor kinetics), and structural-mechanical behavior are employed. The participant should have a basic understanding of one or more of the following areas: heat transfer, fluid flow, reactor physics, structural mechanics, and a working knowledge of FORTRAN. Experience with large-scale scientific computer codes and applications are desirable.

546 PROBABILISTIC RISK ASSESSMENT

Probabilistic Risk Assessment (PRA) activities include development of probabilistic methods for applications to safety analysis of nuclear facilities including consequence analysis; basic plant component failure data analysis; systems reliability modeling with common cause failure; sensitivity theory methods and applications in PRA; use of PRA techniques in support of plants modifications and maintenance, including analysis of human factors in procedures; and applications of PRA methods and models to new facility designs with stress of spent fuel treatment and disposal facilities are carried out.

547 ARTIFICIAL INTELLIGENCE APPLICATION

Large volumes of digitized data from operating nuclear power plants are processed, analyzed, and interpreted using state-of-the-art interactive signal processing techniques on distributed workstations and PCs. Software packages for various numerical, statistical, pattern- recognition and time-series analyses are developed, modified, and maintained using a variety of languages and software-engineering tools. On-line expert systems are being developed that use automated reasoning techniques for assistance with the tasks of surveillance, diagnosis, control and interpretation of physical parameters in advanced nuclear, aerospace, and industrial systems.

548 NUCLEAR WASTE AND REPOSITORY MODELING

The radiological characteristics of spent nuclear fuel and other potential waste forms are evaluated; and the impact of various waste processing techniques is assessed. The performance of nuclear wastes in a deep geological repository is modeled. Repository modeling must account for release of radionuclides from the waste package, and subsequent geochemical transport in the surrounding environment. Probabilistic risk evaluation tools are used to account for model and data uncertainties. Model development and validation requires an ability to integrate performance considerations from a wide variety of scientific fields. Experience with large-scale scientific and PRA computer codes is desirable.

549 FUEL PROCESS MODELING

Various chemical, thermal, and mechanical processes are involved in treating spent nuclear fuel and special nuclear materials to produce suitable waste forms for storage. Simulation of these processes is required to enable proper planning of the sequence of operations and material usage. Activities include development of a simulator for the overall process, including detailed models for the various processing steps, such as electrochemical transport and distillation. Data from the processes will be used to guide development of the models, especially in the area of process losses and material accountability.

550 NUCLEAR CRITICALITY SAFETY

Criticality safety and shielding analyses are performed for complex configurations and operations involving wide ranges of geometries, materials, and neutron spectra. These analysis efforts employ state-of-the-art nuclear data libraries and software and are complemented by ongoing R&D in methods development, software development, critical experimental evaluation, safety analysis report preparation, and nuclear data library validation.

551 ANALYSIS OF COMPLEX, INTEGRAL ENGINEERING SYSTEMS

Development of advanced analysis tools and techniques to address problems involving complex geometric configurations and multi-physics phenomena that are mostly thermally driven. Current applications include thermal hydraulic behavior of full-scale systems and the apparatus used in medium- to large-scale experiments. The commercially available computational fluid dynamics software are used as the base code for advanced model development.

552 COMPUTER STUDIES IN ENGINEERING MECHANICS PROGRAM

The program is concerned with the development of state-of-the-art computational mechanics tools (finite element methods and mesh-free methods) and visualization tools with application to the solution of complex engineering mechanics problems found in industry and reactor safety analysis. Recent research has been performed in coupling a probabilistic engine to our deterministic finite element code to perform physics-based structural reliability analysis and prediction. Currently, we are doing research on the development of finite element computer engines for use on advanced computing architectures including a PC, single workstation, distributed workstations, Beowulf cluster, scalable systems, and massively parallel computers. In addition, research has focused on using virtual reality tools, such as Argonne's immersive virtual reality CAVE and the Nuclear Engineering Division's virtual reality hardware to display computational mechanics results and design concepts. New work on the Computational Material Science Initiative will focus on modeling the behavior of materials at the mesoscale that accounts for various grain boundary mechanisms and the elastic response of the grain interior. Numerical studies are being performed on the response of three-dimensional seismic isolation systems targeted for use with Generation IV reactors. An ongoing research area is the simulation of the response of steel, reinforced concrete, and prestressed concrete structures to static and dynamic overpressure as well as external loading events. Additional research areas include the following: fluid-structure interaction, thermochemical analysis and high temperature response of concrete structures.

553 ADVANCED REACTOR CONCEPT DEVELOPMENT

Opportunities exist for students to participate in development, analysis, and experiment activities supporting innovative concepts for future nuclear power plants. The advanced concepts emphasize passive safety, nonproliferation, long core lifetime, simplicity, low cost, and high reliability. Students will work with experienced researchers to study existing concepts, address new approaches, develop and utilize analytical models, and perform trade-off and optimizing studies. Specific disciplines of interest include heat transfer, fluid mechanics, materials science, heat exchanger technology, steam/gas turbine technology, component design, and cost/efficiency modeling. Students may also select to participate in experiment activities including development of apparatus, assist staff in conducting experiments, interpret results, and compare data with model predictions.

554 COMPUTATIONAL FLUID DYNAMICS

Fluid dynamics, heat, and mass transfer for a variety of large-scale engineering systems. Current efforts focus on, but not limited to, problems related to nuclear safety, electrochemical process modeling, and combustion simulations, aerodynamics, and underhood thermal management. Analytical tools include in-house codes and commercially available computational fluid dynamics software.

555 COMPUTER AIDED DESIGN, MANUFACTURE, AND OPERATIONS SIMULATION

Computational graphics techniques have improved over the last 20 years from simply substituting hand-drawn parts designs with electronic versions of exactly the same figures for plotting by pen-and-ink X-Y plotters to creating 3-Dimensional electronic models of parts that easily can be rotated, modified, assembled to other parts, moved with respect to other assemblies, and even viewed in a virtual reality environment in such a way as to give the impression that the viewer is standing next or even among the pieces modeled. Moreover, these models can be used to provide input to numerically controlled machining centers so that, in principle, parts drawings are no longer needed for manufacture. We are in the midst of converting our engineering, design, and manufacturing to the 3-D modeling in order to reduce the design/drafting time required to verify fit-up of adjacent parts and to avoid interferences between non-adjacent parts and assemblies. Much of our work is directed toward development of equipment and processes that are operated in a high-radiation and inert-atmosphere hot-cell, using hands-off manipulation of components by cranes, electro-mechanical manipulators (the predecessor to robotic arms), and master-slave through-wall manipulators. Thus, we are looking toward extending the modeling to circumvent some of the extensive testing of prototype and actual hardware in a simulated fully operational environment that is normally done to guarantee functionality and accessibility by the various remote handling tools for assembly, operation, and maintenance in this environment. Extension to true robotics is a logical follow-on to our engineering efforts. Opportunities exist for participation in the development of 3-D models of new equipment, of equipment previously designed using 2-D design/drafting tools, of the facilities in which this equipment is used, and of virtual reality models of all of these.

556 PROLIFERATION ASSESSMENT OF FUTURE NUCLEAR ARCHITECTURES

A major issue facing the development and expansion of nuclear power worldwide is the possibility for diversion of the technologies and materials to Weapons of Mass Destruction (WMD). A challenge facing the United States is assessing and understanding the proliferation risks of future nuclear architectures (power plant and fuel cycle designs). A number of sophisticated decision theory techniques are to be considered including fault and event tree methods.

557 RADIATION DETECTION TECHNOLOGY

Advanced radiation detectors are required for both basic science missions and for applied research in such areas as national security. These activities entail the development of advanced gamma ray and neutron detectors and require physics, engineering or computer programming support in the following areas:

- Development of detector materials for gamma-rays and x-rays,
- fast and thermal neutron detectors for detection of nuclear materials,
- development of algorithms for gamma spectroscopy using heavily degraded
- spectra,
- electronics design for small detector packages,
- computer simulations of neutron and gamma detector response, and
- development of algorithms for integrated and distributed detector systems.

558 LASER APPLICATIONS LABORATORY

The laboratory focuses on collaborative research and development activities with industrial partners. The facility includes high-power industrial CO_2 and Nd:YAG lasers, Nano-second pulse width Q-switch Nd:YAG lasers, five-axis workstations, and diagnostic systems for laser beam characterization, plasma analysis and process monitoring/control. Current collaborative research with industry include drilling rocks for petroleum applications, heat treating and glazing of steels, welding of metals and alloys, beam shaping and fiber optics and process monitoring. Other R&D activities include laser surface modification, laser ignition of mixture of natural gas and air and materials testing using laser thermal simulation.

559 GLOBAL THREAT REDUCTION INITIATIVE – REACTOR CONVERSION PROGRAM (GTRI-REACTOR CONVERSION)

The DOE Office of Defense Nuclear Nonproliferation (Office of Global Threat Reduction, NA-21) supports the activities of the Global Threat Reduction Initiative-Reactor Conversion (GTRI-Reactor Conversion) program, previously known as the Reduced Enriched Research and Test Reactor (RERTR) program. The goal of the GTRI-Reactor Conversion program is to minimize and eventually eliminate the use of highly enriched uranium (HEU) in civilian applications. The program achieves its goal by converting research and test reactors to the use of low enriched uranium (LEU) fuels and targets. The program has been very successful, and has developed low-enriched uranium (LEU) fuel materials and designs which can be used effectively in converting the majority of research and test reactors which used HEU to the use of LEU fuel. Current activities focus on development of more advanced, higher density LEU fuels that will allow the conversion of high flux research and test reactors, collaboration with Russian HEU minimization efforts and other international participants in fuel development, development of an LEU-based process to produce Mo-99, and technical assistance to research reactors wishing to convert to LEU.

560 AEROSOL SCIENCES

Participants' primary responsibility will be to contribute to experimental investigations and theoretical modeling in the fields of basic and applied aerosol science. Opportunities also exist in the areas of computerized data acquisition and data reduction. Research applications include aerosol generation, transport, pollution control, sampling, and analysis for both nuclear and fossil power systems. Additional research areas involve the development of novel devices to disperse or collect particles or to develop instrumentation to measure aerosol parameters, pulsed corona applications, and spray generation and characterization. Basic areas of research include electrostatic particle charging, particle formation, transport, agglomeration, deposition, and adhesion mechanisms; radiative heat transfer in particle-laden gages; particle filtration; material erosion by aerosol impaction; aerosol-vapor interactions; and bioaerosol sampling and processing.

561 FUSION BLANKET AND SHIELD STUDIES

This activity is concerned with a general design evaluation of first wall/blanket/shield components of fusion reactors. Various combinations of blanket structural material/coolant/neutron multiplier/ tritium breeding material are being reviewed to develop a well-defined set of design criteria. Experimental and analytical activities on first-wall, blanket, and shield components are underway to develop design tools for reactor first-wall, blanket, and shield including neutronics, thermal hydraulics, structural mechanics, and blanket modules for testing in the International Thermonuclear Experimental Reactor (ITER).

562 FUSION MATERIALS STUDIES

Investigations are conducted to develop an understanding of the effects of a fusion-reactor environment on the properties and performance of candidate blanket materials; structural, breeder, neutron multiplier, first wall tile, and ceramic coating materials. These efforts are focused on low-activation alloys and electrically insulating coatings, and include investigations of irradiation effects, corrosion/compatibility, mechanical properties and welding. This activity includes evaluation and correlations of fission-reactor and ion irradiations to simulate the displacement damage and transmutation reactions characteristic of a fusion neutron spectrum.

563 FUSION BLANKET TECHNOLOGY TESTING

This research involves development and testing of fundamental technologies required for tritium breeding blankets. An important aspect of this effort for liquid metal blanket is the development of electrically insulating coatings on structural materials to mitigate magnetohydrodynamic effects associated with a flowing liquid metal in high magnetic fields. This activity includes development of ceramic breeding materials, neutron multiplier materials, tritium recovery from liquid and ceramic breeding materials and neutronic analysis of tritium breeding capability, activation and afterheat of irradiated materials, structural analyses of the blanket design, and shielding characteristics.

564 SPENT NUCLEAR FUEL PROCESSING

Pilot Scale - Demonstration of electrometallurgical technology for metallic fast reactor fuel from EBR-II is being conducted at the Fuel Conditioning Facility. This technology employs a combination of electrochemical and metallurgical processes to prepare spent nuclear fuel for disposal. Processing takes place in a heavily shielded argon-atmosphere cell. Process control is automated to the extent possible through the use of computer and programmable logic controllers. Areas of research include computer modeling of the pyroprocesses and engineering of improved equipment with faster process rates and greater automation.

565 ROBOTICS

This program supports experimental and theoretical work for improvements and applications of teleoperated robotic systems. Particular emphasis is on implementation of 'teleautonomy' and 'virtual fixture.' In teleautonomy, the robot's autonomous behavior is blended with human instruction for efficient teleoperation. Virtual fixture is an artificially generated surface overlaid on human perception - kinesthetic, visual, and auditory - to help precisely guide the robot motion in teleoperation. The application fields may include inspection, repair, material handling, and decommissioning of nuclear facilities, and other recently emerging application in robotic surgery and service robots. Research topics of interest include dual-arm collaboration, machine vision and sensing, haptic feedback, machine intelligence, and remote control. Examples of activities for participants include programming, simulation, and hardware implementation and testing.

566 NE-INFORMATION TECHNOLOGY AND SECURITY

The focus of this research area is the development of web based database applications for national security programs for the Department of Energy, National Nuclear Security Administration, and the Department of Defense. Multiple information technology projects are conducted by the section in the security, nuclear nonproliferation and defense areas.

567 LIQUID METAL EXPERIMENTS SUPPORTING THE DEVELOPMENT OF THE RARE ISOTOPE ACCELERATOR

A number of studies are under way involving various aspects of liquid metal technology, primarily involving stripper films and targets. These may include studies of thin films, beam interactions with a flowing fluid, materials compatibility, potential lithium vapor transport in a vacuum system, and development of measurement techniques and data acquisition. These studies will closely coincide with ongoing laboratory experimental programs studying liquid metal phenomena. The participants work with staff who are developing the experimental demonstrations and measurement techniques, as well as the assembly and operation of the experimental apparatus.

568 INSTRUMENTATION AND NONDESTRUCTIVE EVALUATION

The Instrumentation and Nondestructive Evaluation (NDE) Section conducts research and development in a broad range of energy-related technologies. Major areas of responsibilities are the development of instruments or NDE techniques for fossil energy, conservation, automobile, textile, waste management, and nuclear technologies, as well as for arms control and verification treaties and homeland security.

The current instrumentation efforts of the Section focus on the development of advanced sensors and control systems. This work encompasses (a) multiphase flow measurement techniques, including in-situ measurement of temperature, fluid level, pressure, density, and viscosity; (b) development of leak detection and location systems for power plants; and (c) a number of projects for arms control to develop sensor/instruments for treaty verification and homeland security. Sensors used in the treaty verification project and homeland security projects are based on acoustic microwave/millimeter wave, submillimeter terahertz, and mass spectrometer techniques. The instruments/sensors are used to detect chemical, biological or nuclear agents as well as explosives. In addition, work has started in developing sensors for biomedical applications.

Our NDE efforts focus on development of techniques and systems for materials characterization and evaluation of component reliability. This work includes (a) characterizing materials, especially ceramics composites, as well as metal, during various stages of fabrication; (b) evaluating the structural integrity of components of a wide variety of energy systems; and (c) pinpointing causes and remedies for improper component behavior through failure analysis. The techniques used to perform this work are based on acoustic, X-ray diffraction and X-ray tomography, NMR spectroscopy and imaging, microwave, neutron diffraction, optical methods, and eddy current.

569 STEAM GENERATOR TUBE INTEGRITY PROGRAM

The structural integrity of pressurized water reactor steam generator tubes containing stress corrosion cracks and similar defects is being experimentally and analytically investigated. Tubes with prototypic stress corrosion cracks are being produced in the laboratory, and these tubes are being tested under simulated operating conditions to determine their failure pressures and leak rates. The structural response of these tubes is also being evaluated using fracture mechanics calculations and finite-element modeling. In addition, existing and advanced eddy current and other NDE techniques for the detection and characterization of flaws in tubes are being evaluated.

570 ANALYSIS AND MODELING OF MATERIALS BEHAVIOR IN ENERGY SYSTEMS

A modern, high-speed, digital computer is employed to simulate the physical behavior of materials used in advanced energy systems (fission and fusion). In the fission area, the thermal, mechanical, and irradiation response of fuel elements for the Reduced Enrichment Research and Test Reactor (RERTR) program are analyzed. Emphasis is placed on realistic models that accurately describe the physical situation. The DART code system is being developed in order to assess the behavior of dispersion fuels for the RERTR. In the fusion area, the thermal, mechanical, and irradiation performance of solid breeders (Li_2O and other ternary oxides) are being modeled. The TIARA code has been developed, verified and validated to predict the tritium inventory in lithium ceramics under fusion reactor operation conditions. Other research activities include the analysis of specific phenomena (e.g. helium-induced swelling) in order to identify key process and/or physical parameters that affect material performance and the thermal and mechanical responses of fusion first-wall structures under novel cooling schemes is being modeled.

571 IRRADIATION PERFORMANCE OF REACTOR MATERIALS

The principal objective of the programs in the Irradiation Performance Section is to assess the behavior of nuclear materials, including cladding and structural components, in the environment of nuclear fission and fusion reactors. These environments result in neutron damage and chemical, metallurgical, and mechanical processes that occur over a wide range of elevated temperatures. The programs fall into the following categories: (1) postirradiation characterization of materials, and (2) postirradiation thermal/mechanical testing of materials. A significant fraction of the Section's activity is devoted to the performance characterization of light-water reactor fuel systems during loss of coolant accidents and spent-nuclear-fuel cask transport accidents. The postirradiation characterization and testing activities utilize the Irradiated Materials Laboratory and other radiological-controlled laboratories to perform examination, testing and analyses. Available research tools include optical microscopes, transmission electron microscope, hydrogen and oxygen determinators, and numerous thermal and mechanical testing instruments. Cooperative research programs are welcome.

572 CORROSION OF MATERIALS IN THE PRESENCE OF DEPOSITS

The program involves experimental studies to establish the mechanisms of corrosion of heat-exchanger and gas-turbine materials in the presence of deposits that are generated during the combustion of coal and coal-derived fuels. The research will require background in the areas of thermodynamics and kinetics of gas-solid reactions and fluid-flow characteristics that influence the type and rate of deposit(s). A background in X-ray diffraction is desirable.

573 STRESS-CORROSION CRACKING OF LIGHT-WATER REACTOR MATERIALS IN SIMULATED COOLANT ENVIRONMENTS

The program involves an experimental investigation of the influence of simulated reactor-coolant environments, under normal and off-normal water chemistry conditions, on the susceptibility of piping and structural materials to stress-corrosion cracking. The effect of microstructure of the materials, water chemistry (viz. oxygen, hydrogen and impurity concentrations, pH), and temperature on the rate and mode of crack growth is being determined for a range of loading conditions. Background in the areas of electrochemistry, electron microscopy, aqueous corrosion, and physical metallurgy are applicable.

574 ALLOY MODIFICATION FOR IMPROVED CORROSION

The program involves experimental studies to establish the composition and microstructure of surface layers (created by ion implantation, surface coating, laser annealing, etc.) that impart improved corrosion resistance in oxygen and oxygen-sulfur-chloride environments. A background in transmission electron microscopy and Auger Electron Spectroscopy is desirable.

OFFICE OF TECHNOLOGY TRANSFER (OTT)

The Office of Technology Transfer (OTT) provides ANL the interface with industry to support the DOE mission of transferring technology through partnerships having the potential to benefit the public, U.S. Industry, and the nation as a whole. Transfer of technology is important to support national policy objectives, improve competitiveness of US industry, and contribute to the national economic and scientific base. Specific activities are technology development, characterization, and marketing leading to Work for Others, Cooperative Research and Development Agreements, licensing, new business startups, and other contracts to facilitate efficient and expeditious deployment of federally developed technology.

575 Characterize Laboratory technology portfolios, identify appropriate potential technology transfer partners and conduct focused marketing activities.

Solicit feedback and perform surveys regarding the effectiveness of OTT activities.

Initiate contact with potential industrial partners and work with them to commercialize new scientific advances.

Develop new license agreements and other innovative approaches for transferring intellectual property into commercial use.

Define and implement action to exploit opportunities for new start-up businesses built on Argonne technology.

PHYSICS DIVISION (PHY)

The Physics Division conducts basic experimental and theoretical research in nuclear, atomic, and molecular physics. We are also involved in the continuing development of the Argonne Tandem-Linear Accelerator System (ATLAS), a novel superconducting heavy-ion accelerator, which is operated as a national facility for nuclear physics research.

576 SUPERCONDUCTING HEAVY-ION LINAC "ATLAS"

The Physics Division is the home of the world's first superconducting ion accelerator, the Argonne Tandem Linac Accelerator Systems, ATLAS. This accelerator is based on superconducting radio-frequency resonators and can accelerate any ion from ones as light as protons (atomic mass 1) to ones as heavy as uranium (atomic mass 238). ATLAS is a Department of Energy National User's Facility that provides high quality ion beams for basic research in nuclear science as described in the next section. The accelerator physics staff based at ATLAS is active in a variety of research and development projects. The topics include superconducting radio-frequency resonator, ion sources based on microwave-heated plasmas, ion beam dynamics simulations, computer control systems, and other related topics. Much of the present research and development is directed towards the components of a proposed advanced accelerator called the Rare Isotope Accelerator, RIA. It is based on extensions of the present ATLAS technology and involves extending superconducting heavy ion linear accelerators to much higher energies and beam power. Topics currently being pursued for this new project also include the design and testing of high-power targets and associated ion sources for the production, extraction, and ionization of short-lived radioisotopes. Novel methods are also being developed for the efficient acceleration of these rare isotopes.

577 NUCLEAR REACTIONS AND NUCLEAR STRUCTURE STUDIES BY HEAVY IONS

Nuclear structure and reactions are studied in collisions between complex nuclei with heavy-ion beams mostly from the Argonne Tandem-Linac Accelerator (ATLAS), a national heavy-ion users facility. The major thrusts of this program are three-fold: (a) the understanding of the nucleus as a many-body system built of protons and neutrons and governed by the strong force, (b) the exploration of the origin of the chemical elements and their role in shaping the reactions that occur in the cataclysmic events of the cosmos and (c) tests of the limits of validity of the Standard Model, the fundamental theory that currently best represents our understanding of the laws and fundamental symmetries of Nature.

The specific current research topics include the development and acceleration of short-lived nuclei and their use in measurements of cross-sections of astrophysics interests as well as in nuclear structure and reaction dynamics studies; the production and study of nuclei at the very limits of stability, including the discovery of new proton emitters near the drip line, and the study of the properties of very heavy elements (actinide and transfermium (Z>100) nuclei), the study of exotic nuclear shapes; the delineation of the essential parameters governing dynamics of reactions between heavy nuclei; tests of current descriptions of the weak force.

These efforts are based on forefront instrumentation available at ATLAS which includes: (1) the Fragment Mass Analyzer, which separates nuclear reaction products from the beam and transprots them to a detection station; (2) the Canadian Penning Trap, which measures nuclear masses with unsurpassed accuracy; (3) a magnetic spectrograph for the detection of high-velocity reaction products; (4) a large, versatile reaction chamber; and (5) a number of gamma-ray detectors including Compton-suppressed germanium spectrometers and NaI and BaF2 scintillators. At the present time, Gammasphere, the national gamma-ray facility composed of 110 Compton-suppressed, large volume Ge detectors is also installed at ATLAS.

There are always opportunities for research participants to be involved in every aspect of the program from the development of detectors to the actual running of experiments, and from the analysis of data to the development of simulations and/or calculations to assist in the interpretation of the results.

578 NUCLEAR PHYSICS AT INTERMEDIATE ENERGIES

The origin of the basic nuclear force between nucleons is explored in our program of Nuclear Physics at Intermediate Energies. In particular, the role of the constituents of the nucleons, i.e. quarks and gluons in a fundamental description of nuclear forces is examined in experiments primarily utilizing electromagnetic probes. A number of studies are currently in progress at the TJNAF (Thomas Jefferson National Accelerator Facility). Physics Division staff members led in the construction of experimental facilities, serve as spokespersons for a number of experiments, and are actively involved in others. Studies of fundamental symmetries that make use of parity violating electron scattering are also performed at Jefferson Lab.

A second major component of our program involves high energy experiments that probe the structure of the quark sea in the nucleon. These experiments will be performed at Fermilab (Fermi National Accelerator Laboratory). .

A third component of our program is the study of the origin of the spin of the nucleon. Physics Division staff have had a major role in HERMES, a broadly based international collaboration devoted to the study of the spin structure of the nucleon using internal polarized targets in the HERA storage ring at DESY (Deutsches Elektronen-Synchrotron), Hamburg, Germany. Although these experiments are completed, analyses of the data are in progress.

More information can be found at http://www.phy.anl.gov/mep/index.html. Opportunities exist for research participants to be involved in all aspects of our work.

579 THEORY RESEARCH

Theory research in the Physics Division addresses a broad range of important problems in nuclear astrophysics, and nuclear physics involving the structure and dynamics of hadrons and nuclei. There is strong emphasis on comparison with data from Argonne's ATLAS facility, from JLab, and from other laboratories around the world; and identifying and predicting phenomena that can be explored with a rare isotope accelerator. The Theory Group has five principal areas of research: (i) the modeling and application of quantum chromodynamics (QCD) to light- and heavy-hadron structure at zero temperature and density, and at the extremes of temperature and density appropriate to the early universe, neutron stars, and RHIC experiments; (ii) the development of reaction theories for use in exploring hadron structure using the data from meson and nucleon-resonance production experiments at JLab, MIT-Bates and Mainz; (iii) the construction of realistic two-and three-nucleon potentials that give accurate fits to nucleon-nucleon elastic scattering data and properties of light nuclei, and their use in detailed many-body calculations of light and near closed-shell nuclei, nuclear matter and neutron stars, and in a variety of astrophysically important electroweak reactions; (iv) the investigation of nuclear processes that take place in stars, in the big bang, and in interstellar and intergalactic space, with emphasis on the basic mechanisms of supernova explosions; and (v) nuclear structure and reaction studies, which include a focus on high-spin deformation and the structure nature's heaviest elements, and coupled-channels calculations of heavy-ion reactions near the Coulomb barrier and calculations of observables in breakup reactions of nuclei far from stability. Additional research is pursued in atomic physics, neutron physics, quantum computing, fundamental quantum mechanics, and tests of fundamental symmetries and theories unifying all the forces of nature, and the search for a spatial or temporal variation in Nature's basic parameters. A significant number of our projects involve major numerical simulations using the massively parallel computer systems at Argonne and NERSC. Many projects also involve collaborators, student and staff, at US and foreign universities, and other national laboratories.

580 LASER TRAPPING AND PROBING OF EXOTIC ATOMS

The ability to control an atom, both its internal and external degrees of freedom, has improved dramatically since the time of the classic Stern-Gerlach experiment. Rapid progress has occurred in recent years due to exciting developments in the field of laser spectroscopy and laser manipulation of atoms. Using precisely controlled laser beams, an atom can be spatially confined in a trap, cooled so that it barely moves, and induced into a quantum superposition of multiple states. We develop new and improve existing methods of controlling atoms, and use these methods to explore scientific problems in the realm of physics and beyond. The following is a brief description of a couple of on-going projects of our group. More details are available at our website: http://www-mep.phy.anl.gov/atta/

Testing time-reversal symmetry in atoms and nuclei. We are searching for a permanent electric-dipole moment (EDM) of the ^{225}Ra ($t_{1/2}$ = 15 d) atom. A positive finding would signify the violation of time-reversal symmetry (T). This experiment provides an outstanding opportunity to search for new physics beyond the Standard Model. We have succeeded in realizing laser trapping and cooling of radium atoms (both ^{226}Ra and ^{225}Ra) for the first time ever. At present, we are developing the techniques and apparatus needed for the EDM measurements with cold ^{225}Ra atoms.

Radio-krypton dating – from dream to practice. The Atom Trap Trace Analysis (ATTA) method has revolutionized our ability to measure radiokrypton isotopes, ^{81}Kr ($t_{1/2}$ = 229,000 yr) and ^{85}Kr ($t_{1/2}$ = 10.8 yr), in samples of natural material. This in turn opens the door to a wide range of new applications in the Earth sciences. ^{81}Kr measurements of groundwater samples from the Nubian Aquifer in the Western Desert of Egypt showed residence times approaching one million years. At present, we are developing the next generation instrument, ATTA-3, which is expected to further reduce sample sizes required for radiokrypton analysis of groundwater and glacial ice.

Our experiments are typically performed by a small team of researchers in a hands-on style. Each participating student can select from a diverse range of projects according to the individual's interests. Projects carried out by past students include developing a discharge source of metastable krypton atoms, making a sensitive photon detector, investigating new ways to reduce the scattering light below the single-atom level, and developing a LabView program for a video processing system.