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).

500 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.

501 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.

502 X-RAY SCIENCE DIVISION

These activities include research, development, and construction of instrumentation needed for the broad range of x-ray microscopy, scattering, spectroscopy, imaging, and time-resolved measurements to be performed at the Advanced Photon Source. Current activities are related to insertion devices, beam-line components, X-ray optics, detectors, novel synchrotron radiation instrumentation, and other experimental equipment useful for various research applications.

503 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.

504 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.

505 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.

506 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.

507 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.

508 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)

Research in this Division is aimed at defining the biological and medical hazards to humans from energy technologies and new energy options. Health-related studies are supported by fundamental research in scientific disciplines, including molecular and cellular biology, crystallography, biophysics, genetics, radiobiology, biochemistry, chemistry, and environmental toxicology. The research involves the integration of findings from investigations at the molecular, cellular, tissue, organ, and whole-animal levels, with the ultimate aim of applying these findings to problems of human health. The Division is organized into three scientific sections (Biophysics, Functional Genomics, and Terrestrial), plus a Structural Biology Center that operates two beamlines at the Advanced Photon Source. Each section comprises several research groups with considerable interaction occurring among all groups. Divisional support facilities include an editorial office, a computer center, a biomedical library, and an instrument design and maintenance shop.

BIOPHYSICS SECTION

509 MACROMOLECULAR INTERACTIONS

A major research goal in biological science is to understand the relationship between the amino acid sequence of a protein and its three-dimensional structure, stability, and function. Because the interactions between the amino acids within a protein obey the same laws of physics that control interactions between proteins, study of the self-association properties of immunoglobulin light chains is relevant to the fundamental properties of all proteins. Antibody light chains are produced in large quantities by patients who have myeloma, a neoplasm. Because the proteins produced by two patients will be similar in three-dimensional structure but will differ in amino-acid sequence, differences in self-association (under various conditions of pH, ionic strength, and temperature) can be related to the physics that determines the protein structure and function. In addition, these studies provide increased understanding of the biophysical properties of these proteins that lead to disease complications in many patients and provide a model system for other, structurally related, protein-based diseases. We are using site-specific mutagenesis, molecular dynamics simulations, and novel bioinformatic approaches to help analyze experimental results.

510 PROTEIN CRYSTALLOGRAPHY AND MOLECULAR MODELING

The principal aims of this program are the expression, isolation and characterization of biologically important macromolecules, the determination of their detailed three-dimensional structures in crystalline state, and the correlation of structure with biological function. The biomolecules under study include cytochromes, bacterial photosynthetic reaction center. The techniques used in this program are taken from a variety of disciplines including molecular biology, protein chemistry, chromatography, protein crystallography, and computer modeling of protein structures. Major equipment includes a rotating anode X-ray generator with an R-axis#2 data collection system and interactive computer color graphics terminals for manipulating macromolecules in three dimensions.

511 SBC/APS USER FACILITY

This program applies modern crystallographic methods to rapidly determine structures of biological macromolecules-proteins and nucleic acids-as single molecules, as multicomponent complexes, and complexed with bound ligands. A significant effort in this program is directed toward improving the methods for crystallographic investigation of macromolecular structure, by developing new and better methods and instruments to measure, process, and analyze diffraction data using cryocrystallography. The program operates two advanced x-ray beamlines at the Advanced Photon Source, for tuned, high-throughput, monochromatic x-ray diffraction data collection that is used to determine crystal structures. Crystal structures are being studied of chaperone proteins which direct the folding of protein receptors, important enzymes from pathogenic and thermolphilic organisms, and nucleic acids. Structures of proteins derived from genomic analysis as part of our structural genomic initiative are being determined at this facility. Major equipment includes undulator and bending magnet beamlines, rotating-anode x-ray generator, with imaging plate detector, modern workstations with large capacity data-storage disks, interactive graphics workstations for molecular modeling, HPLC, FPLC, and ectrophoresis equipment, and all necessary facilities and equipment for molecular biology, molecular genetic manipulations of DNA, protein purification and crystallization, and activity assays.

512 PROTEIN ENGINEERING

This program is aimed at a generalized understanding of how the three-dimensional structure of a membrane protein defines its function. Historically, our work has focused on the bacterial photosynthetic reaction center, a transmembrane protein complex that functions in the process by which light energy is converted into chemical energy. More recently, our research focus has expanded to the development of a generalized system for the heterologous expression, purification, and crystallization of any membrane protein for structure determination or functional characterization. Techniques consistently exercised include gene cloning with plasmid vectors, PCR amplification of DNA sequences, DNA sequencing, protein and DNA gel electrophoresis, protein expression and purification, spectroscopy, bioassay of mutant phenotypes, and protein crystallization. We are in the process of automating many of our routine methodologies using robots recently installed within the division.

513 STRUCTURAL STUDIES OF MACROMOLECULAR ASSEMBLIES

Recognition of biological macromolecules and their interaction and assembly into larger supermacromolecular structures are at the heart of many important processes in molecular and cellular biology. For example, macromolecular assembly occurs in protein biosynthesis, in the recognition of receptors by protein hormones, in the folding of proteins, and in the recognition of and binding to nucleic acids by proteins that regulate the expression of genetic information. We are studying macromolecular assemblies at the atomic and molecular levels by x-ray crystallography, in particular the protein-protein interactions of molecular chaperones of the hsp60 and hsp70 classes, and large oligomeric enzymes, and protein-nucleic acid complexes. Because the crystals of macromolecular assemblies are usually small and fragile and have large unit cell dimensions, they diffract weakly. Furthermore, these crystals have large, complex structures and their structure determination is experimentally demanding. These studies take advantage of the Advanced Photon Source and the Structural Biology Center and the Midwest Center for Structural Genomics facilities at Argonne. The techniques being used include molecular biology and biochemistry, liquid chromatography and electrophoresis, and synchrotron-based x-ray crystallography. Robotic workstations support purification, crystallization, data collection and structure determination.

514 HIGH THROUGHPUT APPROACHES TO STUDY PROTEIN FUNCTION

The abundance of genomic sequence data from different organisms provides an opportunity to accelerate our understanding of protein structure and function. However, optimal utilization of this information requires the development of high throughput methods for the generation of expression clones and the evaluation of protein function. We are developing automated methods for high throughput gene cloning and expression, site-specific mutagenesis, and the study of protein function. A Beckman Coulter Core System with integrated liquid handling stations and supporting devices provides the capability for high throughput production of expression clones for structural genomics and other large-scale programs that aim to characterize protein structure and function. This comprehensive strategy provides an alternative to the single protein approach that has previously dominated cell biology. The current cloning and analysis process spans four days with a maximum linear throughput of 400 targets per production run. The output generated from the expression cloning process is a 96-well plate map that specifies the location of soluble expression clone plasmids. Although developed for structural genomics, the experience gained by implementation of these initial protocols will provide a platform for extension of the system capabilities for application in other growth areas of high throughput molecular biology including site-specific mutagenesis, phage display, and protein interaction studies.

515 BRIDGING BIOSCIENCE AND NANO-SCIENCE: DEVELOPING NOVEL TOOLS FOR UNDERSTANDING PROTEIN-LIGAND INTERACTIONS FOR SYSTEMS BIOLOGY

A key aspect of the functional characterization of genomes is the understanding and consequent mapping of interactions among proteins and between proteins and ligands at systems level. This project is involved in the development of novel methods to make this mapping possible by engaging the combination of bioscience and nanotechnology. Particular research efforts for this project emphasize the use of single molecule manipulation and detection methods (such as scanning fluorescence correlation spectroscopy) to select ligands directly from combinatorial libraries. Since unveiling the mechanism of protein-ligand interactions plays an important role in elucidating protein functionality, we will also develop new tools to solve the protein binding domain structure using surface enhanced Raman spectroscopy.

FUNCTIONAL GENOMICS SECTION

516 PROTEOMICS

Two-dimensional gel electrophoresis coupled with computerized image and data analysis is being used to characterize the normal protein composition of cells and to detect changes in response to environmental pressures. Current studies are focused on the analysis and identification of proteins produced by microorganisms. In addition to two-dimensional gel electrophoresis of proteins (isoelectric focusing combined with sodium dodecyl sulfate polyacrylamide gel electrophoresis), this project involves the use of image and data analysis algorithms, World Wide Web databases, and mass spectrometry. The construction and maintenance of interactive Internet databases is an important part of the data presentation for this project.

517 METALLOPROTEOMICS

Our laboratory is conducting research into the interaction of trace metals such as copper and zinc with proteins and how these interactions change during cellular processes to affect protein activity. It is our contention that metal:protein are regulated dynamically during numerous cellular processes and such regulations may act as a form of post-translational regulation of a protein's structure and function. As a system of study, we are using several models of angiogenesis, the process by which new blood capillaries are formed. It is well-known that angiogenesis is high sensitive, both *in vitro* and *in vivo*, to bioavailable copper. We are employing and developing numerous methodologies to investigate dynamism in the metalloproteome during endothelial cell angiogenesis. These include use of the Advanced Photon Source for high resolution x-ray fluorescence metal mapping *in situ*, development of separative methodologies for metalloproteins, and isolation and identification of novel metalloproteins used by these cells as they undergo morphogenetic differentiation.

518 BIOCHEMICAL TOXICOLOGY

This research program is designed to investigate health effects of toxic metals to which humans may be environmentally or occupationally exposed. One research area focuses on the role of pregnancy, lactation, or ovariectomy in the susceptibility of animals to bone loss after cadmium exposure. Mechanisms of cadmium action on bone are studied in isolated bone cells in culture. Molecular pathways of cadmium action are investigated for specific genes known to influence bone resorption and by gene expression microarray to identify unknown genes. Another research area focuses on the biochemical pathways for toxic heavy metals, including their uptake and tissue deposition. The role of metallothionein, a metal-binding protein, is studied using normal and metallothionein-deficient mice. Measurements of calcium and cadmium content in tissues are performed using atomic absorption spectroscopy.

519 ANTIBODY ENGINEERING

With the recent completion of two hundred sequenced bacterial and six eukaryotic genomes, the scientific community is entering a “post-genomics era”. To add value to this accomplishment, the community's attention is now directed at determining the function of the thousands of gene products, proteins, in each cell. Traditionally, one valuable type of reagent that is widely used to probe cells and learn when the protein is synthesized, where it is localized, and what it is associated with in the cell is the antibody. However, it typically takes two to three months to generate rabbit or mouse antibodies to each individual protein, and there is limited control by the investigator on the quality of the antibodies generated by the immunized animals. To overcome the limitations of antibody generation and to meet the need for thousands of antibodies, we utilize phage-display to isolate high-affinity and selectively generate designer antibodies to any protein. Such antibodies will be used to 1) affinity purify the target proteins from cells, and then identify interacting proteins through gel electrophoresis and mass spectrometry, 2) promote crystallization of proteins for x-ray diffraction studies at the Advanced Photon Source (APS), and 3) format the antibodies as arrays onto glass slides, with which one can measure the concentrations of many proteins simultaneously in cells, as they respond to stimuli or become diseased.

Mortality in over 90% of cancer patients is the result not of the effects of the primary lesion, but the crowding out of normal cells by metastatic tumor cells at secondary sites within the body. Cellular migration of tumors is dependent upon both the successful disruption of cell-cell contacts at the primary site and the erection of proper scaffolding at the secondary site(s). A major step in scaffolding construction must include the attraction of new blood vessels (or angiogenesis) to feed and oxygenate the new tumor. These new vessels are primarily built with a class of cells called endothelial cells, which are one of the very few cell types in mammals that have the ability to migrate post-embryonically. Our group is using a systems biology approach to identify the major protein players involved in endothelial cell migration, differentiation, and morphogenesis in order to develop a new class of side effect-free anti-cancer drugs.

Our recently acquired ability to decode the genomes of both uni- and multi-cellular organisms (including man) has given us the blueprint for understanding biological processes at a level not before possible. The conversion of sequence information into the who, what, where, when, how and why of any one biological process, however, will require the simultaneous application of a number of intersecting methodologies. Knowledge of the three dimensional structure of a protein will in turn frequently translate into functional information, allowing for the elucidation of unexpected links in biological pathways not as amenable to discovery by the more traditional hypothesis-driven research methods.

Small angle x-ray scattering (SAXS) of proteins and macromolecular complexes in solution has been shown to reliably yield information about the size and shape of proteins. More recently it has been demonstrated by our group that wide angle scattering patterns (WAXS) obtained at high flux third generation synchrotron beam lines are not only sensitive to protein conformation states, but the scattering patterns generated can be quantitatively compared to detailed structural models. This data, made possible by third generation synchrotron sources, provides a rich source of structural information that has not yet been exploited. Given the broad range of conditions and particle sizes amenable to solution x-ray scattering, a combination of HTP SAXS and WAXS analysis downstream from a large-scale protein production facility has the potential to generate information on the size, shape and structural class (i.e. fold) of every expressed protein.

This project proposes to establish and standardize a SAXS/WAXS protocol to collect structural data on a large number of proteins; construct a database of small and wide angle scattering patterns; and to use this data to assign a structural class to each of the proteins studied. The long term goal is a high throughput method for experimentally assigning the structural class of every protein that can be expressed from a genome. This work will require the high brilliance focused undulator beams at the Advanced Photon Source (APS) that generate a flux density 100-fold greater than those of second generation sources.

TERRESTRIAL SECTION

Research activities conducted in this area involve both field and laboratory investigations on the transport, fate, and biogeochemical behavior of hazardous wastes, including radionuclides and associated underlying geochemical processes. Other studies address the effects of environmental stresses on terrestrial ecosystems, both natural and managed. Environmental stresses include such things as air pollutants, acidic rain, and ozone. Disturbance effects studies examine changes to ecosystems resulting from stresses associated with energy production and use.

521 TERRESTRIAL ECOLOGY

The ability of plants to adapt or respond to a changing environment is dependent on homeostatic capacities that minimize the cost of growth and biomass allocation. Plants' responses to environmental stresses, such as nutrient limitation or anthropogenic effects such as elevated CO_2, suggest that they have a centralized system of stress response involving changes in nutrient and water use, carbon allocation, hormonal balances, and reliance on mycorrhizal fungi. Our research addresses mechanisms controlling plants with obligate and facultative dependency on the mycorrhizal symbiosis and the relative importance of these mechanisms in various plant life forms. Our overall objective is to determine whether a major mechanism of control is the balance between photo-assimilate supply to the roots and the host's need for nutrients. To address this objective, two general questions will be investigated: (1) what are the mechanisms controlling photo-assimilate allocation to the fungus and nutrient inflow to the plant? (2) Will the host's dependence on supplied nutrients influence its ability to adjust to a changing environment? (3) Does a relationship exist between net C gain of the host and the amount and activity of mycorrhizal fungi?

522 TERRESTRIAL CARBON PROCESSES

Concerns over rising concentrations of atmospheric CO_2 have increased interest in the capacity of soil to serve as a carbon sink. The amount of carbon stored in world soils is estimated at more than twice the carbon in vegetation or in the atmosphere. Thus, even relatively small changes in soil carbon storage per unit area could have a significant impact on the global carbon balance. Soil carbon may be stabilized because of its biochemical recalcitrance or by incorporation into organomineral complexes with clays. Soil structure also plays a dominant role in controlling microbial access to substrates and, thus, relatively labile organic material can be physically protected from decomposition by incorporation into soil aggregates. This project is researching the biological mechanisms involved in the formation, stabilization, and degradation of aggregates and how the aggregation process, in turn, influences soil carbon dynamics. This information is necessary (1) to identify management practices that maximize soil carbon sequestration and (2) to determine the potential for terrestrial ecosystems to serve as a sink for elevated concentrations of atmospheric CO_2. This project involves application of soil physical and biological fractionation techniques and stable isotope measurements to samples obtained from elevated CO_2 experiments and sites with long-term plots representing alternative land management strategies.

523 SYNCHROTRON-BASED ENVIRONMENTAL RESEARCH

This research program in synchrotron-based environmental research is aimed at exploring applications of new advances in x-ray physics to understanding problems in environmental science. The principal goal of this program is to address general issues concerning the bioavailability of contaminants in the environment, with a particular emphasis on the mobility, uptake mechanisms, transformations, and toxicity of metals and organic chemicals in natural soils. Research projects include both the study of bulk samples by using x-ray absorption spectroscopy and the study of microscopic samples and spatial variations on the micron length scale by using x-ray fluorescence imaging, phase contrast imaging, and x-ray absorption spectroscopy with micron-sized spots. Particular research interests within the group include: (1) the investigation of mineral-microbe interactions so as to better understand the role of these interactions in the fate and transport of heavy metal contaminants; and (2) the study of newly created, highly-reactive materials for the selective removal of radioactive contaminants from DOE waste storage tasks.

MICROBIOLOGY

In recent years the genomes of numerous microbes have been determined, making vast numbers of previously unknown proteins accessible. Many of these proteins participate in important biochemical reactions related to the interaction of microbes with the environment. The microbiology group participates in several projects that exploit this new information to improve the understanding of microbes and their proteins, and to engineer them to perform useful functions more efficiently. In collaboration with chemical engineers, integrated fermentation and separation processes are being developed to reduce energy and petroleum consumption in the production of chemicals. Our focus in this effort is metabolic engineering, the genetic modification metabolism to allow the production of chemicals for renewable materials such as corn. A second area of research seeks to improve the understanding of microbial biochemistry by determining the structure of as many of their proteins as possible. Our contribution involves improvements in the production of proteins for crystallographic studies through development of new, high-throughput expression vectors and culture conditions. A third activity deals with the bioremediation of toxic metals through their reduction by microbes under anaerobic conditions. Fundamental physiological studies seek to establish the response of the organisms that carry out these processes to different growth conditions, as well as to develop new methods for the detection and characterization of the proteins involved. Recently, an additional research effort has been initiated, investigation of the formation biofilms in the environment and their role in the biogeochemical cycling of materials.

524 PROTEIN EXPRESSION

A standard approach for characterizing a new protein is to clone its gene and express the protein in a suitable host, such as *E. coli*. Many vectors are available for protein expression, but new ones are often needed for special proteins or special applications. We have developed vectors that (1) allow expression of highly toxic proteins in *E. coli*, and (2) facilitate high throughput cloning, expression and purification of proteins. The latter is currently used in a major project to determine the structures of hundreds of microbial proteins over the next several years. The vector also serves as a platform for the development of additional vectors; it can be modified easily to give variants that should enhance the expression, solubility and purification of proteins.

525 ENZYMOLOGY AND GENETIC ENGINEERING

Many proteins are enzymes, catalyzing the reactions that drive life processes. Purification and characterization of enzymes provides information critical to the understanding of those processes and of great value for harnessing reactions for other uses. We have cloned and purified several enzymes involved in emerging industrial applications that produce chemicals in a more environmentally acceptable way, using renewable biological starting materials and generating fewer pollutants. Where appropriate, genetic engineering is used to alter the specificity of the enzymes by site directed mutagenesis. In related research, “metabolic engineering”, genetically knocking out or adding specific enzymes to alter metabolism, is used to increase the yield of desired products.

526 BIOREMEDIATION

Many critical reactions of bioremediation are catalyzed by metalloproteins. Recent efforts in our laboratory, in collaboration with physicists and proteome biologists, are developing new methods for detecting and analyzing metalloproteins. High intensity X-ray beams available at Argonne’s Advanced Photon Source allow detection of low concentrations of many metals simultaneously. Various protein fractions, ranging from the total protein content of cells to pure individual proteins, are under investigation. The intent is to establish high throughput techniques to separate, detect and identify individual proteins induced under bioremediation conditions. For some proteins, the methods will allow partial determination of the structural environment of the metal in the protein, providing insight into how it contributes to bioremediation.

527 MICROBIOLOGY

Microbes can convert agricultural feedstocks, such as sugars derived from corn, into valuable chemicals, and have long been exploited for this ability. Efforts are now in progress to expand their use to include the production of larger-volume, less-expensive chemicals through new "green" processes. At Argonne, modern techniques in microbiology, genetic engineering, and enzymology are applied in "metabolic engineering", in which metabolic pathways are altered by adjusting gene expression or introducing new enzymes, thereby channeling metabolites to the desired end products. Another major activity of the Microbiology Group involves a collaboration with structural biologists in determining the structures of diverse microbial proteins. This project, funded by NIH, seeks to accelerate greatly the rate at which protein structures can be solved, as well as provide a complete library of potential protein structures. In that effort, we have developed new expression vectors and novel cell culture methods that facilitiate high-throughput production of proteins. Additional vectors under development promise to improve the solubility of expressed proteins and to allow their production in host cells other than E. coli.

Microbes can convert cheap, renewable resources to valuable products and have long been exploited for this ability. Efforts are now in progress to expand their use to include the production of larger-volume, less-expensive chemicals. New processes and products to be developed will reduce both dependency on petroleum and the environmental liabilities of some industrial chemicals. At Argonne, modern techniques in microbiology, genetic engineering, and enzymology, as well as classical approaches, are being applied in this effort. Addition of foreign genes or alteration of gene expression, called "metabolic engineering", attempts to alter the metabolic pathways of the microbes to produce different chemicals. Site-specific mutagenesis of proteins attempts to change the specificity or stability of enzymes to create novel catalysts that will carry out useful reactions not performed by naturally occurring enzymes. Strains developed by these approaches are evaluated in laboratory scale fermentations, which are then optimized for production of the desired metabolites.

CHEMICAL ENGINEERING DIVISION (CMT)

The Chemical Engineering Division is a diverse early-stage engineering organization specializing in the treatment of spent nuclear fuel, development of advanced electrochemical power sources, and management of both high- and low-level nuclear wastes. Currently, we are engaged in the development of several technologies of national importance. Included among them are: advanced lithium-ion and lithium-polymer batteries for transportation and other applications; hydrogen production and fuel cells for transportation and stationary applications; stable nuclear waste forms suitable for storage in a geological repository; and aqueous and pyrochemical processes for the disposition of spent nuclear fuel. Other important programs are focused in catalysis, nanotechnology, and nuclear materials. All Chemical Engineering Division projects are backed up by strong basic research.

FUEL CELL RESEARCH AND DEVELOPMENT

528 POLYMER ELECTROLYTE FUEL CELL DEVELOPMENT

Because of its low temperature and solid electrolyte, the polymer electrolyte fuel cell (PEFC) is being developed for mobile power applications, such as passenger vehicles. Such fuel cells use hydrogen as the fuel (either pure or part of a fuel gas mixture that contains hydrogen) and air as the oxidant for the fuel cell reaction that combines the fuel and oxidant to generate useful electric power, waste heat, and product water. The conventional PEFCs use platinum or platinum alloys as electrocatalysts, which makes them rather expensive. The goal of our program is to develop electrode catalysts that minimize the use of precious metals. This project involves the use of basic electrochemical techniques to determine the oxygen reduction and hydrogen oxidation kinetics, as well as the stability of the catalysts in the acidic fuel cell environment. It also involves the construction and electrochemical testing of fuel cell assemblies and post-test examination of the electrocatalysts and other cell materials by scanning electron microscopy and other techniques. Major equipment includes: electrochemical instrumentation (potentiostat, galvanostat); AC impedance systems; scanning electron microscope; and personal computers.

529 HYDROGEN PRODUCTION FOR FUEL CELLS

Hydrogen is being developed as an energy carrier for transportation, portable power, and stationary power applications. For the fuel cell vehicles, high-purity hydrogen will be produced at the gas stations from available infrastructure fuels. These include natural gas for the near term and renewables, such as ethanol, for the longer term. Similarly, residential fuel cell systems are being developed to operate on a hydrogen-rich gas mixture derived from infrastructure fuels, such as natural gas or liquefied petroleum gas. These hydrogen generators, or fuel processors, are required to match the constraints and needs of the application, which include high energy efficiency, purity, pressure, size/weight, response to changing hydrogen demands, cost, etc. The Hydrogen Production Program at Argonne includes development of advanced catalysts for reforming and purification processes, reactor designs, fuel processor system designs, and demonstration of thermally integrated fuel processor concepts. Major experimental and analytical capabilities include: micro- and bench-scale reactor apparatus, gas chromatographs, mass spectrometers, infrared analyzers, thermal conductivity analyzer for hydrogen, CO chemisorption analyzer, and BET surface area measurement. Material characterizations are performed with scanning electron microscopy, x-ray diffraction, and chemical assay.

530 CERAMIC ELECTROCHEMISTRY

Research activities involve the development of ceramic-based electrochemical devices and components, such as solid-oxide fuel cells and high-temperature steam electrolysis cells. Efforts are directed toward defining materials and fabrication processes that can achieve the desired structures and properties for electrolytes and electrodes, as well as a study of the poisoning effects of chromium in solid-oxide fuel cells. Projects involve characterization of electrochemical ceramic materials and components by means of impedance spectroscopy, DC polarization, x-ray fluorescence, diffraction and near-edge spectroscopy, electron microscopy, and other techniques. Current activities include the synthesis and fabrication of metallic and ceramic components using polymeric precursors and combustion syntheses, spraying, screen-printing, tape casting, slip casting, and extrusion. There is a continuing effort to enhance the understanding of the fundamental mechanisms of cell operation and improve materials and microstructural cell designs.

WASTE MANAGEMENT

531 GLASS HYDRATION STUDIES

When glass is contacted by water vapor or liquid water, alteration reactions occur. Water penetrates into the glass, forming a hydration layer, and displaced atoms diffuse to the glass surface and form minerals. These reactions are of interest to archaeology since hydration aging dating of natural glasses is a subject not well-understood. These reactions are also important to nuclear waste management since such surface alteration will affect the waste form behavior over extended storage periods. This program investigates the kinetics and mechanisms of these reactions using surface analytical techniques such as scanning electron microscopy. Major equipment includes: scanning electron microscope, transmission electron microscope, energy dispersive x-ray analyzer, laser Raman spectrometer, and Fourier transform infrared spectrometer.

532 NUCLEAR WASTE TESTING

The aim of this program is to determine the magnitude and composition of the radionuclide inventory (source term) for nuclear wastes in an environment similar to that expected for the candidate repository site at Yucca Mountain. Projects include tests on unirradiated, spent UO_2 fuels and waste glasses. Tests on irradiated fuel and high-level waste glasses are conducted in hot cells. Analyses of the solid phases, colloids, and solutions are obtained through intermittent sampling of the tests. A participant assisting this group would have opportunity to learn state-of-the-art techniques for studying the long-term corrosion of radioactive waste materials.

533 SEPARATION AND RECOVERY OF METAL IONS

Currently, research is being done on both the chemical and chemical engineering aspects of metal ion separation and recovery for the nuclear industry. Projects include the development of solvent extraction process flowsheets for nuclear waste management. This development will greatly reduce the costs of waste disposal and increase safety by separating radioactive elements from nonradioactive ones. The research uses radioactive tracers and computer modeling, among other methods, to simulate and evaluate potential flowsheets. A participant assisting this group would have the opportunity to learn state-of-the-art techniques in separation science and technology as well as gain practical experience in problem solving.

534 TREATMENT OF SPENT NUCLEAR FUEL

Pyrochemical methods are being developed for treatment of spent nuclear fuel. One of the methods is electrometallurgical treatment, which involves electrorefining the fuel to separate uranium from the fission products. This separation reduces the volume of highly radioactive material that must be placed in a geological repository for disposal. The development work is done with nonradioactive components, which allow hands-on experimental development of the electrorefining process. The electrorefining process is conducted in a high-temperature (500°C) molten-salt electrolyte, and it is applicable to a number of other metals besides uranium. A wide range of experimental activities is possible for further development of this technology.

535 TREATMENT OF ELECTROREFINING WASTE

Zeolite, an alumino-silicate mineral that occurs in nature, is being developed as a medium for isolation of radioactive fission products and actinide elements for permanent disposal. The electrometallurgical treatment of spent nuclear fuels results in molten chloride salts having fission products and actinide elements in solution. These salts can be absorbed in zeolite because the zeolite structure has molecular cages that are suitable for accepting a wide variety of anions and cations. In the present research, the salt-loaded zeolite is mixed with glass powder and sintered. The sintering process converts the zeolite to another mineral, sodalite, which has smaller molecular cages. The smaller cage size inhibits release of the salt, actinides, and fission products to the environment. The research opportunities include testing and characterizing the physical and chemical properties of the sintered sodalite. The results will be used to assist development of the sintered sodalite as a waste form and, eventually, to qualify it for disposal in a geologic repository.

BATTERY RESEARCH AND DEVELOPMENT

536 BATTERY MATERIALS RESEARCH AND DEVELOPMENT

Novel metal oxide and metal alloy materials are being developed and/or modified for use in advanced battery electrodes to improve their performance and life. The research involves the chemical synthesis and processing of these materials and subsequent structural, physical, chemical, and electrochemical characterization. Major equipment includes: x-ray diffractometer, scanning electron microscope, neutron diffractometer, inert atmosphere gloveboxes, furnaces, thermogravimetric and differential thermal analyzers, particle size analyzer, dilatometer, and porosity analyzer.

537 ELECTROCHEMICAL RESEARCH ON ADVANCED BATTERIES

Electrochemical research is being conducted on advanced battery systems, such as Li-polymer and Li-ion. The purpose of this effort is to understand the fundamental electrochemical phenomena in these advanced batteries and identify the processes and/or components that limit cell performance. In these investigations, laboratory cells are built and characterized by a wide variety of electrochemical techniques. Major equipment includes: data acquisition and control systems, potentiostats/galvanostats, AC impedance analyzers, calorimeters, computers, oscilloscopes, and battery cyclers.

538 MODELING AND DESIGN OF ADVANCED BATTERY SYSTEMS

Modeling and design studies are being conducted on advanced battery systems. In this work, algebraic and differential equations describing physicochemical phenomena are developed and solved numerically to characterize and predict cell and battery performance. Fundamental electrochemical transport models on individual cells are developed to fully understand cell performance and add support to the experimental research effort. This work is combined with a relatively applied modeling and design effort to predict the optimum performance of full-sized cells and battery packs.

BASIC AND APPLIED RESEARCH

539 FLUID CATALYSIS

Homogeneous catalytic chemistry and mechanisms associated with the Fischer-Tropsch reaction, ethanol synthesis, the hydroformylation of olefins, and a variety of nanoparticulate catalytic processes are investigated using *in situ* high-pressure spectroscopic and kinetic methods. Parallel synthetic efforts are directed toward the isolation or synthesis of organometallic reaction intermediates and new catalytic species. Catalytic chemistry in supercritical fluids, the surface chemistry of ligand-protected nanoparticles, and magnetically recoverable nanocatalysts are also investigated. In addition, new high-pressure NMR spectroscopic and imaging devices are designed to investigate catalytic processes under industrial process conditions. Major equipment includes: a high-pressure NMR and FT-IR facility.

ANALYTICAL AND ENVIRONMENTAL CHEMISTRY

540 MODERN METHODS FOR INORGANIC ELEMENTAL ANALYSIS

Improved analytical methods are being developed, evaluated, and implemented for the determination of metallic elements in a broad range of sample matrices, including soils, sludges, catalysts, process materials, and waters. Projects involve both conventional and nonconventional sample preparation methods, separations, and state-of-the-art instrumental analysis techniques. Sample preparation schemes can utilize conventional dissolution techniques, more modern dissolution techniques such as microwave digestion procedures, or less common dissolution techniques employing bomb combustions for the destruction of organic matrices. Separations include both batch and column techniques. Instrumentation available for these projects includes: an inductively coupled plasma/atomic emission spectrometer, an inductively coupled plasma/mass spectrometer, and an ion chromatograph.

CHEMISTRY DIVISION (CHM)

Chemistry has been a core capability at Argonne National Laboratory since its founding to explore the peaceful uses of atomic energy. The Chemistry Division conducts a program of long-term fundamental research that addresses problems in the chemical and nuclear sciences that are related to the mission-oriented energy activities of the Department of Energy. The Chemistry Division maintains a large number of laboratories for organic, inorganic, physical chemistries and for work with radioactive materials. Our current research encompasses a wide range of programs including nanoscience, radiation and photochemistry, photosynthesis, catalytic chemistry, theoretical and experiment chemical dynamics, actinide element and separation science, and electrochemistry and computational molecular materials studies. The work is supported predominantly by Basic Energy Sciences, Department of Energy.

541 RADIATION AND PHOTOCHEMISTRY

Argonne addresses the chemistry of novel intermediates and excited states and the roles of solvents and matrices in modulating their reactivity. The development of a terawatt table-top laser system provides a suitable means to study ultrafast phenomena involving electrons, x-rays and plasmas. A dedicated electron linear accelerator has enabled many basic discoveries, including the solvated electron and ion radical chemistry. Argonne scientists are providing basic insights for the safe management of radioactive wastes.

542 PHOTOSYNTHESIS AND BIOINORGANIC HYBRID SYSTEMS

This program is defining the basic principles that govern solar energy conversion via the study of electron transfer reactions within novel structures in natural and biomimetic photosynthesis. Work on the mechanism of charge separation in natural photosystems is being extended to construct novel artificial systems that are optimally tuned to mimic the natural process. Efforts are also underway to explore light-driven processes in integrated biomolecule-semiconductor hybrid molecules, such as linked protein-titanium dioxide systems.

543 CHEMICAL DYNAMICS IN THE GAS PHASE

This program merges theoretical and experimental work on energetic, kinetic, and dynamic processes involved in combustion. Integrated experimental studies are conducted in parallel with theoretical calculations on state- selective chemistry, the chemical kinetics of radical- radical reactions, and photoionization spectroscopy. Group computer facilities (modest linux clusters) and laboratory computer facilities (massively parallel commodity computer) enable several groups in the division to be at the forefront in the development and application of codes for massively parallel machines.

544 ATOMIC, MOLECULAR, AND OPTICAL PHYSICS

This program seeks to establish a refined and quantitative understanding of X-ray interactions with atoms and molecules. Study of weak-field atom — X-ray interactions has been the central theme of research with experiments that test the limitations of first-order approximations, such as the dipole, form factor, and independent electron. In addition, we exploit the properties of atom traps for ultrasensitive trace analysis, electron impact ionization studies and precision spectroscopic measurements. The ultrasensitive trace analysis methods have wide-ranging applications.

545 NANOSCIENCE

One theme of research is inorganic/biological interface. Novel inorganic nanoparticles are coated with organic/biological molecules to produce photochemically active nanostructures whose properties can be tuned. A second research theme is nanophotonics which is dedicated to the understanding of light induced nanoscale interactions in structures that offer the ability to control the propagation of photons below the diffraction limit. Our research encompasses the synthesis, characterization, and theory of nano-optical structures.

546 CATAYLSIS

This research program seeks to understand surface structure, reactivity and selectivity of catalysts at the nanoscale. The experimental work includes synthesis of catalytic materials including clays, nanostructured membrane catalysts, and metal cluster membrane supported catalysts. Catalytic membranes are constructed using anodic aluminum oxidation and atomic layer deposition. Studies include the characterization of clay formation and membrane materials with physical techniques, catalytic reaction experiments for evaluating performance and determining kinetics and mechanisms. Computational simulations complement the experimental investigations by providing theoretical insight at the atomistic level of the catalytic properties of the materials.

547 HEAVY ELEMENT AND SEPARATION SCIENCE

This program conducts pioneering studies on the chemical, structural, and electronic properties of actinide elements in gas, liquid, and solid phases, including f-state energy level structure, thermodynamics, and solid state structure-stability relationships. The goal is to build the comprehensive and predictive knowledge of the chemical and separations properties of heavy elements and fission products that is central to nuclear science chemistry, environmental fate, and role in energy technologies. These studies have also improved the understanding of high-temperature superconductivity and enabled the detection of curium at the near-single-atom level. This program also develops new separation processes for pollution prevention. A central focus is the design of macrocyclic extractants with high selectivity for specific hazardous ions. The TRUEX process was discovered here. This research group also designed the DIPHONEX resins that have proven so useful for waste management and water purification. The whole program benefits from an Actinide Facility that allow radioactive sample preparation with hot cell facilities and transportation of those samples to Argonne's Advance Photon Source for X-ray characterization.

548 COMPUTATIONAL MATERIALS AND ELECTROCHEMICAL PROCESSES

This project uses complementary experimental and theoretical approaches to investigate solid state ion transport/intercalation processes and interfacial electrochemical processes. Scientifically, there is much that remains to be learned about bulk and interfacial electrochemical processes such as solid state ion transport mechanisms and influence of interfacial structure on electrochemical reactions. Technologically, there is a great need for improved electrochemical sources for energy storage and supply, both large and small, such as fuel cells, batteries and electrochemical capacitors. The performance of energy and power systems is largely dependent on the electrochemical processes that occur at an electrode-electrolyte interface, as is the case with a catalyst, or in the bulk of an electrochemically active component, such as an insertion electrode. Fundamental research into these processes will play a key role in the coming years in improving the performance of energy storage and supply systems.

549 INTERFACIAL GEOCHEMISTRY

The Interfacial Processes Group conducts basic research into geochemical processes through the development and application of synchrotron X-ray scattering techniques for in situ studies of mineral-fluid interfaces, taking advantage of the unique properties of the Advanced Photon Source (APS), a third generation X-ray synchrotron source located at Argonne. The characteristics of the APS enable fundamentally new types of in situ experiments for mineral-fluid interfaces to directly observe the structure of the mineral-fluid interface and various molecular-scale processes such as ion adsorption/desorption, dissolution, and mineral growth. These experiments help to define kinetics and reaction mechanisms at the atomic scale in key mineral-fluid systems. Advances in these fundamental areas will yield significant benefits in diverse areas including energy resource exploration and utilization, environmental restoration and waste management.

COMMUNICATIONS AND PUBLIC AFFAIRS DIVISION (C&PA)

550 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.

551 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.

552 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.

553 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.

554 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.

555 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.

556 INFORMATION SYSTEMS

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 current primary technologies delivered from Unix and Windows backend servers are: either Oracle and SQL Server for database management systems, Powerbuilder for Windows application development environments, and Java for web services.

557 TELECOMMUNICATIONS SERVICES

Telecommunication Services provides Argonne-East with a variety of integrated products and services designed to enhance business productivity. Among these services are voice mail, pagers, and telephones.

558 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.

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.

559 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

560 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

561 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.

562 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.

563 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

564 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.

565 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.

566 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.

567 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.

568 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.

569 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.

570 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.

571 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.

572 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.

573 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.

574 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.

575 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.

576 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.

577 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.

578 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™).

579 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.]

580 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.

581 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.

582 INDUSTRIAL HYGIENE

Industrial Hygiene provides sitewide guidance and technical support for 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. Laboratory analyses are performed on workplace, environmental, and biological samples. Other activities involve exposure surveys for 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. Projects are available concentrating on a specific aspect of occupational health. 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 laser-based fibrous aerosol monitors. Optical microscopy is used for particle and fiber analyses.

Projects are available concentrating on a specific aspect of occupational health.

583 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.

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.

584 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.

585 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.

586 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. Aerosols must be characterized chemically to understand their optical and physical properties. Our current studies include the following:

- Use of natural atmospheric radioactive tracers (^{210}Pb and its daughters ^{210}Bi and ^{210}Po) to date submicron aerosols and evaluate their lifetimes.
- Measurement of ^{7}Be and ^{14}C to investigate upper air mixing and the amount of biogenic carbon in aerosols, respectively.
- Measurement of black carbonaceous soot and associated organics during field studies and improvement of methods for these measurements.
- Measurement of organic compounds at the surface and aboard research aircraft during field experiments to investigate direct and indirect effects of aerosols on radiative balance. Indirect aerosol effects include enhanced or reduced cloud formation.
- Determination of the ability of aerosols to take up water through laboratory and field studies and modeling efforts. The hygroscopicity of aerosols and their growth rate determine how quickly they are removed by both wet and dry deposition.
- Measurement of aerosol precursors including ammonia and reactive organic species.
- Measurement of gas-phase species and radiation in conjunction with aerosol measurements to evaluate spatial and temporal variations and the "aging" of the aerosols due to oxidation and photochemical processes.
- Use of numerical models of atmospheric chemistry and transport to interpret and generalize the findings from the observational studies.

587 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

588 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.)

589 HYDROGEOLOGY

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.

590 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.

591 ENVIRONMENTAL SYSTEMS PLANNING, AND COMPLIANCE (includes Denver location)

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.

592 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.

593 LONG-TERM ENVIRONMENTAL STEWARDSHIP

The terms "environmental stewardship" and "long-term stewardship" have been used by several organizations, including the U.S. Department of Energy (DOE) and U.S. Department of Defense, 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 (including at over 100 sites being addressed by DOE). 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.

594 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.

595 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.

596 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.

597 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.)

598 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.

599 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.

600 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.

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 expeirments at nearby Fermi National Accelerator Laboratory. The structure of proton is being studied at the HERA electron-proton collider in Hamburg, Germany. 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.

601 DETECTOR DEVELOPMENT OF THE INTERNATIONAL LINEAR COLLIDER

The International Linear Collider (ILC) will be the next big accelerator project of High Energy Physics. The ILC with a center-of-mass energy of 500 to 1000 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 ILC, 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 tracking calorimeters. We develop Resistive Plate Chambers 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 prepare for the construction of 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.

602 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.

603 EXPERIMENTS USING POLARIZED BEAMS

The Argonne group is working at the Relativistic Heavy Ion Collider (RHIC) 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 systematics 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.

604 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 2007. The CDF II detector includes charged-particle tracking chambers, including 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 electronic readout. Between 2001- 2006 CDF II accumulated over 1 fb^{-1} of integrated luminosity. With current Tevatron luminosities now in excess of 2 10^{32}, it is anticipated that the total accumulated luminosity will increase to 4-8 fb^{-1} by the end of the Tevatron running in 2009.

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 good opportunities for students and faculty to get involved in novel physics analysis of their choice.

INTENSE PULSED NEUTRON SOURCE DIVISION (IPNS)

The Intense Pulsed Neutron Source Division (IPNS) operates an accelerator-based source of neutrons for basic research in condensed matter using neutron-scattering techniques. The IPNS program is operated in a user-oriented mode with thirteen neutron-scattering instruments. Research using these facilities is sponsored by various research divisions.

605 IPNS CONTROLS AND COMPUTING

IPNS uses computers to collect and analyze neutron scattering data and to control the accelerator and Data Acquisition Systems (DAS). The data collection process involves recording the time-of-flight of detected neutrons and binning the data in histograms. Both the data acquisition and accelerator contols use the EPICS software package. Data reduction and analysis is done using the Integrated Spectral Analysis Workbench (ISAW) software plus a few IDL applications. We have upgraded more than half of the old VAX-based DAS systems from old MicroVAX computers with Qbus and Multibus contols to modern Linux systems with Ethernet communication. Old Fortran codes are being rewritten in C or Java. Older Multibus and CAMAC modules are being replaced with VXI/VME modules residing in crates that sit directly on the network and communicate with the outside world using EPICS (Experimental Physics and Industrial Control System). This allows more freedom in the choice of user interface computer and gives the possibility for user interfaces to be developed on a variety of platforms such as Unix, Windows, Macintosh, etc.

The ISAW software is written in the Java language so it will run on any modern computer platform without being recompiled or rebuilt. This will also allow running the software through a web browser. We are collaborating with the University of Wisconsin-Stout, the Spallation Neutron Source, Los Alamos National Laboratory, and Caltech on further software developments.

Research participants would assist in the development of code for experiment control or for data collection, with emphasis on conversion of old VAX Fortran codes to Unix. They might also assist in writing object-oriented codes in Java for setting up data collection or manipulating and displaying data. The students will learn or gain experience in object-oriented programming techniques.

606 IPNS ACCELERATOR SYSTEM

The IPNS accelerator system is an operating facility consisting of an H- ion source, a 750-keV Cockcroft-Walton dc preaccelerator, a 50-MeV Alvarez linac, and a 450-MeV Rapid-Cycling Synchrotron. Computer science projects include work on EPICS[1]-based data acquisition and control systems, development of man-machine interfaces and graphical presentation of data. Particle accelerator technology features high-current regulated magnet power supplies; frequency, amplitude, and phase-modulated high-power rf transmitters; vacuum systems; analog and digital control with feedback circuits; and dedicated computer-control systems. Improvements and modifications to various systems and investigation of beam performance is continually ongoing, providing the participants with a unique experience in computer science, the physics of charged-particle dynamics, as well as a wide variety of engineering specialties.

607 IPNS NEUTRON PHYSICS

The IPNS neutron-generating system consists of a depleted uranium target having nearby liquid and solid methane moderators for slowing the neutrons down to energies appropriate for neutron-scattering studies. Participants will assist senior staff on a variety of measurements to characterize target, moderator, and instrument performance. Target/moderator programs include measurements of pulse shape, neutron spectra, energy deposition, radiation damage in the moderators, and measurement and analysis related to the management of thermochemical instability in solid methane; and energy deposition, delayed neutrons, and shielding of the uranium target. Instrument programs include the design, testing, and characterization of instrument components and systems for neutron detection, shielding and background reduction, analysis of new instrument concepts (based, for example, on time-focusing opportunities) and neutron optics in neutron-scattering instruments.

608 IPNS NEUTRON SCATTERING RESEARCH

The IPNS neutron scattering facility consists of 13 instruments for investigating the structural and dynamical properties of condensed matter. The neutron-scattering instruments include 7 diffractometers (for structures of powders, single crystals, glasses, liquids, and soft materials), 4 spectrometers (for magnetic and chemical excitations, atomic/molecular vibrations and diffusion with energy transfers from 0.05 to 1500 meV), and 2 reflectometers (for interfacial magnetic and atomic structure).

Over 400 experiments are performed per year in various areas of materials sciences, physics, chemistry, biology, and applied technology. Recent studies include:

- Structure and dynamics of electronic and ionic conducting membranes
- Aggregation and surface chemistry of nanophase catalysts
- Short- to intermediate- range structures of glasses, liquids, polymers, superacids and disordered crystals
- Structure, aggregation and organization of proteins in solution
- Structure and dynamics of C60 (bucky balls) and carbon nanotubes
- Intrachain and interchain structures of polymers
- High pressure behavior of gas hydrates, molecular solids, ice, superconductors and colossal magneto-resistance materials

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[1] EPICS (Experimental Physics Instrumentation and Control Systems) is an Argonne/Los Alamos developed system that is now used at over 100 sites.

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 is a major user of the Intense Pulsed Neutron Source (IPNS) and synchrotrons, and operates the high-voltage electron-microscope Tandem-Accelerator System as a national user facility.

609 MAGNETIC NANOSTRUCTURES

This group prepares and characterizes ultrathin films and related magnetic nanostructures with novel properties. The materials are prepared as surfaces, interfaces, heterostructures, sandwiches, superlattices, and array structures using molecular-beam epitaxy, sputtering, lithography and self-assembly techniques. Interest focuses on magnetic, superconducting, optical, transport, structural and elastic properties of predominantly magnetic systems. Characterization techniques include ultrahigh-vacuum electron spectroscopies and diffraction, light scattering (Raman, and Brillouin), 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.

610 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.

611 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.

612 NEUTRON AND X-RAY SCATTERING

Members of the Neutron and X-ray Scattering Group pursue multidisciplinary research programs that are only possible if scattering capabilities are combined with synthesis, materials characterization, and theory. Major research programs include: exotic superconductors, complex oxides with important transport, magnetic, or dielectric properties, orbital correlations, frustration, and self organization, and magnetic behavior in constrained geometries. A second important activity of the group is providing the technical expertise required to develop the advanced neutron and x-ray scattering instrumentation required to fulfill our scientific goals. Scientists in the group play a lead role in the development of novel instrumentation and techniques at Argonne's Intense Pulsed Neutron Source and Advanced Photon Source, as well as the Spallation Neutron Source at Oak Ridge National Laboratory.

613 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.

614 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.

615 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.

616 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.

617 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.

618 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.

619 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.

620 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.

621 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.

622 IN-SITU ALLOY OXIDATION

This program seeks to develop a predictive understanding of the physical and chemical processes that control alloy oxidation. We emphasize studies of model single-phase two-and three-component alloys, including nickel oxide-, alumina-, and chromia-forming systems. While focusing primarily on the early stages of oxidation, which are the most poorly understood, the program also follows the process of oxidation to the mature, "steady state" evolution. A unique combination of *in situ* x-ray and ion scattering tools, state-of-the-art electron microscopy techniques, and multiscale-simulation capabilities are being used to identify and characterize the key interfacial processes and phenomena. The fundamental insights gained from these studies on model alloys will provide valuable guidance in the design of novel, oxidation-resistant alloys. Moreover, insights gained from experiment and simulation on significant atomic-level, interfacial and microstructural processes operating across a wide range of length and time scales will ultimately enable the development of quantitative multiscale predictive models of alloy oxidation. The program utilizes the Electron Microscopy Center (HREM, AEM) , the Advanced Photon Source, and Argonne's expertise in massively parallel computing architectures.

623 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.

624 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.

625 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.

626 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 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.

627 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/L 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.

628 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/*

629 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*

630 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*

631 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/*

632 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

633 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/*

634 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/*

635 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 two-fold: 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

636 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.

637 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 will also be 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/

638 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/*

639 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/mpi/mpich*

640 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.*

641 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.mcs.anl.gov/division/research/applied_math.htm

642 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

643 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/datagrid/*

644 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/mds/*

645 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/security/*

646 ADVANCED CYBERINFRASTRUCTURE FOR CHEMISTRY

The Chemistry programs need to be accessible through a portal infrastructure intended to provide mechanisms to enhance the coordination of research efforts across related subdisciplines in the chemical sciences, focusing research at one scale on obtaining or refining values critical in the next, reducing work performed using limited or outdated values, and enhancing the ability of the community to meet the national research challenges of DOE. Our principal focus is on development of cyberinfrastructure that provides s Web service oriented approach to do the next generation of chemistry. *http://www.cogkit.org*

647 COMPUTATIONALLY MEDIATED EXPERIMENTAL SCIENCE

This interdisciplinary project provides the means of supporting science experiments with the necessary compute power to perform and evaluate the results in real time. The newest generation of advanced scientific instruments will be used. Examples may include state-of-the-art sensor nets to observe earthquake simulations or analytical electron microscopes to observe nanoscale structures. These instruments create a large amount of data that must be analyzed in real time in order to present the scientist with output that can be meaningfully interpreted. The project provides challenges in computer science, data analysis, monitoring, physics, analysis, and presentation of information. *http://www.mcs.anl.gov/~gregor*

648 APPLICATION DEVELOPMENT ENVIRONMENTS FOR SCIENTIFIC COLLABORATION

Grid services offer basic protocols and APIs for integrating scientific instruments, displays, and computational and information resources. We are integrating basic Grid services into existing commodity application development frameworks, environments, and languages. This strategy makes it possible to use more advanced development environments for developing advanced Grid services. High-level development environments of interest are Java, Perl, Python, Web services, and CORBA. With the help of commodity Grid kits, we create sophisticated Grid computing environments. *http://www.globus.org/cog/ or http://www.cogkits.org*

649 EARTH SYSTEM GRID

High-resolution, long-duration simulations performed with advanced DOE climate models will produce tens of petabytes of output. This output must be made available to researchers nationwide, at research laboratories, universities, and other institutions. To this end, we are creating an Earth System Grid (ESG-II): a virtual collaborative environment that links distributed centers, users, models, and data. ESG-II will provide scientists with virtual proximity to the distributed data and resources that they require to perform their research. The creation of this environment will significantly increase the scientific productivity of U.S. climate researchers by turning climate datasets into community resources. *http://www.earthsystemgrid.org/*

650 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 nine 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

651 VIRTUAL DATA AND THE GRID PHYSICS NETWORK (GRIPHYN AND IVDGL)

The Grid Physics Network (GriPhyN) and the international Virtual Data Grid Laboratory (iVDGL) are partners in a pioneering effort to enhance scientific productivity through Grid technology. GriPhyN is developing the new paradigm of *virtual data* to catalog data relationships and workflow “recipes” as they evolve over long periods of time within complex scientific analysis processes; in addition, research focuses on scheduling, resource management, and automated error handling. These computer science challenges are pursued in close collaboration with large-scale experiments in high energy physics, astrophysics, and astronomy. The Virtual Data system is also being applied to science challenge problems in computational biology, Earth systems observation, biomedical applications, and functional MRI. *http://www.griphyn.org* and www.griphyn.org/chimera .

652 NATIONAL FUSION COLLABORATION

The National Fusion Collaboratory (NFC) is a team of fusion scientists and information technology researchers who are designing a network services infrastructure for fusion applications. In particular, NFC addresses the issues of deadline-oriented network service execution and resource management required for the support of fusion experiments, as well as the authorization and use policy requirements necessary to deal with issues of trust in a shared environment. To support these requirements, we are developing a scalable network services infrastructure capable of enforcing use policies in order to provide timely execution in computational Grid environments. *http://www.fusiongrid.org/*

653 GRID SERVICES

The Open Grid Services Architecture seeks to provide a unifying framework enabling a service-oriented view of the Grid. Our work in this area covers the full stack of service interactions and ranges from exploration of diverse hosting environments through investigation of efficient communication protocols, providing efficient basic Grid services (such as job execution and authorization) to complex, high-level services (workflow, execution brokers). We also investigate functionality necessary to support application services. *http://www.globus.org/ogsa.*

654 WIDE-AREA PARALLEL COMPUTING

The Message Passing Interface (MPI) standard is a widely used programming interface for writing parallel programs. It is particularly well suited to applications running on collections of computers that are in different buildings, cities, or countries. This project is enhancing MPICH2, our new implementation of MPI, to provide more efficient and robust communications in the wide-area environment. Projects include quality of service and support, better wide-area network protocols, and exploitation of the topology of the network within which the MPI application is running. *http://www.mcs.anl.gov/mpi/mpich*

655 MULTITHREADING IN NUMERICAL SOFTWARE

Multithreading is a way to exploit multiple CPUs within a symmetric shared-memory processor. It offers the potential for significant performance advantages over other parallelism strategies such as explicit message passing. This project is exploring the use of multithreading in the PETSc numerical library. Because PETSc is aimed at solving large sparse linear and nonlinear systems that arise in the solution of partial differential equations, an effective multithreading implementation must take into account the structure and dynamic nature of the PETSc code. Techniques such as multicoloring and adaptive reordering will be applied to develop an efficient implementation of key routines in PETSc. *http://www.mcs.anl.gov/petsc*

656 FORMAL VERIFICATION OF PARALLEL PROGRAMS

Parallel programming is tricky, and errors can be difficult to detect and debug. This project uses formal methods to verify correctness of parallel MPI programs and of MPI implementations. Verification of multithreaded MPI programs and the development of an MPI-2 test suite are of particular interest.

COMPUTATIONAL SCIENCE

Computational science has joined theory and experiment as a third approach to solving scientific and engineering problems. We are addressing critical problems in areas such as climate modeling, environmental research, materials science, and biology that require the use of high-performance computers and the development of new techniques to exploit those computers effectively.

657 CLIMATE MODELING

Research focuses on the development and application of climate models and on global atmosphere and ocean models. Application areas include simulation of past and future climates. Development focuses on software for building coupled models and analyzing their output as well as on basic development of climate model components. This research is performed jointly with climate and computer scientists at area universities, the National Center for Atmospheric Research, and other national laboratories. *climate.mcs.anl.gov*

658 GRID-ENABLED SERVICE FOR HIGH-THROUGHPUT GENOME ANALYSIS

We are developing the GADU/Gnare systems. GADU is a high-performance, scalable computational pipeline for the data acquisition and analysis of sequenced genomes. It efficiently automates the major steps of genome analysis: data acquisition and analysis by various tools and algorithms, as well as annotation and storage of results. In addition, we are developing Gnare (Genome Analysis Research Environment) to provide a secure collaborative environment where scientists and researchers can discuss, share, and analyze genomic data. Gnare is a public portals-based server that manages workflows running transparently across multiple heterogeneous execution environments and captures the provenance of all the data stored by GADU, including the final relational database of sequence data. *http://compbio.mcs.anl.gov*

659 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 application'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. *http://www.alcf.anl.gov/*

660 CONSTRUCTION OF INTEGRATED BIOLOGICAL DATABASES

We are constructing an integrated system that offers substantially enhanced access to the growing body of genomic information (e.g., chromosomes sequence fragments, enzymes, and rRNA). The project also involves development of new software tools for extracting of information from the integrated system and server. Our goal is to facilitate interpretation of genomes and to provide a valuable tool for scientists internationally.
http://compbio.mcs.anl.gov

661 NUMERICAL ALGORITHMS FOR FLOW SIMULATION

We are developing parallel and high-order methods for computational fluid dynamics. This work includes the development of multilevel iterative solvers capable of scaling to thousands of processors, cache-aware computational kernels, and robust high-order numerical discretizations based on spectral elements. Applications include the study of transitional boundary layers, convection in deep atmospheres, and heat transfer enhancement mechanisms.
http://www.mcs.anl.gov/appliedmath/Flow/cfd.html

662 EVOLUTIONARY ANALYSIS OF METABOLIC SYSTEMS

We are analyzing the evolution of metabolic subsystems in humans and bacteria. The objective is to develop a framework for comparative analysis of such systems and perform phylogenetic analysis of the genes participating in major metabolic pathways. We expect the results of this work to provide new insights about the evolution of functionality of human cells and mechanisms of genetic metabolic diseases. *http://compbio.mcs.anl.gov*

663 PREDICTION AND COMPUTATIONAL CHARACTERIZATION OF POTENTIAL PROTEIN TARGETS FOR ANTIBIOTICS

This project involves the design and implementation of the integrated Tar-Get database and algorithms to support selection of priority targets for high-throughput 3D determination by the Midwest Structural Biology Center. This database focuses on identification and computational characterization of two major classes of proteins: potential targets for antibacterial agents and families of proteins with unique folds. *http://compbio.mcs.anl.gov/targetB/cgi-bin/Homepage.cgi*

664 PROGRAM PERFORMANCE ANNOTATIONS

Achieving the level of performance required by computational science applications often requires system- and compiler-specific modifications to the application code, introducing problems in maintenance, correctness, and development. In addition, the choice of code transformation and modification is often made manually and in an ad hoc fashion, making it impossible to ensure that the code changes help achieve the best performance. This project is developing program annotations, represented as comments, and tools that transparently interface to a suite of code transformation tools such as loop analysis and rewriters and to tools that provide distributed data structures for parallel computation.

665 VIRTUAL FAST REACTOR

This project aims to apply petascale computing resources to the simulation of a full-scale advanced burner reactor. This includes designing and implementing neutron transport, thermal hydraulics, structural mechanics, and fuel behavior models at very high fidelity on relatively complex meshes. Some of the key research issues are techniques to couple the individual physics components (both numerically and in terms of software architecture), validation and verification of the resulting simulations, sensitivity and uncertainty analysis, complex meshing, acceleration techniques for transport equations, and parallel solver frameworks. This project is tightly coupled to the fast reactor design efforts taking place in the Nuclear Engineering Division.

COMPUTING FACILITIES

The MCS Division computational environment features a 2,048-processor IBM Blue Gene/L computer for investigation of highly scalable systems software, tools, algorithms, and applications. MCS also operates a 512-CPU Linux cluster for scalable software work; a distributed systems laboratory; and a virtual environment, featuring several Access Grid nodes and an Active Mural. The local computing environment also has hundreds of desktop computers running Windows and Linux.

666 SYSTEMS ADMINISTRATION

Ensuring that all the MCS computing facilities work smoothly is a complex task, carried out by the MCS Systems Group. Students and visitors in the Systems Group take on special projects to enhance the computing environment, and also assist with day-to-day operations. Participants in the Systems Group can expect to learn a lot about how UNIX, Windows, Mac OS X, and Linux work and how to design and maintain large networks of computers. *http://www.mcs.anl.gov/systems/*

667 NETWORK ADMINISTRATION

The computing environment in the MCS Division is built on top of a modern-day high-performance network. The network includes Infiniband, Myrinet, and various types of ethernet and is implemented by using several different kinds of network equipment. The MCS Systems Group is responsible for building and monitoring the network and for helping it support both production computing and experimental research. Participants in the Systems Group who focus on networking can expect to build tools to help monitor the network, help to expand the network, manage and design network services, and diagnose problems. *http://www.mcs.anl.gov/systems/*

668 SYSTEMS PROGRAMMING

The MCS Systems Group is responsible for managing the MCS computing environment. An important part of this effort involves the design and development of new tools to support large-scale management. Members of the Systems Group who work as systems programmers use languages such as Perl, Python, PHP, Java, C, and various others to build new systems administration tools that are deployed within MCS and eventually released to the world at large. Participants can expect to learn appropriate programming languages, participate in the design of tools to help manage large scalability problems, and learn a great deal about how large environments of computers work.
http://www.mcs.anl.gov/systems/

669 SCIENTIFIC VISUALIZATION AND SIMULATIONS INTERACTION IN VIRTUAL ENVIRONMENTS

Virtual environments provide a powerful human-computer interface that opens the door to new methods of interaction with high-performance computing applications in several areas of research. We are interested in the use of virtual environments as a user interface to real-time simulations used in rapid prototyping procedures. Our projects center on visualization and interaction of models of problems in computational chemistry, biology, materials science, and other disciplines.
http://www.mcs.anl.gov/fl/

670 MULTIMEDIA AND COLLABORATIVE ENVIRONMENTS

We are investigating the use of high-performance networking and computing resources to support collaborative research activities. Research activities include work in on-demand media servers, tools for local and wide-area scientific collaboration, and technology for advanced information resource management, involving toolkits for the development of intelligent agents, compression, indexing, and transaction monitoring for the World Wide Web. *http://www.mcs.anl.gov/fl/*

671 INFRASTRUCTURE FOR ACTIVE SPACES

The Active Spaces project integrates emerging multi-user virtual environment technology and advanced display devices with state-of-the-art interfaces in order to support scientific collaboration. The resulting networked environment, composed of persistent collections of objects and a flexible history mechanism, allows the creation of electronic virtual laboratories and workspaces. These virtual spaces will be networked locations where scientists interact with analytical electron microscopes, high energy physics experiments and data, and, most important, each other. This project is developing the tools to create these active spaces and the scientists' interfaces and will validate these integrated tools in end-user testbeds. *http://www.mcs.anl.gov/fl/*

672 COMPUTATIONAL PHYSICS AND HYDRODYNAMICS

Researcher in the Computational Physics and Hydrodynamics group are studying materials behavior under intense power deposition. The studies have application in diverse cutting-edge scientific fields, including fusion, targets for high-energy and nuclear physics, and design of advanced nanoscale systems. Computational modeling activities involve development of the High Energy Interaction with General Heterogeneous Target Systems (HEIGHTS) simulation package, which is one of the world’s leading civilian-based hydrodynamics and radiation transport codes.

673 PARTICLE AND RADIATION INTERACTION WITH MATTER EXPERIMENTS (PRIME) FACILITY

The PRIME facility, operated by the Computational Physics and Hydrodynamics group, studies the interactions of high-intensity particle interactions with matter. The facility consists of three major experiments: a particle-beam experiment that includes state-of-the-art surface analysis and metrology tools for testing of advanced nanoscale multicomponent thin-film systems, a laser experiment for studying laser-produced plasmas for vacuum ultraviolet and extreme ultraviolet light generation, and a high-density plasma source for studies of high-density plasma/material interactions for energy materials reliability development.

NUCLEAR ENGINEERING DIVISION (NE)

The Nuclear Engineering (NE) Division conducts research and development in engineering, analytical methods, experiments and material sciences, with concentration in nuclear technology and related sciences. Major areas of emphasis include research in nuclear safety technology, reactor fuel cycle analysis, reactor physics, criticality safety, non-proliferation technology, reactor and nuclear facility design, performance and safety evaluation, decontamination and decommissioning of nuclear facilities, and environmental management support.

This Division is responsible for a wide spectrum of technology development programs that require the integration of engineering disciplines in nuclear reactor and fuel cycle technologies. The Division has actively participated in applying its core competencies to programs in other fields of nuclear and non-nuclear technology. The major program areas in which the Division is involved in are development of advanced nuclear energy systems and supporting technologies, international nuclear safety, non-proliferation, and engineering analysis, consisting of advanced computing and simulation, engineering mechanics, and materials behavior in engineered systems.

The Division conducts research and development by applying its analysis and engineering capabilities in reactor physics, criticality safety, engineering design, engineering mechanics, safety experiments, safety analysis, materials, computer simulation, thermal hydraulics and diagnostics.

A major Division mission is in Arms Control, National Security, and Nonproliferation. The Reduced Enrichment for Research and Test Reactors (RERTR) program is an important area of emphasis. A primary objective is the development of high density, low enrichment fuel research and test reactors that can be used to replace the current high-enrichment fuels in these reactors worldwide, thereby reducing the threat that these reactors could be subverted for a weapons program. Other program areas include export control, 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 detector technology, robotics, rad-waste technology and security, and laser applications.

674 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.

675 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 is desirable.

676 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.

677 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.

678 NEUTRON PHYSICS DATABASE APPLICATIONS IN MONTE CARLO

The Laboratory focuses on collaborative research and development activities with industrial partners. The facility includes high-power industrial (CO2) 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.

679 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.

680 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.

681 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.

682 MATERIALS

Efficient and reliable operation of a complex engineering system depends critically on the behavior of the materials from which its components are made. In this activity, the dependability of materials for such systems is established by extracting their key fundamental properties, developing an understanding of those properties in relation to the engineering application, and deriving models and performing experiments that allow extrapolation and prediction of the material's behavior under a variety of service conditions. Methods are explored for tailoring materials to fit particular applications. Historically, much of this effort was directed at the behavior of nuclear reactor fuel and cladding materials subjected to the thermal transients associated with the reactor environment. More recently, efforts have been directed toward a number of other diverse issues, including (1) assessing material properties for safety evaluations of foreign reactor designs, (2) tailoring steel railroad surfaces to mitigate crack propagation, (3) developing ductile titanium aluminide for aerospace applications, (4) studying the behavior of nuclear waste forms, (5) assessing the safety of composite flywheels, and (6) understanding irradiation embrittlement in connection with advanced light-water reactor designs and the extension of the life of existing reactors.

683 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.

684 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.

685 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.

686 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.

687 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.

688 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.

689 INTERNATIONAL WATER RESOURCE MANAGEMENT

The United States Departments of State and Energy support programs to assess and improve the availability of water in developing countries. Lab-wide expertise, including that within the International Nuclear Safety and Cooperation group at Argonne National Laboratory, are developing projects to assist developing countries in these efforts. Opportunities exist in integrated water resource management, including the application of desalination and water purification technologies.

690 NUCLEAR-GENERATED HYDROGEN

The United States Department of Energy has implemented a major research and development program to explore the production, storage, distribution, and use of hydrogen as an alternative to petroleum. The DOE Office of Nuclear Energy Science and Technology is supporting Argonne National Laboratory in the development of hydrogen production options through nuclear heat and electricity. In addition, Argonne is performing system studies to assess the likely paths to successful market penetration of nuclear-generated hydrogen.

691 SPENT FUEL TREATMENT EQUIPMENT DEVELOPMENT

The Engineering Projects section develops treatment equipment for the Argonne National Laboratory-West spent fuel treatment project. Current work includes the scale up of a remote-ized treatment unit for the purification and consolidation of uranium dendrites from an electro-metallurgical treatment unit. This activity involves performing criticality and safety analyses of the treatment unit, thermal analyses of the induction furnace performance characteristics, engineering studies in Pro-Engineer of the treatment unit design, and qualification testing of the unit at ANL-E and ANL-W. A fully functional prototype induction furnace test unit is installed at ANL-E that supports the treatment equipment development and a crucible materials development and testing programs. Crucible materials testing program objective is to develop materials that will survive the harsh thermal environment in the treatment unit are compatible with the materials processed and will reduce the required preparation steps.

692 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:

- planar HPGE detectors for imaging of gamma sources,
- 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 targets for low energy (few MeV) accelerators capable of handling high current.

693 APPLIED ACCELERATOR TECHNOLOGY

These activities entail the development of advanced accelerator technology and require physics, engineering or computer programming support in the following areas: *design and development of accelerator-based neutron and/or photon sources for neutron radiography or boron neutron capture therapy; *design and development of targets for high power accelerators such as the Rare Isotope Accelerator (RIA).

694 INSTRUMENTATION APPLICATIONS

The use of neutrons and photons (gamma rays and x-rays) is being investigated for the nondestructive examination of luggage and cargo containers to detect illicit substances such as explosives, narcotics, currency, and weapons of mass destruction. These projects involve: modeling studies of neutron and photon interaction and transport, visualization of the data, development of algorithms for decision making, evaluation of nuclear data, and system studies. We are also investigating the use of neutrons and photons to characterize radioactive waste. There is also a program to develop radiation detectors and dosimetry methods in support of high-energy accelerator applications such as the Spallation Neutron Source (SNS).

695 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.

696 REDUCED ENRICHMENT FOR RESEARCH AND TEST REACTORS (RERTR)

The DOE Office of Defense Nuclear Nonproliferation supports the activities of the Reduced Enrichment Research and Test Reactor (RERTR) program. The goal of the RERTR program is to minimize and eventually eliminate use of highly enriched uranium (HEU) in research and test reactors. The program has been very successful, and has developed low-enriched uranium (LEU) fuel materials and designs which can be used effectively in approximately 90 percent of the research and test reactors which used HEU of Western origin when the program began. Current activities focus on development of more advanced LEU fuels, collaboration with the Russian RERTR effort 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.

697 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.

698 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).

699 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.

700 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.

701 PLASMA/MATERIAL INTERACTION RESEARCH

A variety of studies are underway to develop physics models and computer codes to study reactor conditions in magnetic-fusion devices. Current emphasis is on plasma materials interactions in tokamak devices, plasma heating and current drive, and overall power balance and operating conditions. Specific studies include sputtering erosion/redeposition, disruption modeling and analysis, and hydrogen isotope diffusion and inventory in first wall and divertor materials.

702 LIQUID METAL TECHNOLOGY FOR FUSION

This project involves several related areas of liquid metal technology for fusion. An electrically insulating coating is needed to reduce the magnetohydrodynamic (MHD) pressure drop in a liquid lithium blanket cooling system. Theoretical modeling of liquid metal flows inside magnetic fields within coolant ducts having electrically non-conducting and conducting walls is being developed. Equipment necessary for applying and testing electrically insulating coatings is being designed.

703 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.

704 ROBOTICS

This program supports experimental and theoretical work with manipulator systems, such as Argonne's dual-arm robotic system, used for applications such as decontamination and decommissioning of nuclear facilities and remote fuel handling. Research topics of interest include dual-arm collaboration, motion and task planning, machine vision and sensing, telerobotic operation, machine intelligence, and remote tool handling. Examples of activities for participants include programming, simulation, and algorithm testing. Skill areas of interest include: familiarity with manipulator control, Telegrip, C/C++.

705 NE-INFORMATION TECHNOLOGY AND SECURITY

The focus of this research area is the development of web based database applications for national security programs in the Department of Energy and National Nuclear Security Administration. The program has successfully resulted in providing the DOE with a nationwide facility clearance system. This system has resulted in the conversion of a highly paper intensive facility clearance process into an efficient, web based electronic system used by federal contractors and federal workers throughout the United States. Web based analytical tools are also under development and training systems will be developed in the future.

706 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, 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.

707 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.

709 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.

710 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.

711 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) materials development for a number of reactor types, (2) postirradiation characterization of materials, and (3) 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 transport. 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 a full array of fabrication equipment, optical microscopes, scanning electron microscope, transmission electron microscope, hydrogen and oxygen determinators, and numerous thermal and mechanical testing instruments. Cooperative research programs are welcome.

712 CORROSION OF MATERIALS IN THE PRESENCE OF

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.

713 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.

714 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.

715 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.

716 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.

717 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.

718 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.

A second major component of our program is the study of the origin of the spin of the nucleon. Physics Division staff play 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.

A third component, high energy experiments to probe the structure of the quark sea in the nucleon, to be performed at Fermilab (Fermi National Accelerator Laboratory) are also in the early stages of planning.

Opportunities exist for research participants to be involved in all aspects of our work.

719 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.

720 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 few 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 atom. A positive finding would signify the violation of time-reversal symmetry (T) and, under the assumption of CPT invariance, the charge-parity symmetry (CP). CP violation was first discovered in neutral Kaon decays, and can be explained by the Kobayashi-Maskawa (KM) mechanism within the framework of the Standard Model. While the KM mechanism gives rise to a negligible EDM, extensions to the Standard Model such as supersymmetry (SUSY), multi-Higgs models, and left-right symmetric models generally predict a relatively large EDM within the reach of this experiment. Therefore, this experiment provides an outstanding opportunity to search for new physics beyond the Standard Model. The ^{225}Ra nucleus is an especially good case because it has the characteristics of octupole deformation, which can lead to large enhancements of the T-violating Schiff moment. The overall scheme is to cool and trap ^{225}Ra atoms in a magneto-optical trap, transfer the trapped ^{225}Ra atoms to an optical dipole trap, polarize them through optical pumping, and perform EDM measurements.

Studying exotic nuclear structure. Although Quantum Chromodynamics (QCD) has been firmly established as the fundamental theory of the strong interaction, it is still technically not possible to calculate the structure of simple nuclei based on QCD. This insufficient understanding offers experimenters the opportunity to participate in the development of nuclear structure models and the possibility of discovering new structure. We are conducting experiments based on precision laser spectroscopy of helium atoms: 1) We have determined the charge radius of the lightest halo nucleus ^{6}He ($t_{1/2}$ = 0.8 s) by performing laser spectroscopy on individual ^{6}He atoms confined in an atom trap. This result helps reveal the structure of this neutron-rich nucleus and constrain models of the three-nucleon force. A more challenging goal for us is to study ^{8}He ($t_{1/2}$ = 0.1 s), which is the most neutron-rich matter on Earth. (2) We have searched for stable, helium-like strangelets in the Earth's atmosphere. The null results set stringent upper limits on the abundance of such anomalous particles.

Radio-krypton dating – from dream to practice. Since radiocarbon dating was first demonstrated by Willard Libby in 1949, the field of trace analyses of long-lived cosmogenic isotopes has seen steady growth in both analytical methods and applicable isotopes. The impact of such analyses has reached a wide range of scientific and technological areas. A new method, named Atom Trap Trace Analysis (ATTA), was developed by our group and used to analyze ^{81}Kr ($t_{1/2}$ = 2.3 10^{5} years, isotopic abundance ~ 1 10^{-12}) in environmental samples. In this method, individual ^{81}Kr atoms are selectively captured and detected with a laser-based atom trap. ^{81}Kr is produced in the upper atmosphere by cosmic-ray induced spallation and neutron activation of stable krypton isotopes. It is the ideal tracer for dating ice and groundwater in the age range of 10^{4}–10^{6} years. As the first real-world application of ATTA, we have determined the mean residence time of the old groundwater in the Nubian Aquifer located underneath the Sahara Desert. We will continue to improve the ATTA method and expand its applications in Earth sciences and nuclear non-proliferation.

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.