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).

In addition, project numbers 204-209 are identified as opportunities for Excite Internships through X-ray Collaboration for Illinois Technology and Education. Applicants for internships must be currently enrolled undergraduate students at accredited two-year or four-year colleges or universities in Illinois. Applicants must be U.S. citizens or permanent resident aliens. Other selection criteria vary according to the APS research groups involved, but include assessment of students' academic records, statements of interest, faculty recommendations, and relationship of students' interest and training to needs of a particular research group. Those considering application are encouraged to consult research group Web pages listed at http://www.aps.anl.gov/cats/cathome.html.

200 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.

201 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.

202 EXPERIMENTAL FACILITIES RESEARCH AND DEVELOPMENT

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.

203 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.

204 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.

205 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.

206 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.

207 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.

208 <u>MATERIALS RESEARCH (MR-CAT)</u>

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.

209 <u>UNIVERSITY-NATIONAL LABORATORY-INDUSTRY (UNI-CAT)</u>

In these sectors, The University of Illinois at Urbana-Champaign is teamed with Oak Ridge National Laboratory, the National Institute of Standards and Technology, and UOP Research and Development. This is a multi-purpose scattering facility capable of high-resolution scattering with excellent energy resolution and beam-focusing optics serving studies in materials, physics, chemistry, biology, and geology.

ARGONNE NATIONAL LABORATORY-WEST (ANL-W)

Argonne National Laboratory-West (ANL-W) is located in Southeastern Idaho on the Idaho National Engineering and Environmental Laboratory site. ANL-W is part of Argonne National Laboratory (ANL) located near Chicago. The ANL-W site is about 35 miles west of Idaho Falls, Idaho. ANL is a non-profit research Laboratory operated by The University of Chicago for the United States Department of Energy. A broad range of national problems are solved through ANL research and development activities.

Research at ANL-W is focused on areas of national concern including those relating to energy, nuclear safety, spent nuclear fuel, nonproliferation, decommissioning and decontamination technologies, and similar work. Typically, basic research is conducted at the main Laboratory near Chicago, with large-scale testing and development at the Idaho site. Nuclear fuel development, post irradiation examinations, characterization, and development of dry storage for spent fuels and other materials are but some of the accomplishments at ANL-W.

210 NUCLEAR MATERIAL SAFEGUARDS AND NONPROLIFERATION

Argonne National Laboratory-West is involved in a number of nuclear material safeguards and nonproliferation activities. Included in these areas are projects involving advanced software development, e.g., expert systems, statistical signal processing, artificial intelligence applications, for safeguard data analysis and material characterization. The Laboratory operates the Safeguard Technology Evaluation Laboratory where evaluation of plutonium monitoring and surveillance systems are evaluated under static and transient conditions. Opportunities exists in the areas of software development, electronic system design and analysis and nondestructive assay and testing of packaged nuclear materials.

211 NONDESTRUCTIVE ASSAY AND NONDESTRUCTIVE EVALUATION

Characterization and examination of radioactive materials is a critical element in a number of priority DOE programs including spent fuel and waste disposition, national security, nuclear nonproliferation and nuclear facility operations. The ANL-West facility infrastructure is well suited for supporting materials characterization through nondestructive assay and nondestructive evaluation techniques. The Hot Fuel Examination Facility (HFEF) hot cell and irradiated material handling capabilities are ideal for performing radiological characterization of highly radioactive materials. In addition, HFEF offers a 14 MeV neutron generator and a 250 kW TRIGA reactor that provide neutron radiography and neutron activation analysis of both hot and cold materials. Other capabilities include gamma-ray spectroscopy, coincidence neutron assay, gamma-ray imaging, and system modeling and computation. This suite of tools is used for both routine safeguards measurements and the development of new assay methods.

212 ADVANCED FUEL CYCLE DEVELOPMENT

Argonne is a leader in DOE's Advanced Fuel Cycle Initiative which has the goal of developing cost effective, safe, and environmentally benign technologies for recycling spent nuclear fuel and stabilizing fission products in durable waste forms. Hot cells at Argonne-West contain laboratory and engineering scale process equipment for oxide reduction, electrorefining, and waste processing. Experimental programs are ongoing to further the fundamental understanding of the chemistry involved with these processes as well as to optimize process parameters. Advanced separations techniques are also actively being studied. The ultimate objective is to develop the knowledge base necessary to design and construct a commercial spent fuel recycling facility.

213 ANALYTICAL CHEMISTRY FOR NUCLEAR WASTE MANAGEMENT

An integral component of the Electrometallurgical Spent Fuel Treatment program at ANL-West is a state-of-the-art Analytical Chemistry Laboratory complex that accommodates analysis of spent fuel isotopic inventories, characterization of hazardous and highly radioactive waste, and evaluation of waste forms. The Analytical Laboratory capabilities include mass spectrometry, inductively coupled plasma-atomic emission spectrometry, atomic absorption spectrometry, chromatography and a variety of radiation detection capabilities. Hot cell and glove box capabilities make it possible for ANL-West researchers to apply these techniques in the study of radioactive and hazardous materials.

214 ADVANCED NUCLEAR FUELS AND MATERIALS

Argonne's long history of fuel development and testing continues with research projects exploring fuels for transmutation systems, research reactor fuels, thorium-based fuels, ultra-long lived fuels and proliferation-resistant fuels. In addition, Argonne is a lead laboratory for the development of Generation IV reactor designs and will help determine the course for next generation fuel design, fabrication and testing. ANL-West is uniquely qualified to design, test and evaluate nuclear fuels. ANL also investigates the performance of structural materials and fuel-cladding materials under service conditions. Such information and expertise will be crucial to the continued development of nuclear energy technology for higher service temperatures and longer exposure tiems for in-core components. The Fuel Manufacturing Facility provides on-site fuel fabrication capabilities and the Transient Reactor Test (TREAT) facility is designed to provide safety-related testing of nuclear fuels. TREAT is an air-cooled reactor that provides short, very intense bursts of nuclear energy and can simulate accident conditions up to and including melting or vaporization of test specimens. The ANL nuclear fuel development loop is closed with a comprehensive irradiated material examination capability in hot cells at locations in Idaho and Illinois. The Electron Microscopy Laboratory at ANL-West includes scanning and transmission electronic microscopes, which are used for imaging and identifying irradiation-induced effects and to provide a better understanding of how irradiation affects mechanical properties in a variety of materials.

215 WASTE MANAGEMENT AND ENVIRONMENTAL TECHNOLOGY

Environmental and waste management issues are among the most pressing for the U. S. Department of Energy. The successful remediation of environmental contamination from the defense nuclear legacy and the proper treatment of radioactive and hazardous wastes from ongoing operations comprise a multi-billion dollar per year set of activities in the U.S. Continued development and deployment of nuclear energy technologies capable of meeting world energy demands with no carbon emissions will depend on the success of these projects and on the development of waste management strategies for future nuclear energy systems. ANL-West is tackling difficult problems related to the characterization, treatment and disposal of mixed and transuranic waste. Specific projects include developing mixed waste treatment methods for high-activity remote-handled spent HEPA filters, studying supercritical fluid extraction techniques for the removal of organics from radioactive waste, applying polymer gels and ion exchange media to liquids treatment, and developing alternatives to incineration for certain waste types. In addition, we are studying radiolytic, chemical and microbial gas production in materials ranging from raw wastes and treatment products to special nuclear materials. Argonne's rich history of fast reactor development has led us into current projects in metallic sodium stabilization, spent fuel storage and collaborative work on the decommissioning of the BN-350 breeder reactor in Kazhakstan. Finally, we are readying our facilities to support critical DOE research initiatives related to vadose zone contaminant study and the demonstration of alternatives to incineration.

216 ENGINEERING SUPPORT GROUPS

The support functions at ANL-West include many site-wide services to the major facilities.

- Engineering provides engineering design and project management support for new buildings, building additions and modifications to the physical plant facilities. The functional specialties include project management, mechanical, electrical, civil, architectural and structural engineering.

- The Environment, Safety and Waste Management (ESM) Department is responsible for the environment, safety and health, and waste management for the ANL-W Site. The mission is to ensure the implementation of all Laws (Federal and State), Regulations, DOE Orders and good practices required to ensure the quality of the environment, safety and health of the employees and general public.

- The Operations Support Group is responsible for providing maintenance engineering, environmental engineering and safety analysis for the day to day activities of the operating facilities. Typical activities include providing technical direction for waste stream analysis, packaging, storage, treatment, and disposal; providing safety analysis for proposed modifications to operating facilities; and providing electrical engineering, instrumentation and controls engineering, and mechanical engineering support to the maintenance crafts and facility managers.

The safety responsibilities include radiation protection, fire protection, industrial hygiene, and industrial safety. Environment and waste management includes the control of hazardous radioactive and radioactive mixed waste; control of emissions; and ESM manages the DOE Environmental Restoration and Waste Management. (ER/WE)_ Five Year Plan which designates funding and established the context within which environmental cleanup, waste operations and research and development activities at DOE sites are performed.

217 ADVANCED NUCLEAR ENERGY CONVERSION TECHNOLOGY

Argonne is involved in a number of areas related to advanced nuclear energy systems. Included in this is hydrogen production from nuclear energy and corrosion control in salts used in nuclear fusion reactors. The ability to produce hydrogen from water and energy sources that do not emit greenhouse gases is a critical element to the transition to a hydrogen economy. Argonne is currently in the process of evaluating a number of different thermochemical water splitting cycles that could potentially be linked to a nuclear power plant to produce environmentally-benign hydrogen as a transportation fuel. The development of nuclear fusion as a power source is one of the greatest technical challenges of researchers today. The extremely high temperatures needed in order to drive the process results in a tremendous challenge to find appropriate means of confinement. Molten fluoride salts have been proposed for years to act as both a coolant and a neutron blanket for fusion reactors. However, the high flux of neutrons into these fluoride salts results in the formation of corrosive tritium fluoride. Argonne is looking at the inclusion of a redox agent in the fluoride salt which would minimize the tritium fluoride concentration and reduce corrosion to an acceptable level.

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 two scientific sections (Biophysics, and Functional Genomics), 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

218 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.

219 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 and aqueous phases, and the correlation of structure with biological function. The biomolecules under study include various antibodies, enzymes, cytochromes, and the bacterial photosynthetic reaction center. The techniques used in this program are taken from a variety of disciplines including molecular biology, protein chemistry, chromatography, immunochemistry, 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.

220 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 smaller molecules. 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 studies 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, several 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.

221 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.

222 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 at Argonne. The techniques being used include molecular biology and biochemistry protein crystallography, x-ray diffraction, high-performance liquid chromatography, and electrophoresis.

223 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.

224 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

225 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.

226 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 and in the RNA isolated from bones. Molecular pathways of cadmium action are investigated with reverse transcriptase-polymerase chain reaction for specific genes known to influence bone resorption and by differential display to identify unknown genes. Another research area focuses on the biochemical pathways for metabolizing 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.

227 ANTIBODY ENGINEERING

With the recent completion of sequencing two hundred 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 2-3 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 generating antibodies and to meet the need for thousands of antibodies, we utilize phage-display to isolate high-affinity and selective generate “[3”]designer antibodies”[2”] 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 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. Although a large number of antiangiogenic drugs with significant *in vitro* anti-cancer activity are presently in clinical trials, their mechanism of action is not well understood. Our laboratory is presently engaged in the construction of recombinant bacterial viruses which carry portions of proteins derived from endothelial cells on their surface. By studying the interaction of antiangiogenic molecules with these viral particles, we hope to identify the means by which this class of drugs inhibits the neovascularization of tumor tissue.

A second related project within this laboratory is analysis of the mechanism by which small molecules bind to proteins. In spite of the fact that multiple three dimensional pictures have been obtained of protein-ligand pairings, the pace of rational drug design has been hindered by a lack of global coherent rules underlying small molecule-protein interactions. By studying the pattern of virally-presented combinatorial peptides binding to common metabolites such as ATP and glucose, and correlating those sequences with three dimensional structures of known metabolite/protein pairs, we aim to create a database of peptide sequences which are predictive for metabolite binding in known protein sequences. Information derived from this work can eventually be extended to combinatorial chemistry-derived drugs to predict potential targets within the human body prior to clinical trials.

BIOTECHNOLOGY (BTC)

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. Engineers promote industry processes to produce environmentally friendly "green" solvents, support an emerging agriculture-based chemical industry, and develop biocatalytic systems for the production of chemicals from renewable resources through numerous industry/government partnerships. And to help clean the environment, researchers continue to develop and test novel technologies to remove, detoxify, and recover heavy metals and other unwanted entities from pipelines, soils, groundwater, and aqeuous waste streams.

HEALTH

229 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.

230 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™).

231 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.]

INDUSTRY

232 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.

[Also, see related listing under the Energy Systems Division, Center for Industrial Technology Systems.]

233 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.

[Also, see related listing under the Energy Systems Division, Center for Industrial Technology Systems.]

234 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.

[Also see related listing under the Energy Systems Division, Center for Environmental Restoration Systems]

CHEMICAL ENGINEERING DIVISION (CMT)

This 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, including advanced lithium-ion and lithium-polymer batteries for transportation and other applications; fuel cells, including the use of an oxidative reformer and gasoline as the fuel supply; stable nuclear waste forms suitable for storage in a geological repository; and aqueous and pyrochemical processes for the disposition of spent nuclear fuel. Our programs in basic science are engaged in smaller research projects, such as catalysis, hydrogen production, and superconductivity, that have the potential to impact future energy systems. All Chemical Engineering Division projects are backed up by strong basic research.

FUEL CELL RESEARCH AND DEVELOPMENT

235 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 are not based on 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.

236 FUEL PROCESSING FOR FUEL CELLS

Low-temperature polymer electrolyte fuel cells are being developed for use in light-duty vehicles and stationary applications. These fuel cells operate best with hydrogen. However, the lack of a hydrogen supply infrastructure and the low energy density of hydrogen storage technology have created a need for compact and lightweight fuel processors that can convert available liquid fuels or natural gas into hydrogen-rich gas. These fuel processors involve a number of unit operations and processes and require new and more advanced technologies (catalysts, reactor designs, integration methods, etc.) for the various applications. This project undertakes the development of all aspects of the fuel processor and includes the catalytic reforming process, sulfur and carbon monoxide (a byproduct of the reforming reaction) removal and cleanup, and the integration of all of the components into a compact hardware. All of these activities are pursued through mathematical modeling and experiment. Major experimental equipment includes: a gas chromatograph, mass spectrometer, IR analyzer, thermal conductivity analyzer for hydrogen, CO chemisorption analyzer, apparatus for BET surface area measurement, and catalytic reactor test stands. Material characterizations are performed with scanning electron microscopy, x-ray diffraction, and chemical assay.

237 METAL-SUPPORTED SOLID-OXIDE FUEL CELL DEVELOPMENT

Research activities are concentrated on the development of a new type of solid-oxide fuel cell. Efforts are directed toward defining materials and fabrication methodology that will achieve the desired structure and properties for the electrolyte, electrodes, and interconnects. The project involves the characterization of high-temperature inorganic materials by means of x-ray, surface area, electron microscopy, and other techniques. The project also involves the fabrication and characterization of metallic and ceramic structures using tape casting, slip casting, extrusion, complex impedance measurements, and other techniques. There is a continuing effort to enhance understanding of the fundamental mechanisms of fuel cell operation and to improve fuel cell design and operation. Major equipment includes: tape caster, furnaces, AC impedance system, computer, and scanning electron microscope.

238 NOVEL MATERIALS FOR USE IN SOLID-STATE FUEL CELLS

This research effort is directed toward the development of new materials for use in a moderate-temperature-range (500°–800°C) fuel cell. Studies are currently being conducted to find new, highly conductive materials for use as the anodes, cathodes, electrolytes, and interconnects. Effort involves synthesis of materials, sintering and processing of materials, and characterization of electrochemical and chemical properties. Major equipment includes: frequency response analyzer, differential thermal analyzer, dilatometer, optical microscope, scanning electron microscope, electrochemical analytical equipment, and computer-controlled data acquisition and reduction.

WASTE MANAGEMENT

239 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.

240 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.

241 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.

242 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.

243 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

244 BATTERY MATERIALS RESEARCH AND DEVELOPMENT

Novel oxide, nitride, sulfide, salt, 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.

245 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.

246 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

247 FLUID CATALYSIS

Homogeneous and heterogeneous catalysis chemistry and mechanisms associated with the activation of methane, dihydrogen, carbon dioxide, carbon monoxide, and dinitrogen are explored using *in situ* spectroscopic and kinetic techniques. Parallel synthetic efforts are directed toward the isolation or synthesis of organometallic reaction intermediates and new catalytic species. Catalytic reactions in supercritical fluids and catalytic C-H bond activation chemistry, catalytic formation of preceramic organometallic polymers, and shape-selective macrocyclic catalysts are also investigated. In addition, new high-pressure NMR spectroscopic and NMR imaging techniques are developed to investigate organometallic systems. Major equipment includes: high-pressure multinuclear NMR facility, high-pressure Fourier transform infrared spectroscopy, liquid and gas chromatographs, and high-pressure autoclaves.

248 ION TRANSPORT PROPERTIES

This program uses *in situ* magnetic resonance imaging to better define electrode-electrolyte interfaces and solid-state ion transport mechanisms. Areas of interest include the analysis of the chemical composition at the electrode-electrolyte interface, ion concentration gradients within solid-state batteries, conformational dynamics of polymeric electrolytes, and ion penetration depths within graphite insertion electrodes. Special emphasis is placed on measuring ionic diffusion coefficients as a function of distance from the working electrode to probe the mechanism of ion transport in lithium-polymer electrolyte battery materials. Major equipment includes: multinuclear NMR facility, NMR-electrochemical imaging cells, magic angle spinning, Fourier transform infrared spectroscopy, and liquid and gas chromatographs.

249 TRACE-ORGANIC ANALYSIS OF ENERGY AND ENVIRONMENTALLY DERIVED MATERIALS

A wide variety of chemical carcinogens and toxins with potential health and safety implications are analyzed. Chemicals responsible for hazards are identified and measured. Methods used include gas chromatography, combined gas chromatography/mass spectrometry, high-performance liquid chromatography, high-performance liquid chromatography/mass spectrometry, supercritical fluid chromatography, Fourier transform infrared spectrometry, wet chemistry, and computer analysis. In some cases, chemicals present below the parts-per-billion level are detected. Sophisticated computer-controlled analytical equipment is used.

250 METHOD DEVELOPMENT IN TRACE-ORGANIC ANALYSIS

A variety of analytical problems are encountered in trace-organic analysis for which methods are not currently available. Methods are being developed to meet these needs. Recent and ongoing method development examples include PCB and dioxin analysis, as well as air sampling. Recent instrumentation development includes gas chromatography/matrix-isolation/Fourier transform infrared spectrometry, multidimensional gas chromatography, capillary gas chromatography, and mass spectrometry. Major equipment includes: gas chromatograph, supercritical fluid chromatograph, high-performance liquid chromatograph, mass spectrometer, mass spectrometer/mass spectrometer, and Fourier transform infrared spectrometer.

251 MODERN METHODS FOR TRACE ELEMENT ANALYSIS

Improved analytical methods are being developed, evaluated, and implemented for the determination of trace elements in a broad range of sample matrices, including soils, sludges, coals, solid and liquid wastes, 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: atomic absorption spectrophotometers (flame, graphite furnace, hydride generation, and cold vapor), an inductively coupled plasma/atomic emission spectrometer, an inductively coupled plasma/mass spectrometer, and an ion chromatograph.

252 DETERMINATION OF LONG-LIVED ACTINIDES IN ENVIRONMENTAL MEDIA

Procedures have been developed to efficiently determine the amount of small (10^{-12} Ci) quantities of radionuclides such as plutonium and uranium in soil, water, and other environmental media. It is necessary to characterize large numbers of U.S. Department of Energy sites not only to assess contamination levels for subsequent treatment, but also to determine sites that can be safely released to the public. The actinides are determined using alpha-pulse analysis after dissolution and chemical separations.

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 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, metal clusters, theoretical and experiment chemical dynamics, carbon chemistry, actinide element and separation science, and electrochemistry and computational molecular materials studies. The work is supported predominantly by Basic Energy Sciences, Department of Energy.

253 RADIATION AND PHOTOCHEMISTRY

Argonne addresses the chemistry of novel intermediates and excited states and the roles of solvents and matrices in modulating their reactivity. A dedicated electron linac 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.

254 PHOTOSYNTHESIS

This program is defining the basic principles that govern charge separation in molecules via the study of electron transfer reactions within novel structures. Remarkable progress has been made since the first demonstration of the Marcus inverted region at Argonne. Work on the mechanism of charge separation in natural photosystems is being extended to construct novel artificial systems to mimic the natural process.

255 CLUSTER STUDIES

This program investigates metal clusters and cluster-molecule complexes. Argonne achieved many breakthroughs in studying these systems. Now, closely linked experimental and theoretical explorations are elaborating their structure, electronic properties, and chemical reactivity.

256 CHEMICAL DYNAMICS IN THE GAS PHASE

This program merges theoretical and experimental work on energetics, kinetics, and dynamics. 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.

257 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.

258 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 nanoscale interactions in structures that offer the ability to control the propagation of photons below the diffraction limit. Our research encompasses the generation, characterization, and theory of nano-optical structures.

259 CHEMICAL TRANSFORMATION MECHANISMS

This research program seeks to understand thermal transformations and their effect on catalysis-related phenomena. Aspects of heterogeneous catalysis, molecular processes, and structure-activity relationships in chemical systems of large complexity are addressed. Another area of interest is the elucidation of mechanisms that are critical to molecular and nanomaterials synthesis. Studies include the phenomena of clay formation and soot formation together with spectroscopic molecular characterization, molecular interactions at surfaces and interfaces, soot particle growth mechanisms, and electronic interactions of organic molecules at the clay interfacial surface. The studies of structure at surfaces and interfaces are of relevance to catalytic transformations.

260 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. These studies have 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.

261 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.

COMPUTING AND INSTRUMENTATION SOLUTIONS DIVISION (CIS)

The Computing and Instrumentation Solutions 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.

267 SYSTEMS MANAGEMENT

Systems managers manage the performance of high-performance distributed workstations. Other activities include software installation and configuration, testing of new systems, and necessary programming modifications to address special needs.

268 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.

269 HIGH-SPEED NETWORKING

Scientific computation demands increased data transmission speeds through high-speed networks to enable the transfer of large data files, effective distributed processing, remote visualization capabilities, and other high-volume electronic communication. ECT is developing fiber-optic networks with standard protocols to meet these increasing demands. ANL also participates in the planning, development, and operation of several high-speed national networks.

270 LOCAL-AREA NETWORKING

Distributed computing plays an increasingly prominent role in both scientific computing and administrative business systems. The distributed environment at ANL can be characterized as networks of Unix scientific workstations and networks of personal computers integrated via a Laboratory-wide network. Ongoing activities include the design and upgrade of these networks, the development of network servers and services, and the provision of a client-server framework for new scientific and administrative network applications.

271 ELECTRONICS AND INSTRUMENTATION

This section designs and implements computer- and microcomputer-based real-time systems, real-time applications software, distributed-intelligence networks, data links and specialty electronics. In addition, Electronics and Instrumentation designs equipments and systems for nuclear reactors, particle accelerators, telemetry systems, and research programs. Calibration services traceable to the National Bureau of Standards are also provided. This section also develops new instruments and techniques for radiation detection and imaging, pulse spectrometry, and nondestructive analysis. The fabrication facility provides quick turnaround construction of prototype instruments. Systems are developed for applications in synchrotron-light research, neutron scattering studies, environmental monitoring, national security related specialty electronics and nuclear physics.

272 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.

273 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.

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.

262 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

263 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 Monitoring (ARM) program
- Develop petabyte-scale scientific data access and storage solutions for the Large Hadron Collider at CERN

264 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.

265 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.

266 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 Evaluation Section and the Chemical and Biological Section 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.

CHEMICAL AND BIOLOGICAL TECHNOLOGY SECTION

274 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.

275 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. In addition, we are investigating the development of novel natural gas resources, especially the methane hydrates distributed in ocean sediments throughout the world.

276 PROCESS EVALUATION SECTION

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, (3) recovery of materials from aluminum salt cake (recovery of salt by electrodialysis, conversion of oxides to value-added products), and (4) evaluation of non-consumable anodes for molten salt electrowinning of metals.

CENTER FOR ENVIRONMENTAL RESTORATION SYSTEMS

The Center for Environmental Restoration Systems 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.

277 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.

278 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.

279 SPATIAL ANALYSIS AND DECISION SUPPORT SYSTEMS

Environmental research requires the ability to collect, manipulate, analyze, evaluate, and display data on three-dimensional characteristics and spatial variables at both small and large scales. Geographic information systems (GIS), computer aided design (CAD) software, data base systems frameworks, visual simulation capabilities, remote sensing/satellite imagery collection, and multimedia techniques are used individually and in combination to solve environmental problems. Current studies include global scale simulation of continental drift through geologic time, developing expert systems utilizing input from GIS sources to guide brownfield redevelopment, coupling risk models to GIS, incorporating distributed sensor networks into spatially based decision support tools, and coupling geophysical data to related GIS information.

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.

280 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.

281 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.

282 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.

283 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.

284 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.

ENERGY TECHNOLOGY DIVISION (ET)

The Energy Technology Division provides an integrated, state-of-the-art approach to the design, fabrication, and testing of highly-reliable materials, components, and instrumentation. The Division is particularly strong in the areas of ceramic superconductors, high-temperature properties of metals and ceramics, corrosion, radiation effects, nondestructive evaluation techniques, materials processing, thermal hydraulics, engineering mechanics, instrumentation and control, and components and systems testing. For energy technologies, the Division's programs emphasize safe and reliable design, efficient performance, and inherent safety of components and systems, as well as gathering basic engineering data and developing applicable new methods of analysis.

285 ADMINISTRATION

The Energy Technology Division has opportunities for students interested in cost accounting, project management, human resources, purchasing, computer science, network administration, and data management. The challenge is to reduce large amounts of data to manageable reports. Strong background in database applications such as Access and/or Excel will be very beneficial.

286 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.

287 COMPUTATIONAL PHYSICS AND HYDRODYNAMICS

The research in this group covers a wide range of applications in computer simulation and physics of materials behavior under harsh environments. The HEIGHTS computer simulation package developed in this section has unique worldwide capabilities. One major research area is to simulate material behavior under intense power deposition from various sources. This includes detailed models of heat transfer, phase change, thermal hydraulics, magnetohydrodynamics, plasma physics, photon radiation and radiation transport. Models of material erosion and destruction due to laser, ion and electron beams, and plasma radiation are being developed and benchmarked using worldwide powerful facilities. The HEIGHTS package is currently being used for fusion applications, nuclear and high energy physics programs, and space applications. Potential applications include defense, industrial, and medical applications. Other research areas include particle transport and diffusion, flow and solidification of metals in castings, and single/multiphase fluid flow in various engineering systems.

288 THERMAL MECHANICAL SCIENCES

Research in this group relates to many diverse areas involving structural dynamics, thermal-hydraulics, heat transfer, fluid flow, and vibrations. Program emphasis is placed primarily on experimentation and testing, but also extends to modeling. The group operates several test facilities. These include the Flow-Induced Vibration Test Facility (an 8,000-gpm water flow loop), the Flow and Heat Transfer Test Facility (a computer-controlled, thermal-hydraulic, transient, nonisothermal, 2,200-gpm water loop), a low-velocity water channel, a slurry test facility, an adiabatic two-phase flow apparatus, small-channel flow boiling and condensation heat transfer test apparatus, and a 500-gpm water loop. The group performs fundamental research, component development, and performance testing and consultation. Current activities include research in the areas of flow-induced vibration, multiphase flow and heat transfer in compact heat exchanger geometries, ice-slurries for district cooling, and chaos associated with fluid-structure interaction. In addition, vibration studies are performed in support of accelerator facilities.

289 TRANSPORTATION OF HAZARDOUS MATERIALS

This group provides technical assistance to the Department of Energy (DOE) in performing technical reviews and confirmatory analyses of Safety Analysis Reports for Packaging (SARPs) and transportation of radioactive materials. The SARPs are reviewed and evaluated to verify compliance of the packaging designs with the safety requirements specified in DOE Orders and in NRC, DOT, and IAEA regulations. The group also provides technical assistance to DOE on other nuclear waste management and transportation issues, including training, satellite tracking, and production and distribution of public information videos. The group provides technical support to the Nuclear Regulatory Commission (NRC) in plant aging management and license renewal, including the development and update of the Standard Review Plan for License Renewal (SRP-LR), NUREG-1800, the Generic Aging Lessons Learned (GALL) report, NUREG-1801, and the review of license renewal applications for the ANO-1, Peach Bottom, St., Lucie, V. C. Summer and Dresden and Quad Cities nuclear power plants. The group also provides technical support to NRC on regulation improvement activities and plant licensing actions such as the Diablo Canyon steam generator alternative repair criteria for primary water stress corrosion cracking.

290 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 conductor development using high-T_C ceramic superconductors. The Ceramics Section staff have fabricated wires and other technologically useful shapes for motors, bearings, sensors, etc. as well as synthesized superconducting compounds. Other areas include whisker-or fiber-reinforced ceramic matrix composites that are being studied for a variety of high-temperature applications; ionic conductors for batteries, fuel cells, sensors, and gas-separation; and advanced refractories for iron and steel making and for the containment of nuclear waste. 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 differential thermal analysis, mechanical properties measurements, and for the superconductors, determination of critical current density and critical temperature. For composites, neutron diffraction is used to characterize the internal stress distribution. Those interested in hands-on ceramics laboratory work should apply for a position in this section.

291 ANALYSIS AND MODELING OF MATERIALS BEHAVIOR IN ENERGY SYSTEMS

In the area of nuclear fission, the thermal, mechanical, and irradiation response of nuclear fuel elements for the reduced enrichment research and test reactor (RERTR) is being analyzed. Emphasis is being placed on realistic models that accurately describe the physical situation. In the fusion area, the thermal and mechanical responses of fusion first-wall structures under novel cooling schemes is being modeled.

292 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.

293 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) is 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. Finally, the response of plasma-facing components in fusion reactors to plasma disruption events is being analyzed.

294 IRRADIATION PERFORMANCE OF REACTOR MATERIALS

The principal objective of the programs in the Irradiation Performance Section is to assess the behavior of materials, including fuel, cladding and structure components, in the environment of nuclear fission and fusion reactors. These environment results in neutron damage and chemical, metallurgical, and mechanical processes that occur over a wide range of elevated temperatures. The programs falls into the following categories: (1) fuels and materials development for a number of reactor types, (2) postirradiation characterization of fuels and materials, and (3) postirradiation thermal/mechanical testing of fuels and materials. A significant fraction of the Section's activity is devoted to the performance characterization of light-water reactor fuel systems. The developmental activities include design and fabrication of test fuel or material for irradiation testing in a reactor. The postirradiation characterization and testing activities utilize the Section's Alpha-Gamma Hot Cell Facility and the Irradiated Materials Laboratory to perform examination, testing and analyses. Available research tools include a full array of fabrication equipment, optical metallographs, scanning electron microscope, Auger microscope, electron microprobe, hydrogen and oxygen determinators, and numerous thermal and mechanical testing instruments. Cooperative research programs are welcome.

295 OXIDATION-SULFIDATION BEHAVIOR OF MATERIALS

The program involves experimental studies to establish the mechanism of oxidation-sulfidation of model metallic and ceramic materials exposed to complex and multicomponent gas environments. The research will require background in the areas of thermodynamics and kinetics of gas-solid reactions and use of optical and electron microscopy techniques to elucidate the corrosion mechanisms.

296 CORROSION OF MATERIALS IN THE PRESENCE OF DEPOSITS

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

297 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.

298 ALLOY MODIFICATION FOR IMPROVED CORROSION RESISTANCE

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.

299 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.

300 ELECTROMECHANICS AND SUPERCONDUCTIVITY APPLICATIONS SECTION

Research in this area involves the design, development, and analysis of macro-scale devices, such as motors, energy storage coils, power transmission lines, fault-current limiters, bearings, levitated vehicles, etc., using high-temperature superconductors. The group also investigates high-efficiency conventional electric motors, active magnetic bearings, the use of pulsed magnets in aluminum forming, and the use of ac magnets to contain and stir liquid metals. Fabrication and experimental testing of prototypes are conducted in most instances. Major past projects have included the development of superconducting current leads that require an order of magnitude less refrigeration than conventional leads, and a superconducting bearing that holds the world's record for the lowest coefficient of friction. Present projects include the use of superconducting bearings in flywheel energy-storage systems with a goal of 90% efficiency on a diurnal basis. One of our previous students won second prize in the national Apparatus Competition of the American Association of Physics Teachers for a superconducting motor that he built while working in our group.

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.

301 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.

Ergonomic evaluations of workstations and workplace are also conducted by the Industrial Hygiene Group. Recommendations for modifications are made to reduce the incidence of repetitive strain injuries.

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

302 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 response 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. 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 including the design, development, testing for efficacy, and application of such methods as Computer-Based Training (CBT) and Web-Based training (WBT).

ENVIRONMENTAL ASSESSMENT DIVISION (EAD)

The Environmental Assessment Division has developed a broad program of interdisciplinary, applied research and development, undertaken from a system's perspective. 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.ead.anl.gov.

303 ATMOSPHERIC SCIENCES

Construction and operation of energy technology systems and other industrial activities are evaluated to assess their potential impacts on ambient air quality, climate, meteorology, and acoustic environment. The effectiveness of control technologies and related government regulations in mitigating these impacts is 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

304 ENVIRONMENTAL RESTORATION AND WASTE MANAGEMENT

The Division also conducts special environmental analyses and remediation studies to support the cleanup or environmental restoration programs of federal facilities. The work includes analyzing cleanup alternatives at different sites with regard to possible contamination of air, soil, surface water, and groundwater. Regulatory impacts on waste management and environmental remediation are also analyzed. Restoration studies include remedial investigations, feasibility studies, risk assessment, hydrogeologic studies and modeling, and the development of sampling and remedial design strategies. The evaluation and implementation of innovative cleanup methodologies and technologies at federal facilities play an important role in the Division’s activities. Pollution prevention studies emphasize improved waste management practices including material disposition studies.

305 ENVIRONMENTAL DATA MANAGEMENT AND COMMUNICATIONS

In keeping with the Division's mission to advance informed environmental decision making, it 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 in the analysis and communication of spatial data. Advanced visualization, including virtual reality systems, is utilized to communicate environmental data and the results of environmental modeling to technical and non-technical audiences. In addition, the Division makes extensive use of World Wide Web technologies in almost all of its environmental studies. The applications range from public information dissemination to secure working Web sites where data integration and analyses support distributed decision making. Web-based software has been developed by the Division to enhance access to spatial and other data over a Web browser.

306 HYDROGEOLOGY

Analytical and numerical models of surface flow, groundwater flow and solute transport are developed and used to evaluate environmental contamination problems. Impacts to human health, endangered species, and the environment are quantified. 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 involving a wide range of skills and knowledge. The interaction of water, geologic materials, and contaminants is a general part of most environmental issues.

307 NUCLEAR MATERIAL TRANSPORT

This activity involves the assessment of radiological impacts resulting from the releases of radioactive materials from transportation of radioactive nuclear waste materials. The assessment requires the modeling of the transport of radioactive materials via various environmental pathways that would eventually lead to radiation exposure to humans. Modeling includes computer simulation of radiation transport, atmospheric dispersion, radionuclide pathways, and radiation health effects.

308 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. Specific activities include both analytical studies and field work such as development of planning and guidance materials; audits of environmental compliance at federal facilities and associated corrective action plants; presentation of workshops on environmental laws, regulations, and compliance; preparation of baseline surveys and emission inventories; development of database management expert computer systems, and web-based systems for environmental compliance information, and preparation of NEPA documents and management of the NEPA process for specific projects. Planning may include entire environmental management systems including natural and cultural resources.

309 LONG-TERM ENVIRONMENTAL STEWARDSHIP

In the DOE, the terms “environmental stewardship” and “long-term stewardship” refer to the mechanisms necessary to ensure both short- and long-term protection of the public and the environment from residual contamination after initial cleanups at over 100 sites in the DOE Complex have been completed. These mechanisms include physical and institutional controls, information management, environmental monitoring, and risk assessment. The U.S. Department of Defense faces similar issues in the postclosure period of its cleanups. Stewardship encompasses many daunting technical issues, 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 accessing changes in site risks over decades.

310 ECOLOGICAL AND GEOGRAPHICAL SCIENCES

Analyses are conducted on the effects of 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, radiological and chemical contamination, and cumulative impacts. Ecological risk assessments are performed for contaminated sites to develop cleanup criteria and evaluate 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 systems. Recent projects have examined the effects of dam operations on aquatic and terrestrial ecosystems, biodiversity and habitat evaluations, ecological risk assessments at contaminated sites, and wetland and prairie restorations.

311 ENVIRONMENTAL POLICY ANALYSIS (Washington, DC location)

The environmental, technological, and economic implications associated with developing and implementing national environmental laws, regulations, and policies are assessed to identify areas for improvement. Multidisciplinary and focused assessments are conducted on environmental topics such as the management practices for controlling air and water pollutants and managing wastes. The environmental, energy, and economic effects of these practices and the impacts of different strategies to minimize the effects are also assessed. Policy makers use these assessments in their decision making on issues of national importance.

312 NATURAL RESOURCES

Natural resource management plans are prepared for federal facilities that identify goals and objectives for a five-year period. An integrated approach is taken to develop the plans that examines planned facility missions and programs, potential impacts associated with each program, and current baseline physical and natural environment. Program activities are considered together with objectives for 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 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, probabilisitc risk assessments, cumulative risks from combined exposures to multiple contaminants, and risk communication.

313 ENVIRONMENTAL IMPACT ASSESSMENT

Proposed federal actions are assessed according to the requirements of the National Environmental Policy Act (NEPA). Environmental effects are analyzed and presented in environmental impact statements and other documents. Activities include conducting public involvement activities, gathering information and data, evaluating environmental impacts, development of databases and multi-media tools, response to issues of public concern, examination of regulatory issues, information retrieval and archiving, development of management tools, and report preparation. These activities are performed by closely integrated multi-disciplinary teams.

314 RISK ASSESSMENT

Risk assessment is used as a tool in determining environmental management objectives and in evaluating a wide range of technological and environmental issues in various land-use and demographic settings. In conducting these assessments, an extensive set of analytical tools are used to quantify the hazards or sources of risk, the pathways or mechanisms by which sensitive human or ecosystem populations become exposed, and the nature and extent of the resulting impacts. One such tool is the RESRAD computer code which determines site-specific cleanup guidelines on the basis of the calculated exposures to hypothetical residents or workers on the site. Other focus areas include evaluations of transportation risks, risks to the ecosystem, probabilistic risk assessments, and risk communications.

ENVIRONMENTAL RESEARCH DIVISION (ER)

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. Current emphasis is on the environmental effects of hazardous wastes (e.g., identification, amelioration, and remediation) and atmospheric responses to energy production and use (e.g., induction of smog and alteration of global climate). The Division is organized into two scientific sections (Atmospheric Research and Terrestrial Research), each with several research groups, as well as three major additional program groupings (Environmental Management and Surveys, Photophysics and Photochemistry, and Radiation Physics). An interactive and collaborative approach to the investigation of these complex environmental issues is the hallmark of the Division.

ATMOSPHERIC SECTION

Research activities include investigation of the physics and chemistry of the lower atmosphere, particularly with regard to the processes of transport, chemical transformation, diffusion, and deposition of airborne trace substances. Related activities involve studies of climate change, terrestrial water and carbon cycles, and aquatic environments in freshwater lakes. Measurements are made with a view toward the development of descriptive theoretical and numerical models. Particular attention is paid to the changes in the atmosphere that are brought about by human activities, such as emissions from the burning of fossil fuels.

315 ATMOSPHERIC PHYSICS

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 CARBON CYCLE studies, The heat, water vapor, and carbon dioxide 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. 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.

316 ATMOSPHERIC CHEMISTRY

The chemistry transformations and fates of energy-related air pollutants released into the atmosphere are studied over urban and regional areas. The research concentrates on the behavior and formation fine aerosols and their radiative effects. The turbulent air-surface exchange of the substances is measured in dedicated field experiments, parameterizations of the exchange rates are developed, and models are developed to use satellite data to describe the exchange rates over urban regions and global scales. Observations of organic compounds are taken at the surface and aboard research aircraft during field experiments and the data are used to evaluate the processes that generate aerosols in the atmosphere. Measurements are also made to determine aerosol lifetimes and optical properties. Aerosol species are important in air quality and in global and regional climate considerations. Many of the aerosols studied such as black carbonaceous soots have important radiative properties that can contribute to Earth's overall radiation balance. Many of the findings from the observational studies are interpreted and generalized with the use of numerical models of atmospheric chemistry and transport.

The chemistry transformations and fates of energy-related air pollutants released into the atmosphere are studied over urban and regional areas. The research concentrates on the behavior and formation of ozone and other oxidants (particularly peroxyacyl nitrates or PANs), nitrogen oxides, sulfur oxides, volatile organic compounds, hazardous air pollutants, and fine aerosols. The turbulent air-surface exchange of the substances is measured in dedicated field experiments, parameterizations of the exchange rates are developed, and models are developed to use satellite data to describe the exchange rates over urban regions and global scales. Observations of organic compounds are taken at the surface and aboard research aircraft during field experiments and the data are used to evaluate the processes that generate ozone, PANs, and other oxidants in the atmosphere. Laboratory and field studies of PANs and organic oxidants are carried out by using novel analytical instrumentation developed for these compounds. The organic oxidants, which are key secondary pollutants that play important roles in gas-, aerosol-, and aqueous-phase chemistry in the troposphere, can be toxic to plants and animals. Measurements are also made to determine aerosol lifetimes and optical properties. Both the gas and aerosol species are important in air quality and in global and regional climate considerations. Many of the gases and aerosols studied have important radiative properties that can contribute to Earth's overall radiation balance. Many of the findings from the observational studies are interpreted and generalized with the use of numerical models of atmospheric chemistry and transport.

317 AQUATIC PROCESSES

A variety of techniques are used to study both climatic effects and contaminant transport and exchange processes in the Great Lakes and the Great Lakes region. These include analysis of data obtained from satellites, collection of *in situ* observations of the benthic boundary layer, numerical modeling, and statistical analysis of water-quality data. Emphasis is placed on the application of advanced computational and statistical methods to interpretation and analysis of observational data.

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.

318 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.

319 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?

320 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.

321 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.

ENVIRONMENTAL PROGRAMS

322 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.

323 APPLIED GEOSCIENCE AND ENVIRONMENTAL MANAGEMENT AND FIELD RESEARCH

Argonne's program in applied geosciences and environmental management is adapting nonintrusive geophysical and geochemical techniques used in petroleum exploration and mining to produce data sets that can, for example, be integrated with geology to identify contamination and predict directions of contaminant migration in field sites. Nonintrusive techniques being adapted include seismic refraction and electromagnetic surveys, geochemical analysis, and analysis of stable isotope tracers. The integrated results are used to prioritize potential sampling locations on the basis of their potential usefulness in pinpointing contaminants, thus limiting the need for costly drilling, analytical works, and hazardous waste disposal. The process has been used in environmental site characterization programs for many hazardous waste sites. Initially, sound geologic and site history models are developed to guide the selection of investigative techniques. Then a multidisciplinary team of scientists conducts a field investigation and integrates the results to determine the extent of contamination. The process is quick and cost-effective, and it results in identification of principal controls on subsurface migration pathways for contaminants, improved geochemical sampling programs, better delineation of the aquifer system, identification of relevant subsurface features, and reduced requirements for long-term site monitoring. The Argonne system for expedited environmental site characterization is the basis for the American Society for Testing and Materials standard ASTM D6235. The process is being marketed commercially as the QuickSite® system.

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 addition research effort has been initiated, investigation of the formation biofilms in the environment and their role in the biogeochemical cycling of materials.

324 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.

325 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.

326 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.

HIGH ENERGY PHYSICS DIVISION (HEP)

The Division conducts research into the nature and properties of elementary particles -- the building blocks of matter. The program includes colliding beam and neutrino experiments at nearby Fermi National Accelerator Laboratory. 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.

327 LEPTON SCATTERING EXPERIMENTS

Physicists from Argonne's High Energy Physics Division, together with colleagues from 50 institutions from different parts of the world, are involved in studies of high-energy electron-proton collisions. The experiment, ZEUS, is located at the HERA colliding beam facility at the DESY Laboratory in Hamburg, Germany. With energies of 27 GeV for the electrons and 920 GeV for the protons, the structure of the proton is being probed with an unprecedented accuracy. A large variety of physics topics are being addressed: structure functions of the proton, photon, and pion, diffractive scattering, searches for exotic particles, etc.

A group of US institutions was responsible for the design and construction of the barrel calorimeter, one of the major components of the experiment. In an effort to improve the performance of the ZEUS detector, the Argonne group built a preshower counter that is located in front of the barrel calorimeter. The group is also involved in a major upgrade of the forward tracking system, for which it is building the front-end readout system. There are opportunities for students as well as faculty to become involved in both data analysis and hardware upgrades.

328 MINOS LONG BASELINE NEUTRINO EXPERIMENT

Recent results from underground cosmic-ray experiments give convincing evidence that the phenomenon of neutrino oscillations occurs in Nature. This implies that a neutrino which is produced 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 is building a neutrino beam and two massive particle detectors for the MINOS experiment. These will be 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.

329 EXPERIMENTS USING POLARIZED BEAMS

This program consists of two experiments, one studying the spin dependence of proton-proton interactions at high energies, and the other kaon-proton interactions producing lambda and sigma hyperons at the intermediate energies. Both of these experiments are international collaborations involving many physicists.

The Argonne group is involved in the Relativistic Heavy Ion Collider (RHIC) spin experiments at Brookhaven National Laboratory. Detailed tasks include design and construction of a polarimeter for RHIC and an endcap electromagnetic calorimeter for one of the large RHIC detectors (STAR). The primary physics issues that will be studied at center of mass collision energies from 100 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° production; and (3) measurements with transversely polarized beams. To achieve these physics goals, there will be detection of jets, direct photons, $W^{\pm}$'s, and Z°'s; the endcap calorimeter will play a crucial role in these measurements.

The group is also participating in studies of kaon-proton interactions at Brookhaven using the SLAC Crystal Ball detector. This detector consists of 672 NaI detectors covering almost 4π solid angle for measurement of photon and neutron angles and energies. From this information, various reactions can be identified and interpreted in forms of lambda and sigma resonant states. Some decay channels allow the determination of spin asymmetries due to the weak decays of hyperons. Many challenging pattern recognition problems are being studied.

330 PROTON-ANTIPROTON COLLIDER EXPERIMENTS

This activity is part of an international collaborative effort to study proton-antiproton collisions using the Collider Detector at Fermilab. The 2800 GeV center-of-mass collision energy is the highest currently available in particle physics, and has opened up new possibilities for studying phenomena. The detector contains a large solenoidal magnet with extensive charged particle tracking devices, including microvertex detectors, completely surrounded by calorimeters. The central electromagnetic calorimeter design and construction was led by the Argonne group. More than 110 pb^{-1} of integrated luminosity has been obtained in early running at the Tevatron Collider.

This old sample continues to be used to make a precision measurement of the W gauge boson mass and, following the discovery of the top quark, determining its mass and studying production properties. Our group is also involved in studying the strong interaction and proton structure using direct photon production and in aspects of b-quark physics.

The Collider Detector at Fermilab has completed an extensive upgrade program, preparing for the higher intensities which will come from accelerator upgrades, including the new Main Injector. The Argonne group is involved in new electronics for the electromagetic calorimeter, the new central drift chamber, and other areas. Data taking, now underway, will eventually provide samples more than 100 times more sensitive than those currently available; enhanced trigger capability will produce new b physics opportunities.

331 ACCELERATOR PHYSICS GROUP

Experimental and theoretical studies are in progress to develop new and better techniques for particle acceleration. Such techniques will be required to permit future explorations of physics at the highest energies. Argonne pioneered a new experimental technique which uses a precisely timed relativistic electron beam to probe high-gradient electric fields, "wake fields", which are produced by a leading high-current "drive" pulse. With it, new insights have been gained about wake fields in plasmas and in a wide variety of passive structures.

The first phase of a new facility is now operating which will extend experiments beyond "proof of principle" into technologically interesting levels. It includes a high current (up to 10 kA) laser photocathode based electron gun, a special rf linac to handle the large current, a separate low intensity gun which forms the "probe" beam, and a well-instrumented experiment section. With it, accelerating gradients of 100-300 MeV/m will be studied and demonstrated.

Many technical subjects are relevant to this project, including laser and particle beam physics, microwave properties of materials, magnet and cavity design, accelerator theory, and computer simulation.

332 ATLAS DETECTOR AT LHC

Argonne physicists have joined the large collaboration planning to build the ATLAS detector at the LHC (Large Hadron Collider), the next accelerator to be built at CERN, the European Organization for Nuclear Physics. ATLAS will be a large general-purpose detector with several major subsystems: inner (tracking) detector, superconducting solenoid, electromagnetic calorimeter, hadronic calorimeter, and muon system. The high energies that will be available at LHC are expected to provide insight into several of the puzzles of current particle physics, including the origin of electroweak symmetry breaking and the hierarchy of particle masses. Argonne had a major role in the design and prototyping of the hadronic calorimeter which is based on scintillating tile technology. These tasks are now essentially complete and construction proper commenced in January 1999 with the construction of the first sections (submodules) of the absorber structure. Construction of the submodules and modules will continue until 2002. In the summer of 1999, we commenced construction of the first modules, which are assembled from the submodule section as well as its instrumentation and testing using light and/or radioactive sources. The first of these production modules will be tested at CERN with high energy particle beams in late summer 2000. This construction activity will continue until mid-2003.

Argonne physicists are also involved with detector triggering and with offline computing development. Ongoing activities include tests of prototype hardware, both as components and as elements of a partial trigger system as well as simulation of the triggers to be implemented.

For offline computing, the group is investigating new software architectures based on Object-Oriented methods and has written prototype sections of the software system. The prototype work carried out in 1999 and early 2000, has been developed into a full implementation for use in analysis of data taken in the beam tests of the first production calorimeter modules. Further development based on this first experience in the field will continue into 2001.

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.

333 IPNS DATA ACQUISITION AND ANALYSIS

IPNS uses computers to collect and analyze neutron scattering data. The data collection process involves recording the time-of-flight of detected neutrons and binning the data in histograms. This is done through a dedicated microprocessor. We are in the process of converting the control of this system from a MicroVAX system to a Linux system. Old Fortran codes are being rewritten in C or Java. We are currently in the process of modernizing the data acquisition hardware and software. Older Multibus and CAMAC modules are being replaced with VSI/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, VMS, etc.

We are also in the process of developing a network-based data display and visualization program. The software is being 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.

Research participants would assist in the development of code for experiment control or for data collection, with emphasis on conversion of 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.

334 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.

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

335 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.

336 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 300 experiments are performed per year in various areas of materials sciences, physics, chemistry, biology, and applied technology. Recent studies include the high-temperature conducting properties of ceramic 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 and carbon nanotubes; intrachain and interchain structures of polymers; high pressure behavior of gas hydrates, molecular solids, ice, superconductors and colossal magneto-resistance materials.

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.

337 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.

338 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.

339 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, 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, 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.

340 NEUTRON AND X-RAY SCATTERING

Members of the neutron and x-ray scattering group pursue multidisciplinary research programs of the nature that are only possible if scattering capabilities are combined with other experimental work. Major research programs include: high-T_c superconductors, colossal magnetoresistive materials, ceramic membrane reactor materials, negative thermal expansion materials, magnetic response of strongly correlated electron systems, and multilayer and amorphous magnetic systems. A second important goal of the group is to provide the technical expertise required to continue the development of a future advanced pulsed neutron source. Scientists in the group play a lead role in the development of new instrumentation and user-based research programs at the Intense Pulsed Neutron Source (IPNS) and serve as instrument scientists for five instruments at the IPNS. Members of the group are becoming involved in the development of instrumentation for the Spallation Neutron Source at Oak Ridge National Laboratory and are also active in developing new x-ray scattering instrumentation and techniques for use at the Advanced Photon Source and other synchrotron x-ray sources.

341 SYNCHROTRON RADIATION STUDIES

The synchrotron radiation studies group utilizes a variety of X-ray scattering techniques ranging from single-crystal and powder diffraction for structure determination, x-reflectivity and standing-waves for the study of surfaces; to X-ray absorption spectra (EXAFS and XANES), photoelectron spectromicroscopy, and angle-resolved UV photoemission measurements for the study of electronic structures of materials. These studies are carried out with in-house X-ray scattering instrumentation and at synchrotrons at Brookhaven (NSLS), Cornell (CHESS), Stoughton (SRC) and the Advanced Photon Source at Argonne, to provide information on the structural and electronic aspects of materials of interest to both group members and other researchers in the Materials Science Division. Of particular interest are chemical and electronic structures of high-temperature superconductors and the study of structures of surfaces and interfaces. Participants are invited to join with a group member in research of mutual interest or to contribute to on-going research efforts.

342 CONDENSED MATTER THEORY

Projects are available in a variety of areas involving analytical and numerical simulations of simple models of the behavior of condensed matter. Past participant projects included studies of various properties of superconductors: microscopic and phenomenological theories, vortex lattices, high T_C, heavy fermions, etc.; electronic structure and properties of strongly correlated metals., magnetic multilayers, quantum effects in electronic kinetics, particularly, in strong magnetic fields. Participant responsibilities include analytical solution of simple problems, programming and running the simulations and participating in discussions of their scientific implications. Participants will have the opportunity to use supercomputers and parallel processors.

343 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.

344 INTERFACES IN ADVANCED CERAMICS

This program addresses interface (epitaxy, grain- or phase-boundary) related properties of advanced ceramics and ceramic composites, with particular emphasis on atomic-level investigations of the structure and chemistry of the interfaces in these materials. Advanced ceramic materials are used, for example, as electronic-packaging materials, in structural applications, in advanced batteries and fuel cells, as ceramic-coating materials or as high-T_c superconducting materials. 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 atomistic simulations (the latter involving lattice statics, lattice dynamics, molecular dynamics and Monte Carlo techniques). This enables us to address fundamental issues of relevance to the processing and mechanical performance of advanced ceramics. Among these issues are, for example, (a) the relationship between microstructure, atomic structure and interface chemistry (incl. non-stoichiometry and interfacial phases) as a function of processing conditions, (b) the role of amorphous interface phases and (c) point-defect and mechanical properties. The program draws heavily on three major Argonne facilities, the Electron Microscopy Center (HREM, AEM) and, in the near future, the Advanced Photon Source, as well as Argonne's expertise in massively parallel computing architectures.

345 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.

346 LASERS IN SURFACE SCIENCE

An extremely sensitive method of examining the chemical composition of a surface is to ionize and detect neutral atoms and molecules ejected from a sample during ion-, electron-, or photo-stimulated desorption. For most surfaces >99.9% of the desorbed atoms and molecules are charge neutral, and therefore undetectable in conventional mass spectrometers. Intense lasers can ionize nearly all of the desorbed material, thereby dramatically increasing the detection efficiency. These laser ionization and particle ejection methods have been combined with recent advances in mass spectrometer design and optical imaging to produce several surface analysis instruments that feature capabilities found nowhere else in the world.

These instruments are being applied to a multitude of fundamental and applied surface analysis problems. Presently under investigation are (1) the origins of the universe as revealed through isotopic anomalies in meteorites, (2) the fundamentals of particle-solid interactions as studied via the yield and energy distribution of sputtered clusters, (3) ways of making better plastics by understanding diffusion of additives in polymers, (4) methods for directly measuring the solar wind composition by trace element analysis of collectors returned from space, (5) new techniques for making flat panel displays using self-assembled monolayers on surfaces, and (6) techniques for chemical imaging of various organic and inorganic materials, such as fracture surfaces.

347 MOLECULAR SIEVE MATERIALS--HETEROGENEOUS CATALYSTS

Molecular sieve materials in the aluminosilicate zeolite family and in the newer metalloaluminophosphate families are synthesized. Mechanistic aspects of their crystallization from gels are being investigated. Materials characterizations and studies of intrinsic properties are made with a variety of techniques, including X-ray diffraction and spectroscopy, neutron scattering, magnetic resonance spectroscopies, infrared spectroscopy, and electron microscopy. Molecular dynamics computer-simulation methods are being applied to the analysis of framework dynamics and to the siting and diffusive microdynamics of adsorbates in the intracrystalline pores. These properties control molecular shape-selectivity in both adsorption and catalysis. Ab-initio molecular-orbital theory is being used to investigate the Bronsted acid catalytic activity of the zeolites and their isomorphously-substituted analogues and conformations of molecules used as templates during gel crystallization. Materials made by intracrystalline encapsulation of transition-metal chalcogenide clusters or metallic clusters are being tested as novel catalyst formulations.

348 DIAMOND FILMS FROM FULLERENES

Diamond is an important material because of its exceptional hardness, high thermal conductivity, low electrical resistivity, chemical inertness, etc. Thus, there are many important applications where diamond films could be utilized, and a substantial amount of research is being conducted to learn how to produce high-quality thin diamond films. Such films are commonly grown using a hydrocarbon precursor in hydrogen gas. Hydrogen is generally believed to be necessary for the diamond thin-film growth process. However, hydrogen in varying amounts is inevitably incorporated in the growing diamond lattice, leading to structural defects. The growth of diamond films using fullerene (C_{60}) precursors in an argon microwave plasma without the addition of hydrogen or oxygen has recently been accomplished at Argonne National Laboratory. The gas mixtures were produced by flowing argon gas over fullerene-containing soot at high temperatures. Optical spectroscopy reveals that C_2 is present in the discharge, giving direct evidence that it is one of the products of C_{60} collisionally induced fragmentation. The nanocrystalline diamond films are characterized with scanning and high-resolution transmission electron microscopy, x-ray diffraction, and Raman spectroscopy.

349 THIN FILM GROWTH AND CHARACTERIZATION

The fabrication of thin film layered structures of multicomponent materials such as high-temperature and alloy superconductors, and ferro-electric and electro-optic materials, and the development of hybrid technologies incorporating some or all of these materials into a single device requires a detailed understanding of film growth and interface properties. In addition, the fabrication of reliable devices utilizing currently developing thin films technologies will require control of film properties at extremely sharp interfaces (one or two atomic layers). We have developed an instrument for performing pulsed beam time-of-flight ion scattering and recoil spectroscopy (TOF-ISARS) that permits real-time, in situ characterization of the growth layer of multicomponent oxide thin films with submonolayer resolution. This instrument is being used, for example, to study the deposition of Pb, Zr, Ti, and Ru using a sequential layer-by-layer deposition method under ambient oxygen pressure conditions appropriate for the growth of $PbZr_{1-x}Ti_xO_3$ films. Our measurements have shown layer-by-layer as well as two-dimensional and three-dimensional island growth during deposition. This and other systems of technological importance are currently under investigation.

350 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.

351 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 100 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, (3) anodic film formation in Mg electrowinning, and (4) isotopic analysis of meteorite grains.

352 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.

353 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.

354 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.

355 NANOSCALE THERMAL TRANSPORT

The goal of this program is to develop an understanding of how confinement and proximity effects, which arise due to the prevalence of grain boundaries, phase boundaries, and surfaces in nanostructures, lead to novel thermal transport processes. Key issues addressed include: (i) the effects of spatial confinement on phonon propagation, (ii) the factors that control interfacial resistance to thermal transport, (iii) the proximity effects associated with coupling of different thermal transport mechanisms, and (iv) thermal transport at hard-soft interfaces. The insight and guidance into the control of thermal transport that is being provided by these studies is driving advances in a number of areas, including improved thermoelectric devices, thermal barrier materials, heat transfer fluids, novel MEMS and NEMS devices, micro- (and eventually nano-) electronic devices, and biomedical applications.

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.

356 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/*

357 SENSITIVITY ANALYSIS AND DESIGN OPTIMIZATION

Sensitivity analysis is concerned with determining 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*

358 <u>COMBINATORIAL PROBLEMS IN SCIENTIFIC COMPUTING</u>

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; 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*

359 <u>PERFORMANCE BOUNDING TOOLS</u>

We are developing tools that can be 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. We invite students and faculty to help develop performance-bounding tools that use source analysis to extract application signatures sufficiently detailed to establish realistic performance bounds for applications.
http://www.mcs.anl.gov/performance

360 <u>OPTIMIZATION</u>

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 in the use of TAO for 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

361 <u>OPTIMIZATION TECHNOLOGY CENTER</u>

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/*

362 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/*

363 COMMON COMPONENT ARCHITECTURE

Many computational science simulations require a range of tools to address areas such as meshing, numerical partial differential equations, optimization, sensitivity analysis, and visualization. The integrated use of software libraries for these areas remains a challenge because of data management and interoperability issues. Within the CCA project at Argonne, we are developing component-based infrastructure to enable integrated use of software developed independently by different groups, with particular emphasis on parallel and distributed computing. Potential projects include developing interfaces to libraries that support optimization, mesh generation, visualization, and collaboration. Additional projects support the interaction with other tools, such as computational differentiation and integrated computational workbenches. *http://www.mcs.anl.gov/cca/*

364 COMPILER SUPPORT FOR RUN-TIME REORDERING TRANSFORMATIONS

Run-time data and computation reorderings have been shown to improve the performance of programs that operate on sparse matrices. Using a framework developed for composing run-time reordering transformations at compile time, we are developing ways to automate the analysis and code generation for legal transformation compositions. This research includes investigating the data dependence question from a new perspective, the use of automated theorem provers to show transformation legality, and the generation of optimized inspectors and executors that implement run-time reordering transformations. The focus will be on the sparse matrix and vector computations that occur in the solution of nonlinear PDEs and numerical optimization. Applicants should have completed at least one compilers course (multiple semesters preferred) and have a working knowledge of C/C++ or Python. An understanding of automated theorem provers is also desirable.

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.

365 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/*

366 PARALLEL-PROGRAMMING LIBRARIES

As parallel computers become more widely deployed and incorporate more complex architectures, the need for a software technology that allows a straightforward use of the next generation of parallel machines also increases. The focus of our research is the design of portable parallel libraries (e.g., MPI, MPICH), the integration of multithreading and communication, and the design and implementation of high-level languages and advanced programming models. We also investigate applications in areas as diverse as environmental science, collaborative environments, computational chemistry, and medicine. *http://www.mcs.anl.gov/mpi or http://www.globus.org/*

367 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://www.mcs.anl.gov/compbio or http://compbio.mcs.anl.gov.*

368 AUTOMATED REASONING

Investigations are under way to develop new concepts and new applications for automated reasoning. Our emphasis is on the formulation of more effective ways of reasoning (inference rules) and more powerful strategies to control that reasoning. We also study various applications, including program verification and open questions from mathematics and logic. *http://www.mcs.anl.gov/AR/*

369 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

370 PARALLEL I/O

We are investigating scalable input/output techniques for high-performance computer systems. Research topics include the development of software support for high-performance I/O from scientific and other projects. Projects under way include the following: (1) developing scalable parallel I/O software for large (approximately 1000-node) Linux clusters, building on the PVFS system; (2) combining techniques in parallel I/O and databases for large-scale scientific data management; and (3) experimenting with multiterabyte parallel data clusters. *http://www.mcs.anl.gov/romio* and *http://www.mcs.anl.gov/~rross*

371 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 a 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/*

372 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/*

373 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/*

374 CHEMISTRY COLLABORATORY

The Collaboratory for Multiscale Chemical Science and its portal are 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 active thermochemical tables that provide a computational representation of the relationships between molecular-scale data and derived thermochemical properties of molecules. The results are presented as a Web service to the chemistry community. *http://www.mcs.anl.gov/scidac/index.html#chemistry*

375 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*

376 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*

377 NEESgrid

NEESgrid is a virtual laboratory for the earthquake engineering community. The goal of the project is to develop a systems design for integrating experimental and computational facilities for use by three communities of researchers: structural engineering, geotechnical engineering, and tsunami research. *http://www.neesgrid.org/*

378 EARTH SYSTEM GRID

High-resolution, long-duration simulations performed with advanced DOE climate models will produce tens of petabytes of output. To be useful, this output must be made available to global change impacts 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/*

379 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 and to test these advances at large scale in demanding data-intensive physics experiments. GriPhyN's mission is to solve two fundamental challenges: to create mechanisms that can track the lineage of experiment data at petabyte scales for auditability and reproducibility, and to make petascale data grids as easy to use for scientists as a desktop workstation. To meet these challenges, GriPhyN is developing the new paradigm of virtual data to catalog data relationships as they evolve over long periods of time within complex scientific analysis processes. This effort is supported by research into achieving transparent Grid usability through policy-driven scheduling, resource management, and automated error handling. GriPhyN researchers also are developing mechanisms that transparently select locations for process execution and automate data delivery distribution. These computer science challenges are pursued in close collaboration with large-scale experiments in three areas of physics: the CERN LHC HEP experiments CMS and ATLAS; the Laser Interferometer Gravitational Wave observatory (LIGO); and the Sloan Digital Sky Survey (SDSS) and National Virtual Observatory (NVO). *http://www.griphyn.org/*

380 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 requirement 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 computation Grid environments. *http://www.fusiongrid.org/*

381 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.*

382 WIDE-AREA PARALLEL COMPUTING

The Message Passing Interface (MPI) standard is a widely used programmer's 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 MPICH, the most widely used 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*

383 <u>MULTITHREADING IN NUMERICAL SOFTWARE</u>

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*

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, chemistry, materials science, and biology that require the use of high-performance computers and the development of new techniques to exploit those computers effectively.

384 <u>CLIMATE MODELING</u>

Research focuses on the development of global and regional climate models, programming methodologies, algorithms, and graphics tools, including the CAVE, to support climate modeling on large parallel machines. This research is performed jointly with climatologists at Midwest universities and at the National Center for Atmospheric Research, with the aim of understanding the effect of global change on climate at the global and regional scales and on decadal time scales from the distant past to the future centuries. *http://www-climate.mcs.anl.gov*

385 <u>EXPERIMENTAL STUDY OF TEMPORAL ORGANIZATION OF CYANOBACTERIAL METABOLIC CYCLE</u>

This project is intended to experimentally support development of mathematical models of cyanobacterial cells describing circadian changes in the metabolism and gene expressions. The experimental study will involve synchronous cultivation of cyanobacteria and measurement of metabolic and gene expression changes occurring under periodic control of the circadian cell clock. The ultimate goal of this experimental study and its simulation counterpart is to understand the elusive clock mechanism and its role in the periodic temporal organization of a single cyanobacterial cell and populations of such cells interacting with each other via their cultivation medium.

386 <u>COMPUTATIONAL CHEMISTRY</u>

We are working with quantum chemists in several projects involving large-scale modeling and simulation for chemical dynamical simulations. These projects include linear algebra and preconditioning methods for reaction rate calculations, higher-dimensional datafitting for potential energy surfaces (interpolated moving least-squares), and large-scale parallel software for multireference configuration-interaction methods to conduct molecular geometry optimization. The project in linear algebra deals with the use of numerical linear algebra software tools and parallel libraries to calculate reaction rates for high-dimensional problems. We also develop preconditioners of potential use with the PETSc numerical library.. *http://www.mcs.anl.gov/scidac/beskinetics*

387 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://wit.mcs.anl.gov/compbio or http://compbio.mcs.anl.gov*

388 NUMERICAL ALGORITHMS FOR FLOW SIMULATION

We are exploring the development of 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 upon 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*

389 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 that the results of this work will provide new insights about the evolution of functionality of human cells and mechanisms of genetic metabolic diseases. *http://wit.mcs.anl.gov/compbio or http://compbio.mcs.anl.gov*

390 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: (1) potential targets for antibacterial agents and (2) families of proteins with unique folds. *http://compbio.mcs.anl.gov/targetB/cgi-bin/Homepage.cgi or http://www-wit.mcs.anl.gov/target*

COMPUTING FACILITIES

The MCS Division computational environment includes a 512-CPU Linux cluster for investigating scalable computer science; a distributed systems laboratory; and a virtual environment, featuring several Access Grid nodes and an Active Mural. Additionally, the computing environment consists of hundreds of UNIX computers and PCs running 2000, NT, and Linux.

391 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 and 2000, NT work and how to design and maintain large networks of computers.
http://www.mcs.anl.gov/computing or http://www.mcs.anl.gov/systems/

392 NETWORK ADMINISTRATION

The computing environment in the MCS Division is built on top of a modern-day high-performance network. The network includes ATM, HIPPI, 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/computing/*

393 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 Perl, Java, C, and various scripting languages 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/computing/ or http://www.mcs.anl.gov/systems/*

394 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/*

395 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/*

396 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/*

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. A primary objective is the development of high density, low enrichment fuel research and test reactors that can be used to replace the current HEU fuels in these reactors worldwide, thereby eliminating a significant nuclear proliferation pathway.

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 the fusion area, principal areas of work are liquid metal technology, advanced materials and first wall/blanket/shield design. In addition, there are a number of other areas in which technology development is being undertaken. These include detector technology, robotics, and laser applications.

397 LARGE-SCALE COMPUTER CODE DEVELOPMENT

Large-scale computer codes for the analysis of steady-state performance and applied operational and accidental transients in reactor power plants are developed. Activities include (1) development of understanding of basic physical phenomena, (2) formulation of mathematical models, (3) development of numerical solution techniques for coupled, non-linear partial differential equation systems, (4) computer code programming (FORTRAN) and verification, (5) code and modeling validation (experiment analysis), and (6) code performance, improvement, maintenance, and graphics.

Model development and validation requires proficiency in one or more of the following disciplines: heat transfer, single and two-phase fluid dynamics, reactor physics, fuel management, nuclear data and engineering mechanics. Computer code development activities include numerical analysis methods, programming, and code verification and maintenance.

398 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.

399 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.

400 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.

401 NEUTRON PHYSICS DATABASE APPLICATIONS IN MONTE CARLO

Nuclear interaction datasets for continuous-energy Monte Carlo calculations are developed and enhanced. These are based on the Evaluated Nuclear Data File (ENDF) data, and require conversion of neutron resonance cross section parameters to rigorous continuous-energy cross section data and probability tables. Secondary energy and angle distributions must also be converted to probability tables for use in Monte Carlo simulation. Work is underway to perform the file conversions and to validate the new data by a variety of means, including comparison with benchmark critical assemblies and visual comparison of plots against standards. Activities include application of nuclear data processing codes, visualization tool development, and benchmarking of Monte Carlo simulations against experiment.

402 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.

403 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.

404 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.

405 SAFEGUARDS ANALYSIS OF FISSILE NUCLEAR MATERIAL

The safeguards activities include the development and testing of methods for the assessment and quantification of the precision and accuracy of instruments, the quantity and the probability of the material unaccounted for is accessed in light of possible diversion or in-process holdup. Of particular interest are nuclear facilities based on the electrometallurgical processing of spent nuclear fuel.

406 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.

407 HEAT TRANSFER AND FLUID DYNAMICS

Analytical and experimental studies are being performed on a wide variety of heat-transfer and fluid dynamics driven phenomena mostly relevant to nuclear reactor design and safety. Areas currently under active investigation include development and application of advanced computational methods for fluid and heat transfer, safety analysis, and multi-phase flow.

408 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.

409 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 particle methods) and visualization tools with application to the solution of complex engineering mechanics problems found in industry and reactor safety analysis. Recently work has been performed in coupling a probabilistic engine to our deterministic finite element codes in order to perform 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, a workstation cluster, 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 to display computational mechanics results. Work in concurrent engineering is also being done. Another active research area is the development of numerical methods for evaluating the structural integrity of modern lightweight materials, such as fiberglass composites for potential use in automobiles and civil structures. Recently, work on the Computational Material Science Initiative has focused on modeling of the behavior of materials at the mesoscale (various grain boundary mechanisms and the elastic response of the grain interior are being incorporated into a unified computer code). Work is being done in seismic analysis with a particular focus on seismic isolation and sloshing of liquid-filled tanks. 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, thermomechanical analysis and high temperature response of concrete structures.

410 LIGHT-WATER REACTOR SAFETY ANALYSIS

A number of studies are under way involving various aspects of nuclear-reactor technology. These include studies of foreign reactor systems, studies of U.S. plant features, and modeling of the physical processes of postulated reactor accidents. In many cases, the modeling activities closely coincide with ongoing laboratory experimental programs studying accident phenomena. The thermal-hydraulic, chemical interaction, and aerosol behavior of the real or simulated-core-melt materials are modeled in computer routines. The participants work with staff who are developing the physical models, creating computer routines, and integrating the computer models into large-scale, integrated computer codes.

411 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, 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.

412 QUANTITATIVE IMAGE ANALYSIS

Examination of nuclear fuels, containment materials, and crucibles makes use of quantitative metallography performed on a PC-based image analysis system. Participants will measure metallurgical features observed in optical micrographs and electron-beam images and create figures for publication of the test results. Video clips of analytical and test results will be digitally captured from existing 8mm and VHS format videotapes and edited for presentation on the division’s world wide web home page and at various meetings.

413 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.

414 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.

415 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.

416 INTERNATIONAL NUCLEAR SAFETY

The United States Departments of State and Energy support programs to promote nuclear safety development worldwide. These programs range from specific projects to upgrade the safety of operating reactors to collaborative nuclear safety research and development. The International Nuclear Safety and Cooperation group at Argonne National Laboratory carries out safety R&D projects with a number of countries, including those of the Former Soviet Union. Opportunities exist in Soviet-designed reactor safety improvement, safety research and development, and international project management.

417 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.

418 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.

419 ILLICIT SUBSTANCE DETECTION

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, nuclear materials, and chemical warfare agents. These projects involve: experimentation in passive and active interrogation methods, modeling studies of neutron and photon interaction and transport, data visualization, 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.

420 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 low energy (few MeV) accelerators capable of handling high current.

421 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).

422 LASER APPLICATIONS LABORATORY (CLAUDE)

The laboratory focuses on collaborative research and development activities with industrial partners. The facility includes high-power industrial CO_2 and Nd:YAG lasers, five-axis workstations, and diagnostic systems for laser beam characterization, plasma analysis and process monitoring/control. A range of detectors are available for diagnostics and aerosol or spray characterization. Current collaborative research with industry include 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 cladding, laser cutting and ablation in decommissioning and decontamination and materials testing using laser thermal simulation.

423 REDUCED ENRICHMENT FOR RESEARCH AND TEST REACTORS (RERTR)

The DOE Office of Nonproliferation and National Security 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.

424 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.

425 ARMS CONTROL AND NONPROLIFERATION TECHNOLOGY AND POLICY

Argonne's multidisciplinary work in the field of arms control and nonproliferation technology and policy is coordinated through the Arms Control and Nonproliferation Program, which is run from the Technology Development Division.

Within this program, people with many skills, including chemists, physicists, engineers, material scientists, and even attorneys, work together to support U.S. government efforts to control weapons of mass destruction and to prevent their spread. Program staff support arms control treaty negotiation, implementation, and verification. They develop technology for on-site inspection and remote sensing, material/item identification, tracking shipments, and detection and prevention of nuclear proliferation.

426 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).

427 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.

428 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 a vanadium alloy structure 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.

429 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.

430 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.

431 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.

432 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++.

433 SPALLATION NEUTRON SOURCE (SNS) – INSTRUMENT DEVELOPMENT

The Spallation Neutron Source (SNS) is a collaborative project involving six Department of Energy National Laboratories. When completed, SNS will be the most powerful spallation neutron source in the world. Argonne National Laboratory has primary responsibility for developing the neutron scattering instrumentation and for working closely with Oak Ridge National Laboratory to develop the experimental facilities.

The SNS Instrument Systems group is currently developing neutron scattering instruments as part of the SNS. Students will work with engineering staff to develop mechanical 3-D models for design visualization and verification purposes. Emphasis on machine design using Pro/Engineer CAD software.

OFFICE OF PUBLIC AFFAIRS (OPA)

434 JOURNALISM AND PUBLIC RELATIONS OPPORTUNITIES

The Office of Public Affairs 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 Office of 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 Logos, a quarterly scientific review. 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.

OFFICE OF TECHNOLOGY TRANSFER (OTT)

The Office of Technology Transfer (OTT) supports the DOE mission of transferring technology through partnerships having the potential to benefit U. S Industry and the nation through support of national policy objectives, improved competitiveness, and contribution to the national economic and scientific base. This will be accomplished through technology characterization and marketing leading to Work for Others, Cooperative Research and Development Agreements, licensing and other contracts to facilitate efficient and expeditious development, transfer, and commercialization of federally owned or originated technology.

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

Develop and perform surveys regarding the effectiveness of OTT activities.

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

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.

436 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.

437 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.

438 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.

439 THEORETICAL PHYSICS

Theoretical research in the Physics Division addresses a broad range of problems involving the structure and dynamics of hadrons and nuclei. There is a strong emphasis on comparison to data provided by experimental groups at Argonne and at other facilities around the world. The principal areas of research include: hadronic structure with quarks and gluons, nuclear dynamics with sub nucleonic degrees of freedom, nuclear many-body theory with realistic force models, and heavy-ion structure and reactions.

We also pursue some research in atomic physics, neutron physics, fundamental quantum mechanics, and quantum computing. Several of our projects require major numerical simulations using state-of-the-art computers, including Argonne's massively parallel IBM SP, SGI Origin 2000, and VA Linux systems.

440 CATCHING RARE ATOMS WITH LIGHT

We are developing a new method of ultrasensitive trace-isotope analysis based upon the technique of laser manipulation of neutral atoms. Using this method, we can count individual 81Kr atoms present in a natural krypton sample with an isotopic abundance of 6x10-13. In other words, we can detect and measure rare atoms below the parts-per-trillion level. Isotope analysis of 81Kr can be used to determine the age of ancient polar ice that holds critical information on the history of earth climate.

In the experiment krypton atoms in a sample are injected into a vacuum chamber to form an atomic beam. The atoms of a particular isotope are selectively captured in an atom trap formed by six laser beams, and cooled down to about 1 milli-Kelvin. The individual atoms in the trap appear as bright dots, and can be counted with a photo-diode.

Our experiments are typically performed by a team of 2-3 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.

For more information on our team and projects, please visit our website at: www-mep.phy.anl.gov/atta/