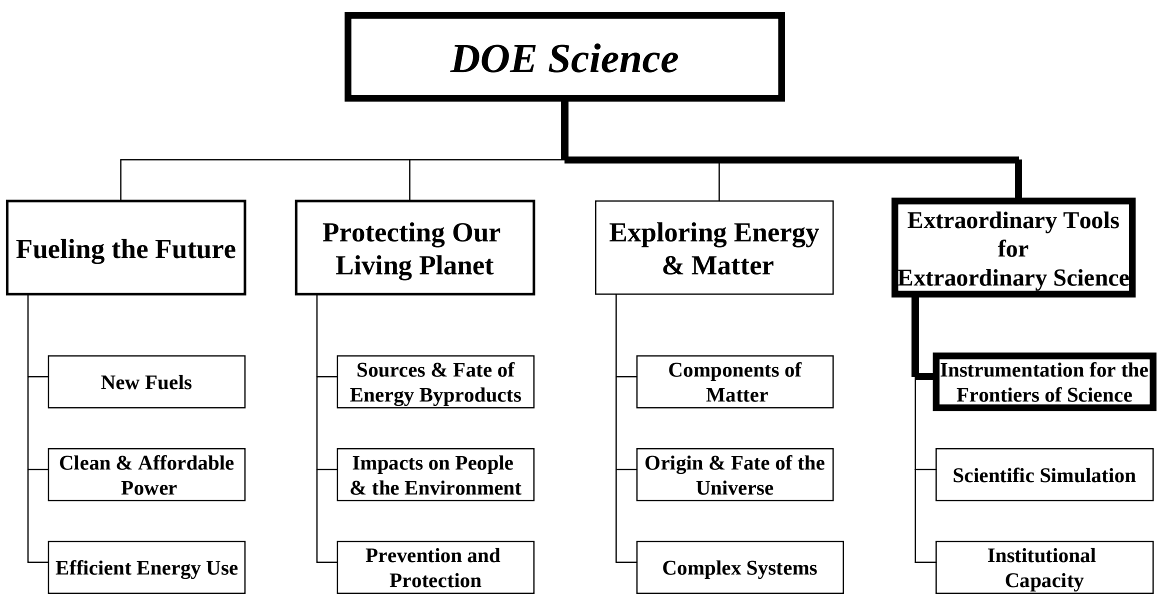
Chapter 11
Instrumentation for the Frontiers of Science

Scientific Challenge: ***To provide research facilities that expand the frontiers of the natural sciences.***



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Conceiving and constructing the instrumentation of scientific research is at least as challenging as developing or proving any scientific theory and occupies a significant fraction of the research activity. A distinctive contribution of the Department of Energy and its predecessor agencies to science in the United States has been the construction and operation of leading-edge facilities for scientific research. Through universities and national laboratories, the Office of Science has maintained the United States' world leadership position in developing accelerators, reactors and accelerator-based neutron sources, synchrotron light sources, electron beam microcharacterization centers, plasma physics devices, supercomputers, and other special-purpose facilities such as the Joint Genome Research Institute, the Combustion Research Facility, and the William R. Wiley Environmental Molecular Science Laboratory.

These facilities enable scientists to acquire new knowledge required to achieve the Department's missions and, more broadly, to advance the U.S. scientific enterprise. The Office of Science continues to explore the frontiers of research through its stewardship of the most advanced scientific facilities in the world.

Accelerators for High Energy and Nuclear Physics

Description, Objectives, and Research Performers

Over the past 70 years each generation of accelerators has allowed scientists to answer a set of questions, make fundamental discoveries, and establish the questions to be answered by the next generation of accelerators. The Berkeley Bevatron, for example, was built in the 1950s to discover the anti-proton, long predicted by the Dirac Equation, and went on to become the discovery site for a host of new "particles." They were, in fact the first clues to the existence of quarks, but were not recognized as such until 1964 when the Omega-Minus particle was discovered at the Brookhaven AGS, a much more powerful accelerator than the Bevatron. The Bevatron itself was combined with a heavy ion linear accelerator in the 1970s to initiate the field of heavy-ion nuclear physics at intermediate energies. In more recent times, the discovery of the J/ψ meson and the tau lepton at SPEAR, the discovery of the W and Z bosons at the CERN Sp p S, and the discovery of the top and bottom quarks at the Fermilab Tevatron have established the Standard Model of particle physics. The discovery potential of these machines has been dramatically increased by colliding energetic beams of protons with one another or with anti-proton beams. This greatly increases the energy available for the creation of new particles, or new physics.

Alongside the development of high-energy proton accelerators has been the extension of electron accelerators to higher energies. The electron linac at the Stanford Linear Accelerator Center (SLAC) produced the second line of evidence for quarks as the basic constituents of neutrons and protons when researchers discovered the scaling phenomena in deep inelastic electron-proton scattering. SLAC has also been a pioneer in electron-positron collisions for particle physics with the SLAC Linear Collider (SLC), which accelerates electrons and positrons to 50 GeV and then brings them into collision with one another.

Today two new major nuclear physics accelerators are beginning operations: the Continuous Electron Beam Accelerator Facility (CEBAF) in New port News, Virginia; and the Relativistic

Heavy Ion Collider (RHIC) at Brookhaven National Laboratory. Each is a unique, world-class facility that promises new knowledge about the nature of nuclear matter and structure.

Research Challenges and Opportunities

High energy physics accelerators enable a wide range of inquiry: observing and understanding charge conjugation-parity (CP) violations; characterizing and determining the nature of neutrinos; observing rare particles in the collisions of protons and antiprotons, or of electrons and protons; measuring high energy phenomena in the universe from the early moments of the Big Bang and those observable today from distant stars and galaxies; and similar complex endeavors.

A specific challenge for research personnel at high energy physics accelerators is to build vertex and tracking systems that can withstand the high particle fluxes and high radiation exposure near beam pipes and interaction points. These conditions are expected with improved Fermilab Tevatron Run II-III upgrades and with the Large Hadron Collider (LHC) at CERN. Work on LHC detectors (ATLAS and CMS), BaBAR at SLAC, and Run II upgrades of CDF and D-Zero at Fermilab includes new developments in silicon pixel imagers, silicon vertex detectors, micro-strip gaseous detectors, radiation hard electronics for signal and data processing, and advances in superconducting magnet technology. Advances in science will require international collaboration in the construction and operation of future accelerators and detectors.

Researchers will continue to exploit the highly successful B-factory at SLAC, achieving luminosity beyond design for the asymmetric electron-positron collisions, reducing unwanted background radiation in the experimental zone, and maintaining the high level of operational readiness in order to further the experimental goals of the program. The linear accelerator will be operated to supply positrons and electrons simultaneously to the B-factory, End Station A, and the advanced accelerator physics experiments. Related challenges are the production of a highly polarized, extremely stable beam of particles to study Moller scattering in a hydrogen.

Other challenges for researchers using the high energy physics accelerators include using lasers, plasmas, and very high frequency radio sources to accelerate charged particles; applying advanced superconducting materials and new geometrics to build superconducting magnets for particle beam optical systems that operate with pole tip fields in excess of 16 Tesla; developing new high frequency, high power radio frequency sources; to develop higher current, higher brightness particle beam sources; formulating advanced software for computer modeling and simulation; and pushing forward theoretical charged particle beam dynamics and plasma physics as related to charged particle acceleration and control.

Nuclear physics accelerators are the sites for researchers to pursue various major challenges: investigating the quark/gluon substructure of nuclei: creating and understanding nuclei taken to their limits of deformation, excitation, and isotopic stability; understanding stellar burning and supernovae processes; performing nucleosynthesis of elements; studying the structure of nuclei that are far from beta stability, previously unavailable for experiment; investigating neutrino oscillation; and studying polarized ion nuclear reactions for unique high resolution spectroscopic information. A specific challenge is to provide electron and photon beams needed to probe various aspects of nucleon, meson, and nuclear structure. The nuclear physics accelerators will provide heavy ion beams needed to probe and understand the structure of nuclei and the various phases of nuclear matter, and a variety of unstable and stable particle beams needed to probe various aspects of nuclear astrophysics and nuclear structure.

Research Activities

At Fermilab, experiments are ongoing to study neutrinos, B-mesons, known and new particles, and unusual states of matter. Fermilab has a large and well-equipped facility for assembling silicon microdetectors, a world-class data processing center, and an active group of theoretical physicists. It also serves as the host center for the U.S. efforts on the CMS detector and on the magnet development program for the LHC accelerator. Brookhaven National Laboratory serves as the host center for U.S. efforts on the ATLAS detector for the LHC accelerator. SLAC research facilities produce electrons and positrons, support the operation of the B-factory, and detect and measure the particles resulting from the collisionstherein. The Alternative Gradient Synchrotron (AGS) facility accelerates protons at 24 GeV, providing the world's highest intensity proton and kaon beams. These beams are used for forefront high energy and nuclear physics fixed target research aimed at understanding the fundamental structure of matter and energy.

Four major accelerators have either just started operations or will be operating by the year 2000: the CEBAF at the Thomas Jefferson National Accelerator Facility (TJNAF), which will open a new window on the role of quarks in nuclei; the RHIC, which will collide gold nuclei at 100 GeV per nucleon in search of the quark-gluon plasma which existed a hundredth of a second after the Big Bang; the Main Injector at Fermilab, which by raising the intensity of the beam by a factor of 5-10, will provide the opportunity to exploit the discovery of the top quark and search for other new particles such as a light Higgs; and the B-Factory at SLAC, which is studying the properties of the interaction that breaks the symmetry between matter and anti-matter, called charge-parity violation. Together, these leading-edge facilities will allow a significant improvement in the fundamental understanding of the nature of matter.

Modern physics research, in many cases, requires probe particle beams of great energy (billions and trillions of electron volts), very high currents, and exceptionally precise optical control. The science and technologies fundamental to building and operating such machines are highly specialized; ongoing R&D supports continual improvements in advanced computer modeling simulation and control software, and instrumentation for measuring particle beams.

Accomplishments

- Researchers at Stanford developed a germanium transition edge sensor that will be used for the search for galactic dark matter.

- The Tevatron collider is Fermilab's major accomplishment: 1000 superconducting magnets, all operating flawlessly, cooled by a 4-mile liquid-Helium system with refrigeration capability; and industrial-strength antiproton beams. During Run I of the Tevatron collider, which ended in 1996, there were about 1013 proton-antiproton collisions. Run I produced a tremendous amount of data, which led to the discovery of the top quark.

- The g-2 experiment at BNL usesthe largest superconducting magnet ever built, 15 meters in diameter, with field uniformity of 1 part per million along its circumference and a stability of 1 part per 10 million.

- The introduction of Lie Algebra techniques and symplectic (area preserving in phase space) requirements into the computation of accelerator and collider optical systems by a researcher at the University of Maryland enabled the modern million-turn simulation of storage rings that is now considered a major contribution to defining new machines.

- The demonstration of critical current densities of 5000 amperes per square centimeter in magnetic fields of 5 Tesla by a researcher at the University of Wisconsin shows the room for additional performance improvement over the current commercially available superconductor, which operates at about 3000 amperes per square centimeter.

- The invention of the laser wakefield and laser beat wave plasma acceleration concepts by researchers at the University of California at Los Angeles has opened up an entirely new means for charged particle acceleration.

- The proof-of-principle demonstration of the self-modulated, laser-driven plasma wakefield accelerator at accelerating gradients of greater than 100 GeV per meter and the laser driven plasma beat wave accelerator at accelerating gradients of 3 GeV per meter open a possible new path to ultra high gradient charged particle acceleration and the possible construction of accelerators of energy otherwise not economically feasible.

- The proof-of-principle demonstration of the particle driven plasma wakefield accelerator showed an alternative to lasers which does not require the development of optical channeling techniques to accelerate over long distances.

- Successful proof-of-principle demonstration of the Inverse Free Electron Laser shows that this device can provide very short (millionth of a meter) long bunches, and can probably be used as a quasi-linear, radiation-based transverse beam cooler.

- Successful proof-of-principle demonstration of inverse Cerenkov acceleration shows that by using a medium to control phase velocity of the laser, acceleration can be achieved at high gradients over centimeter distances.

- The successful application of NbTi superconductor technology in the construction of Fermilab's 1000 GeV Tevatroncontributed significantly to the industrialization of the underlying superconducting magnet technology later adapted for use in MRI imaging devices.

- The world's first full superconducting electron accelerator facility was completed at the Thomas Jefferson National Accelerator Facility (TJNAF). The high intensity, continuous wave, 4 GeV accelerator is being used to study the transition from the hadronic picture to the quark-based picture of nuclear physics.

- Major instrumentation has been built for the three experimental halls at TJNAF (with high resolution superconducting spectrometers, the CEBAF Large Acceptance Spectrometer (CLAS), a high momentum superconducting spectrometer, and a short-orbit spectrometer for measurement of short-lived reaction products.

- The Relativistic Heavy Ion Collider (RHIC) was completed and in FY1999 and is now being commissioned. The world's highest energy heavy ion collider facility will be used to search for the quark-gluon plasma, the state in which nucleons are melted into a soup of quarks and gluons—a state that only occurred previously at the instant after the Big Bang.

- A major upgrade and accelerator improvements to the pulse stretcher ring at the MIT Bates Linear Accelerator have recently been completed. The ring will be used to provide circulating continuous wave polarized beams for a new program of few-nucleon studies using internal gas targets.

- A new world-class Gammasphere detector is now in use to observe, with high precision, rare nuclear processes involving the emission of many gamma rays.

- The Sudbury Neutrino Observatory, located in a 7000-foot-deep mine, will be available for experiments in FY1999. The observatory will be used to resolve the question of the existence of a neutrino mass.

- At Oak Ridge National Laboratory, the Radioactive Ion Beam facility is enabling the first-time measurements of nuclear reactions that fuel the explosion of stars.

- The Next Linear Collider Test Accelerator (NLCTA) is used to demonstrate several technologies for use in high-frequency, microwave-driven linear accelerators and will be adapted as a gneral user facility for advanced accelerator physics and technology research.

- At the Multi-Particle Spectrometer Facility at Brookhaven National Laboratory scientists discovered the first definitive examples of exotic states: particles that are not totally composed of quarks.

- At the positive kaon spectrometer at Brookhaven National Laboratory scientists have recently discovered the rarest Standard Modelallowed decay ever observed at a branching ratio of 1 part in 100 billion. Another rare kaon experiment made the first observation of a decay that holds promise for determining a key quark mixing parameter of the Standard Model.

Light Sources and Neutron Beam Facilities for Natural and Life Sciences

Description, Objectives, and Research Performers

All science depends on advanced instrumentation to enable scientists to see structure and phenomena they have not observed before. The understanding of the behavior and properties of materials undergirds every major technology area. The sciences that focus on condensed matter, or materials research in general, are interdisciplinary, involving materials sciences, major areas of physics and chemistry, the earth sciences, biology, and medicine. Products of condensed-matter science, such as the transistor, the integrated circuit chip, and liquid crystal displays, have revolutionized our lives through their use in television, calculators, electronic watches, personal computers, appliances, autos, and innumerable other applications.

Light sources and neutron beam facilities improve our understanding of the fundamental interactions of photons, neutrons, electrons, and ions with matter, pending knowledge that can be used to design probes for materials sciences and related disciplines. Such information has made it possible for researchers to build the advanced machines and instrumentation necessary to create, manipulate, focus, and detect a large variety of beams of electromagnetic radiation and particles. As a result, new complex spectroscopic, scattering, and imaging techniques have been developed. These techniques further basic research in a wide variety of disciplines. Examples of investigations at the facilities include materials characterization, processing, and design; chemical kinetics, reaction dynamics, and reaction diagnostics; the molecular basis of geochemistry and environmental chemistry; and understanding materials under extremes of temperature and pressure for geophysical and earth sciences.

Research Challenges and Opportunities

Major challenges include understanding the physical mechanism that makes high temperature superconductivity possible and understanding giant or colossal magnetoresistance.

Photochemistry presents opportunities for altering chemical reaction pathways so that high volume industrial intermediates and specialty chemicals can be produced by less polluting processes. Research challenges include the spectroscopic investigation of natural photosynthetic systems at short times following the absorption of light to determine the nature of the excited electronic states involved in the energy conversion process.

Recently, scientists have used a Magnet Optical Trap (MOT) to trap atoms and form an atomic cloud known as a Bose-Einstein Condensate (BEC). A judicious use of multiple laser pulses can increase the number of atoms trapped in a MOT. A laser, other than those used to trap the atoms, could be used to modify the shape of the electron cloud in rubidium (Rb) atoms leading to an increase in number of trapped species. The modification in the shape of the electron cloud causes the atoms to attract rather than repel one another during a collision. In addition to the MOT’s use as a testbed for quantum statistics, possible technological applications include developing an atom laser that can, conceptually at least, be used to "write" structures of atomic dimensions on a substrate, thus greatly reducing the size of microelectronic integrated circuits.

Progress in the biomedical sciences and in biotechnology increasingly depends upon understanding the relationship between the structure and function of biological molecules. Continued progress in meeting this demand will depend not only on efficient operation of the facilities but also on overcoming serious limitations in the capabilities of the best currently available instrumentation.

Research Activities

Synchrotron radiation can provide an intense source of light over a broad spectral range from the visible ultraviolet to the hard x-ray regions of the spectrum. The very precise properties of bremstrahlung, or synchrotron radiation, are used as a tool for other sciences, especially materials science, chemistry and biology. One of the best research tools available to science is the x-ray beam, a highly penetrating light ideally suited to a broad range of applications. Most of what we know about the three-dimensional arrangement of atoms in DNA, RNA, and viruses has come from x-ray research. X-ray light sources have also allowed scientists to conduct molecular-level examinations of ceramics and semiconductor materials, both of which are essential to the development of designer materials for new technologies.

The Stanford Synchrotron Radiation Laboratory (SSRL) was built in 1974 to take the intense x-ray beams from the Stanford Positron Electron Accelerating Ring (SPEAR) storage ring that was built for particle physics by the SLAC laboratory. Over the years, the SSRL grew to be one of the main innovators in the production and use of synchrotron radiation with the development of wigglers and undulators that form the basis of all third-generation synchrotron sources. The facility is now composed of 25 experimental stations and is used each year by over 700 researchers from industry, government laboratories, and universities. These include astronomers, biologists, chemical engineers, chemists, electrical engineers, environmental scientists, geologists, materials scientists, and physicists. The success of the SSRL and SPEAR has led to the development of new generations of light sources at other national laboratories:

- Advanced Light Source (ALS) at Berkeley is one of the world’s brightest sources of ultraviolet light and soft x-rays, and a powerful source of higher energy x-rays, serving as an excellent probe of the electronic properties of atoms, molecules, surfaces, and condensed matter. It is also a powerful tool for determining the structure of macromolecules.

- National Synchrotron Light Source (NSLS) at Brookhaven provides intense focused light from the infrared through the x-ray region, probing crystal structure, molecular bonding, phase transitions, and many other properties germane to a wide range of sciences. It has 2,300 users from 350 institutions, including 50 corporations.

- Advanced Photon Source (APS) at Argonne is a third-generation hard x-ray source and one of only three of its kind in the world. It has 2000 users and covers a wide range of science and technology research from condensed matter physics and structural biology to lithography and micromachining.

Neutrons are a unique and effective tool for probing the structure of matter. Synchrotron light is an electromagnetic wave, but neutron beams behave as particles with mass which scatter off various objects, but also like quantum-mechanical waves as they move through space. Because the neutron is uncharged electrically, it can penetrate deeply into materials and give precise information about the positions and motions of individual atoms in the interior of a sample—a tool invaluable in nondestructively measuring the internal strain in a material.

The neutrons are especially sensitive to the presence of certain isotopes of light elements, such as hydrogen, carbon, and oxygen, which are found in many important hydrocarbon and biological molecules; for example, the contrast between hydrogen and deuterium has revolutionized polymer physics. Beams of neutrons are particularly well suited for measurement of the positions as well as the fluctuations in these positions of atoms (phonons), and the structure (position and direction) of atomic magnetic moments in solids as well as the excitations in this magnetic structure (spin waves). Such studies allow physicists to take measurements leading to an understanding of phenomena such as melting, magnetic order, and superconductivity in a variety of solids.

Proton machines have not only advanced in energy, but also in the intensity of their beams. Typical currents have been in the microamp region, but some machines, in particular the LANSCE (Los Alamos Neutron Science Center) (formerly the LAMPF), accelerate a milliamp of protons to energies of 800 MeV. Originally built as a meson factory to produce pions and use them to study the properties of nuclei, this accelerator is now used in conjunction with the Proton Storage Ring (PSR) as a pulsed neutron spallation source for use in materials science and other fields for scientific and national security purposes.

A much more intense version of this machine, the Spallation Neutron Source (SNS), at the somewhat higher energy level of 1 GeV, will be built at Oak Ridge National Laboratory as a collaboration of five national laboratories. Initially the machine will operate at 1 milliamp, and eventually at 5 milliamp.

Argonne National Laboratory is also the location of the Intense Pulsed Neutron Source (IPNS), which uses protons from a linac plus rapid cycling synchrotron (the injector system for the late ZGS) and fires them into a depleted uranium source. It has been a highly innovative user facility for the study of materials from high-temperature superconductors through biological materials.

Reactors are well-established neutron sources. The High Flux Isotope Reactor (HFIR) at Oak Ridge National Laboratory is a light-water-cooled and -moderated reactor. It provides state-of-the-art facilities for neutron scattering and materials irradiation. The High Flux Beam Reactor (HFBR) at Brookhaven National Laboratory will be permanently closed. The nuclear research reactor was used for more than three decades by over 200 scientists annually for groundbreaking discoveries in physics and biology. The department is upgrading all of its neutron science facilities and is building the Spallation Neutron Source, which will help to alleviate the loss of HFBR.

Accomplishments

- The combination of intense, bright sources, tunability, and high photon energies has allowed vastly improved resolution and many orders of magnitude increases in signal, enabling the study of weak scattering from small samples and surfaces, novel spectroscopies such as magnetic and inelastic scattering, real-time studies, and studies using the coherent properties of the beam. These experiments have forced scientists to rethink their basic understanding of semiconductors, metals, superconductors, alloys, composite materials, liquid crystals, surfaces and interfaces, magnetism, dynamic processes, elementary excitations, electronic structure, and factors controlling phase equilibrium.

- Experimental results from the APS include a new structural determination and biochemical analysis of the human fragile histidine triad (FHIT) protein, which derives from a chromosome that is commonly disrupted in association with cancers.

- Clifford G. Shull, long supported by the Department at Oak Ridge National Laboratory, was a co-winner of the 1994 Nobel Prize in physics for his work on experiments in which neutron waves fall on the crystal and scatter elastically (losing no energy) in a process called diffraction.

- The High Flux Isotope Reactor (HFIR) is the world's leading source of elements heavier than plutonium for research, medicine, and industry.

- Charge-coupled device detectors (CCDs) developed for structural-biology research, have become the standard detectors for protein crystallography. The program's Structural Biology Center at Argonne and Beamline 9 at SSRL were the first to routinely achieve sub-Ångstrom resolution of protein structures.

- High-precision area detectors for thermal neutrons have been developed based on helium 3 and on microelectronics. These detectors are essential for neutron scattering studies in structural biology and materials science, and are particularly well suited to neutron spallation sources.

Plasma and Fusion Energy Facilities

Description, Objectives, and Research Performers

Plasma and fusion energy sciences provide various facilities for the study of plasmas under various conditions and magnetic fields. Each of the three large fusion devices, as well as smaller facilities located at universities, provides a focus for participation by extended collaborative teams. Research is conducted at national laboratories, universities, and industrial firms.

Research Challenges and Opportunities

The main challenge of the National Spherical Torus Experiment (NSTX) is to integrate the research goals into a well-structured experiment. The spherical torus plasma regime is significantly distinct from most tokamak experiments. The magnetic fields are not large; the expected plasma parameters allow the exploration of new methods for starting the plasma and maintaining the necessary plasma currents. These innovative methods have been explored on small devices, but applicability to a larger system remains to be demonstrated. The potential for long-pulse operation, in which self-generated currents sustain the plasma, has been predicted.

High plasma pressures have been achieved on one small system. Calculations predict excellent confinement of the plasma in a spherical torus because of the unique plasma configuration. There are also predictions of improved (relative to conventional tokamaks) particle and power handling which would reduce requirements on plasma facing components.

The mission of the DIII-D national program is to establish the scientific basis for optimizing the tokamak approach to fusion energy production. The challenge is to improve the performance of heating and current drive tools such as electron cyclotron heating; the fueling tools; high speed pellet injectors; plasma facing components, such as carbon tiles for power exhaust; and plasma control systems. The associated challenge is to utilize these tools reliably and for long pulses. The R&D for the improvement of these hardware tools also advances the related engineering sciences.

The physics of plasma edge transport is enormously complicated because of the plethora of plasma, sheath, and atomic physics phenomena that can play a crucial role in the edge plasma. The behavior of power and particle exhaust depends on these phenomena. Understanding transport in high temperature plasmas, which are subject to many modes of micro- and macroscopic instability, represents another challenging task.

Alcator C-Mod is the newest, most advanced world-class tokamak, built to explore the physics of plasmas in a compact, high field environment. Alcator's high confining fields let researchers experiment with plasmas hotter and denser than those in machines of similar size. Alcator C was the first device to produce the density and confinement of hot plasma necessary for a useful fusion reaction. Alcator C-mod experiments help to increase our understanding of the principles governing the transport of particles and energy in high temperature plasmas. Divertor physics, plasma control, and plasma heating issues will continue to be explored in Alcator C.

Research Activities

The NSTX is being built as an innovative confinement concept in which the magnetic fields are not large. It began operating in 1999, with full scale experimental operations starting in 2000. The DIII-D facility is the largest operating magnetic fusion experiment in the United States that focuses on the advanced tokamak concept and has a 2.2 Tesla (T) field. By contrast the Alcator C-Mod facility is a high-field (8-9 T) user facility with currents much like DIII-D, namely 2.5 MA. Medium-grade experiments exploring alternative concepts are located at various universities, including the University of Wisconsin and UCLA.

Accomplishments

- During the past decade, the DIII-D program has made substantial contributions to the world fusion program on issues such as the optimum plasma shape, different modes of operations for higher performance plasmas and transport barrier formation, power exhaust plasmas, current drive by radio waves externally for continuous operation of fusion plasmas, and profile control for plasma stability.

- Alcator C-Mod has achieved high confinement that does not saturate at high density regimes as was feared in view of results of a previous generation of high field experiments. This result bodes well for self-sustaining fusion reactions in compact high field tokamaks.

- Operation of high performance plasmas with radio frequency auxiliary heating alone has been established; this offers technological advantages over traditional neutral beam heating systems.

- Asymmetries in disruption halo currents first observed in Alcator C-Mod have become a critical consideration for the engineering design of future tokamaks. Alcator C-Mod engineers have also developed highly robust real-time algorithms for effective plasma control. The C-Mod approach has been adopted by other experiments.

Single-Purpose and/or Multi-Disciplinary Facilities

Description, Objectives, and Research Performers

DOE supports several different facilities of this type: *The William R. Wiley Environmental Molecular Science Laboratory (EMSL)* is a unique national scientific user facility. With over 100 leading edge instrument and computer systems in one facility, the EMSL provides users with the capability to undertake molecular-level research on environmental issues in an interdisciplinary environment. The EMSL is focused on basic research that can lead to significant improvements in the efficacy and cost of cleaning up contaminated environments, with emphasis on assisting the Department meet its responsibilities in environmental remediation and waste management. In 1999, over 800 users from academia, government laboratories, and industry used the EMSL instrument and computer systems.

Electron beam michrocharacterization centers provide essential tools for characterizing and analyzing the geometrical packing configurations of atoms in solids and crystals, defects and imperfections, and other properties of materials. They work at the scale of 1-2 Ångstroms; this scale determines the performance and detailed behavior of materials for many practical purposes. There are four Centers, located at Argonne, Lawrence Berkeley, and Oak Ridge National Laboratories, and the University of Illinois; they are networked and interfaced with one another. Serving over 1000 users annually, they provide world-class facilities for the physical sciences and engineering communities in scanning and transmission spectrometry and atomic force microscopy and related tools.

The Combustion Research Facility at Sandia-Livermore serves a broad array of university users exploring theoretical and experimental combustion systems. *The Materials Preparation Center* is a national user facility at Ames Laboratory. It provides unique, specialized equipment for the synthesis, processing, and analytical characterization of special materials, and it annually serves several hundred users from industry, universities, and other national laboratories. Centers that bring together scientists from different backgrounds working on common problems include the Centers for X-Ray Optics and Advanced Materials at Lawrence Berkeley National Laboratory, and the Surface Modification and characterization Facility at Oak Ridge National Laboratory, as well as the 100 Tesla Pulsed Field Magnet and the actinide photospectrometer at Los Alamos National Laboratory. Photochemistry and radiation facilities studying the capture of solar energy at the molecular level are located at several national laboratories as well as one at the University of Notre Dame.

Research Challenges and Opportunities

Research challenges at the Combustion Research Facility are to improve theory and obtain confirmatory experimental measurements of the dynamics and spectroscopy of vibrationally and electronically excited species relevant to combustion systems. This will enable predictions of reaction rates under a wide variety of conditions, including high temperatures and pressures, energy transfer phenomena, and spectra for diagnostic probes.

Research Activities

Collectively, the electron beam microcharacterization centers embrace transmission, scanning, scanning-transmission, analytical, high and atomic resolution, high voltage, and environmental electron microscopies; atom probe and field ion microscopies; mechanical properties or microindentation instruments; atomic force microscopy; and nuclear microanlaysis. Dedicated capabilities include high spatial resolution x-ray energy dispersive chemical analysis for heavy elements, electron energy loss spectroscopy chemical analysis for light elements, extended x-ray absorption fine structure analysis, electron beam holography, atomic and sub-atomic spatial image resolution (with appropriate computer simulation interfacing and analysis), and various kinds of electron diffraction analyses. Various in situ capabilities allow real time experiments under extremes of high and low temperature, controlled gaseous environments, magnetic field-free and applied magnetic fields, various kinds of concurrent in situ particle irradiation, and controlled types and amounts of applied stress, all with a variety of multi-axis tilt-goniometric capabilities that have a critical effect on diffraction contrast imaging capabilities of crystal defects. The activities among these four user Centers are coordinated and interactive with one another via the Electron Beam Microcharacterization Collaboratory 2000 Telepresence Microscopy, which permits remote access and operation via the world wide web.

Accomplishments

- EMSL scientists have used cutting-edge fluorescence microscopy and spectroscopy to study the reaction dynamics of individual enzymes that degrade organic contaminants in real time and under different local environments. Using these tools, the change in the active site of a single biodegradative enzyme from an oxidized state to a reduced state can be observed.

- Research on nanoscale ice films has received national recognition because of its potential importance in research on solvation in aqueous solutions, cryobiology, and desorption phenomena in cometary and interstellar ices.

- EMSL scientists recently resolved a scientific controversy over the effect of the metal-coated fiber tip used in near-field scanning microscopy on fluorescence lifetimes by finding that fluorescence lifetime can be lengthened or shortened depending on the height of the aluminum tip above the molecule.

- Automated crystallographic texture mapping techniques have resulted in a thorough understanding of the role of grain boundary character on percolative current flow in high temperature superconductors.

- Determination of interfacial chemistry by state-of-the-art analytical electron microscopy techniques has clarified the operative toughening mechanisms in whisker-reinforced and self-reinforced ceramics.

- Microchemical composition analysis of the fine (Ångstroms) precipitates in stainless steels enabled development of new alloys with improved high-temperature creep resistance.

- Collective high-resolution electron microscopy, image simulations and microanalysis have been used to identify the major constituent in a new aluminum matrix mullite composite that is now being used in automotive applications.

- Modeling of a balance between interfacial and strain energies revealed that nanometer-sized precipitates in aluminum alloys could take only certain restricted or discrete sizes. This explanatory hypothesis was then used to optimize the behavior of hardened aluminum alloys used for automotive and aerospace applications.

- Recently scientists at the Combustion Research Facility have designed and refined a novel and elegantly simple experiment that allows the interaction of chemistry and turbulence to be examined in quantitative and verifiable detail for the first time. This experiment has unequivocally demonstrated an error in current models of basic combustion processes.

- Technologies that have been enabled as a consequence of the Materials Preparation Center include lead-free solder, freon-free refrigeration, recyclable lightweight automotive composite materials, nanocrystalline neodymium-iron-boron magnet alloys with matching crystallite and magnetic domain sizes, and quasicrystal coatings produced by plasma-arc-spray that have superior wear resistance and reduced surface friction.

Biological and Environmental Research Facilities

Description, Objectives, and Research Performers

Dedicated special facilities comprise key biological and environmental resources. Some are special beam lines and equipment stations at synchrotron light and neutron sources, and others are partially devoted to this area of research. Others are observation stations dispersed over large areas, taking regular readings of climatic conditions. Climate observation facilities are located in three climatologically significant regions, the largest concentration of instruments and facilities comprises the ARM Southern Great Plains Site – over 300 continuous data streams collected by instruments spread across an area of ~55,000 square miles.

Research Challenges and Opportunities

The accuracy of the data that will be produced through the Atmospheric Radiation Monitoring (ARM) program will be essential in bringing about resolution of the most important unresolved question in climate prediction, the role of clouds and solar radiation in climate. Furthermore, to enable decade-to-century climate prediction and understanding of climate variability, necessary to address long-term energy needs and distributions, measurement must be made over the span of a decade. In order for ARM to achieve its goals, its three sites must be maintained with both state-of-the-art instrumentation and data systems capable of transferring gigabytes of data with efficiency, accuracy, and timeliness. Not only are the three sites located in areas that have unique and critical climatological sites from the scientific viewpoint, but the climatologies also pose different challenges to the equipment.

Progress in the biomedical sciences and in biotechnology depends both on efficient operation of the facilities and on overcoming serious limitations in the capabilities of the best currently available instrumentation. Thus, a critical part of DOE stewardship includes the development and operation of experimental stations at the major facilities such as synchrotron light sources, neutron sources, and ultra high field mass spectrometers and nuclear magnetic resonance spectrometers, as well as research into new instrumentation such as detectors and data management and analysis systems.

Research Activities

Structural biology research facilities at the Argonne National Laboratory, Lawrence Berkeley Laboratory, and SSRL light sources investigate the sub-Ångstrom structures of proteins; other laboratories investigate PET scanning magneto encephalography and magnetic resonance imaging for single cell analysis on a fast time scale. At reactors located at MIT and McClellan Air Force Base, neutron beams are being used for clinical studies of boron neutron capture therapy. In the area of environmental studies, Field Research Centers are being established to study bioremediation of sites polluted with radionuclides. Other stations monitor carbon dioxide flow, atmospheric radiation, and water vapor through the ARM program. These efforts involve collaboration with other government agencies including NASA, NOAA, and the Department of Agriculture.

The Production Sequencing Facility (PSF) is devoted to the high-speed, automated sequencing of the human genome and is a key element of the DOE Joint Genome Institute. It is a high-throughput DNA sequencing factory that will utilize and integrate advances in sequencing technology and automation, drawing on the sequencing, automation and information management expertise of DOE National Laboratories and leading experts at universities. The PSF will begin operation in FY 1999.

The ARM infrastructure supports climate observatories in three climatic regions: the U.S. Southern Great Plains, the Tropical Western Pacific, and the North Slope of Alaska. These observatories gather data on clouds and on the local radiation budget, making total radiance as well as high resolution spectroscopic measurements of both the solar (incoming) and infrared (outgoing) atmospheric radiation. These data are used to improve the modeling of clouds and radiation in General Circulation Models, the primary tool with which climate predictions are made.

Accomplishments

- Charge-coupled device detectors that were developed for structural-biology have become the standard detectors for protein crystallography. The program's Structural Biology Center at Argonne and Beamline 9 at SSRL were the first to routinely achieve sub-Ångstrom resolution of protein structures.

- The world's highest resolution and fastest 3D PET instrument was constructed.

- A nuclear medicine camera device for small animal and breast-specific imaging has been developed.

- Merging of PET's electronic radio tracer detectors, and magnetic resonance imaging's (MRI's) powerful magnetic fields has been accomplished.

- Development of a laser-based technology for single cell analysis enabled measurement of cellular enzyme substrates within a second time scale has been accomplished.

- High impact advances have been made in single atom and single molecule analysis schemes. To date, 52 R&D-100 Awards have been received for technologies developed by the researchers in the Measurement Sciences Program. Microscopic imaging of the contents of single cells using magnetic resonance tomographic methods has been demonstrated; this technology was applied to the analysis of tank waste sludges from the Savannah River Site, providing important practical insights on why a new treatment system had failed.

- More than 70 structures have been solved at the ALS Macromolecular Crystallography Facility, which has served more than 180 scientists in its first year of operation.

- The ARM North Slope of Alaska/Adjacent Arctic Ocean Site (NAS/AGO) is collecting data from a second site, inland from the Barrow site, at Atquasuk.

- The ARM Program atmospheric observatory at the Southern Great Plains site is being used for surface characterization and hydrology experiments by Department of Agriculture and NASA, for calibration and validation of NASA's Earth Observing System, and for storm studies conducted by the National Oceanic and Atmospheric Administration.

Computing and Computational Support

Description, Objectives, and Research Performers

Computing and the computational support essential to the success of all the programs is provided by state-of-the-art facilities and networking. These include the NERSC computing center at

Lawrence Berkeley National Laboratory and the ESNet, as well as Advanced Computing Research Facilities (ACRFs) at various DOE laboratories. In addition there are grand challenge efforts and collaboratory efforts involving the various programs.

Research Challenges and Opportunities

Massively parallel computers are difficult to program efficiently. New tools, as well as underlying system software support, are required to make this possible. Petascale data archives from advanced simulation as well as next generation experimental facilities require development of new technologies because current approaches do not scale. Other challenges include providing ultra high speed network access to massively parallel computers; development of tools to enable applications to effectively use network performance and status diagnostics; and integrating software produced by multiple groups into a single framework.

Research Activities

NERSC**,** located at Lawrence Berkeley National Laboratory, provides high performance supercomputers and associated software support for investigators supported by the Office of Science. The Center serves 2500 users working on about 700 projects; 35% of users are university based, 60% are in National Laboratories, and 5% are in industry.

ACRFs support advanced computational hardware testbeds for scientific application pilot projects and fundamental research in applied mathematics and computer science. ACRFs are located at Los Alamos National Laboratory (based on SGI/Cray Technology); Argonne National Laboratory (Intel-Based Clusters); and Lawrence Berkeley National Laboratory (SGI/Cray T3E and IBM-SP Technology). Related capital equipment such as high speed disk storage systems, archival data storage systems and high performance visualization hardware are also supported.

ESnet provides worldwide access to Office of Science facilities, including advanced light sources, neutron sources, particle accelerators, fusion reactors, spectrometers, ACRFs, and other leading-edge science instruments and facilities. ESnet provides the communications fabric that links DOE researchers to one another and forms the basis for fundamental research in networking, enabling R&D in collaboratory tools and applications testbeds such as the national collaboratory pilot projects.

Supporting research aims to develop the most powerful and effective mathematical and computational tools for modeling, analyzing, and simulating complex phenomena in the core disciplinary and technology areas of DOE. This R&D applies the results of fundamental research in applied mathematics and computer science to an integrated set of tools that can be used by scientists in various disciplines to develop high performance scientific applications. Research is underway in computer science; high performance computer networks, their protocols, and methods for measuring their performance; software to enable high speed connections between high performance computers and both local area and wide area networks; software to make effective use of computers with hundreds or thousands of processors as well as computers that are located at different sites; large-scale scientific data management and visualization; and the underlying mathematical understanding and numerical algorithms to enable effective description and prediction of physical systems.

Accomplishments

- Various computational and communications tools have been completed: the Message Passing Interface (MPI-2) standard, development of Dynamic System Instrumentation tools and Applications Program Integration (API), Sandia University of Mexico Operating System (SUNMos) lightweight operating system kernal, Parallel Virtual Machine (PVM), and Globus to integrate geographically distributed computations and information resources.

- Tertiary tape storage systems have been integrated with distributed disk cache systems and object oriented database systems.

- The High Performance Parallel Interconnect (HiPPI) 6400 standard was completed.

- The Internet Engineering Task Force (IETF) accepted proposed differentiated services architecture, and these services were demonstrated.

- Software was interoperated by Argonne National Laboratory and Lawrence Livermore National Laboratory to build a framework that accelerated real application by a factor of more than 20.

- A modular electronic logbook framework was developed and widely deployed inside and outside DOE.

Portfolio Summary

This portfolio area, "Instrumentation for the Frontiers of Science," encompasses research from many programs and supporting activities that crosscut the research topics covered above. The table below summarizes specific core research activitiesthat strongly support or moderately support Instrumentation for the Frontiers of Science, including accelerators for high energy and nuclear physics, light sources and neutron beam facilities for natural and life sciences, plasma and fusion energy facilities, single-purpose and multidisciplinary facilities, biological and environmental research facilities, and computing and computational support. The funding totals for these areas are an analytic tool reflecting the highly crosscutting, leveraged aspects and implications for individual research areas within DOE's science portfolio. **Because research areas may appear in multiple chapters, there will be significant instances of multiple counting, and the chapter totals will not sum to the overall science budget.** Additional details on these research areas are presented in the Research Summary Matrix and the corresponding Research Summary Profiles.

Strongly Supportive Core Research Activities
Adv. Particle Accelerator Concepts
Advanced Computing and Communications Facility Operations
Advanced Medical Imaging
Alcator C-Mod Facility Operations
Atmospheric Radiation Measurement (ARM) Program Infrastructure

Atomic, Molecular, and Optical Science Boron Neutron Capture Therapy Carbon Cycle Research Chemical Physics Research DIII-D Facilities Operations Ecological Processes Engineering Behavior Environmental and Molecular Sciences Laboratory (EMSL) Experimental Fusion Physics Support Experimental Plasma Research (Alternatives) Facility Operations: AGS Facility Operations: Fermilab Facility Operations: SLAC General Technology: Accelerator R&D General Technology: Detector R&D Heavy Ion Facility Ops. & Constr. High Performance Computer Networks Low Energy Facility Ops. & Constr. Medium Energy Facility Ops. & Constr. Natural and Accelerated Bioremediation Research Program Neutron and Light Sources Facilities NSTX Facility Operations Photochemistry and Radiation Research Production DNA Sequencing Facility Science Education Support Scientific Computing Application Testbeds Structural Biology Research Facilities Structure of Materials TFTR Facility Theory & Simulations of Matter, Engineering Physics
Moderately Supportive Core Research Activities Advanced Computing Software and Collaboratory Tools Catalysis and Chemical Transformations Chemical Energy and Chemical Engineering Computer Science to Enable Scientific Computing CP Violation - B-Meson System CP Violation - K-Meson System Electroweak Interactions Experimental Condensed Matter Physics General Purpose Plant & Equipment (GPP/GPE) Geosciences Hadron Spectroscopy Heavy Element Chemistry High Energy Physics Theory Materials Chemistry Mechanical Behavior and Radiation Effects Multiprogram Energy Lab Facilities Support (MELFS) Neutrino Mass and Mixing Neutron and X-Ray Scattering

Nuclear Structure & Astrophysics - Low Energy Nuclear Physics Nuclear Structure/Dynamics ... Phase Trans. - Heavy Ion Nuclear Physics Oak Ridge Landlord Particle Astrophysics & Cosmology Physical Behavior of Materials Quark/Gluon Substructure of Nuclei - Medium Energy Nuclear Physics Resources and Tools for DNA Sequencing and Sequence Analysis Search for Higgs & Supersymmetry Separations and Analysis Spin Structure of Nucleons Strong Interactions, Supersymmetry & Particles
NOTE: Please see Appendix A for more information on the budgets, the research performers, and other related information for eachCore Research Activity.