DOE Business Plan for the Office of Science's Argonne National Laboratory

Mission and Overview

Argonne National Laboratory (ANL) was founded in 1946 and traces its scientific legacy directly to nuclear physics research teams led by Nobel Laureate Enrico Fermi. ANL was largely responsible for the science behind the emergence of the U.S. nuclear power industry and today has transformed itself into a multipurpose laboratory with a mission focus and deep capabilities in basic and applied materials, chemical science, energy technologies and analysis, high-performance computation, physics, and biosciences. ANL also leads research in other scientific areas of importance to the Department of Energy such as the environmental and national security. ANL has retained strong capabilities in the design, construction and management of major scientific facilities. As a DOE steward of critical national research infrastructure, the laboratory provides access to university, industry and government researchers on a competitive basis. These research facilities include the Advanced Photon Source (APS), which provides x-ray beams for research ranging from materials to structural biology; the Intense Pulsed Neutron Source (IPNS), which has achieved many "firsts" in the field of neutron scattering; the Center for Nanoscale Materials (CNM), which focuses on exploring the nanoscale physics and chemistry of nontraditional electronic materials; and the Argonne Tandem-Linac Accelerator System (ATLAS), a superconducting linear accelerator for heavy atoms. The ANL user community now includes over 3,500 scientists and engineers.

Laboratory Focus and Vision

Six core competencies underpin activities at ANL:

1. Materials science, nanoscience, chemistry, and structural biology.
2. Synchrotron radiation science and technology for the study of materials of all kinds.
3. Energy related research, including transportation science and engineering, and nuclear fuel cycle and reactor design.
4. Integration of modeling, fundamental science, engineering and economic expertise for energy and environmental issues.
5. Advanced software tools, massively parallel computer

Lab-at-a-Glance

Location: Argonne, IL

Type: Multi-program lab

Contract Operator: University of Chicago

Responsible Site Office: Argonne Site Office (Bob Wunderlich)

Website: http://www.anl.gov/

Physical Assets:

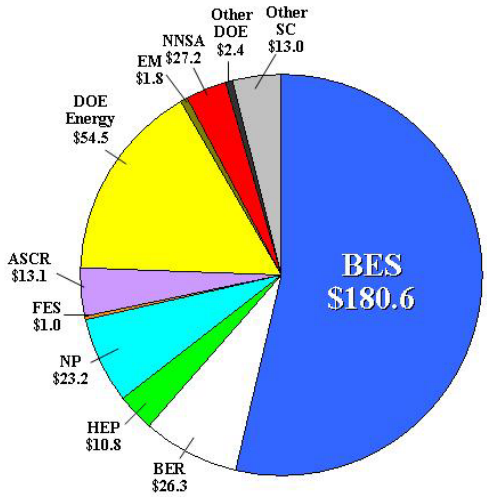
- 4.8M square feet of facilities; 100 buildings
- 1,500 acres

Human Capital:

- 2635 employees
- 600 Students (Undergraduate and Graduate);
- 3500 Facility Users and Visiting Scientists

FY 2005 Total DOE Funding: $353.9M

FY 2005 DOE Funding by Source
PALS data (BA in Millions):



FY 2005 Non-DOE Funding: $138M

architectures and large-scale computational sciences.

6. Fundamental nuclear physics tied to cosmology and the origins of the elements.

The Office of Science believes that these six competencies will enable ANL to deliver its mission and customer focus, to perform a complementary role in the DOE laboratory system, and to pursue its vision for scientific excellence and pre-eminence in the areas of:

- Pursuing the limits of high spatial and temporal resolution for materials research at the nanoscale.
- Capturing the frontiers of low-energy nuclear physics, particularly for the study of rare and unstable isotopes.
- Integrating materials science, computational science and other sciences to create a sustainable and secure energy future.
- Creating the world's leading core accelerator technology development capability.
- Advancing computational science (architectures and applications) to tackle national R&D challenges requiring petascale capabilities.
- Developing nano-bio capabilities to dramatically increase chemical energy conversion.

Business Lines

The following capabilities, aligned by business lines, distinguish ANL and provide a basis for effective teaming and partnering with other DOE laboratories, universities, and private sector partners in pursuit of the laboratory mission. These business lines and the distinguishing capabilities outlined in the table below provide an additional window into the mission focus and unique contributions and strengths of ANL and its role within the Office of Science laboratory complex. Items in italics within the column, Distinguishing Capabilities, identify research facilities that convey particular, strategic strengths and capabilities to the Lab. Descriptions of these facilities can be found at the website noted in the Lab-at-a-Glance section of this Plan.

Business Lines	Distinguishing Capabilities	Distinguishing Performance	Mission Relevance
Primary Business Lines			
Materials Science	• **Biological & Inorganic Materials Synthesis & Characterization;** • **Hard X-ray Nanoscale Research;** • ***Advanced Photon Source;*** • ***Center for Nanoscale Materials;*** • ***Electron Microscopy center;*** • ***Intense Pulsed Neutron Source.***	International leader; most highly cited papers in materials science; Unrivalled co-location of photon, neutron, electron, and ion based materials analysis facilities; High caliber staff as indicated by 2003 Nobel Prize in Physics.	Understand materials structure for energy, health and national security applications; Lead portions of the nanoscale revolution.
Mathematics & Computer Sciences	• **Advanced Architecture Research** • **Applied Modeling & Simulation** • **Computational Mathematics**	Leader in fundamental architecture for massively parallel computer systems; DOE top 10 scientific achievement for large-scale massively parallel optimization; Partner with ORNL to establish	Providing computational tools to advance the forefront of science.

Business Lines	Distinguishing Capabilities	Distinguishing Performance	Mission Relevance
		leadership class computing for open scientific research.	
Advanced Biosciences	• **Imaging** • **Structural Biology/Genomics: biomolecular structure determination** • **Bioinformatics** • ***Structural Biology Center***	Top 3 world-wide in production & characterization of protein structures Unique capabilities based on the APS, IPNS, and protein crystallization center	Increase bio-defense capabilities, develop new energy sources and environmental technologies, and advance medical sciences.
Fundamental Physics	• **Nuclear structure and astrophysics with stable beams;** • **Laser trapping of individual atoms;** • **High energy physics experiments and theory;** • ***Argonne Tandem-Linac Accelerator System***	World leader; experimental & theoretical nuclear physics Most highly cited nuclear theory paper of past decade Worldwide roles in CDF and ATLAS experiments	Understand fundamental matter and forces and master connections between high energy & nuclear physics, astrophysics & cosmology.
Energy & Environmental S&T	• **Nuclear Fuel Cycle & Reactor Design;** • **Transportation Science;** • **Integration of Economics, Computing, Engineering and Sciences;** • ***Cloud and radiation testbed;*** • ***Engine Research Facility for Diesels;*** • ***Advanced Powertrain Test Facility for Hybrid-vehicles;*** • *Electrochemical Analysis and Diagnostics Laboratory.*	International leadership in fuel cycle & reactor technologies as evidenced by CEA & JNC partnership. World leader; vehicle testing confirmed by Toyota, Hyundai, GM, Ford, others. World's most widely used greenhouse gas and total fuel cycle model (GREET). Shared leadership of Atmospheric Radiation Measurement User Facility with ORNL and PNNL. Internationally recognized expertise in environmental assessment as evidenced by Alaska Pipeline EIS.	Support next generation nuclear reactor design efforts. Advance integrated approaches to energy & environmental challenges. Advance the frontiers of large-scale, systems-level-modeling and simulations as applied to energy and environmental technologies
Secondary Business Lines			
Accelerator Design	• **Accelerator R&D for low velocity beams** • **Superconducting RF Design** • **Synchrotron Radiation Sources**	World's first superconducting ion accelerator. New classes and performance standards for RF cavities World-leading development of synchrotron operations	Maintain DOE lead in accelerator design, construction and operations.
National Security	• **Infrastructure Assurance** • **Nuclear Risk Mitigation** • **Bioagent Detection**	National leader in energy infrastructure risk mitigation National leader in detection and deterrence of radioactive threats National leader in bio-micro-arrays for agent detection	Reduce homeland security threats.

Major Activities

Following is a set of major activities that ANL would like to pursue to support aspects of the DOE mission and build on core strengths and capabilities of the laboratory. The Office of Science is examining all of these potential activities and they are at different stages of development. Some are currently underway and some are mere concepts at this time. For those that are still in the conceptual phase, ANL has indicated significant interest and is viewed to have current supporting research and mission focus to pursue such activities. Budgets, the Office of Science's strong commitment to a fair and competitive funding process and technical advice from its major scientific advisory committees will ultimately contribute to decisions about which activities can be pursued and at which sites. The companion documents, the DOE's Five Year Plans, provide greater insights into these activities in terms of various five-year budget scenarios.

The major activities are:

1. Advanced Photon Source (APS) Optimization & Upgrade
2. Integrated Energy, Environment & Economic Research
3. A Next Generation Facility for Nuclear Structure and Astrophysics
4. Petascale Computing

1. APS Optimization & Upgrade

- **Summary:** Create the capability to see nanostructures in real time and in real environments and deliver unprecedented one picosecond time resolution x-ray pulses through major upgrades to the APS accelerator.
- **Expectations:** The unique characteristics of an optimized APS will open up new frontiers of scientific discovery and investigation, and enable exploration of: complex chemical and biological reactions in real time; orders of magnitude capacity improvements for materials studies; and *in-situ* studies of self-assembling nanoscale semiconducting materials.
- **Benefit Perspective:** Potentially *Transformational* Benefits
- **Risk Perspectives:**
  - Technical: *Moderate risk* because technical issues are addressed within planned contingency,
  - Market/Competition: *Low risk* given the large user community. The upgrade will be necessary to keep the APS among the best of the hard x-ray facilities, and ensure that its performance and scientific output continue to be ground-breaking.
  - Management/Financial: *Low risk* given incremental nature of funding.

The APS has delivered a return on the investment during its past ten years of operation serving approximately 3,000 users per year who conduct leading edge experiments that have made lasting contributions to the U.S. economy and social well-being. Ensuring that the APS remains at the forefront of scientific discovery over the next two decades will draw upon ANL's competencies in synchrotron radiation sources and will build upon the capabilities of the new Center for Nanoscale Materials, which is utilizes the APS's x-ray sources as a primary tool. The APS upgrade will replace and upgrade major components to the accelerator to further increase performance in the hard x-ray region of the spectrum.

ANL's optimization plan enhances DOE's potential to dramatically impact energy source diversity, efficiency, sustainability and security goals. For example in materials research, the APS upgrade addresses the need to observe unique *in-situ* pictures of controlled self-assembly of new nanomaterials under real conditions, and to study the critical failure modes of these and other lightweight materials so necessary to improve transportation energy efficiency. This is created by providing access to one picosecond x-ray pulses as well as high flux pulses in nano-focused spots at high energies. This will create capabilities for imaging and inelastic, high energy and time-resolved x-ray scattering, which will be an order of magnitude greater than any other existing or planned machine in the world. This upgrade will also fill the gap in time resolution between new ~3 GeV storage rings being constructed and FELs offering a unique combination of flux and time resolution for hard x-rays.

2. Integrated Energy, Environment & Economic Research

- **Summary:** Combine ANL's expertise in decision science, computational, fundamental and applied research with social/economic science capabilities to develop a suite of products and tools that advance DOE's mission to provide a more diverse, sustainable and secure energy future for the Nation while mitigating environmental impact.
- **Expectations:** An integrated analytical energy/environment/economic modeling framework to provide the DOE with a new capability designed to: inform policy and investment decisions leading to a more diverse, sustainable and secure energy future; develop new technology options, primarily in the transportation, transmission and nuclear generation sectors; and integrate R&D programs from basic to applied to deployment.
- **Benefit Perspective:** Potentially *Substantial* Benefits
- **Risk Perspectives:**
  - Technical: *Moderate risk* in terms of developing a decision-support framework; *High* in terms of developing specific technologies due to uncertainties in basic research.
  - Market/Competition: *High risk* because many different organizations (public and private) will be competing for market in this area.
  - Management/Financial: *Low risk* because the program will be implemented incrementally.

The DOE currently lacks an integrated approach to the analysis of the impacts that technology options have on energy utilization and production, the economy and the environment. ANL's ability to draw upon the systems and decision modeling expertise, as well as the basic and applied scientific talent contained within the lab and the social/economic sciences capabilities of the University of Chicago (together with its partner universities Northwestern University and the University of Illinois) present an opportunity to provide analytical capabilities that DOE has never before had available.

This investment exploits ANL's capabilities in materials characterization and synthesis, nuclear fuel cycle and reactor design, transportation science and engineering, computational sciences, integration of computing, science, engineering, and large-project delivery. This investment is anticipated to have broad impact and significant returns: a reduction in petroleum use to save $4.5B/year in trade balance, and $6B/year in consumer costs. Diesel engine work at ANL if successful targets 30-40% reduction in average diesel vehicle fuel use; this target also reduces emissions of greenhouse gases by 30-40%.

3. Next Generation Facility in Nuclear Structure and Astrophysics

- **Summary:** A next generation facility in nuclear structure and astrophysics will be a powerful research tool dedicated to producing and exploring new rare isotopes that are not naturally found on earth, will help answer long standing questions of nuclear physics and astrophysics, and is viewed as the top priority of the nuclear physics community.
- **Expectations:** Research conducted at a facility with exotic beam capabilities will have far-reaching results, including: uncovering the origins of heavy elements in the periodic table; determining how galaxies, stars and plants form and evolve; producing isotopes for biomedical applications.
- **Benefit Perspective:** Potentially *Transformational* Benefits
- **Risk Perspectives:**
  - Technical: *Moderate risk* because technical uncertainties are mitigated by planned contingency.
  - Market/Competition: *High risk* due to intense competitive pressures.
  - Management/Financial: *High risk* given the scope of the project, but potentially reduced through State of Illinois participation.

ANL will leverage existing capabilities in nuclear physics, including scientific talent and the ATLAS facility, to develop the world's leading exotic beam facility. This activity draws on Argonne's experience with accelerator research & technology, especially Argonne's long history in building and operating ATLAS; and development of specific technologies for rare isotope beam capabilities, fundamental physics, materials, computational sciences; and large project management. Given the complexity of this undertaking, ANL intends to partner with other DOE labs as well as those of the Nation's leading universities and industry, including joint efforts with the University of Chicago and the NSF Physics Frontier Center focusing on nuclear astrophysics.

A facility with exotic beam capabilities will provide the means for the next generation of researchers within nuclear physics and laboratory astrophysics to answer some of the most important and fundamental questions of our time and to train the next generation of nuclear physicists. Fundamental physics research in the U.S. will rise further in pre-eminence and U.S. leadership in low-energy nuclear physics will not be lost to Europe. Important applications in stockpile stewardship and nuclear medicine will be addressed. The proposed Illinois Accelerator Institute will bring together many of these partners and capabilities.

4. Petascale Computing

- **Summary:** ANL will focus on advanced architecture deployment and integration at the petascale to support DOE's missions, including ANL activities in nanoscale materials research, reactor simulation, systems biology, accelerator designs, and the modeling of complex energy and environment systems.
- **Expectations:** Development of petascale computing capabilities for: creation of "designer" nanomaterials for industrial, medical, and other applications; modeling of whole microbial cells for bioengineering and synthetic biology applications in support of energy and environmental research; and fission and fusion reactor modeling that will significantly help reduce design margins and shorten development schedules by streamlining experimental and licensing requirements.
- **Benefit Perspective:** Potentially *Transformational* Benefits
- **Risk Perspectives:**
  - Technical: *Moderate risk* due to commercial risk as well as semiconductor design and software risk. This risk is mitigated by the particular choice of application.

- Market/Competition: *High risk* because of intense competition of several players for this market.
- Management/Financial: *High risk* due to close coupling with business plans of computer vendors who may or may not stay in the market.

ANL is a partner with ORNL to develop leadership class computing capabilities to support forefront science, and while supporting broad classes of advanced architectures, aims to focus especially on architectures with substantial promise to reach petascale levels of computing capability within the next five years. This activity builds on ANL's strengths in High Performance Computing (HPC) software, advanced hardware architectures, and application expertise; and enables forefront research, engineering, and facilities**.** The proposed Theory and Computer Science (TCS) building would provide the needed space and facilities support. The TCS building also leverages ANL's plans for co-locating the high energy physics division with the nuclear physics division.

Major technical hurdles involve the development of a computer architecture that achieves high application performance with reasonable cost and power consumption. ANL is working with IBM and other vendors to achieve this goal, in collaboration with researchers at other DOE laboratories and at universities. ANL also must ensure that applications software with appropriate scientific content, efficiency and reliability is available to meet the community's needs. In addition to hiring new staff, ANL will collaborate with other DOE laboratories (especially ORNL and LBNL), the University of Chicago, Northwestern, and the University of Illinois and other universities to build strong software development teams.

Financial Outlook

Detailed information regarding the financial outlook for the Argonne National Laboratory is subject to 1) competition and merit review, 2) the availability of appropriated funds and 3) programmatic decisions. The first two factors can not be predicted or estimated in advance. The third, programmatic decisions, are developed in accordance with the planning targets reflected in the Department of Energy programmatic Five Year Plans, a companion document to these strategic laboratory business plans. In addition, because of the Office of Science commitment to competition and merit review, there is often a time lag between programmatic decisions and the determination of which research provider can best deliver the greatest value in conducting the research. Thus, it is not always apparent how programmatic decisions unfold for particular laboratories. Nevertheless, some decisions, such as the plans for large scientific user facilities, show clear paths to individual labs and therefore inform their business plans.

Support for Non-DOE funded work is a vital role our national laboratories, contributing to national security, energy security, environment stewardship, scientific discovery, and more fundamentally, the competitiveness of the U.S. economy. For the Argonne National Laboratory, this is no exception. The Office of Science is supportive of this work and although it is not addressed in any detail within the accompanying Five Year Plans, the Office of Science believes it is sufficiently important and appropriate to address within this strategic laboratory business plan. A brief perspective and financial outlook is therefore provided.

Argonne's non-DOE funded work engages both the Federal and private sectors and represents approximately 25% of the laboratory's total budget. The major ANL non-DOE federally funded activities are primarily supported by the Department of Homeland Security, focused on infrastructure assurance; the National Institutes of Health, emphasizing but not limited to protein

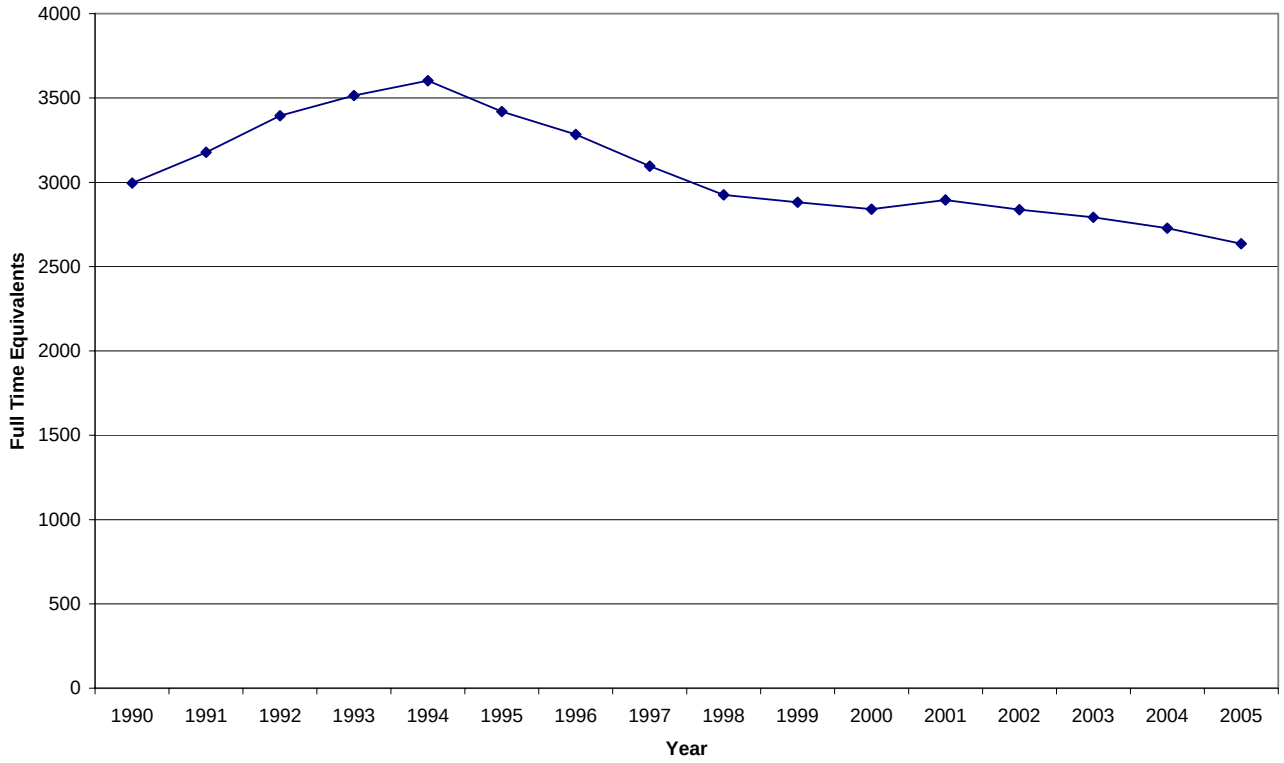
characterization; the Department of Defense, covering a broad range of specialized technical (and often classified) assistance, infrastructure assurance, environmental assessments and nuclear related issues; the Department of Agriculture, for hazardous waste assessments; the Department of State, in support of IAEA; and the Nuclear Regulatory Commission, providing a technical basis for regulatory decisions. It is anticipated that each of these areas will continue to grow. Also anticipated is that the Intelligence Community will become a key sponsor over the next five years. Argonne's work for the private sector is varied and is typically a much smaller effort per project and of shorter duration than that for the Federal sector. Typical current work examples include locomotive engine combustion studies for GM Electromotive and DUV lithography support for Intel.

Uncertainties and Risk Management

External Factors: Over the next five years, ANL will have a number of concerns driven by external forces. A primary concern is the stability of funding for core scientific programs new facilities, such as petascale computing and the Advanced Photon Source's upgrade. The priority placed by DOE on petascale computing will determine whether or not sustained funding will be provided that is needed to make the program a success. ANL's future is directly coupled with Federal support for a broad science and technology program. In addition, the upcoming competition for ANL's contract brings with it a degree of uncertainty for ANL employees, who have always been a part of the University of Chicago system.

S&T Workforce: ANL's ability to recruit and retain scientific staff and maintain relationships with external partners (universities, other labs, private industry) is vital to its ability to maintain core science and technology programs. The Office of Science has requested that ANL, along with other laboratories, explore and/or expand such incentives as onsite daycare and flexiplace working arrangements to attract the best and brightest to replace its aging workforce and Argonne has accepted these specific recommendations and has undertaken additional activities mentioned in the following discussion of diversity.

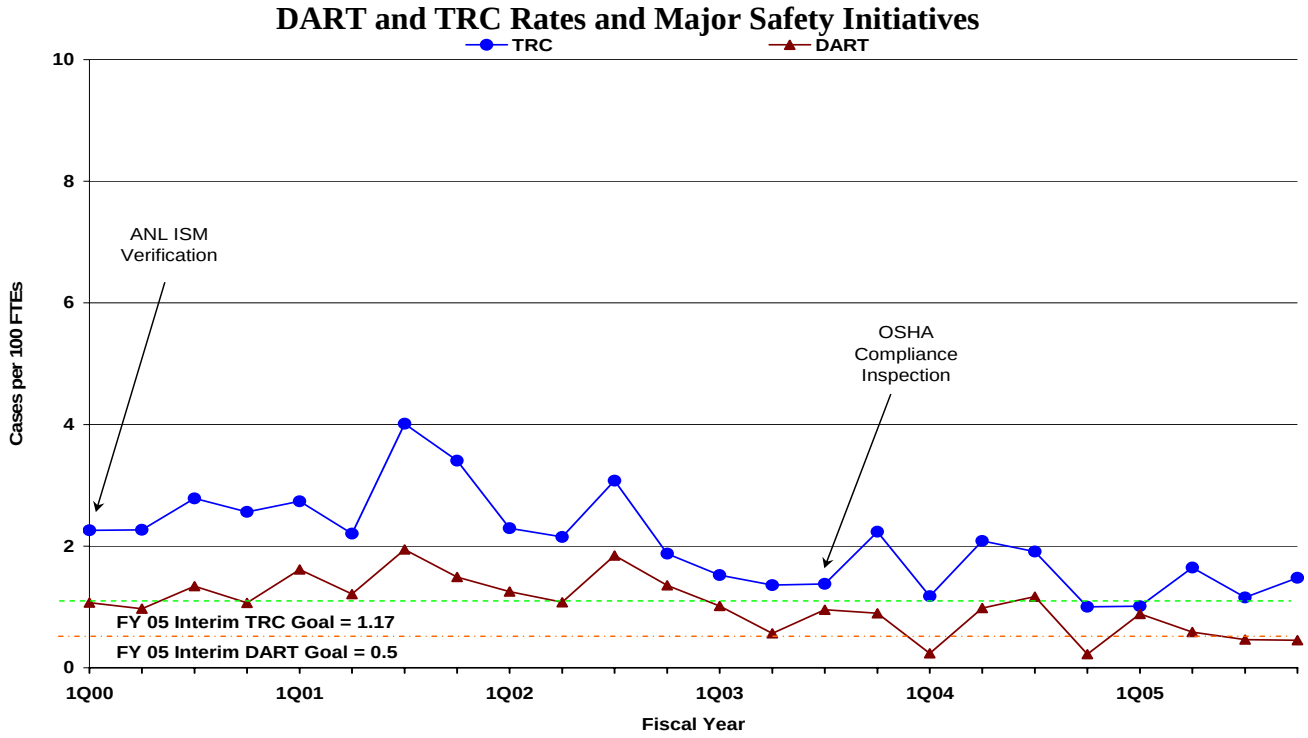
Workforce Trends



Workforce Diversity: As with most DOE labs, ANL must make significant progress in the recruitment and retention of under-represented populations, particularly African American and Hispanic scientific staff. In particular, Argonne is committed to pacing the rapidly increasing representation of women and underrepresented minority science and engineering PhD's graduating from tier 1 universities as evidenced in for example, "A National Analysis of Diversity in Science and Engineering Faculties at Research Universities" by Donna, J. Nelson, January, 2005. ANL, working with the University of Chicago, has organized a regional coalition of national research universities to assist with recruitment and is taking other steps to improve and retain workforce diversity and strength. These include; developing a "rolodex" of potential diverse candidates in all scientific and in particular for senior role model scientific and management fields; identifying and cultivating potential employees early via summer schools and focused workshops; insisting on qualified diverse candidates for each posting; encouraging employee affinity groups; and addressing exit issues critical to retaining a diverse workforce. Argonne is committed to hiring in a manner that reflects the diversity of tier 1 university science and engineering PhD's now, and a population of National scientific and engineering diversity by 2015. Based on national availability projections for the scientific and engineering PhD's, Argonne's goal is an S&T workforce consisting of 18% female, 4.3% African American, 3.5% Hispanic, and 0.5% Native American. Critical to the success of this commitment is realization of constrained ideal funding projections as well as maintenance of the diverse workforce development pipeline, a core educational activity of Argonne.

FY05 Data	All Employees			All Employees					
	Male	Female	Total	Caucasian	African American	Hispanic	Native American	Asian	Total
Scientists & Engineers	861	158	1019	836	13	17	3	150	1019
Management & Administration	457	225	682	604	13	15	2	48	682
Technical support	215	26	241	205	15	13	1	7	241
Clerical & Secretarial	19	324	343	280	30	25	0	8	343
Other	301	49	350	260	65	18	3	4	350
Total	1853	782	2635	2185	136	88	9	217	2635

Safety: Argonne takes safety very seriously. In 2003 Argonne provided DuPont STOP™ training for its support operations significantly reducing safety incidence in operations. Argonne has implemented rigorous safety walk-throughs for all programmatic areas of the laboratory and is actively removing safety obstacles.



Physical Infrastructure: ANL is located on a 1,500 acre Federal reservation near Chicago, Illinois. Established in the late 1940s, it has 1.4M sf of space in 119 buildings. Fifty six percent of its space, as well as most of its utility systems and roads, are over 40 years old. ANL's AUI is 0.964 (good).

Maintenance, recapitalization, and modernization are supported both with overhead (maintenance and Institutional General Plant Projects [IGPP]), operating, and GPP funds, and with line item funding (projects which cost $5M or more). ANL will attain a maintenance investment level of 2% of replacement plant value (excellent) in FY 2006, which will be continued in FY 2007 and the outyears. ANL's deferred maintenance backlog is $58.5M resulting in an ACI of 0.96 (good). A deferred maintenance reduction initiative was initiated in FY 2006, and will be continued in FY 2007 with funding of $2.6M. The proposed FY 2007 funding for the clean-up and demolition of excess facilities funding is $500,000. The FY 2007 GPP funding request is for $5.6M. The laboratory will begin funding $2M of IGPP in FY 2007 to address roofing needs.

Funding for one new line item project is requested in FY 2007 - Building Electrical Services Upgrade, Phase II. This project will upgrade critical portions of the electrical power distribution system in twelve research buildings and support facilities, including the Canal Water Plant supplying cooling water for site experiments. ANL's future recapitalization and modernization challenges include laboratory space modernization, roads/parking/lighting upgrades, fire safety improvements, and central heating plant upgrades as well as the clean-up and demolition of numerous contaminated facilities.