Ames Laboratory

Site Utilization and Management Plan

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I. Ames Laboratory Mission in the DOE Laboratory System

The Department of Energy Office of Science (DOE-SC), Ames Laboratory (Ames) is a government owned laboratory operated by Iowa State University (ISU), it's current contractor, on the university campus located in Ames, Iowa. The Laboratory's mission within the SC's Basic Energy Sciences is to provide key advances in materials science research, especially in materials theory, synthesis and characterization, of benefit to DOE missions

Beginning in 1947 as part of the Manhattan Project, Ames Laboratory today provides expertise to the DOE laboratory system in materials science, engineering, analytical instrumentation and chemical sciences, with applications in energy, human health and environmental improvement. Ames operates the Materials Preparation Center (MPC), a DOE user facility which provides the highest purity materials to the research community. Ames receives international recognition in such fields as condensed-matter physics, analytical chemistry, metallurgy, solid-state inorganic chemistry, catalytic science, instrument development and cluster computing; and is noted for assembling world-class teams of researchers representing various disciplines to solve large multifaceted problems facing the nation such as energy and the environment. Ames has received fifteen 15 R&D-100 awards since 1984.

Materials sciences have historically been a broad strength at Ames where scientists' foci range from synthesis and processing of rare-earth materials with unique purity, structures and properties, to finding new synthetic routes to known and unknown materials including metastable oxides, nitrides and silicides of metals, ductile intermetallics, electroluminescent organic materials and electrocatalysts. Ames is the recognized center of quasicrystal research in the U.S. Ames scientists have developed a novel, high-pressure gas atomization process that produces microscopic metal powders to produce a variety of important materials from lightweight structural composites to permanent magnet materials. Other focuses include high-Tc superconductors, bioinspired materials, and magnetic molecules. Ames leads the world in the theoretical design of novel optical materials including photonic band gap crystals and "left-handed" materials. In the chemical sciences, researchers are studying the chemical kinetics and reactivity of transition metal complexes, new synthetic routes to inorganic catalytic materials and molecular "stepping stones", to contribute to the ultimate goal of performing chemical transformations with minimum energy requirements and zero waste generation. Ames has a longstanding strength in the development of analytical instrumentation of ever greater sensitivity and increased throughput. Commercial examples of Ames-developed instrumentation can be found in analytical labs around the world. Despite the fact that Ames is largely dedicated to fundamental research, it recognizes practical applications, such as the recently developed lead-free solder and highly successful commercialized separations technologies. Normalized to current funding levels, its licensing program is one of the most successful of the DOE laboratories.

The Lab's primary DOE customer is SC. Additional DOE partners include the Offices of Fossil Energy, Energy Efficiency and Renewable Energy, and Nonproliferation and Verification. The main non-DOE federal partners are the National Institutes of Justice, which has provided funds for the Midwest Forensics Research Center, and the National Institutes of Health. Secondary partners include the Department of Defense, the Federal

Bureau of Investigation, and various corporate entities, specifically, metals manufacturers, automakers and agri-business.

II. Current and Future Business Plans

Ames business plans, including both current and future initiatives, center on two business lines: "Fundamental Materials Research" and "Analytical Techniques and Instrument Development". These business plans support the mission of the Office of Science and are expected to remain viable at least during the next five years of the operation of the Ames Laboratory. Five areas of core competency underpin activities within these two business lines at Ames:

1. Materials design, synthesis and processing
2. Analytical instrumentation/device design/fabrication
3. Condensed matter theory (including photonic band gap and other novel materials)
4. Materials characterization, x-ray and neutron scattering, solid-state NMR, spectroscopy/microscopy
5. Separation science

<u>Business Line: Fundamental Materials Research</u>

From its beginning Ames has dedicated itself to performing fundamental research in the materials sciences. The next generation of technology will demand an ever-increasing refinement of materials tuned by compositional complexity, structural tailoring and the manipulation of physical properties. Examples of emerging technologies include:

- Devices that manipulate light, in the same manner that current semiconductor technology manipulates electrons, for huge potential gains in processing speed and energy savings;
- Advanced magnetic devices and magnetic nanomaterials with properties for sophisticated sensors and control applications and dynamic large scale data storage;
- Structural technologies based on materials with finely tuned compositional and structural properties for light weight, enhanced strength, and high temperature applications;
- Novel bio-inspired technologies for medical and agricultural applications involving the marriage between biological processes and materials science; and
- Catalytic agents for chemical transformations that can be carried out with safer chemicals, avoiding toxic, flammable or explosive reactions for enhanced safety, environmental protection and energy savings.

These new and refined materials will be used to benefit:

- Manufacturing concerns, from basic structural materials to sophisticated electronic and photonic devices;
- Energy-based industries, for the development and optimization of new technology for energy production and conservation;

Health-related industries and pharmaceutical applications such as directed drug delivery;
Chemical industries with more efficient, safer routes for synthesis and production;
Educational institutions and labs that depend upon the discovery and synthesis of new materials to fuel scientific exploration; but
Ultimately, the beneficiaries of all the technological and scientific advances made possible through fundamental materials research is the American public.

Fundamental Materials Research - Product Line Examples

- Novel Optical Materials:
  Ames has established theoretical research on certain new optical materials slated to become the "optical semiconductors" and "superlenses" of the future.

  Materials Preparation, Synthesis and Processing
  Ames' MPC houses unique synthesis, processing and characterization facilities to enable fundamental research and the development of materials-dependent technologies.

  Magnetic Materials and Correlated Electron Systems
  Potential applications for magnetic molecules include novel designs for magnetic memory, fast switching devices and quantum computing. Ames has a history of success in the areas of magnetic materials and correlated electron systems including the development of new routes to the synthesis of superconducting MgB_2 and in magnetic superconductors and magnetic refrigeration materials.

  Complex Intermetallic Compounds
  Ames is recognized for work in the area of aperiodic crystals and for structural and property investigations of glassy and complex crystalline materials. Complex intermetallic compounds are of fundamental scientific interest in elucidating the nature of interatomic interactions in solids and they have potential in applications ranging from "nonstick" frying pans to agricultural machinery due to their low surface friction, high strength, unusual elastic properties and low thermal and electrical conductivity.

  Catalytic Materials
  Ames is developing novel catalytic materials to gain fundamental chemical and engineering insights about selective oxidation, desulfurization, denitrogenation and dehalogenation reactions. Ames has demonstrated success in the development of silica-based mesoporous catalysts with controlled, nanostructured morphology and surface properties. These systems will have a significant impact on catalysis and will serve in the construction of systems for such diverse tasks as self-healing polymers and drug-delivery vehicles.

Two Major Initiatives in Fundamental Materials Research: 1. Bioinspired Materials and Materials and 2. Materials Discovery Synthesis and Processing

1. Bioinspired Materials

Ames management is directing efforts in material sciences to the synthesis and characterization of novel materials that mimic living systems. These materials possess the ability to switch among several states in response to the environment and self-assemble into structures and are expected to become a very significant part of materials science. Over the next several years, Ames expects to build and strengthen this overall program in support of the DOE mission and in keeping with the future vision for the laboratory. This building process will involve creating teams of bioengineers, theorists, synthetic chemists, biologists and experts in chemical characterization.

Funding plan: Ames plans to grow this initiative in funding modules consisting of $400K/year projects derived from the funding of individual peer-reviewed projects. It is anticipated that the initiative will consist of four such projects at any given time with a total funding for FY2005-FY2010 of $7.9M. This approach will establish a reasonable rate of growth to accommodate the necessary addition of staff and instrumentation.

2. Materials Discovery, Synthesis And Processing

Significant efforts are needed to strengthen U.S. research in design, discovery and growth of novel materials for basic research. Ames has the physical and intellectual infrastructure to lead this DOE materials effort. The proposed funding for this initiative ($7.0 M over 5 years) will enable the Lab to establish new outreach programs and collaborations with universities, laboratories and industry across the country and to increase staffing and add new research programs in the relevant areas. Critical areas in need of attention include coordination of the nation's crystal growing efforts, and providing well-characterized and high quality crystalline samples for facilities including DOE's synchrotron and neutron sources.

Funding plan: The Lab has proposed funding for this initiative ($7.0 M over FY2006-FY2010) to establish new outreach programs and collaborations across the country. The funding will be used to increase staffing in the Lab's programs in materials synthesis, processing and characterization, fund new materials synthesis and processing programs within the MPC, provide opportunities to scientists for visits and training, and increase opportunities for graduate students and postdoctoral scientists from across the U.S. for additional training.

Business Line: Analytical Techniques and Instrument Development

Ames has strengths in development of analytical techniques and instrumentation. Continued scientific and technological advancements will be fueled by the ability to manipulate processes at nanometer length scales. Fundamental insights into factors that affect structure-function relationships and approaches to quantitatively probe these relationships at unprecedented levels of detail are needed. Advances in analytical instrumentation which allow convenient, accurate and rapid analyses of the chemical components of, for example, single cells and the behavior of individual molecules will be essential. There is an ever-increasing need for analytical instrumentation which will allow rapid analyses of massively complex systems such as the thousands of chemicals

in the dynamic cellular compositions in plants and animals, and of the hundreds of various pollutants of our Nation's waterways. Development of analytical instrumentation capable of tackling these tasks will require simultaneous development of systems consisting of integrated separation, analysis and computational units. The customers for these technologies include those engaged in health science research, the emerging biotechnology industry and environmental monitoring services.

Analytical Techniques and Instrument Development - Product Line Examples

- Mass Spectrometer Techniques and Instrument Design
  Ames continues to conduct research in mass spec development and instrument design. These strengths are now being focused on a novel program of mass spectral imaging of plant metabolites in order to map metabolite distributions within plant tissues, which will become an integral part of the Plant Metabolomics Initiative.

- Single-Cell Analysis
  Ames' efforts continue in developing novel techniques to add to the number of cellular components that can be separated and identified. The ability to acquire images of living cells at a high rate and at a resolution below the diffraction limit of light is needed to gain new insights into a variety of biophysical and biochemical processes that are relevant to fundamental cell biology, the diagnosis of diseases, and/or the assessment of the efficacy of treatment.

- Single-Molecule Analyses
  Recent advances in instrumentation have allowed the imaging of individual molecules at time scales characteristic of chemical transformations and enable observation step by step of the progression of single physical or chemical events.

- Electrochemically Modulated Liquid Chromatography (EMLC)
  Ames scientists are developing a new format for performing liquid chromatographic separations: EMLC, which will reduce the time required for chemical separations and allow the use of environmentally benign solvent, water. EMLC is an intriguing variant of high performance liquid chromatography.

- Surface-Enhanced Raman Scattering
  Ames is developing a strategy to overcome issues of low sample throughput and large sample volumes associated with the single assay formats that are barriers to the widespread application of multiple biomarker profiling by applying surface enhanced Raman spectroscopy.

- Solid-State NMR Techniques for Heterogeneous Polymers
  Development and application of this analytical technique is crucial to the success of various Ames projects ranging from biomembranes to catalytic surfaces to heterogeneous polymers, where it can provide information on sizes of domains, heterogeneities, and interfaces below the resolution limit of electron microscopy

Two Major Initiatives in Analytical Techniques and Instrument Development: 1 Distributed Electrostatic Levitation User Facility and 2. Plant Metabolomics

1. Distributed Electrostatic Levitation User Facility

This proposed facility enables an important new class of investigations of the high temperature structure and properties of materials by removing the constraints of containment in vessels. Recent advances in electrostatic levitation (ESL) have made this possible, but the only two ESL units in the U.S. are not available to the growing list of potential users. This initiative involves establishing an ESL User Facility in the Ames MPC, coupled with ESL facilities designed for high-energy x-ray scattering measurements at the APS and neutron scattering measurements at the SNS. Together, the proposed facilities will provide a powerful complement of tools for fundamental studies, the discovery of new metastable phases, and advanced materials manufacturing methods. The facility would be unique in the world and would bolster U.S. dominance in the study of high temperature structure and properties of materials. Ames would serve as the operational base for these facilities with partners at major research universities, industry, other national laboratories and private foundations being actively sought to share in the cost.

Funding plan: The total cost for this effort (3 ESL chambers and associated equipment) is estimated at $12M over a 5 year period. The Lab is actively seeking partners at major research universities, industry, other national laboratories and private foundations to share the cost of the construction and operation of these facilities. In the absence of full funding, the number and sophistication of chambers could be scaled down, but still accommodate pioneering research efforts with some concomitant reduction in efficiency and duty cycle.

2. Plant Metabolomics

It is proposed to combine efforts excellence in analytical chemistry, computational chemistry and virtual reality engineering in Ames with the plant science research at ISU for this initiative. Plant metabolomics is the determination of all of the metabolites (chemical products) in a cell or tissue, and their roles in the genetic, developmental, physiological and environmental activities of the plant. The importance of this field is in articulating the cellular pathways and networks that regulate and define a biological trait or phenomenon. This initiative will culminate in the first comprehensive center for plant metabolic research in the world, a facility having state-of-the-art analytical instrumentation and the source for development of the next generation of instrumentation. This facility will enable interaction of leading chemists, engineers and biological scientists to focus on this multifaceted problem.

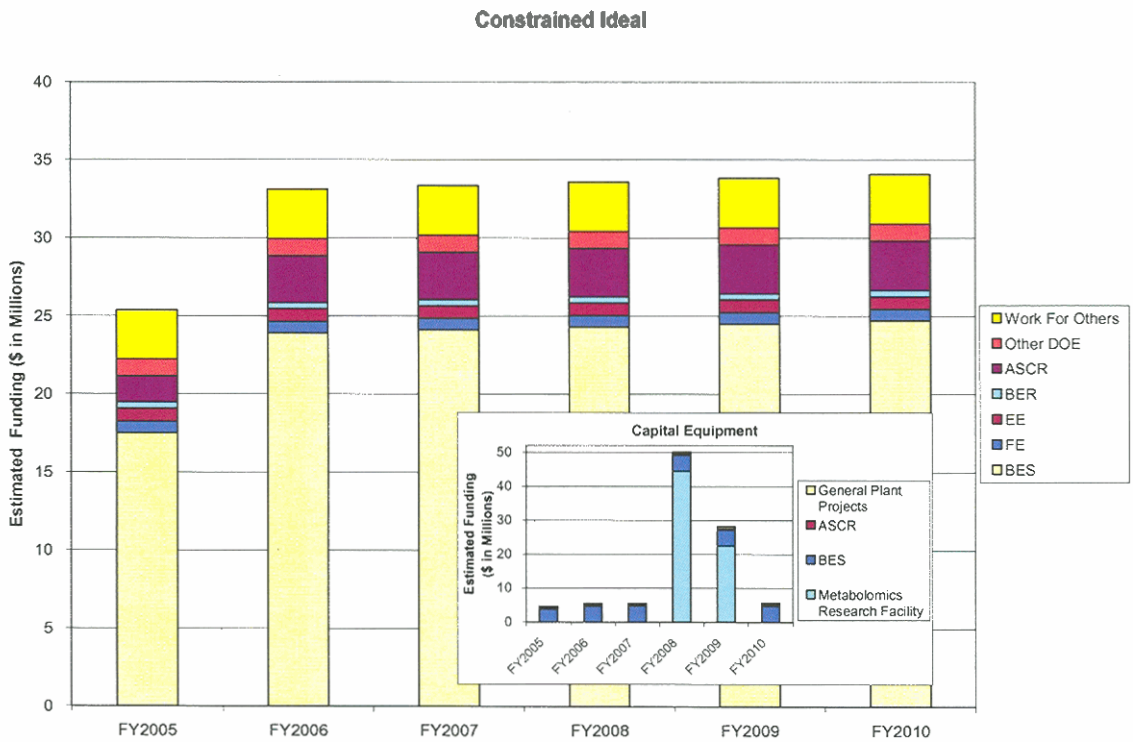
Funding Plan: Funds to be requested of DOE are $37.5M for the proposed building, $19.1M for analytical instrumentation, and $10.5M to equip the computational portion of the facility. If funding for the building is unavailable, the Lab would carry out the instrument development projects in various laboratories in the existing facilities. This would result in a loss of the coherence of the research activities and a loss of crucial human interactions, including the collaborating visitors from academia, industry and government labs.

III. Budget Projections

Ames total funding in FY 2004 was $32.8M and the FY 2005 budget $31.2 M. The Lab's primary DOE customer is SC Basic Energy Sciences, which accounts for about 70% of the Laboratory's total funding. DOE partners outside SC include the Offices of Fossil Energy, Energy Efficiency and Renewable Energy, and Nonproliferation and Verification. The main non-DOE federal partners are the National Institutes of Justice, which has funded the Midwest Forensics Research Center, and the National Institutes of Health.

Table 1 shows the preferred budget scenario based upon the "constrained ideal". Ames envisions the "constrained ideal" scenario to be maintaining the programs of the Lab roughly as is with the addition of the four initiatives fully funded as described above. Under a flat budget projection from FY 2005 levels, the Laboratory would not propose major programmatic changes, but would absorb cuts necessary due to inflation in a roughly homogeneous fashion and would mitigate the effects by increasing efforts to gain funding from other federal sources.

Table 1 Preferred Budget – Based on the "Constrained Ideal"



IV. Management Approach

Organization

The Laboratory operates under a single executive management system to carry out the mission. There are no separate "directorates" based on program support or other designation. The Laboratory Executive Management has the responsibility to fund, operate and manage all facilities and program to accomplish the DOE mission activities. This responsibility extends from the Laboratory Executive Management through the Ames Site Office to the SC.

Workforce:

The workforce for Ames remains relatively stable from year to year and there is no anticipation of major reductions in force or other downsizing over the next five years. Any reductions will likely be from attrition. The projected levels of full time equivalent (FTE) employees over the next five years, (both direct funded research FTEs and total FTEs) based upon the constrained ideal and a flat budget projection are detailed in **Error! Reference source not found.** and Table 3.

Table 3. Personnel. Total Direct Funded Research FTEs.

Budget Scenario	FY2005	FY2006	FY2007	FY2008	FY2009	FY2010
Flat	207.2	201.5	194.1	186.9	180.0	173.2
Constrained Ideal	207.2	254.2	246.8	239.6	232.7	225.9

Table 3. Personnel. Total Laboratory FTEs (both Direct and Overhead funded).

Budget Scenario	FY2005	FY2006	FY2007	FY2008	FY2009	FY2010
Flat	317.0	308.0	292.0	287.0	277.0	266.0
Constrained Ideal	317.0	364.0	357.0	350.0	343.0	336.0

Graduate Program:

A key element of the mission of Ames Laboratory is to train scientific and engineering professionals. Graduate assistants generally represent about 20% of the workforce. Many of the Ames Laboratory researchers hold joint appointments with ISU, serving as faculty advisors and teaching classes. Over 2900 masters and Ph.D. degrees in science and engineering have been awarded to Ames students since 1947.

Personnel Training:

The Ames Training Program provides Laboratory employees with a variety of training and developmental opportunities. The contractor, ISU, provides programs which permit Ames staff members to expand their education and training through formal coursework and other experiences.

Security Posture:

Ames security posture is mature, stable, and well-equipped for future changes in local and national security conditions. The Laboratory has implemented an Integrated Safeguards and Security Management System. The unclassified Design Basis Threat policies were reviewed by DOE. Ames is categorized as Threat Level 4 because of its very limited inventories of: nuclear materials, high hazard chemicals, and sensitive information. Ames continues to maintain an excellent record of protection of facilities and property. Threat Level 4 requirements will continue to be met through Order compliance and administrative controls, as described in the Site Security Plan. The Laboratory has a formalized Cyber Security Protection Program, implemented through dedicated staff and a network of line management representatives equipped with cyber protection tools. Current and future system upgrades and administrative policies are designed to minimize and protect system access points, while ensuring system configurations employ up-to-date protection strategies. The cyber security system is reviewed periodically by DOE.

Integrated Safety Management (ISM):

The Laboratory has a mature and comprehensive ISM system in place that governs all work at Ames. The FY2004 Total Recordable Case (TRC) rate was 1.54 (5 cases) and the Days Away, Restricted or Transferred (DART) rate was 0.62 (2 cases). During FY2005, Ames exceeded the SC goals. The FY 2005 TRC for Ames was 0.62, surpassing the SC goal of 1.10 and the DART was 0.21 surpassing the SC goal of 0.50. Management's commitment to continuous improvement to safety, in addition to a comprehensive and mature Integrated Safety and Environmental Management System provides the basis for a solid safety record at the Laboratory. Ames is planning to continue to improve safety performance with multiple strategies, including: contractual performance measures, readiness reviews, application of internal and external lessons learned, safety walkthroughs by upper management, and strengthening of the concept of line management's responsibility for safety.

Relationships - within the Community, Industry, and with State, Local and Federal Regulators:

The Laboratory maintains public trust and excellent relationships within the local Ames community, with industrial partners, and with federal and state regulators. The Laboratory works to strengthen these relationships through educational outreach activities, and working in partnerships. For example, regulators such as the Iowa Environmental Protection Agency and the Iowa Department of Public Health have worked with the Laboratory on recent joint efforts. Scientists participate in with local school science activities, and the Laboratory jointly hosts both regional middle school and high school science bowls.

Budget, Finance and Resource Management:

The Laboratory continues to provide budget and financial data to the DOE Ames Site Office (AMSO) and the Integrated Service Center (ISC) staff in accounting and finance in a responsive and accurate manner. Ames has an established internal audit program. Systems have been working effectively and DOE rated the Ames performance in budget and finance department as "outstanding" for the past four years. Procurement and property systems are DOE-approved and have also been highly rated by DOE.

V. Infrastructure and Facilities Planning

Ames occupies approximately 325,000 gross square feet in government-owned buildings located on approximately 10 acres of ISU land, leased to the federal government on a long-term (99-year) basis. The facility is integrated into the campus in such a way that ISU provides and maintains the site-wide infrastructure (e.g. heating plant, chilling plant, roads, sidewalks, parking and grounds). The government-owned buildings at Ames are adjacent to, or even physically connected by hallways, to university-owned buildings. Ames has 12 buildings, including three laboratory buildings, one office building, three shop buildings and five storage buildings. There are no temporary structures and all facilities are operational. The last major addition was the construction of the Technical and Administrative Services Building in 1994 that houses most of the management, administrative, and technical support groups of the Laboratory.

The Ames buildings were well-designed and built and have been maintained over their lifetimes such that maintenance problems have not compounded. The average age of the Ames facilities is 37 years. The Laboratory meets the SC goal that all "mission critical" facilities are rated Good or better and all "Mission Dependent", not Critical" facilities be rated Adequate or better. The overall Facility Condition Index (FCI) is 2.6% (good) and is improving (<2% is excellent). This rating has been accomplished with modest maintenance expenditures of approximately 1.5% to 1.7% of replacement plant value. Capital improvement funds have been used judiciously to make betterments to the facility. Many of the high maintenance utility generation and distribution systems are provided and maintained as part of the contractor's campus infrastructure. Maintenance expenditures are evaluated and set in conjunction with other resource requirements to maximize the overall mission effectiveness of the Lab. The condition rating of the facilities is further validated by occupant survey results where 70% of the respondents rate the facilities as "outstanding".

Internal Concerns that May Impact Site Operations:

Ames has identified and documented potential issues of concerns related to environment, safety and health (ES&H) resulting from historical activities. Although the Assistant Secretary for Environmental Restoration and Waste Management (EM) funded the remediation of a closed Chemical Disposal Site (CDS) at Ames during the early 1990's, the uncertainties associated with the long-term stewardship could be a concern for DOE. Another concern is legacy contamination in a DOE-owned laboratory research building. During the late 1940's and early 1950's, research activities involving Thorium-232 and Beryllium were conducted in Wilhelm Hall which generated legacy contamination, which remains in certain interstitial spaces. Characterization studies

indicate that the contamination does not pose a health hazard to current occupants of the building and protective controls are in place. The Laboratory continues to document actions related to legacy contamination and assess alternative approaches to minimize worker exposures and long-term liabilities. Gilman Hall, an ISU-owned building utilized during the late 1940's for Manhattan Project work involving thorium, uranium and beryllium indicates beryllium contamination in limited areas of restricted access mechanical spaces. Ames has established control practices in these areas.

VI. Contractual Management and Configuration

AMSO has direct DOE line responsibility for the administration of the performance-based management and operating contract between the DOE and ISU, operating contractor for Ames. It is the responsibility of the AMSO to ensure that the Laboratory has systems in place to accomplish the assigned mission in a safe and environmentally-sound manner in accordance with the terms of the prime contract. The DOE Contracting Officer's primary responsibilities include work authorization, obligation of funds, and oversight of the contractor's compliance with the contract's terms and conditions. DOE extended the performance-based Contract W-7405-ENG-82 with ISU for two years in December of 2004. The current contract will expire on December 31, 2006 and a competition is underway to select a contractor for the period of January 1, 2007 thru December 31, 2011.

In accordance with the performance-based contract with DOE, ISU is responsible for the management and operation of Ames. This contract requires that DOE establish formal expectations and perform an annual performance evaluation of ISU for the work specified. The annual payment of fee to ISU is contingent on the results of the annual DOE evaluation. ISU and DOE have agreed to use a performance-based management system to measure contractor performance. The parties agreed, to the extent possible, to utilize objective performance measures as the basis against which the contractor's overall performance would be determined. In addition, the parties also agreed that the contractor would conduct an ongoing self-assessment program to assess the effectiveness and efficiency of operational systems and procedures. The DOE SC developed a common set of Performance Goals and Objectives for the SC laboratories, including Ames. The Ames Performance Evaluation and Measurement Plan uses the standardized set of Performance Goals and Performance Objectives and applies weightings to each. AMSO and the HQ program offices, in coordination with the Contractor, developed Performance Measures and as applicable, targets for each Performance Objective. The Performance Measures and Targets identify significant activities, requirements, and/or milestones important to the success of the corresponding Performance Objective and will be the primary means of determining the Contractor's success in meeting the Performance Objective. Since the inception of the performance-based contract in 1995, ISU has been rated highly by DOE. Over the past five years, ISU has been rated at the excellent to outstanding level for both its science and technology programs and operations for Ames. As a result of the contractor's research efforts in the last available rating cycle of CY 2004, a performance rating of "Outstanding" was achieved in the area of Science Programs.