Office of Advanced Scientific Computing Research

State of the Office

Michael R. Strayer
Associate Director

Energy Policy Act of 2005

Advanced Scientific Computing Research Program

The Energy Policy Act (EPAct) of 2005

- **Established Under Secretary of Science position**

- **Requires the Department of Energy (DOE) to:**

  - **periodically review all of the science and technology activities of the Department in a strategic framework that takes into account both the frontiers of science to which the Department can contribute and the national needs relevant to the Department's statutory missions; and**

  - **develop a plan to improve coordination and collaboration in research, development, demonstration, and commercial application activities across Department organizational boundaries**

- **Facilitated the President's American Competitiveness Initiative (ACI) and Advanced Energy Initiative (AEI) in the FY 2007 request**

Under Secretary for Science

Advanced Scientific Computing Research Program

On May 26th, Ray Orbach was confirmed in his new position as Under Secretary for Science

  – Is currently "dual-hatted" as Acting Director of the Office of Science.

Secretary of Energy Bodman, in his July 3, 2006 Memorandum for the Under Secretary for Science stated that,

"the primary responsibility of the Under Secretary for Science is to advance the science portfolio at the Department of Energy and to strengthen the contributions of science to all of the Department's activities in collaboration with the Under Secretary and the Under Secretary for Nuclear Security."

Under Secretary for Science Role and Responsibilities

Advanced Scientific Computing Research Program

According to EPAct Section 1006(4), The Under Secretary for Science shall—

- **serve as the Science and Technology Advisor to the Secretary**

- **monitor the research and development programs of the Department**

Role and Responsibilities (cont.)

Advanced Scientific Computing Research Program

- **advise the Secretary with respect to**
  - **any undesirable duplication or gaps in the programs**
  - **the well-being and management of the multipurpose laboratories under the jurisdiction of the Department**
  - **education and training activities required for effective short- and long-term basic and applied research activities of the Department;**
  - **grants and other forms of financial assistance required for effective short- and long-term basic and applied research activities of the Department**
  - **long-term planning, coordination, and development of a strategic framework for Department research and development activities**
- **carry out such additional duties assigned to the Under Secretary by the Secretary relating to basic and applied research**

Under Secretary for Science (cont'd.)

Advanced Scientific Computing Research Program

- **Is involved in all aspects of the science mission of the Department, including the science functions of NNSA.**

- **Identifies crosscutting research areas between the Office of Science and the Department's applied programs.**

- **Is committed to maintaining the integrity of the basic and applied research programs in the Department.**

- **Will work to improve the coupling between basic and applied research and to strengthen applied research programs.**

FY06 DOE Program Reviews (Energy Policy Act Report 994)
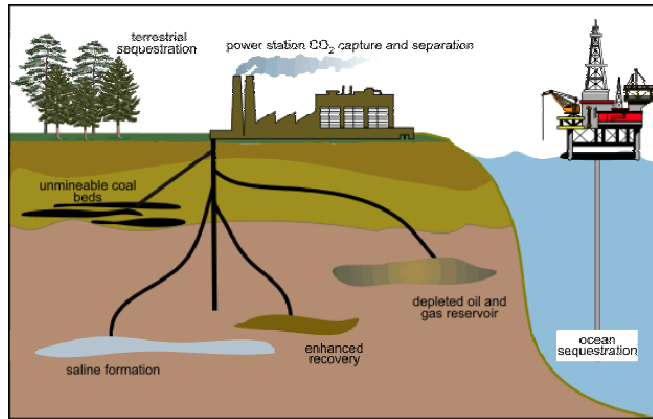
Advanced Scientific Computing Research Program

- Crosscutting Issues
  - **Radiation-Resistant Materials**
  - **Energy Storage**
  - **Advanced Mathematics for Optimization of Complex Systems, Control Theory, and Risk Assessment**
  - **Building Synergies With Work-for-Others, Laboratory Directed Research and Development (LDRD), and DOE University-Sponsored Research**

Advanced Mathematics for Optimization

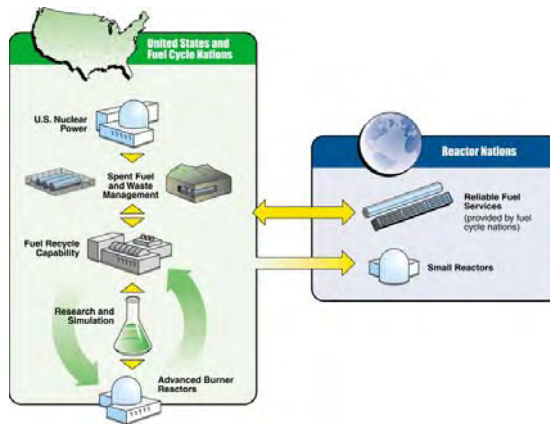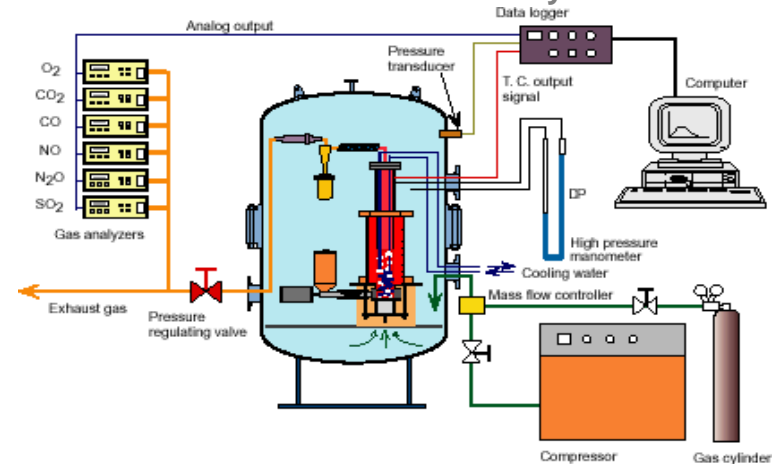**Advanced Scientific Computing Research Program**

Carbon Sequestration

Electric Power Grid

Nuclear Power Systems (GNEP)

Advanced Combustion Systems

Examples of Collaboration and Coordination

Advanced Scientific Computing Research Program

– **Advanced nuclear energy systems in support of the Global Nuclear Energy Partnership (GNEP)**

– **Alternative energy, including genomic approaches to cellulosic ethanol and solar to fuels processes**

– **Hydrogen**

– **Materials for fission, fusion, energy storage, superconductivity, and combustion**

– **High-performance computing across the government**

– **Carbon sequestration and understanding the terrestrial carbon cycle**

Workshop on Simulation and Modeling for Advanced Nuclear Energy Systems

Co-sponsored by

Office of Nuclear Energy

Office of Advanced Scientific Computing Research

U.S. Department of Energy

Context

Advanced Scientific Computing Research Program

- **One of three August workshops sponsored by DOE in support of the Global Nuclear Energy Partnership (GNEP)**
- **15-17 August (Tue-Thu) in Washington DC**
  - **Half-day of plenary presentations**
  - **Day-and-a-half of parallel breakouts for approximately 80 specifically recruited participants, plus others**
  - **Preliminary reports drafted on third day by breakout leaders**
- **Output – Report outlining modeling and simulation challenges for Nuclear Energy Research**

Charge

Advanced Scientific Computing Research Program

"Conduct a workshop to obtain community input on the role of computational science and high performance computing in the advanced fuel cycle initiative. Explore the entire spectrum of opportunities, both short and long term. Ensure close coupling of the workshop discussions and activities to the science and engineering needs of the Office of Nuclear Energy (NE). Reference the workshop findings and recommendations to both those NE needs as well as to current and expected future capabilities of the Office of Science, and in particular, its Office of Advanced Scientific Computing Research (ASCR). Prepare a preliminary letter report within one week of workshop completion and follow with a full report within 30 days of workshop completion."

Overall goals

- **For the "enabling technologists"**
  - **Learn driving issues, vocabulary, and needs of the applications researchers**
  - **Communicate opportunities and imperatives to migrate to relevant state-of-the-art computational practices (*algorithms, software, hardware* – as brought together in applications-oriented frameworks and demonstrated, e.g., in SciDAC and ASC)**

- **For the applications researchers**
  - **Communicate the driving issues and identify known computational science challenges**
  - **Learn what expertise and infrastructure is available already, from related computational applications**

Advanced Scientific Computing Research Program

ASCR

U.S. Department of Energy

Office of Science
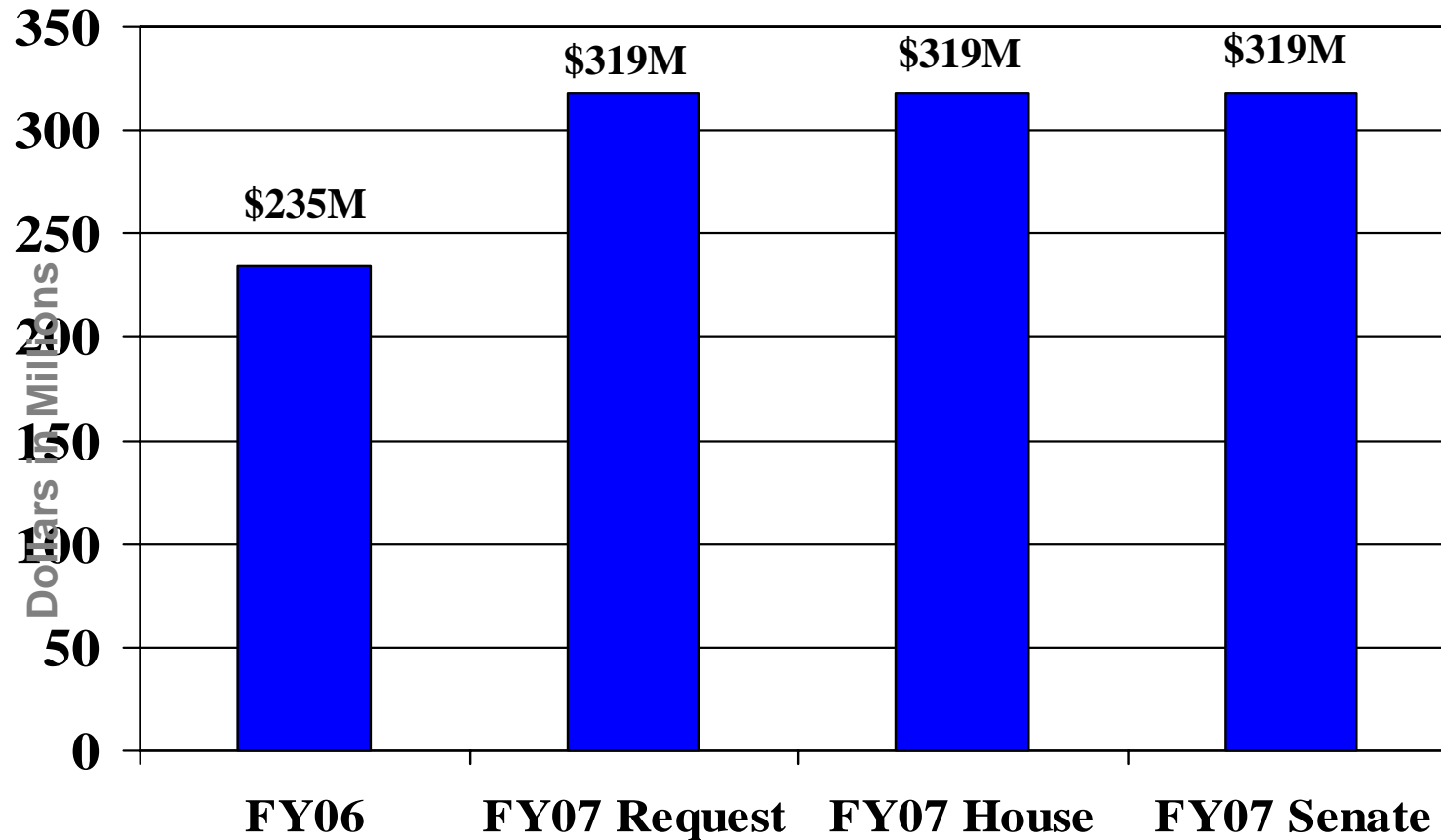
FY 2007 - House

Advanced Scientific Computing Research Program

FY 2007 House Energy and Water Development Appropriations Bill passed both the Appropriations Committee and the House

Report language:

> " *The Committee commends the Office of Science and the Office of Advanced Scientific Computing Research for their efforts to provide cutting-edge capabilities to meet current scientific computational needs, and at the same time to extend the boundaries of that cutting edge into the next generation of high-performance scientific computers and supporting software."*

FY 2007 - Senate

Advanced Scientific Computing Research Program

FY 2007 Senate Energy and Water Development Appropriations Bill passed the Appropriations Committee

Report language

"...*The Committee is concerned with the relationship between the Office of Science and the NNSA. As an example, the ASCR strategic plan discusses the need to work with other Federal agencies including several defense agencies, but only discusses in general terms three areas of research where NNSA and the Office of Science cooperated. In the area of basic research,* the strategic plan states that it is an area that is `not important enough to justify ASCI investment at this time.' *The Committee is also aware that the Office of Science has budgeted $13,000,000 for the DARPA to support a petaflop computer deployment by 2010. The Committee believes this funding would be better spent within the Department to support a petaflop initiative.* The Department is directed to divide the funds equally between the Office of Science and the NNSA Advanced Simulation and Computing activities to support development of component architecture for high-performance software and storage"

FY 2007 ASCR Budget Current Status

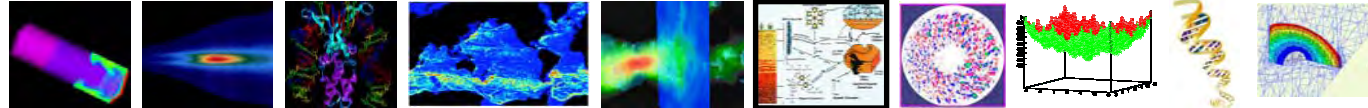**Advanced Scientific Computing Research Program**

- It appears increasingly likely that the Department will be operating under a continuing resolution (CR) for part of FY 2007.

- The effects of any CR depend on how it is drafted. We will need to quickly assess the CR to see how they may affect the implementation of the President's ACI and AEI.
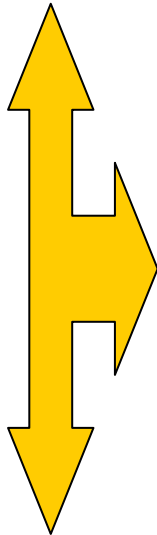
Path to Petascale

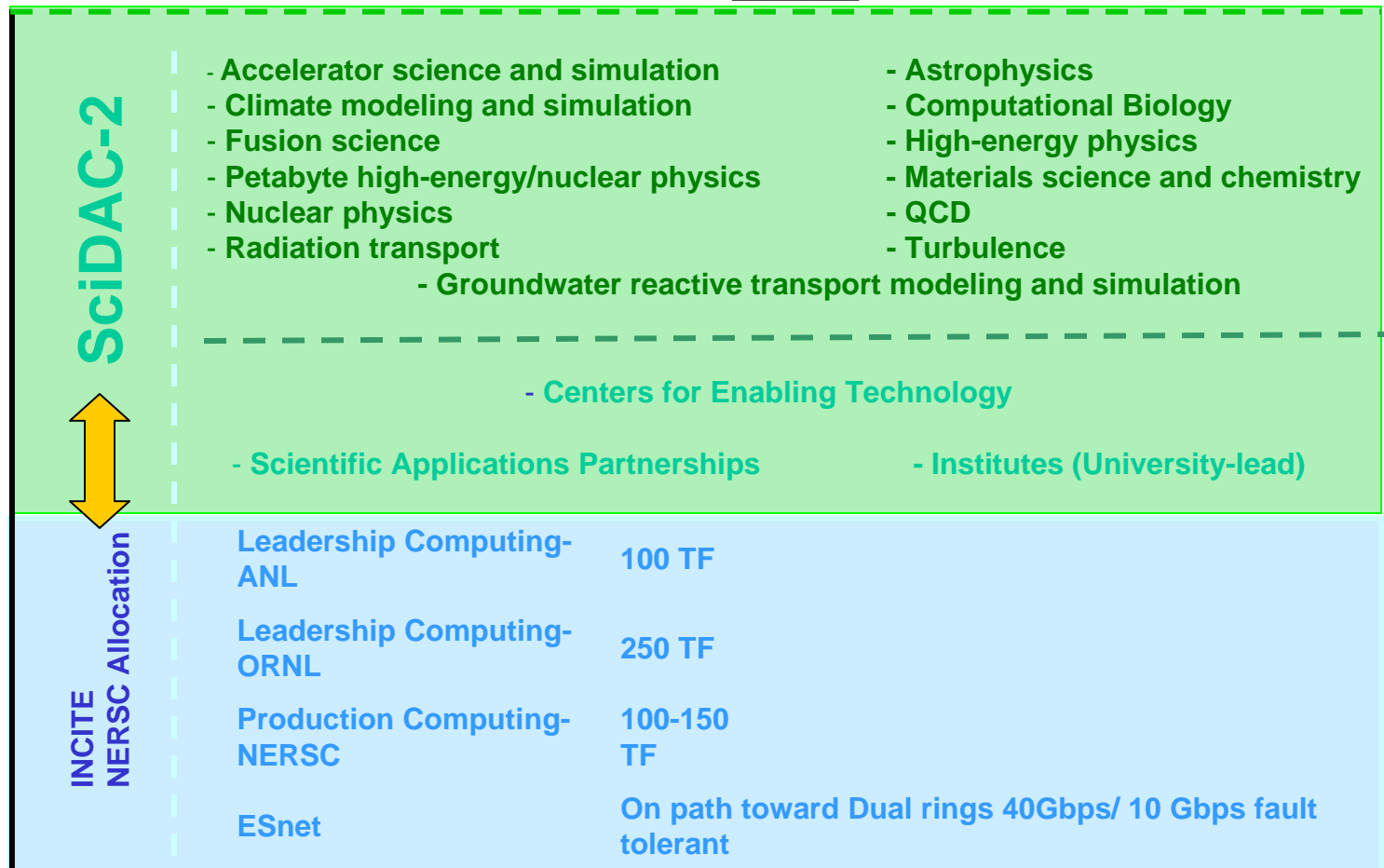**Advanced Scientific Computing Research Program**

Scientific Discovery

Applications

SciDAC-2

- Accelerator science and simulation
- Climate modeling and simulation
- Fusion science
- Petabyte high-energy/nuclear physics
- Nuclear physics
- Radiation transport
- Astrophysics
- Computational Biology
- High-energy physics
- Materials science and chemistry
- QCD
- Turbulence
- Groundwater reactive transport modeling and simulation

- Centers for Enabling Technology

- Scientific Applications Partnerships

- Institutes (University-lead)

Computing/ Networking

INCITE NERSC Allocation

Leadership Computing-ANL	100 TF
Leadership Computing-ORNL	250 TF
Production Computing-NERSC	100-150 TF
ESnet	On path toward Dual rings 40Gbps/ 10 Gbps fault tolerant

Facilities Update

Advanced Scientific Computing Research Program

- **NERSC – delivery of NERSC-5 in FY 2007**

- **LCF at ORNL –**
    - **Upgrade Cray XT3 upgrade**
        - **Now: 25Teraflop → 50Teraflop**
        - **By the end of 2007: 50Teraflop → 250Teraflop**
    - **Acquire 1 Petascale Cray Baker system by end of 2008**

- **LCF at Argonne –**
    - **Acquire 100 Teraflop IBM Blue Gene/P in FY2007**
    - **Upgrade to 250-500 Teraflop IBM Blue Gene/P in 2008**
    - **On path to a Petascale IBM Blue Gene /Q by end of the decade**

Because of cost thresholds, ASCR's facility acquisitions and upgrades will under recently signed DOE Order 413.3A, *Program and Project Management for the Acquisition of Capital Assets*

Innovative and Novel Computational Impact on Theory and Experiment- INCITE

**Advanced Scientific Computing Research Program**

- Initiated in 2004
- Provides Office of Science computing resources to a small number of computationally intensive research projects of large scale, that can make high-impact scientific advances through the use of a large allocation of computer time and data storage
- Open to national and international researchers, including industry
- No requirement of DOE Office of Science funding
- Peer-reviewed
- 2004 Awards: 4.9 Million processor hours at NERSC awarded to three projects
- 2005 Awards: 6.5 Million processor hours at NERSC awarded to three projects

INCITE 2006

Advanced Scientific Computing Research Program

Wired Magazine, August, 2006, pg. 42
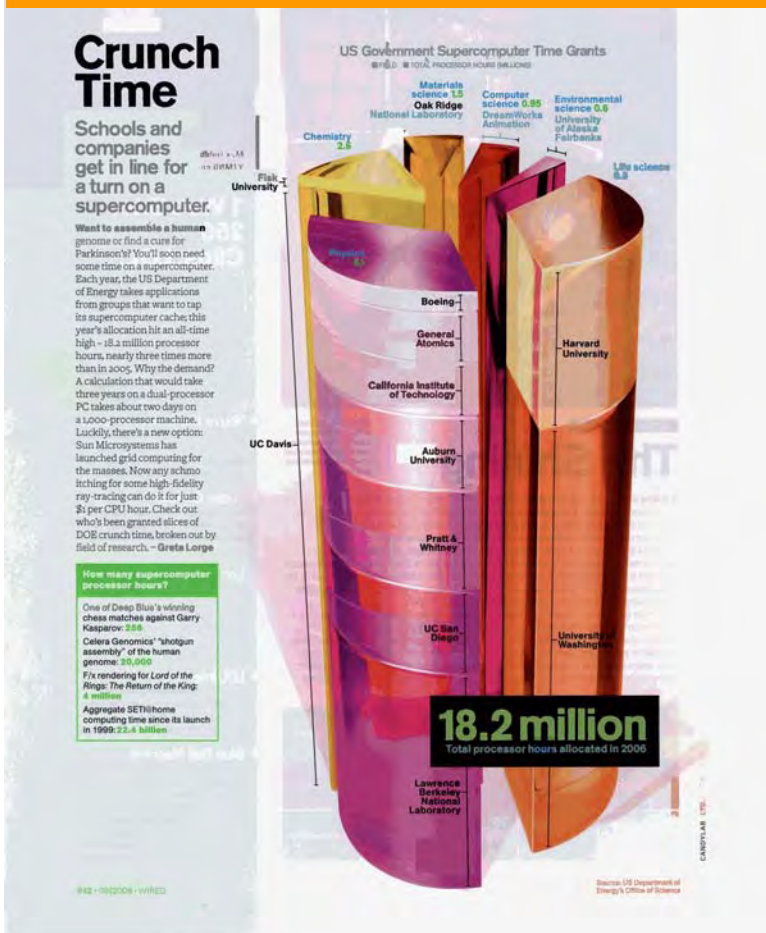
- **Expanded to include SC high end computing resources at PNNL, ORNL and ANL in addition to LBNL and multiple year requests.**

- **Received 43 proposals requesting over 95 million processor hours.**
  - **60% from Universities**
  - **40% had funding from other federal research agencies**

- **15 Awards for over 18.2 million processor hours**

INCITE 2007

Advanced Scientific Computing Research Program

- **Expanded in 2007 to include 80% of resources at Leadership Computing Facilities in addition to 10% of NERSC and 5% of PNNL**
- **Call issued July 27, 2006**

http://hpc.science.doe.gov

- **Proposals due September 15, 2006**
- **Award announcements in mid-December**

Advanced Scientific Computing Research Program

Staffing

ASCR Staffing

Advanced Scientific Computing Research Program

	FY1996	FY2001	FY2006
Budget	$118M		$235M
Program Attributes	• Base Research • ACRTs • NERSC • ESnet		• Base Research • R&E Testbeds • SciDAC-2 • NERSC ESnet • LCF (at ORNL; at ANL in FY2007)
Staff			
Federal	13	10	Current: 10 End of FY 06: 14
IPAs	2	3	Current: 3 End of FY 06: 4
Detailees	1	0	Current: 3 End of FY 06: 4
Total	16	13	**Current: 16 End of FY 06: 22**

Duties and Responsibilities Acquired Since FY1996

IT Reporting	**Performance Measures**
New Program Activities	**Budget growth**
Advisory Committee	**Peer review of laboratory activities (research and facilities)**
Laboratory Annual Appraisals	