Office of Advanced Scientific Computing Research

State of the Office

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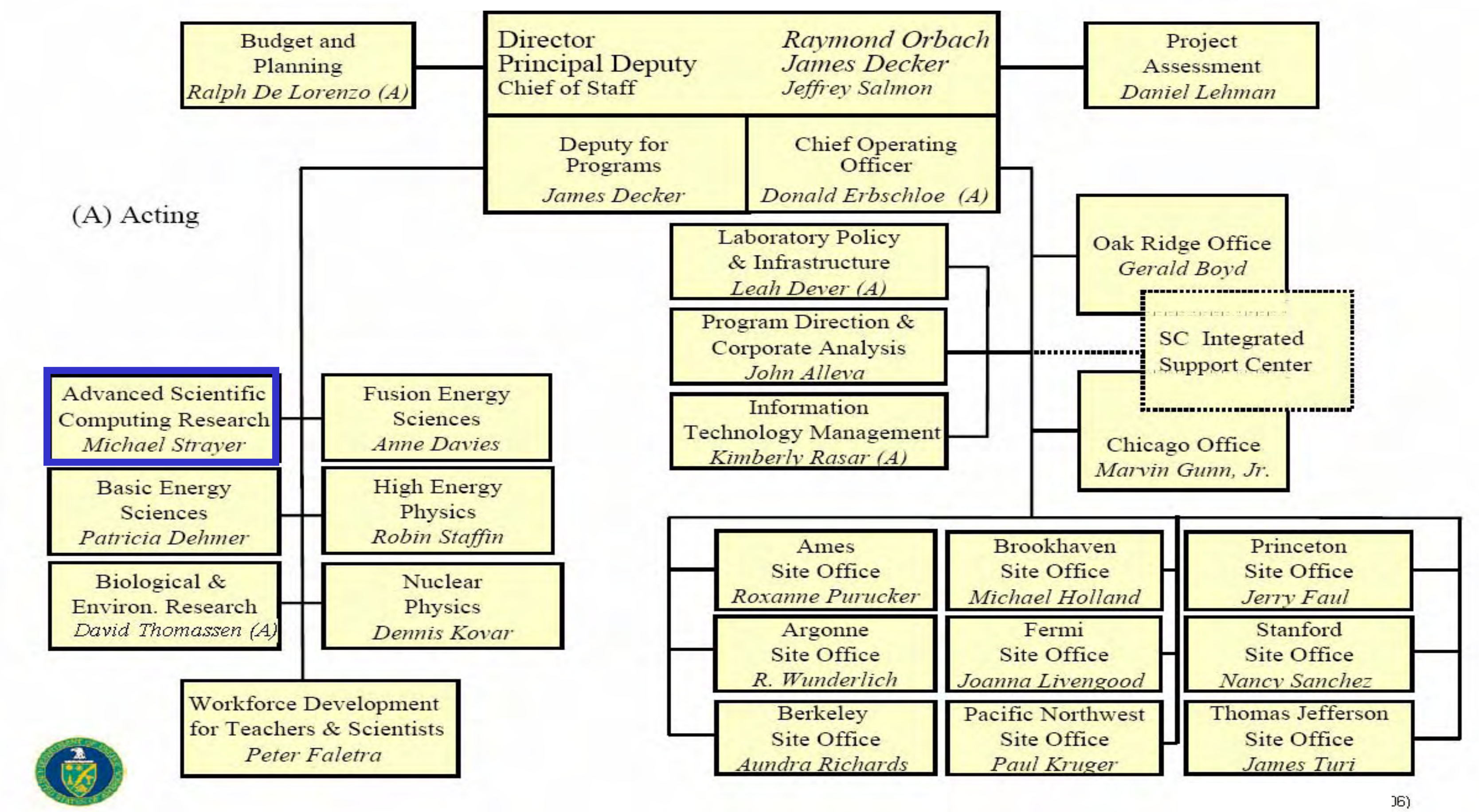
Associate Director

U.S. Department of Energy

Office of Science

Office of Science

Advanced Scientific Computing Research Program



Mission

Secretary Samuel Bodman, House Committee on Science Hearing, February 15, 2006

"The Office of Science plays a critical role in ensuring America's scientific leadership and economic dynamism…"

The mission of the Science program is to deliver the discoveries and scientific tools that transform our understanding of energy and matter and advance the national, economic, and energy security of the United States.

In support of it's mission, the Science program has responsibilities in three main areas: selection and management of research; operation of world-class, state-of-the-art scientific facilities; and design and construction of new facilities.

"Investment in these facilities is much more than bricks and mortar: it is an investment in discovery, and in the future of our nation."

American Competitiveness Initiative

In the President's State of the Union Address on January 31, 2006, President Bush stated,

"I propose to double the federal commitment to the most critical basic research program in the physical sciences over the next ten years. This funding will support the work of America's most creative minds as they explore promising areas such as nanotechnology, supercomputing, and alternative energy sources."

Secretary Bodman, Ibid

"Developing revolutionary, science-driven technology is at the heart of the Department of Energy's mission. To ensure that America remains at the forefront in an increasingly competitive world, our Department is pursuing transformational new technologies in the cutting-edge scientific fields of the 21st century—areas like nanotechnology, material science, biotechnology, and high-speed computing."

Vision

First in Computational Science

"Best in class in advancing science and technological through modeling and simulation"

Facilities

Enabling Technologies

Computational Partnerships

Scientific Discovery

"In the last decade the power of computation - our ability to model and simulate experiments that we have not conducted in a laboratory – has become so great that it must now be considered a third pillar, along with theory and experiment, in the triad of tools used for scientific discovery." ***Dr. Raymond L. Orbach, SciDAC Review, spring, 2006***

"SciDAC is unique in the world….There isn't any other program like it anywhere else, and it has the remarkable ability to do science by bringing together physical scientists, applied mathematicians, and computer scientists who recognize that computation is not something you just do at the end…" ***Dr. Raymond L. Orbach, SciDAC Review, spring, 2006***

"SciDAC, together with ASCR facilities, could provide powerful resources and the nexus of a new global village for computing that could take computational science and scientific discovery to wholly new levels."

20 Year Outlook

Facilities for the Future of Science: A Twenty-Year Outlook 2

Facilities for the Future of Science:
A Twenty-Year Outlook

Contents

Facilities

- Upgrade the Oak Ridge Leadership Computing Facility to provide more than 250 teraflops peak capability by the end of FY 2007, and 1,000 teraflops by the end of FY 2008

- Acquire a 100 teraflop IBM Blue Gene P high-performance computer system at the Argonne National Laboratory in FY 2007, creating the Argonne Leadership Computing Facility, and increasing to a capability in the range of 250–500 teraflops by the end of FY 2008

- Upgrade NERSC to a peak capacity in the range of 150 teraflops by the end of FY 2007, and to 500 teraflops peak capacity by the end of the decade

- Evolve ESnet over a 5 year period to dual backbone rings at 40 Gb/sec with fault tolerant 10 Gb/sec connections to most major SC laboratories and higher bandwidth connections to NERSC, the LCFs, and other sites with exceptional data requirements

Research

- Research efforts in applied mathematics and computer science are focused and strengthened to deliver the operating systems, programming models, software tools, and mathematical algorithms and libraries needed for scientists to make effective use of petascale computing

- The Scientific Discovery through Advanced Computing (SciDAC) program, will strengthen activities at the software centers initiated in FY 2006 for petascale computing. In addition, SciDAC will initiate research investments in applied mathematics and computer science to accelerate efforts in modeling and simulation on the petascale computing facilities

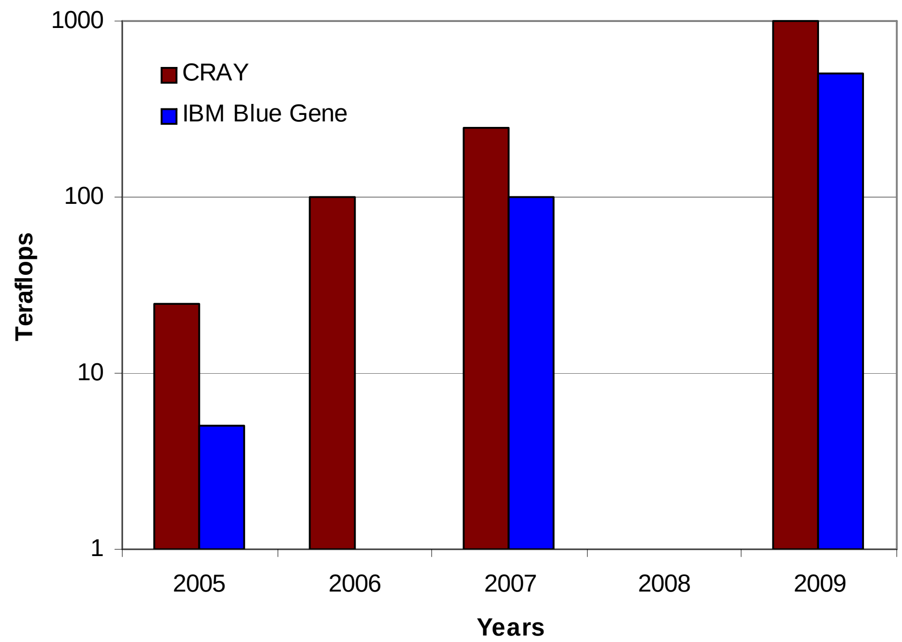
- The Research and Evaluation Prototype effort will be coordinated with the National Nuclear Security Administration (NNSA) and focused on the Defense Advanced Research Projects Administration (DARPA) High Productivity Computing Systems (HPCS) program partnership

Road to Petascale Computing

Plan for LCF

Identify problems that can effectively utilize petascale computing

Currently, *most* applications scale to 1,000 processors, *some* scale to 10,000 processors, and a *few* will scale to 100,000 processors

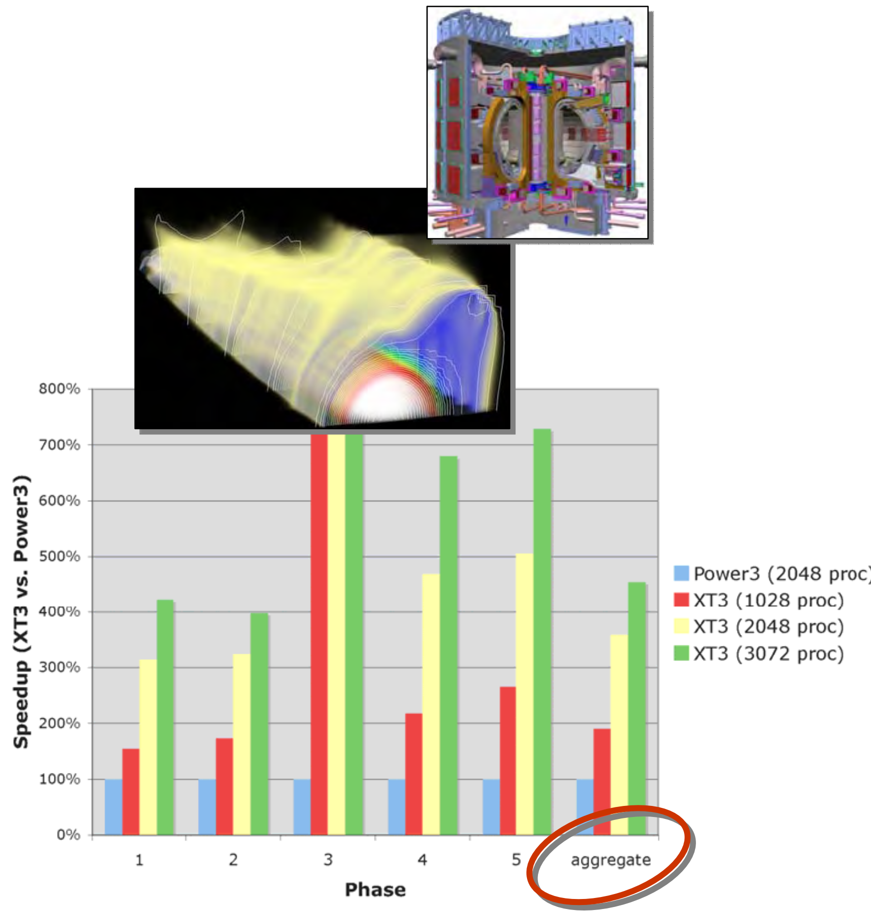


Road to Petascale Computing

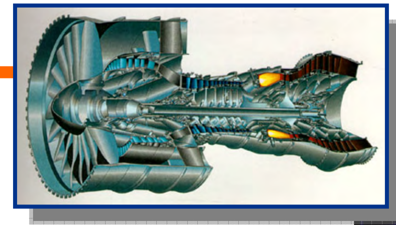
Fusion

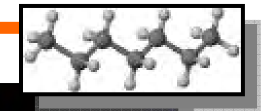
Largest plasma wave simulation for fusion based research

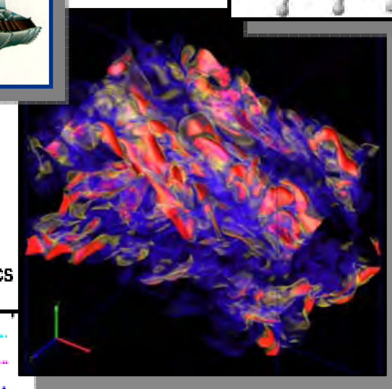
Using 4,096 processors of Cray XT3 at LCF (ORNL) largest, most-detailed simulation ever done of plasma control waves in a tokamak, the reactor that will eventually form the core of the multinational ITER reactor



Road to Petascale Computing



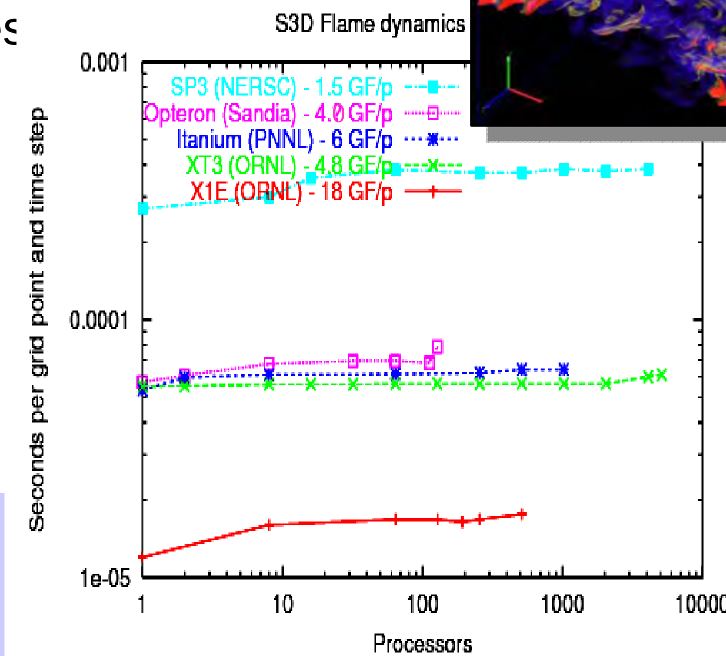




Combustion

Underlying science for improved fuel efficiency of gas turbines and technologies for transportation

Petascale computing will enable simulations in parameter spaces relevant to engines



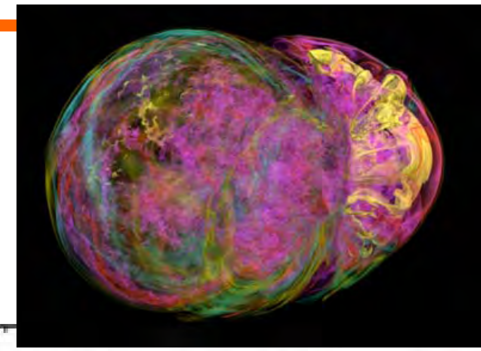
A 50% increase in efficiency of automobiles could save 21% of U.S. oil consumption for *transportation*

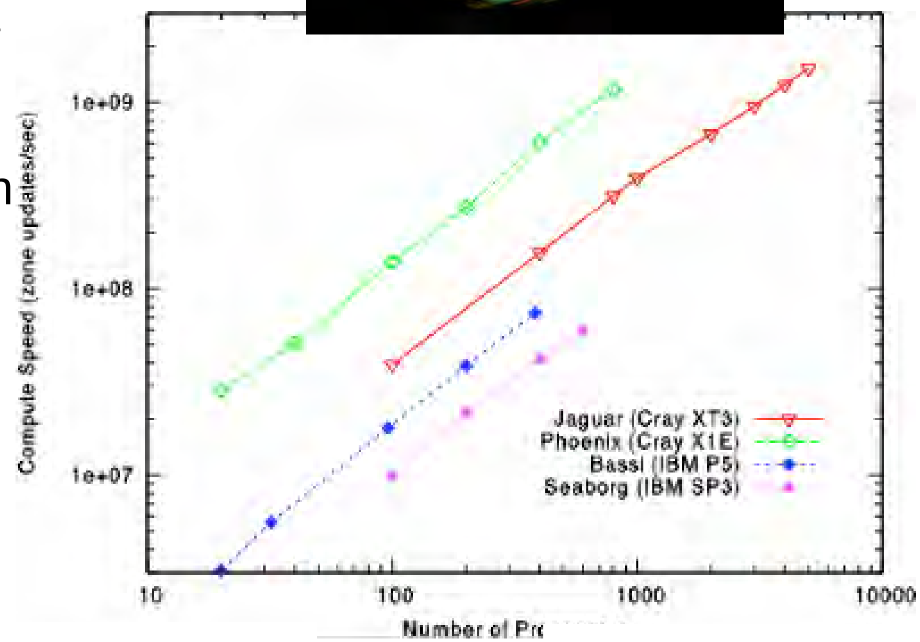
Road to Petascale Computing

Astrophysics

Discovery of a new instability important to core collapse supernovae – the supernova shock wave instability (SASI) and a plausible mechanism for generating the initial neutron star spin required to give birth to pulsars

10 TF: Hydrodynamics only
100 TF: Multifrequency neutrino transport
1 PF: Multifrequency and multiangle neutrino transport *(pin down explosion mechanism and all observables)*





Road to Petascale Computing: Modeling for Reactor Design

Researchers at Argonne National Laboratory recently developed a *Portable, Extensive, Toolkit for Scientific* (PETSc) numerical library used in dozen of scientific applications world-wide.

PETSc encapsulates the complexity of underlying parallel algorithms and presents them in terms of numerical abstractions familiar to scientists. It has been used to extend fully compressible flow codes, most notably the *pressure-oriented implicit continuous Eulerian* (PCICE) scheme developed at INL.

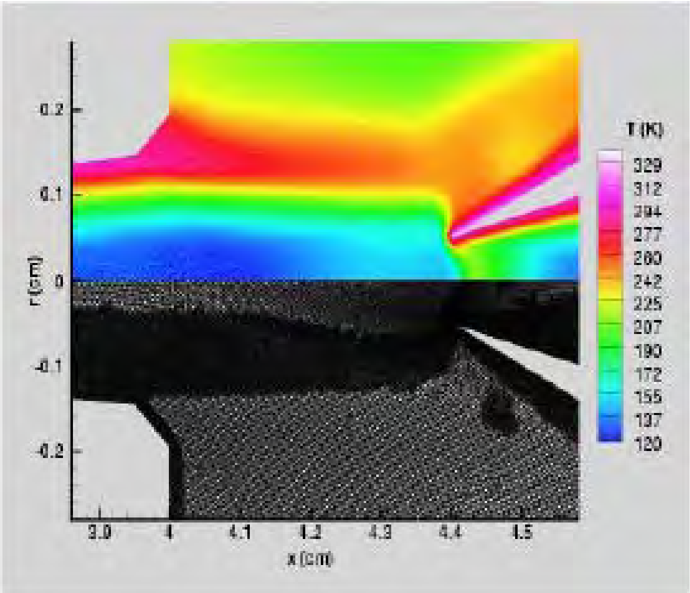
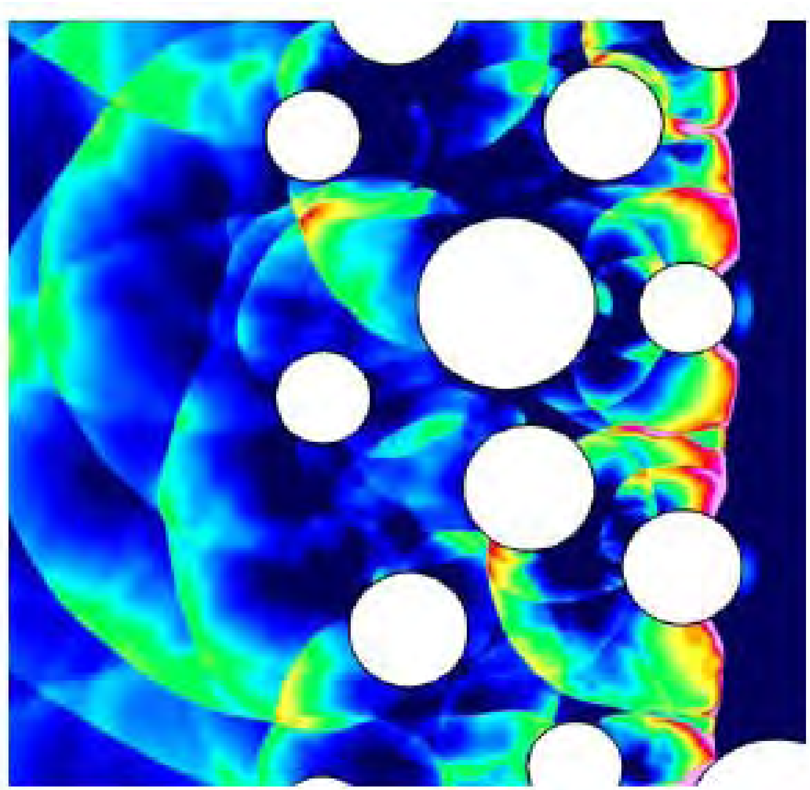


Figure 1. Temperature distribution obtained with PCICE in a nozzle subject to flow through it. Courtesy of Richard Martineau, INL.

Road to Petascale Computing

Researchers at Lawrence Livermore National Laboratory recently develop a suite of fast and scalable adaptive algorithms for modeling the interaction between fluids and embedded solid particles. Accurate simulations moving particles immersed in fluid or gas is computationally challenging.

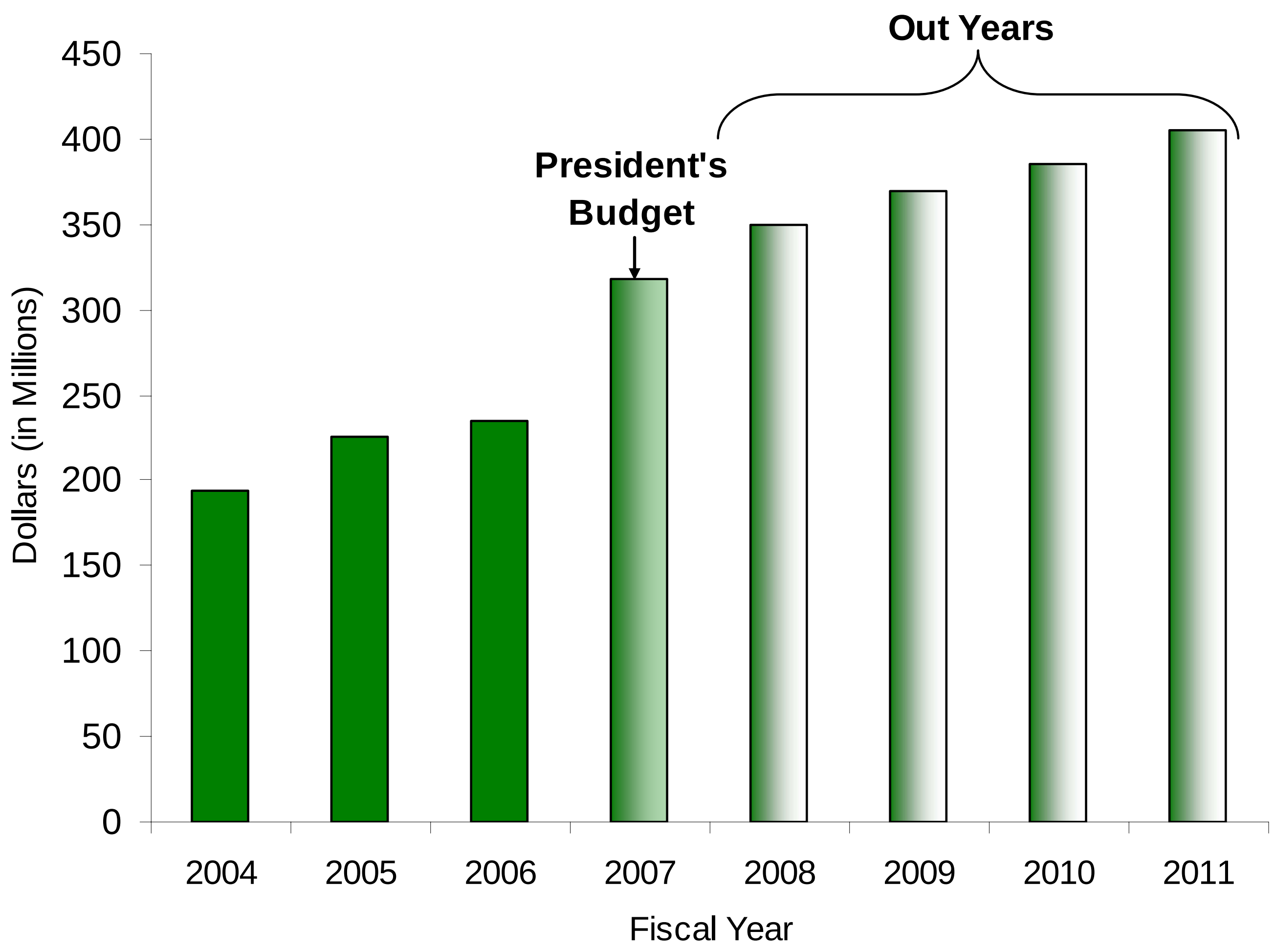
This new algorithm based domain decomposition approach combines locally optimal representation of the dynamically evolving regions occupied by fluids.



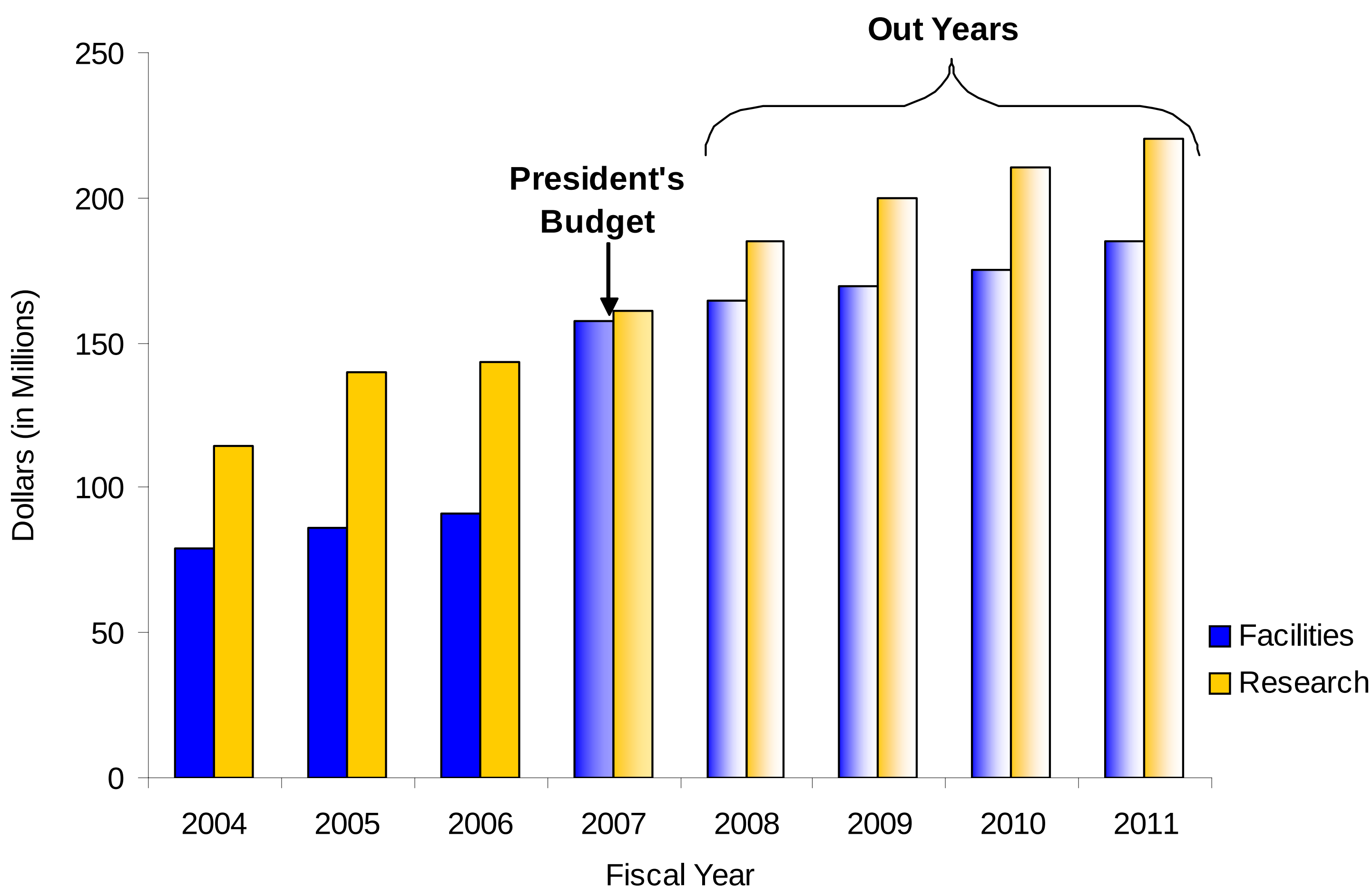
Research Opportunities Distributed Network Environment

- **Distributed Data Management**
  - Gigabit networks and services for interconnecting data analysis and management centers associated with Petascale computers and with experiments generating massive datasets
- **Cybersecurity**
  - accelerate the development of approaches for operational cybersecurity
  - Scalable distributed authentication and authorization systems
- **End-to-End performance**
  - Inter-domain interfaces and issues
- **High performance middleware**
  - Network caching and computing
  - Fault tolerance and error handling
- **Partnerships**
  - Exploit collaborations among scientists and network/middleware researchers to increase scale and productivity of science in areas like bioinformatics and nanotechnology
  - Integrated testbeds and networks

ASCR Budget Comparison FY 2004 – FY 2011



ASCR Budget Comparison: Facilities and Research

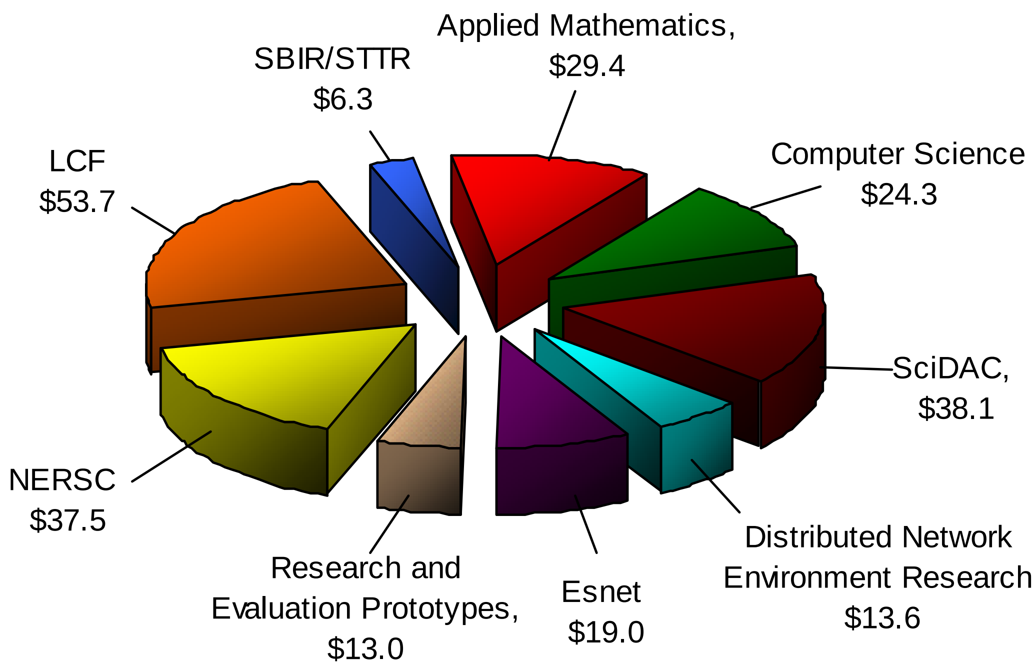


ASCR Budget

B/A (dollars in thousands)

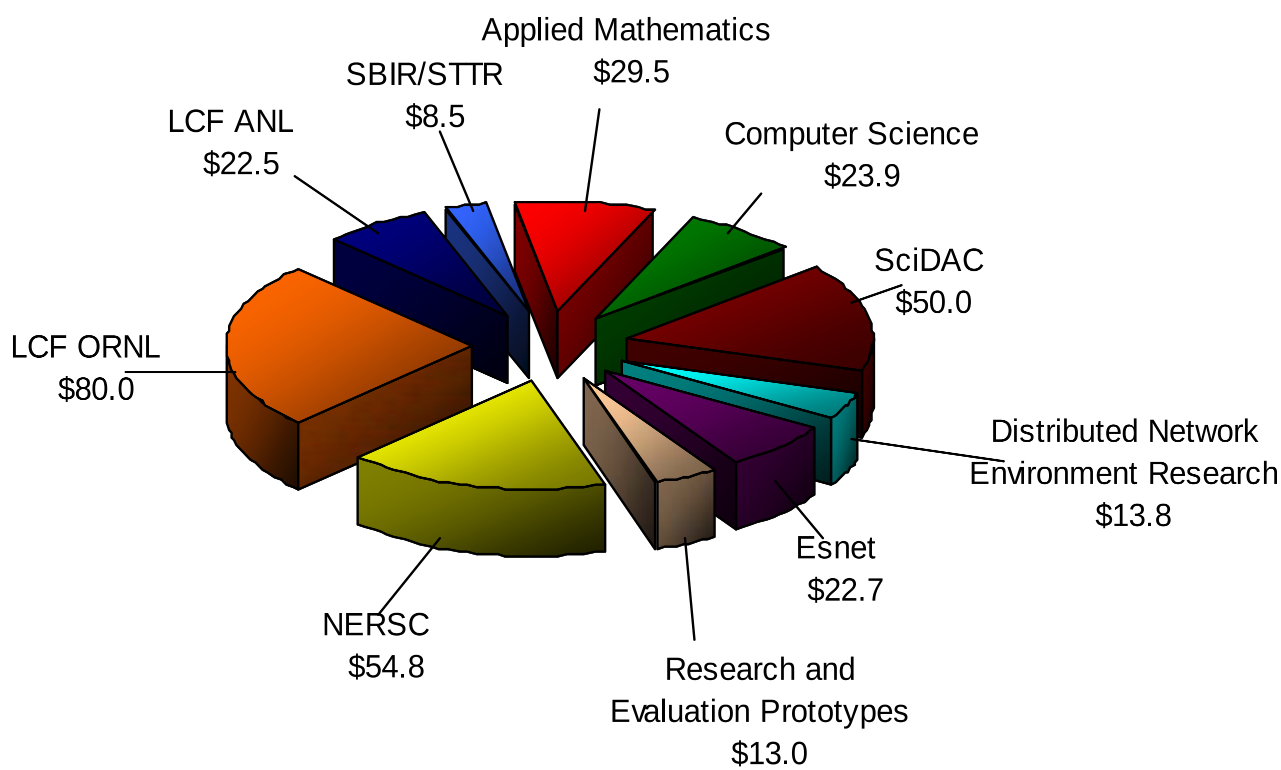
	FY 2006 Approp.	FY 2007 Request	FY 2008	FY 2009	FY 2010	FY 2011
User Facility Operations	91,191	157,294	164,790	169,790	174,790	185,000
Research	143,493	161,360	185,210	200,210	210,210	220,000
Total, ASCR	234,684	318,654	350,000	370,000	385,000	405,000

FY 2006 ASCR Budget



FY 2007 ASCR Budget Request

Advanced Scientific Computing Research Program



The Power of Partnerships
Today and Tomorrow

Advanced Scientific Computing Research Program

ASCR

BES	Methane Flames	Diesel Combustion Ultrafast Science
BER	GCM Performance	Clouds Simulation of Microbes
FES	Plasma Core	Full Simulation of Burning Plasma
HEP	Weak Matrix Elements	Increased Accuracy
NP	Performance of Supernova codes Accelerator Design	Elements beyond Fe LCLS System Design
NE	Neutron Transport	Advanced Fuel Cycles
EM		Groundwater Transport
NNSA	Libraries & Algorithms	Science Based Materials
Industry	Improvements in Mesh Generation	Virtual Prototypes

Role of Advisory Committee

- Meetings of the full committee are public
- Provide advice to the office
  - By means of written reports
  - In response to charges
- Reports written by sub-panels
  - Due two weeks before voting
  - All sub-panel members need not be members of ASCAC
  - Interim report (outline) due at the ½ way point
- Full meeting discusses reports and accepts or rejects by vote
- ASCR office supports the activities of the Committee
- There are currently two charges

Performance Measurement

CHARGE #1

The sub-panel should weigh and review the approach to performance measurement and assessment at these facilities, the appropriateness and comprehensiveness of the measures, and the science accomplishments and their effects on the Office of Science's science programs. Additionally, the sub-panel should consider the evolution of the roles of these facilities and the computational needs over the next three – five years, so that SC programs can maintain their national and international scientific leadership.

In addition to the above, the sub-panel is asked to provide input for the Office of Management and Budget (OMB), evaluation of ASCR progress towards the long-term goals specified in the OMB Program Assessment Rating Tool (PART). See attachment. Note that the OMB guidelines specify ratings of excellent, good, fair, poor, or not acceptable. In addition to these ratings, comments on observed strengths or deficiencies in the management of any component or sub-component of ASCR's portfolio and suggestions for improvement would be very valuable.

Interim report due: July 30, 2006
Draft report due: October 30, 2006

ESnet

CHARGE #2

The sub-panel should weigh and review the organization, performance, expansion, and effectiveness of the current operations of ESnet. The sub-panel should consider the proposed evolution of ESnet, its appropriateness and comprehensiveness in addressing the data communication needs of SC that will enable scientists nationwide to extend the frontiers of science. Furthermore, the sub-panel needs to make suggestions and recommendations on the appropriateness and comprehensiveness of the networking research programs within ASCR with a view towards meeting the long-term networking needs of SC.

Interim report due: October 30, 2006
Draft report due: October 30, 2007

ASCR Staffing

	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	10
IPAs	2	3	3
Contractor	1	0	1
Total	16	13	13

Duties and Responsibilities Acquired Since FY1996

IT Reporting

New Program Activities

Advisory Committee

Laboratory Annual Appraisals

Performance Measures

Budget growth

Peer review of laboratory activities (research and facilities)