OFFICE OF CYBERINFRASTRUCTURE $220,080,000

The FY 2009 Budget Request for the Office of Cyberinfrastructure (OCI) is $220.08 million, an increase of $34.75 million, or 18.8 percent, over the FY 2008 Estimate of $185.33 million.

Office of Cyberinfrastructure Funding
(Dollars in Millions)

	FY 2007 Actual	FY 2008 Estimate	FY 2009 Request	Change over FY 2008 Estimate Amount	Percent
Cyberinfrastructure	$182.42	$185.33	$220.08	$34.75	18.8%

The Office of Cyberinfrastructure supports research, development, acquisition and operation of advanced shared and connecting cyberinfrastructure that enables otherwise unrealizable advances in 21st century science and engineering research and education. OCI capitalizes on a broad range of fundamental scientific research support by the Computer and Information Science and Engineering (CISE) Directorate as well as application and social research in other directorates to create and expand the next generation of deployed cyberinfrastructure. This cyberinfrastructure is especially relevant to converting data to knowledge, understanding complexity through computational simulation and prediction, and creating more systematic, principled knowledge about the social and technical issues of powerful virtual organizations.

OCI was created in July 2005 in an organizational realignment that moved the CISE Division of Shared Cyberinfrastructure (SCI) into the Office of the Director. At the same time, a Cyberinfrastructure Committee (CIC), composed of members of NSF's senior management, was created. The CIC provides integration and strategic vision across NSF's portfolio of cyberinfrastructure activities. In FY 2007, funds were added to the OCI budget to begin the acquisition of a leadership-class high-performance computing (HPC) system optimally configured to enable *petascale* performance (computing at sustained rates on the order of 10^{15} floating point operations per second (petaflops) or working with very large datasets on the order of 10^{15} bytes (petabytes)) on important science and engineering problems.

OCI-supported cyberinfrastructure includes information technology resources and tools such as supercomputers, high-capacity mass-storage systems, system software suites and programming environments, scalable interactive visualization tools, productivity-enhancing software libraries and tools for scientific programming, large-scale data repositories and information management systems, networks of various reach and granularity, an array of software tools and services that enhance the usability and accessibility of computational, observational and experimental infrastructure, and virtual environments that make it possible for geographically distributed researchers and educators to collaborate. OCI supports socio-technical research on the way cyberinfrastructure is used and on ways of improving its effectiveness. It supports activities that develop ways of using cyberinfrastructure to augment learning as well as training in the development and use of cutting-edge cyberinfrastructure. OCI also supports the scientific and engineering professionals who create and maintain these IT-based resources and systems, and who provide the Nation's researchers and educators with essential cyberinfrastructure services. OCI makes investments that improve the cyberinfrastructure for science and engineering research, funding the deployment of cyberinfrastructure and innovative developments in cyberinfrastructure. In doing so, it both leverages and complements investments made by other agencies. For example, some of NSF's high-end computing investments take advantage of expertise at laboratories funded by the Department of Energy (DOE) and hardware and software developments funded by the Department of Defense's Defense Advanced Research Projects Agency (DARPA). In addition, OCI investments in petascale applications and tools complement those of DOE's SciDAC program, and OCI's TeraGrid infrastructure is used by researchers funded by NIH, DOE and other agencies.

OCI activities directly respond to the President's advanced networking, high-end computing and cyberinfrastructure priorities, and are key components in the Networking and Information Technology Research and Development (NITRD) priority. The technologies developed and the systems deployed by OCI facilitate discovery and innovation and bolster national competitiveness. The American Competitiveness Initiative (ACI) describes the goal of providing world-leading, high-end computing capability, coupled with advanced networking, to enable scientific advancement through modeling and simulation at unprecedented scale and complexity across a broad range of scientific and engineering disciplines. OCI investments in high-performance computing for research and education, the TeraGrid infrastructure, and international network connections directly contribute to this goal.

OCI will participate in the NSF-wide Cyber-enabled Discovery and Innovation (CDI) investment through the development, deployment, and use of enabling cyberinfrastructure, made in collaboration with NSF's research directorates.

The FY 2008 appropriation will reduce funding available for new activities presented in last year's budget request. Among these are: a $7.50 million reduction in the funds available for the acquisition of a new high-performance computing system; a roughly 40 percent reduction in investment for a new activity designed to respond to the growing need for innovative approaches to the long-term curation of digital data; a 40 percent reduction in OCI's ability to invest in the new Cyber-enabled Discovery and Innovation program; and the deferral to FY 2009 of the start of a planned new activity aimed at the integration of research and education through cyberinfrastructure.

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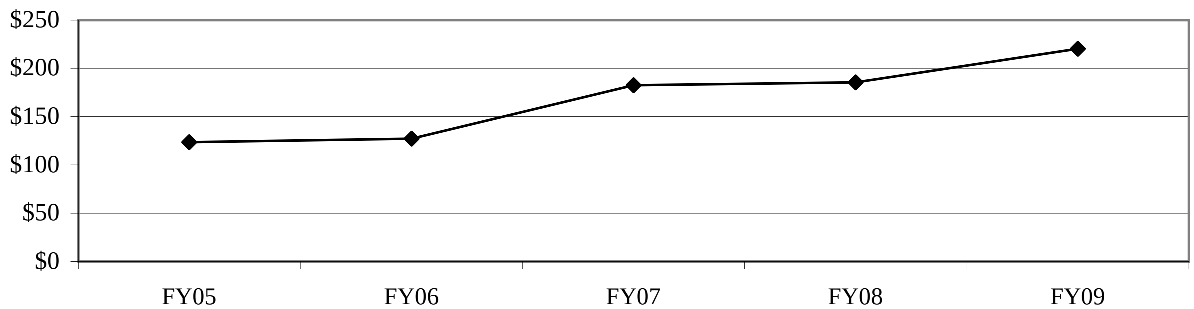
OCI Subactivity Funding
(Dollars in Millions)



RELEVANCE

What happens to space-time when two black holes collide? What impact does species gene flow have on an ecological community? What are the key factors that drive climate change? What are the mechanisms operating within cellular signaling pathways? How do we design nano-materials with useful electrical, optical, or mechanical properties? How does major technological change affect human behavior and structure complex social relationships? By combining the analysis of the huge datasets that will be generated by the next generation of astronomical instruments with advanced cosmological modeling, can we determine the distribution and effects of dark matter in the cosmos?

Advances in computing and related information technology are providing us with the ability to answer these and other questions that were previously beyond our reach, either directly through computation or as a result of the new modes of collaboration and analysis enabled by digital technology. The ability of modern observing technology to produce unprecedented quantities of empirical data, in fields of research such as particle physics, astronomy, and the environmental sciences, drives the development of new ways of managing, analyzing, visualizing, and representing data. The availability of data in digital form prompts the development of new approaches to querying and melding diverse datasets that permit interdisciplinary groups to collectively address much more complex research questions.

The Office of Cyberinfrastructure's investments are guided by NSF's *Cyberinfrastructure Vision for 21st Century Discovery* (www.nsf.gov/dir/index.jsp?org=OCI), a comprehensive cyberinfrastructure strategic plan for the Foundation; by the American Competitiveness Initiative, by the America COMPETES Act, and by the opportunities identified by the academic and industrial research community through workshops and white-papers. It also responds to OSTP's and OMB's memo of August 14, 2007, on R&D budget priorities which stated that, "High-end computing should be increasingly used to support research for transformational solutions to complex problems in energy, climate and weather, human health, new materials and national security."

OCI supports the development and deployment of cyberinfrastructure that is shared by all scientific and engineering disciplines, making possible potentially transformative basic research in areas such as nanotechnology, physics, chemistry, materials science, and engineering, as called for in the ACI. It also promotes interoperability between components of cyberinfrastructure both here in the U.S. and abroad. About two-thirds of NSF's investments in cyberinfrastructure are made by the directorates and offices responsible for fundamental domain specific research and education in science and engineering, with the remaining one-third provided by OCI. Through coordinated planning and investments facilitated by NSF's Cyberinfrastructure Council, OCI provides economies of both scale and scope, ensuring that NSF's cyberinfrastructure portfolio delivers the highest returns on the Nation's investment.

Summary of Major Changes in Office-wide Investments ***(Dollars in Millions)***

FY 2008 Estimate, OCI…..……………………..……………………………………………$185.33

Discovery +$12.75

Software and Services for Complex Science and Engineering (+$13.23 million).

OCI will extend its support of this area for the development and provision of software and services that facilitate complex science and engineering research (+$6.98 million). These include: innovative approaches to the management of data collections; software and practices that enhance the semantic interoperability of data and tools; robust middleware that supports distributed applications, distributed collaboration, interactive remote observation, and the tele-operation of instruments and experimental facilities; cybersecurity test-beds; as well as advanced data analysis and multi-modal visualization tools. Advances in the analysis and management of data from observations, experiments, and computational models are critical to advancing ACI goals in data-intensive areas such as nanotechnology, materials science, weather and climate prediction, and the prediction of hazards from events such as earthquakes and hurricanes. OCI will continue to provide opportunities to researchers who wish to exploit new ideas emerging from computer science and elsewhere and to explore whether these have the potential to be the next revolutionary strategic technologies in cyberinfrastructure. As such technologies mature, they will contribute to strengthening the capabilities of computing systems and advanced networks as highlighted in the ACI, and to the provision of new tools for basic research.

OCI will increase its investment in the development and provision of software and services that facilitate complex science and engineering research through the Cyber-enabled Discovery and Innovation initiative (+$6.25 million). (Addition OCI investments in CDI are described under Research Infrastructure.) Additional areas of emphasis include: the use of *in situ* computation in sensor networks; virtual organizations that are built around specific complex science and engineering research foci and that leverage other NSF investments such as those in the TeraGrid, in observing systems, and in specialized experimental equipment; research aimed at improving the effectiveness of collaborative digital environments; novel modeling methodologies that include the flow of uncertainty in predictive simulations; research on ways of programming novel computational architectures; and the development of more robust approaches to fault-tolerant computing in science and engineering.

Accelerating Discovery in Science and Engineering through Petascale Simulations and Analysis (PetaApps) (-$6.84 million).

After successfully stimulating the development of petascale application software, the pace of new investments in such software will be reduced in FY 2009. There remains a need for additional software for petascale computing (e.g. new scalable algorithms, new programming models, better debugging techniques, tools for analyzing extremely large datasets, and multi-scale, multi-physics models). These are being partially addressed in an ad hoc fashion through various NSF programs. A further PetaApps solicitation is being discussed and it is likely that this activity will be resumed when sufficient funds are available.

Cyber Services (+$6.36 million).

Some OCI activities consist of the provision of cyber-services and access to cyber-resources; others are explorations of new directions in technology development; and some involve the development or deployment of cyberinfrastructure prototypes. In the first two years of OCI's existence, most of these activities were classified as infrastructure. However, based on the experience of the last two years, it seems more appropriate to include those activities associated with research, development and prototyping of new cyberinfrastructure within the Discovery strategic outcome goal. These are activities in which cyberinfrastructure is the main object of research.

<u>Learning</u> -$6.00

Integration of research and education through cyberinfrastructure (+$4.0 million).

In collaboration with other directorates and offices across the Foundation, OCI will support the development of innovative technologies that will facilitate the integration of research and education, creative explorations and demonstrations of the use of these and other cyberinfrastructure to integrate research with education, and research on how educators and students interact with cyberinfrastructure. One aim of this support is to connect students and educators with the types of science and engineering that are themselves being facilitated by cyberinfrastructure, and that are difficult or ineffective to reproduce in a school laboratory or informal education setting using traditional methods.

Cyberinfrastructure Training, Education, Advancement and Mentoring (-$10.0 million).

This activity, having successfully achieved its objective of stimulating new collaborations between domain scientists and cyberinfrastructure experts and encouraging them to initiate learning and workforce development activities that complement ongoing NSF investment in cyberinfrastructure, has reached the end of its planned lifetime.

<u>Research Infrastructure</u> +$27.30

High Performance Computing: Acquisition, Operations and Maintenance (+$24.42 million).

Increased funding is for the acquisition, operations, and maintenance of high-performance computing (HPC) systems and for the national open science and engineering research community. These leading-edge computational resources, together with advanced networking capabilities, serve to maintain NSF's national supercomputing grid, the TeraGrid, as the world's leading high-end computing environment for open research. They are used in innovative research in areas ranging from biology, materials science and physics to engineering and social science. This activity is directly responsive to the ACI's goal of providing a "world-leading high-end computing capability (at the petascale) and capacity, coupled with advanced networking, to enable scientific advancement through modeling and simulation at unprecedented scale and complexity across a broad range of scientific disciplines." OCI's investments in this area are coordinated with those of other federal agencies, primarily through the High-End Computing Inter-agency Working Group.

Digital preservation and analysis (+$3.0 million).

OCI will increase its investments in DataNet, an activity launched in FY08. These investments are aimed at stimulating exemplar data research infrastructure organizations. By integrating library and archival sciences, cyberinfrastructure, computer and information sciences, and broad science expertise, these investments will develop a prototype infrastructure for providing reliable digital preservation and analysis capabilities for science and/or engineering data.

Cyber-enabled Discovery and Innovation initiative (+$6.24 million).

OCI will support the development and deployment of cybertools for pattern recognition, feature extraction, and feature tracking in streaming data, for mining, analyzing, and representing very large, multi-variate spatiotemporal datasets, and for model generation and validation through the Cyber-enabled Discovery and Innovation investment. (See also Discovery.)

Cyber Services (-$6.36 million).

See above under Discovery.

<u>Stewardship</u> +$0.70

A number of activities are funded directly from NSF's programs to advance NSF's Stewardship goal. These include Intergovernmental Personnel Act appointments, NSF-wide studies and evaluations, and mission-related information technology investments. As is discussed further in the Stewardship chapter of this Request, in FY 2009 NSF has realigned IT investments to tie mission-related activities more directly to NSF's programs.

Subtotal, Changes +$34.75

FY 2009 Request, OCI……………………………………………………………..……… $220.08

QUALITY

OCI maximizes the quality of the projects it supports through the use of a competitive, merit-based review process. The percent of funds that were allocated to projects that undergo external merit review was 99 percent in FY 2007, the last year for which complete data exist.

To ensure the highest quality in processing and recommending proposals for awards, OCI convenes a Committee of Visitors, composed of qualified external evaluators, to review each program every three years. These experts assess the integrity and efficiency of the processes for proposal review and provide a retrospective assessment of the quality of results of NSF's investments. The next OCI Committee of Visitors is scheduled for FY 2008. The OCI Committee of Visitors (COV) is charged with assuring that the programs administered in OCI meet NSF's high standards of program management and to ensure openness to the research and education community served by the Foundation and that attempts are made to improve performance. The COV will focus on two specific areas, in the context of OCI's four focus areas of High Performance Computing, Data, Virtual Organizations, and Learning and Workforce Development: (1) assessments of the quality and integrity of program operations and program-level technical and managerial matters pertaining to proposal decisions; and (2) comments on how the outputs and outcomes generated by awardees have contributed to the attainment of NSF's mission and strategic outcome goals. While all OCI awards will be under consideration, this particular OCI COV will pay particular attention to the OCI high-performance computing portfolio due to its importance to the science and engineering community.

OCI's activities are guided by the document, *Cyberinfrastructure Vision for 21st Century Discovery*, developed by NSF based on input from the research and education community, and by national priorities highlighted in the American Competitiveness Initiative, the America Competes Act, and the August 2007 memo on R&D priorities from OMB and OSTP. In partnership with NSF's directorates and offices, OCI receives advice from the Advisory Committee for Cyberinfrastructure (ACCI) on such issues as: the mission, programs, and goals that can best serve the science and engineering community; how OCI can promote quality graduate and undergraduate education in the computational sciences and engineering; and priority investment areas in cyberinfrastructure. The ACCI meets twice a year. Members from both academe and industry represent a cross section of the science and engineering field, with representatives from many different disciplines. The ACCI includes a balanced representation of women, underrepresented minorities, and individuals from a range of geographic regions and institutions. Internally, mechanisms to maintain integration across NSF's cyberinfrastructure activities include the executive-level Cyberinfrastructure Council, which includes the Director, the Assistant Directors and the Office Heads, and the Cyberinfrastructure Coordinating Committee composed of program officers representing the directorates and offices and chaired by the Office Head for OCI.

PERFORMANCE

The FY 2009 Budget Request is aligned to reflect funding levels associated with the Foundation's four strategic outcome goals highlighted in the FY 2006-2011 Strategic Plan. These goals were designed as a mechanism to better enable assessment of program performance and to facilitate budget and performance integration.

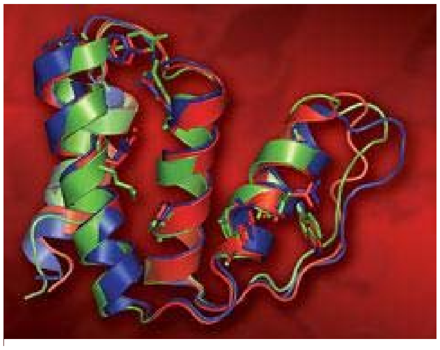
Office of Cyberinfrastructure
By Strategic Outcome Goal
(Dollars in Millions)

	FY 2007 Actual	FY 2008 Estimate	FY 2009 Request	Change over FY 2008 Estimate Amount	Change over FY 2008 Estimate Percent
Discovery	$3.99	$14.75	$27.50	$12.75	86.4%
Learning	0.57	10.10	4.10	-6.00	-59.4%
Research Infrastructure	176.28	158.43	185.73	27.30	17.2%
Stewardship	1.58	2.05	2.75	0.70	34.1%
Total, OCI	$182.42	$185.33	$220.08	$34.75	18.8%

Totals may not add due to rounding.

Recent Research Highlights

► **Speeding Simulations for Drug Design:** Proteins are the building blocks of the body, and biologists have learned that the myriad ways they function--from fighting off infection and building new bones to storing a memory--depend on the precise details of their 3-D shapes. But determining the shapes of proteins has been a slow and exacting process. To speed up this important science, researchers at the NSF-funded San Diego Supercomputer Center helped biologists from the University of Washington begin to harness the power of massive supercomputers. After working to adapt the computer code, they used one of TeraGrid's supercomputers to compute a protein structure in just three hours, something that normally takes weeks. By dramatically accelerating scientific research, modern supercomputers are opening the door to medical advances such as rational drug design.



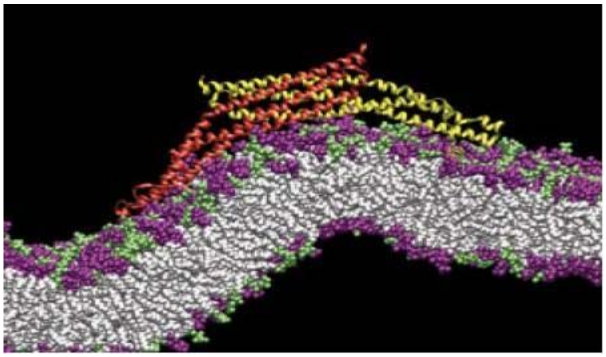
Three-dimensional structure of a protein, one of the building blocks of life. *Credit: R.C. Walker, SDSC/UCSD and S. Raman, University of Washington.*

► **Long Time Modeling of Type Ia Supernovae:** Among the brightest objects in the sky, Type Ia supernovae are also of paramount importance in cosmology, serving as "standard candles" that help scientists accurately mark off distance across the universe. To harness new precision cosmology to better calibrate these standard candles, scientists at the ASC Flash Center at the University of Chicago have used their enhanced TeraGrid simulation code to conduct the longest, self-consistent, 3-D, numerical simulation of a Type 1a supernova explosion ever performed. The computations extended from supernova ignition through the active explosion phase, following the evolution for 11 days and revealing a longer-than-expected evolution with distinct stages. Such simulations are an important complement to the observations. The simulations' capability allows researchers to make meaningful comparisons of their theoretical and numerical models with observations.

Cross-sections through one eighth of a star's volume, showing the distribution of material that has undergone nuclear fusion (from white – fully burned – to dark red – unburned) at two different times (left - two seconds after ignition; right - after 77 minutes). *Credit: Dr. Alexei Poludnenko, ASC Flash Center, Dept. of Astronomy & Astrophysics, University of Chicago.*

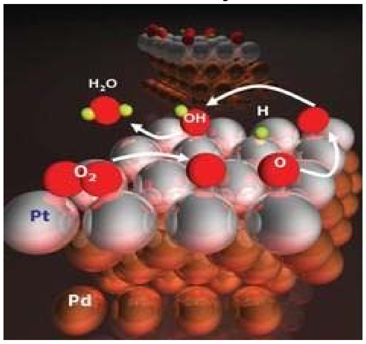
► **Securing Urban Water Supplies:** Urban water distribution systems cover hundreds of square miles and include thousands of miles of pipe. But in most cases, drinking water is largely unmonitored after it leaves the treatment plant, making it possible to intentionally contaminate a water supply using simple equipment. With this in mind, and to help improve water quality, researchers have developed new methods of locating the source of contaminants and testing approaches to limiting their impact. Working with data from sensor networks in large metropolitan areas, they used evolutionary computation to search through the large number of possible solutions until the contaminant distribution in the computational model matched the real-world sensor data. This procedure used hundreds of processors simultaneously on TeraGrid systems. The researchers expect these techniques will prove useful to cities that are installing networks with hundreds of thousands of sensors. Current simulations already are showing officials how to cope with problem situations. Extensions of these techniques may help assess the vulnerabilities of urban water systems to deliberate contamination and evaluate strategies for detection and mitigation.

► **How Proteins Induce Curvature in a Cell Membrane:** Using a range of TeraGrid resources, researchers at the University of Utah modeled and observed for the first time how proteins induce curvature in a cell membrane. Their findings provide new details about an essential cellular process involving BAR. BAR domains are a family of banana-shaped proteins that bind to cellular membrane as it curves--a process by which cells absorb material from outside. The researchers used TeraGrid systems to explore how long a stretch of membrane they needed for curvature to occur. Their final simulations included the protein interacting with a 50-nanometer length of membrane--probably the longest patch of membrane ever simulated. Their results confirm experimental findings and show that the orientation of the BAR domain as it attaches to the membrane determines the degree of curvature.



Close-up of the midsection of a 50-nanometer length of membrane after 27 nanoseconds of simulation showing the curvature produced by the BAR domain (orange and yellow helices) molded to the membrane surface. *Credit: Gregory Voth, University of Utah.*

► **Better Fuel Cells:** Splitting oxygen molecules into oxygen atoms and the subsequent formation of water are currently the rate-limiting step in getting energy from fuel cells, the reaction that restricts overall power production. Researchers at the University of Wisconsin and Brookhaven National Lab are exploring the oxygen reduction reaction, and the catalyst that provokes it, by using the TeraGrid resources at the National Center for Supercomputing Applications. They found that palladium with a platinum monolayer offered the best overall performance characteristics, improving the overall efficiency of the oxygen reduction reaction by 33 percent.



Possible reaction pathway for the oxygen reduction reaction on a catalytic surface. *Credit: Manos Mavrikakis, UW-Madison.*

► **The Roots of Entrepreneurial Success**: Economists have long debated the factors leading to entrepreneurial success: are entrepreneurs uniquely optimistic and more willing to assume risks, or are environmental factors, such as bankruptcy laws and the availability of credit, more significant? Economics researchers at the University of Illinois at Urbana-Champaign have developed a model that considers individual differences in willingness to bear risk and optimism. The model can also evaluate the effect of bankruptcy rules on small firms. Researchers applied the model to data from the Survey of Small Business Finance. Using TeraGrid computing resources they were able to quickly determine if the behavioral predictions of a particular theory could be reconciled with economic data. This necessitated computing many integrations of an economic model, varying a large number of policy parameters. Their results indicate that the environment in which businesses operate influences success more than personal characteristics, and that entrepreneurs are not excessive risk-takers.

Other Performance Indicators

The table below shows an estimate of the number of people benefiting from OCI funding based on the types and number of awards. However, OCI investments directly impact a much larger number of researchers and educators within the U.S. and around the world who use OCI-supported cyberinfrastructure facilities, resources, and tools.

Number of People Involved in OCI Activities

	FY 2007 Estimate	FY 2008 Estimate	FY 2009 Estimate
Senior Researchers	206	245	360
Other Professionals	577	515	525
Postdoctorates	16	22	25
Graduate Students	114	150	190
Undergraduate Students	51	70	95
Total Number of People	964	1,002	1,195

OCI Funding Profile

	FY 2007 Estimate	FY 2008 Estimate	FY 2009 Estimate
Statistics for Competitive Awards:			
Number	70	71	72
Funding Rate	23%	23%	23%
Statistics for Research Grants:			
Number of Research Grants	43	50	55
Funding Rate	19%	18%	18%
Median Annualized Award Size	$450,000	$400,000	$400,000
Average Annualized Award Size	$511,682	$440,000	$440,000
Average Award Duration, in years	2.2	2.5	2.5