# Scientific Discovery through Advanced Computing

## the U.S. Department of Energy's SciDAC Program

**Lali Chatterjee**

Office of Advanced Scientific Computing Research (OASCR)

- **Thanks to RIKEN HPC Center**
- **Recognize Japanese Earth Simulator for its contribution to HPC**
- **Good wishes from Dr. Michael Strayer, Director SciDAC and Director OASCR**

# Overview of Talk

- SciDAC Highlights
- OASCR, Office of Science, DOE
- SciDAC Science Application Partnerships
- SciDAC Centers for Enabling Technology
- SciDAC Institutes
- SciDAC Science
- OASCR and SciDAC
- Outreach and Education
- Acknowledgements and Future Perspectives

**"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, mathematicians, applied mathematicians, and computer scientists who recognize that computation is not something you do at the end, but rather it needs to be built into the solution of the very problem it is that one is addressing."**

**Dr Raymond Orbach, Under Secretary for Science and Director, Office of Science, US Department of Energy**
**in SciDAC Review, Issue 1**

# SciDAC



## First Issue of SciDAC Review Publication

# SciDAC

**Continuing the quote…**

**"SciDAC has strengthened the role of high-end computing in furthering science. In good part this is due to the fact that it is unique and brings together teams that are able to create a structure for addressing what previously have really been intractable problems."**

http://www.scidac.gov

# SciDAC

## SciDAC Goals:

**Breakthrough science enabled through HPC and tripartite partnerships between Computer Scientists, Applied Mathematicians and Discipline Scientists.**

**Characterized by large multi – institutional collaborations**

**Funded in partnership by**

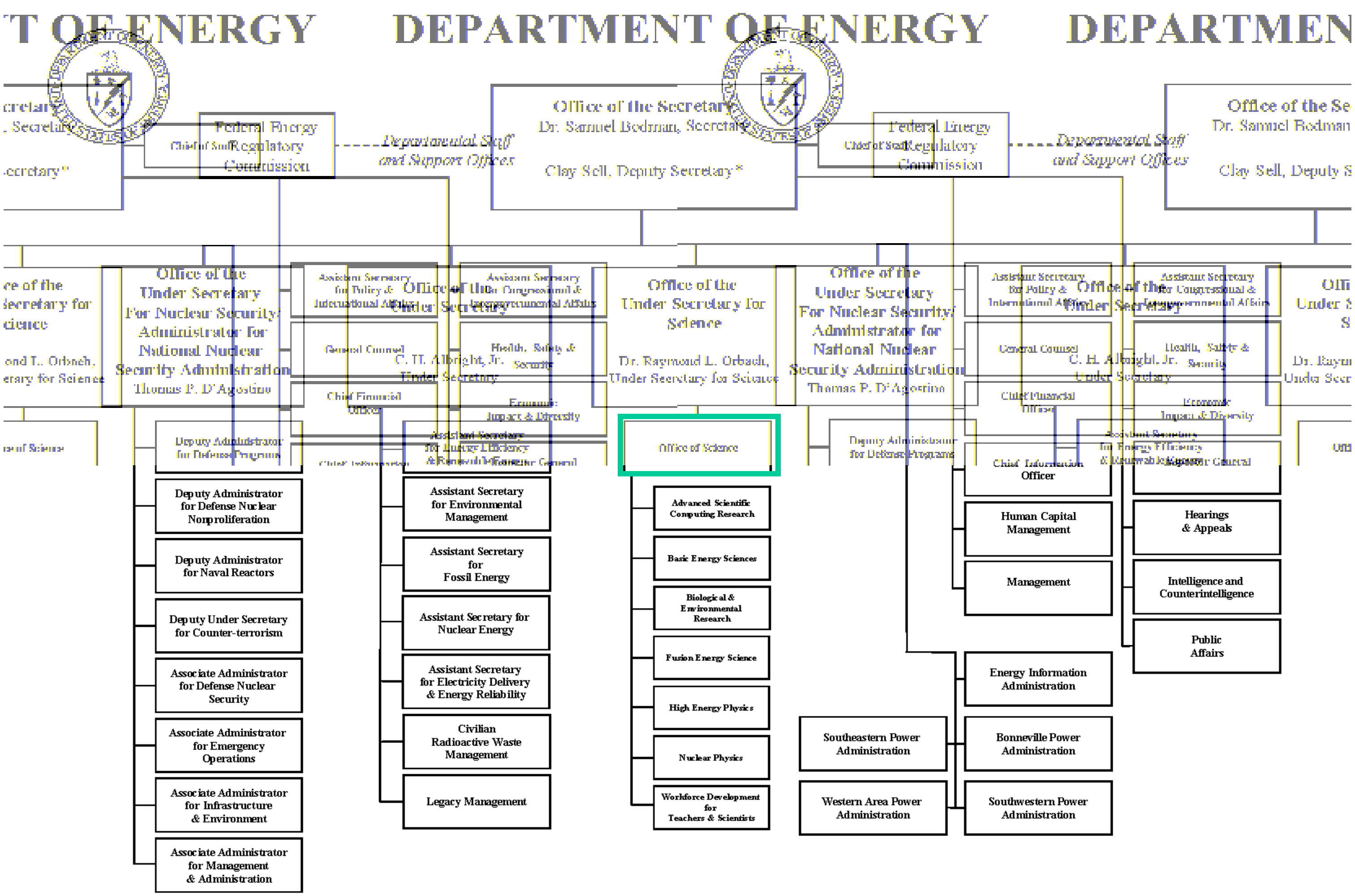
- **Office of Science, Department of Energy (DOE)**
- **National Nuclear Security Administration, DOE**
- **and by the National Science Foundation for the Grid Projects**

U.S. Department of Energy

Office of Science

# Department of Energy Organizational Structure

## Advanced Scientific Computing Research Program




* The Deputy Secretary also serves as the Chief Operating Officer

06 Feb 08

# SciDAC and U.S. DOE

- **U. S. Department of Energy**
- **Office of Science (www.science.doe.gov)**

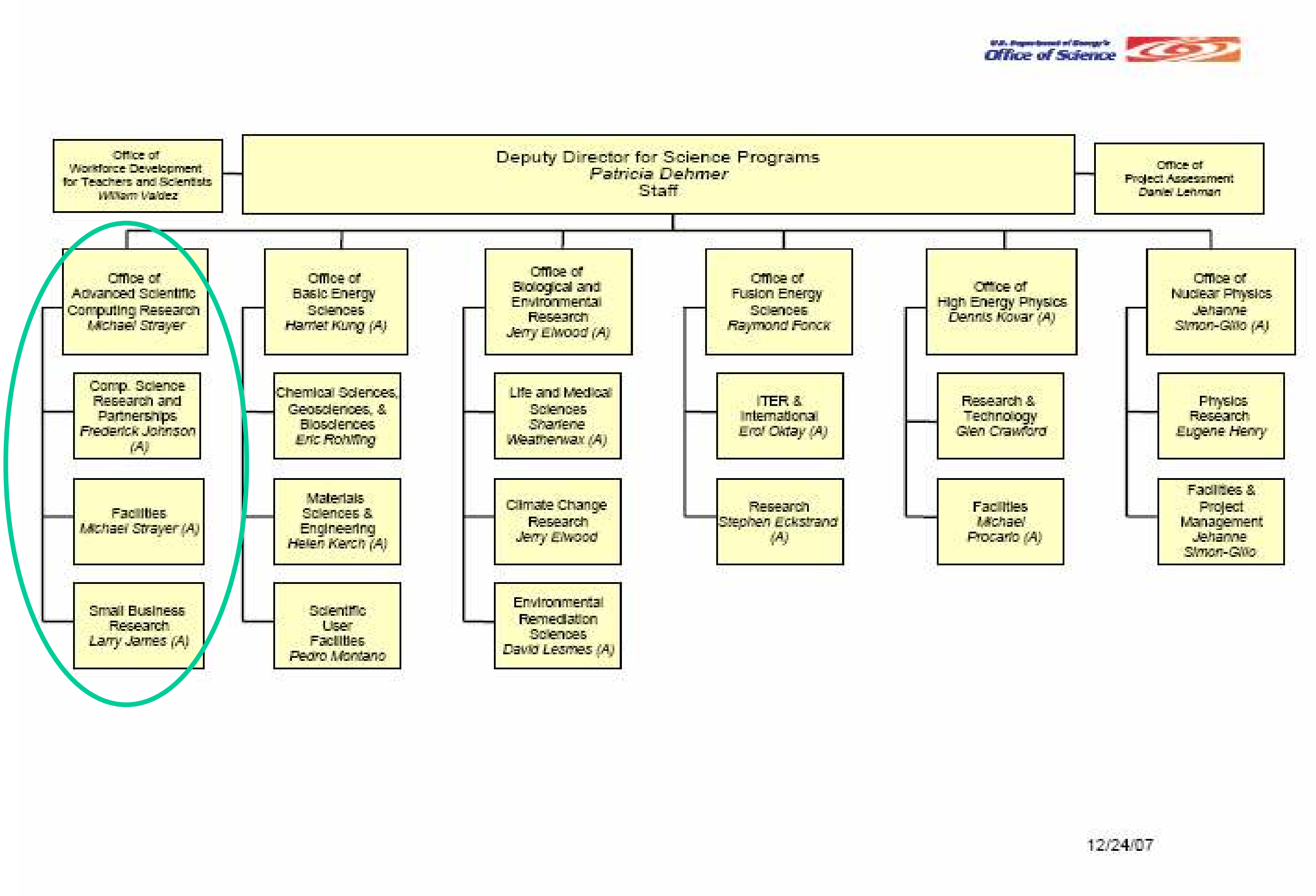
| Advanced Scientific Computing Research | Basic Energy Sciences | Biological and Environmental Research | Fusion Energy Sciences | High Energy Physics | Nuclear Physics |
|---|---|---|---|---|---|

**and**

- **National Nuclear Security Administration**

# Office of Science Science Programs

Advanced Scientific Computing Research Program



U.S. Department of Energy
Office of Science

# OASCR Organization

Advanced Scientific Computing Research Program

**Office of Advanced Scientific Computing Research**
**Director – Michael Strayer**

**Facilities Division**

**Computational Science Research and Partnerships Division (SciDAC)**
**Division Director: Frederick Johnson**

**Small Business Research Division**

**Scientific Discovery through Advanced Computing (SciDAC)**
**Director – Michael Strayer**
(Office of Science (SC) wide Partnership Program)

# How OASCR affects SciDAC Research

**Facilities** - Leadership Computing Facilities (LCF), National Energy Research Scientific Computing Center (NERSC), ESnet

**Research** – Applied Mathematics, Networks, Computer Science, and Science Application Partnerships

**Outreach & Education** - Publications, Fellowships, Student Research

**Workshops** – Explore New Initiatives and Partnerships.

# SciDAC

SciDAC started in 2001 and program is now in its second phase after a successful round of SciDAC 1.

New Awards in 2006 (SciDAC-2) build on successes of past and promote new areas with potential for high quality science through HPC and tripartite partnerships.

Selected by combination of peer reviews by mail, peer review panels and crosscut panels.

# SciDAC - 2 Awards

Centers for Enabling Technologies (9)

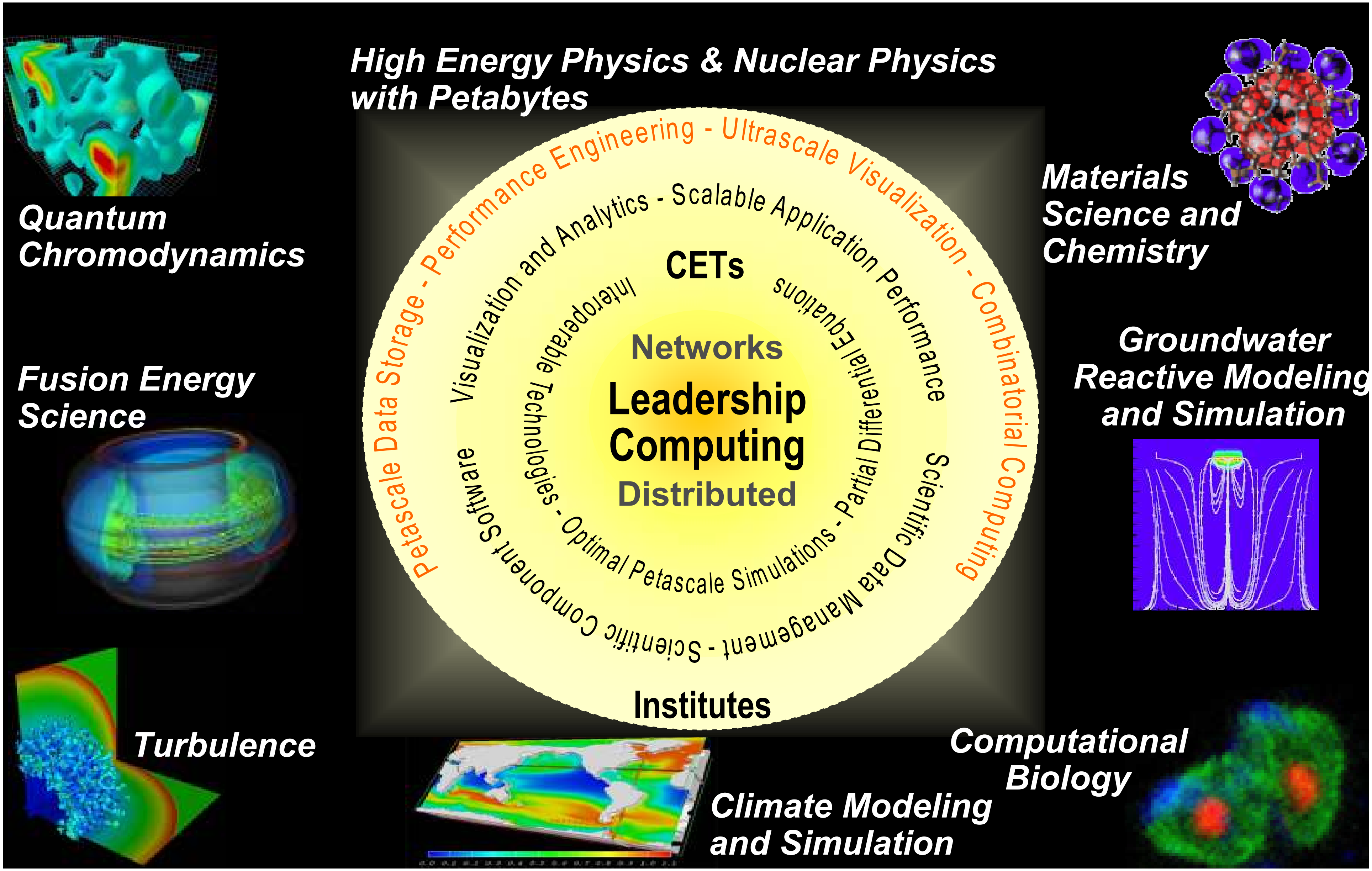
SciDAC Institutes (4)

Science Applications and

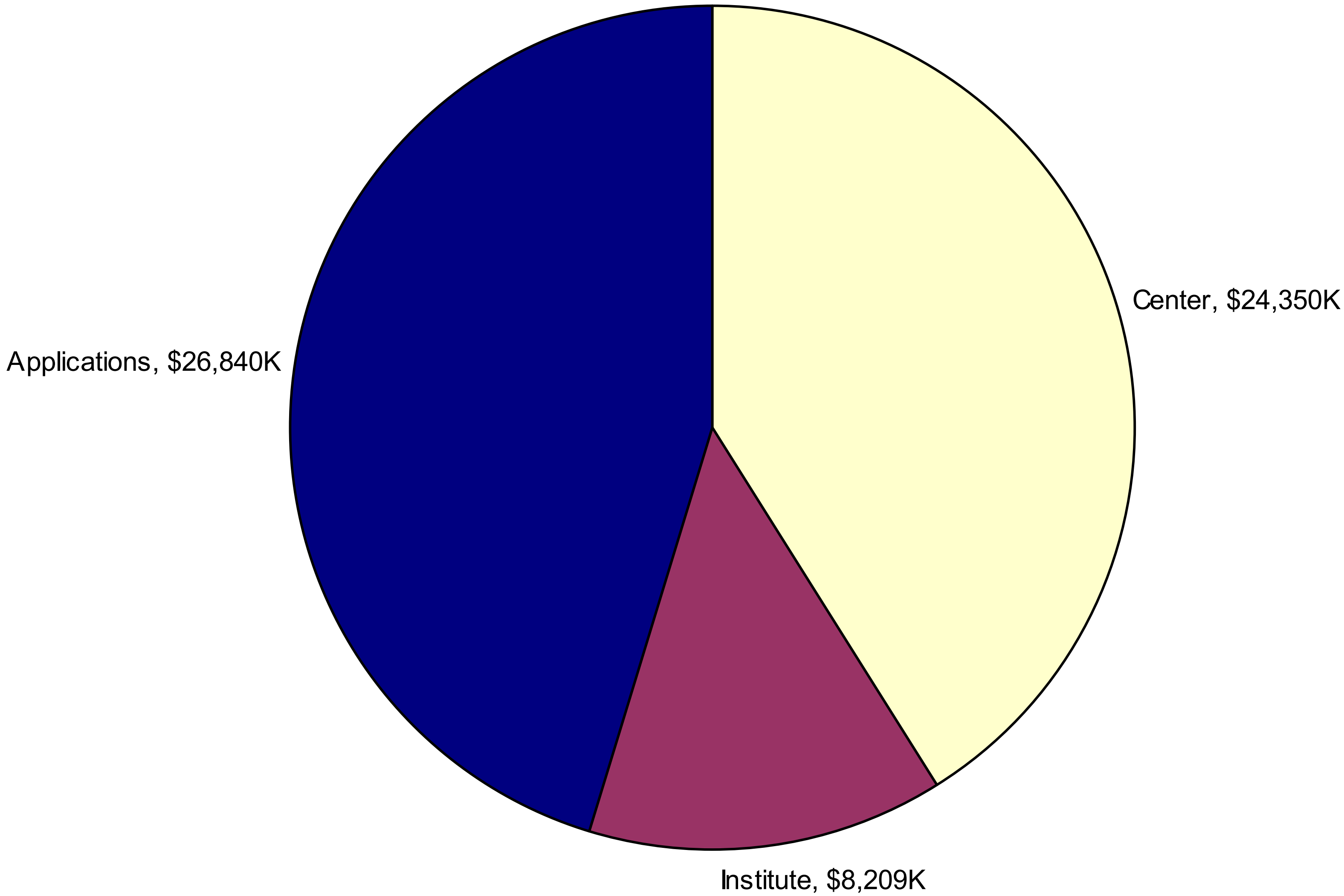
Science Application Partnerships (17)

- Climate, Fusion, Groundwater, Materials, Chemistry, High Energy Physics, Nuclear Physics, Astrophysics, Biology……

# SciDAC-2 Awards



# SciDAC-2 Awards
## (~$60M annualized)



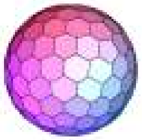
# Science Applications and Partnerships (SAPs)

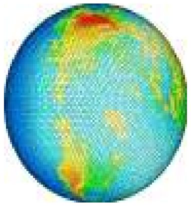
- This SciDAC program element supports projects with partnerships between computational mathematics, computer science and a science domain.
  - Focus on a specific scientific application with challenging computational needs that would benefit from petascale computing.
    - High Energy and Nuclear Physics with Petabytes, Accelerator Physics, Radiation Transport, Nuclear Physics, Astrophysics, Quantum Chromodynamics, Material Science and Chemistry, Biology, Climate, Turbulence, Groundwater, and Fusion
  - May provide the insertion of new technologies directly into application codes or explore new programming and/or modeling methodology for petascale applications.
  - Science Applications (SA)s may have Science Application Partnerships (SAP)s that focus on the applied math and computational challenges of the science **embedded** in the project or **linked** to the project.
  - In either case, the project must be a cohesive one with a shared goal and coordination strategy or management plan. Each institution and investigator must clearly identify their contribution towards this goal.

# Science Application Partnerships

Global Climate Research including Role of Clouds

Petascale Communications for Open Science





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Quantum Simulations and predictive modeling of materials and stress corrosion

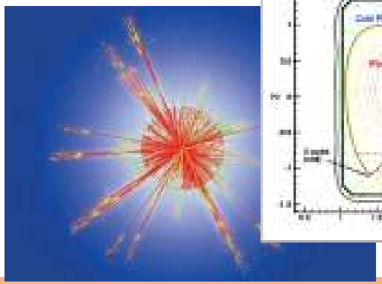
Building an Energy Density Functionional validated by existing data for predicting critical unknowns – nuclear physics

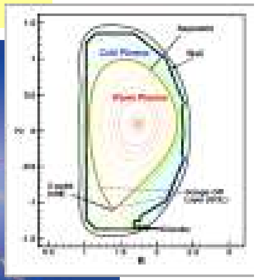
Modeling for Accelerator Design including Beam Dynamics, Electromagnetics, and Advanced Accelerator concepts

Fusion Simulations towards Integrating Systems

Subsurface Flows and Biogeochemical Processes

Quarks on the Lattice and Exploding Supernovae



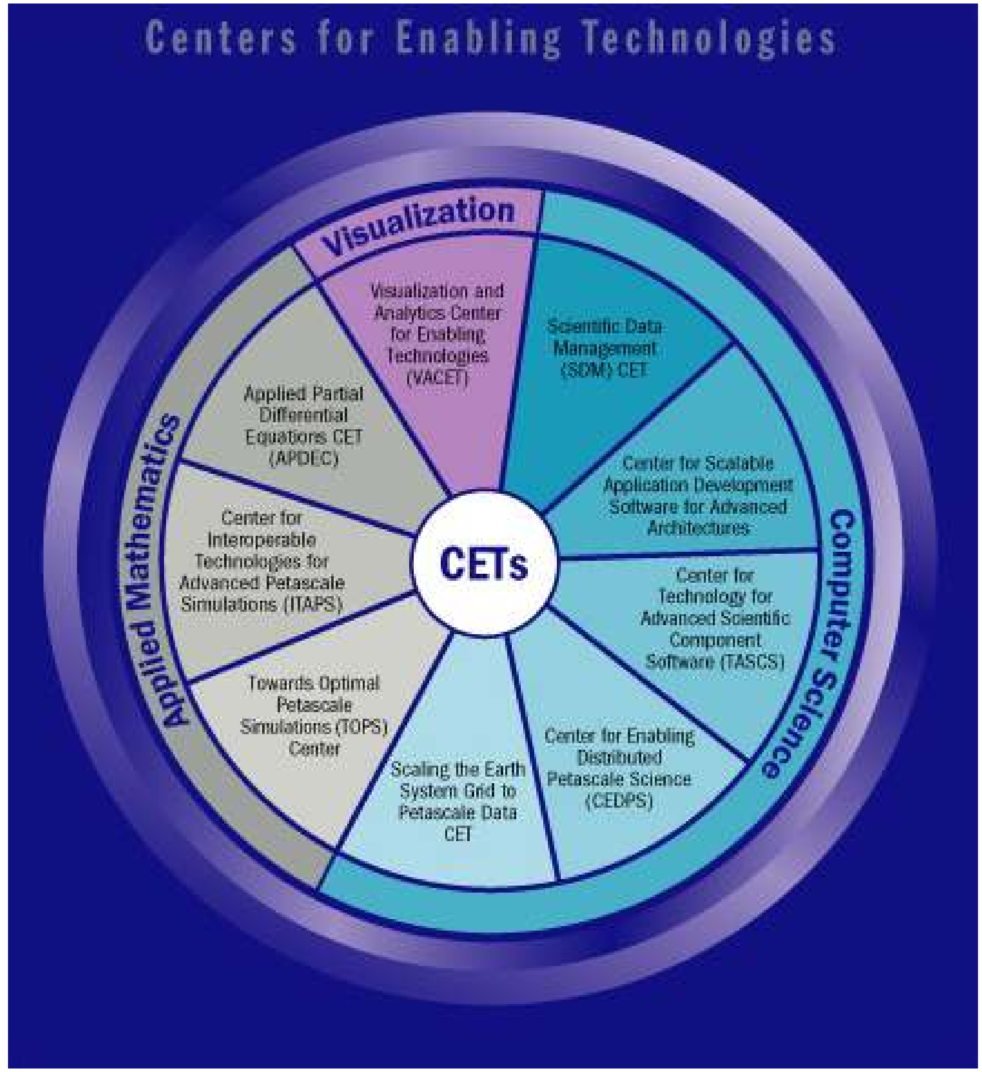


Turbulence and Shock Waves, Computational Chemistry & Life Sciences

# Centers for Enabling Technologies (CETs)

**SciDAC-2 grant awards support nine Centers for Enabling Technologies**

**www.scidac.gov**



# Centers for Enabling Technologies (CETs)

CETs provide the essential computing and communications infrastructure for support of SciDAC applications. The CET effort encompasses a multi-discipline approach with activities in:

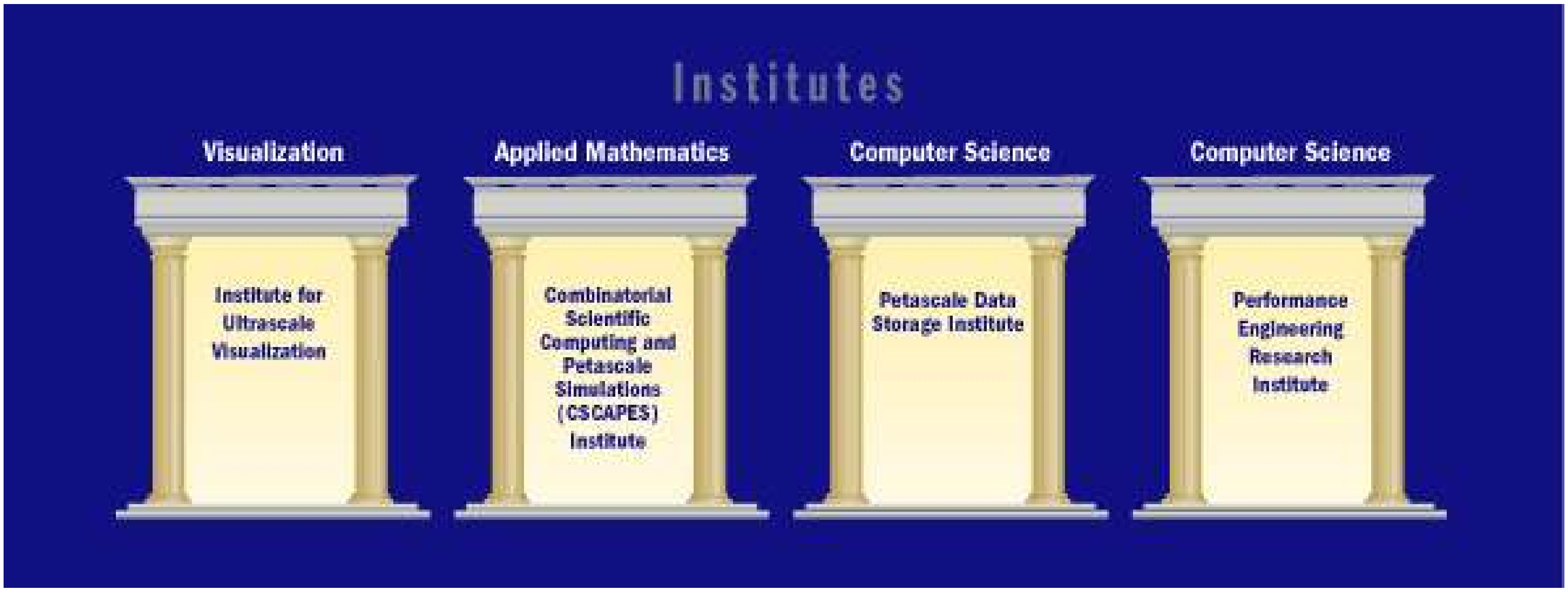
- Algorithms, methods, and libraries.
- Program development environments and tools -- terascale and petascale program development and tools provide maximum ease-of-use to scientific end users.
- Systems software that provides system stability and functionality needed by users for tera- to peta- scale simulations.
- Visualization and data management systems.

CETs work directly with applications on:

- Development and application of computing systems software that allows scientific simulation codes to take full advantage of the extraordinary capabilities of terascale and petascale computers.
- Ensuring that the most critical computer science and applied mathematics issues are addressed in a timely and comprehensive fashion.
- Addressing all aspects of the successful research software lifecycle including transition of a research code into a robust production code and long term software evolution and maintenance and end user support.

# SciDAC Institutes





# SciDAC-2 Institutes

The SciDAC Institutes are university-led centers of excellence intended to complement other efforts by focusing on major software issues through a range of collaborative research interactions. Activities include software methods or techniques that are important to a number of specific science problems.

– Develop, test, maintain, and support optimal algorithms, programming environments, systems software and tools, and applications software.
– Focus on a single general method or technique – e.g. visualization.
- Forge relationships between experts in software development, scientific application domains, high performance computing, and industrial partners.
– Reach out to engage a broader community of scientists in the activities of scientific discovery through advanced computation and collaboration.
– Have a dimension of training and outreach in high performance computing topics, including for graduate students and postdocs.

# SciDAC Science

- SciDAC Science spans multiple disciplines involving complex and multi-scale phenomena.
- The following slides showcase some of these applications and exciting developments
- These are only glimpses of the depth and expanse of SciDAC science and discovery.

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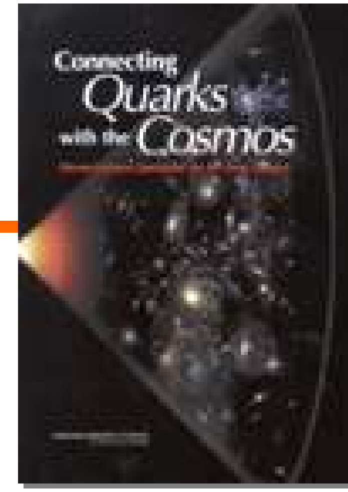
Office of Science

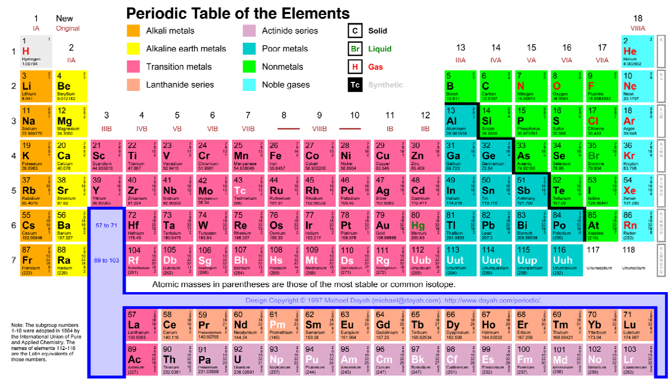
**Advanced Scientific Computing Research Program**

## Turner Report: Eleven Science Questions for the New Century

⇨ How were the elements from iron to uranium made?




The deaths of massive stars in stellar explosions known as core collapse supernovae are the dominant source of elements in the Universe between oxygen and iron and there is growing evidence they are responsible for the production of half the elements heavier than iron.




Key question being addressed computationally:

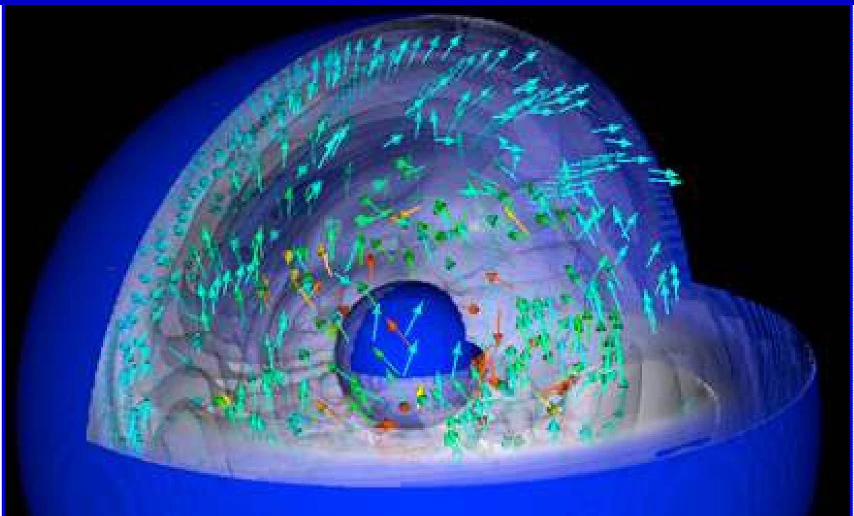
- *How do these stars explode?*
- *What elements are synthesized in these explosions and in what abundance?*

*At right, different colors correspond to different elements.*

*Cas A Supernova Remnant (Chandra Observatory)*

# Discovering the Elusive Core Collapse Supernova Explosion Mechanism

***Researchers glean unprecedented insight into the shock waves that blow apart a 10- to 20-solar mass star***



*MHD SASI simulation using new 3D GenASiS code*

**Researchers can now simulate ~1 second after 'post-bounce'. Petascale systems will allow longer simulations: tens of seconds after the explosion and will allow inclusion of neglected yet important physics such as magnetic fields.**

- ❑ **Achieved longer run simulations and, 0.8 seconds after explosion, saw the initial shock wave revived by turbulence of in-falling material**
- ❑ **CHIMERA used to investigate multiple stellar models, effect of both Newtonian and Einsteinian gravity, and impact of recently discovered subatomic physics**
  - **>12K cores used in current 3D simulations**
- ❑ **Current 3D spatial resolution**
  - **78x156x312 (Chimera)**
  - **256x256x256 (Genasis)**

**LCF liaison contributions**
- **Implementing efficient, collective I/O**
- **Pencil decomposition of 3D flow algorithm**
- **Preconditioning of the neutrino transport equation**

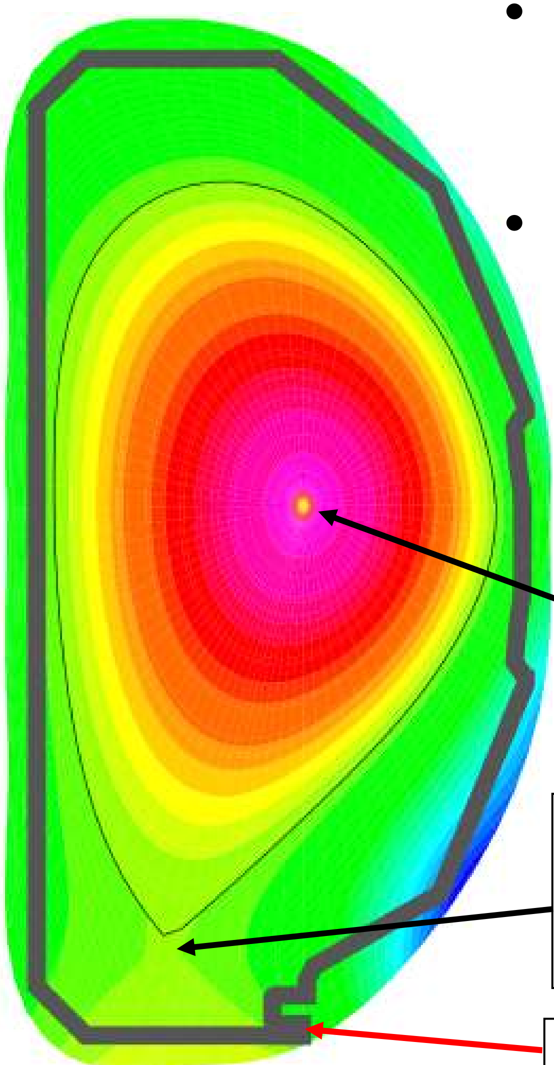
# FACETS: Framework Application for Core-Edge Transport Simulations

**Fusion project -** funded January 15, 2007

**Preparing for whole device simulations**

- Multi-institutional, interdisciplinary project: Tech-X (Lead)
- Massively parallel to produce rapid, whole-device modeling capability
- Core to wall modeling of transport in 5 years. Rough timeline:
  - core/fluid-edge coupling with simplified transport models; dynamic wall model developed
  - core/fluid-edge/wall
  - equilibrium coupled
  - core transport coefficients from core gyrokinetic turbulence code (primary thrust of GA-ORNL SAP) &
  - edge transport and turbulence from edge gyrokinetic code

# FACETS addressing parallel computations for whole device modeling



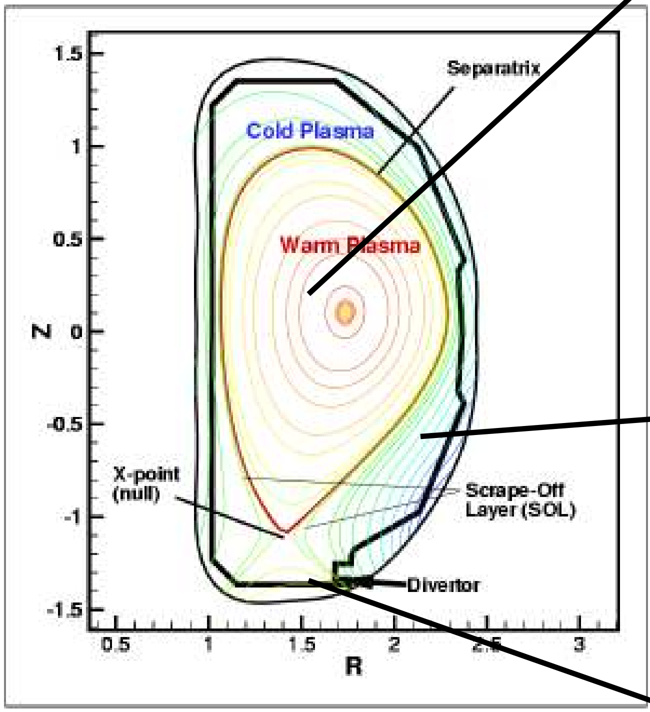
- **Computations must combine software components describing different regions**
- **Parallelism homogeneous across regions:**
  - **task based**
  - **domain decomposed**

Hot central plasma: nearly completely ionized, magnetic lines lie on flux surfaces, 3D turbulence embedded in **1D** transport

Cooler edge plasma: atomic physics important, magnetic lines terminate on material surfaces, 3D turbulence embedded in **2D** transport

material walls, embedded hydrogenic species

# FACETS will integrate the core-edge-wall interaction



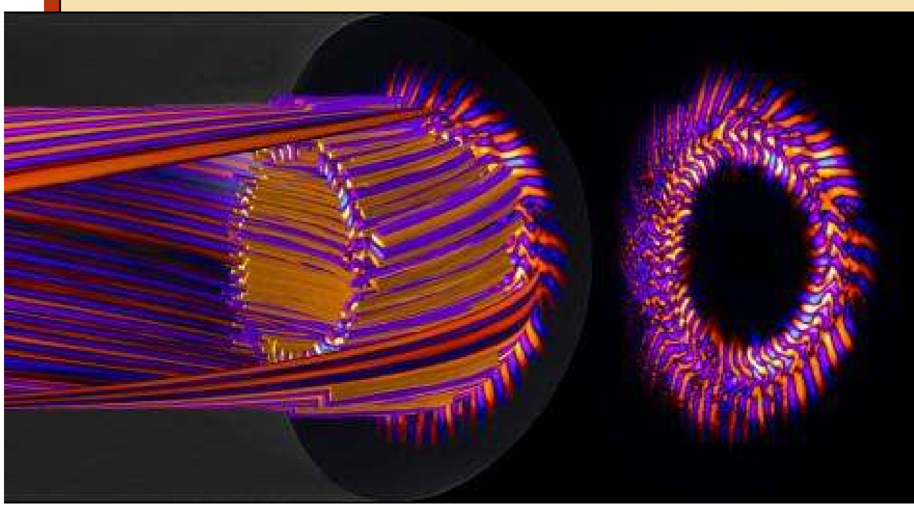

**Closed field lines: slow perpendicular + fast parallel transport**
⇒Quantities 1D, but embedded 3D turbulence
**Hot plasma**
⇒Collisionless, little significant atomic physics (except beams)

**Open field lines: so parallel transport must balance perpendicular**
⇒Quantities are 2D, but embedded 3D turbulence
**Cool plasma**
⇒Collisional, atomic physics is important

**Wall: absorption and release of hydrogenic species**
⇒Multiple 1D (into wall) equations
⇒Materials science important

# Gaining Understanding of Cause and Effect of Core Plasma Turbulence

- Simulation of experimental discharges (NSTX and others) has shown the behavior of microturbulence to be intimately related to geometry and shaping
- Recent improvements to GTC-S allowed more realistic simulations of electron temperature gradient (ETG) drift instabilities, ion temperature gradient (ITG) drift instabilities with non-adiabatic electrons, and trapped electron modes (TEM)

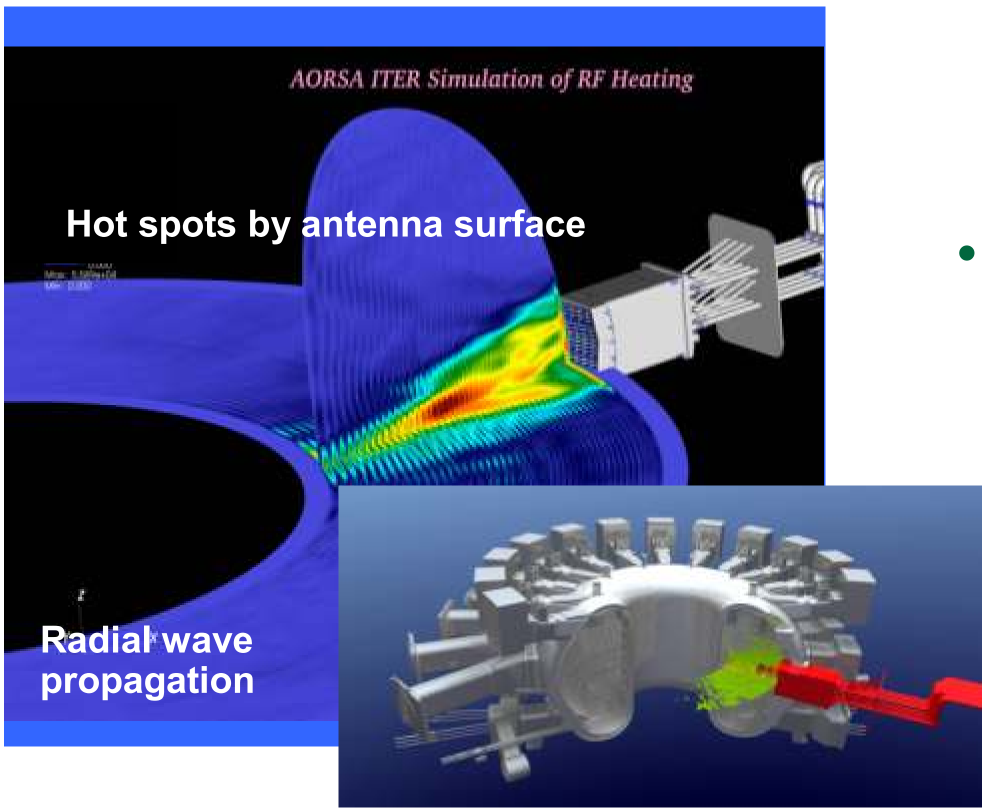


- The number of particles included in recent simulations allows this project to reduce the amount of statistical noise and explore core turbulence at levels of fidelity never seen before

# Producing New Insights for RF Heating in ITER Plasmas

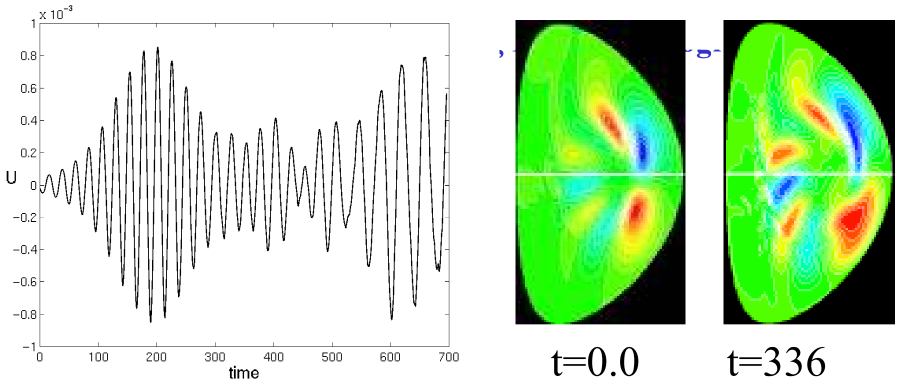
***Fully 3-dimensional simulations of plasma shed new light on the behavior of superheated ionic gas in the multibillion-dollar ITER fusion reactor***

***"Until recently, we were limited to two-dimensional simulations. The larger computer [Jaguar] has allowed us to achieve three-dimensional images and validate the code with observations."*** *– Fred Jaeger, ORNL*

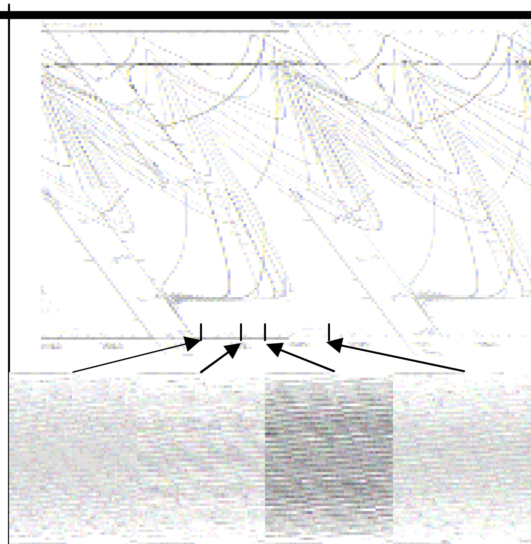



- 3D simulations reveal new insights
  - "Hot spots" near antenna surface
  - "Parasitic" draining of heat to the plasma surface in smaller reactors
- Work pushing the boundaries of the system (22,500 processor cores, 87.5 TF) and demonstrating
  - Radial wave propagation and rapid absorption
  - Efficient plasma heating
- AORSA's predictive capability can be coupled with Jaguar power to enhance fusion reactor design and operation for an unlimited clean energy source

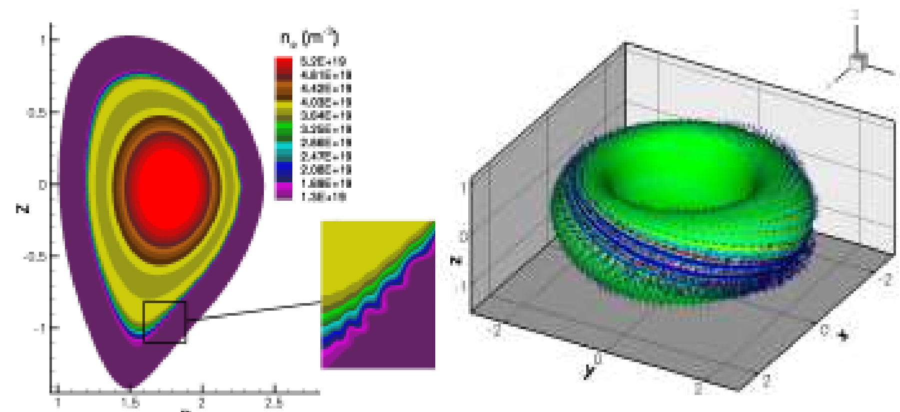
# The Center for Extended Magnetohydrodynamic Modeling (current activities)




**Beam-driven modes in NSTX show nonlinear frequency chirping**

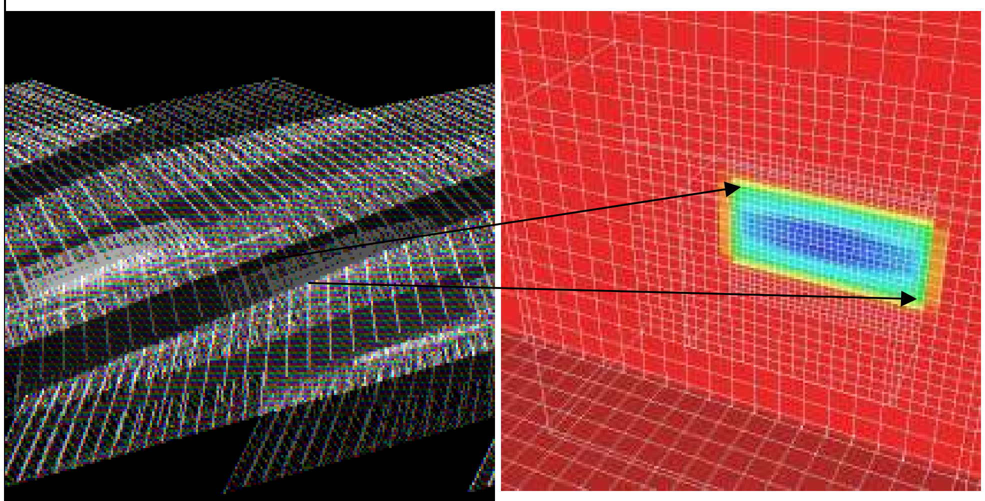


- Repetitive sawtooth cycles in CDX-U show periods of stochastic field lines
- M3D and NIMROD predict similar but different behavior. Now trying to understand differences in non-linear results




ELM Theory Milestone: with n>40modes:

- shows helically localized ripple structures
- $T_e$ perturbations less than $n_e$ perturbations



AMR simulation of Pellets predicts difference between inboard & outboard launch

# Accelerating Climate Science

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Advanced Scientific Computing Research Program

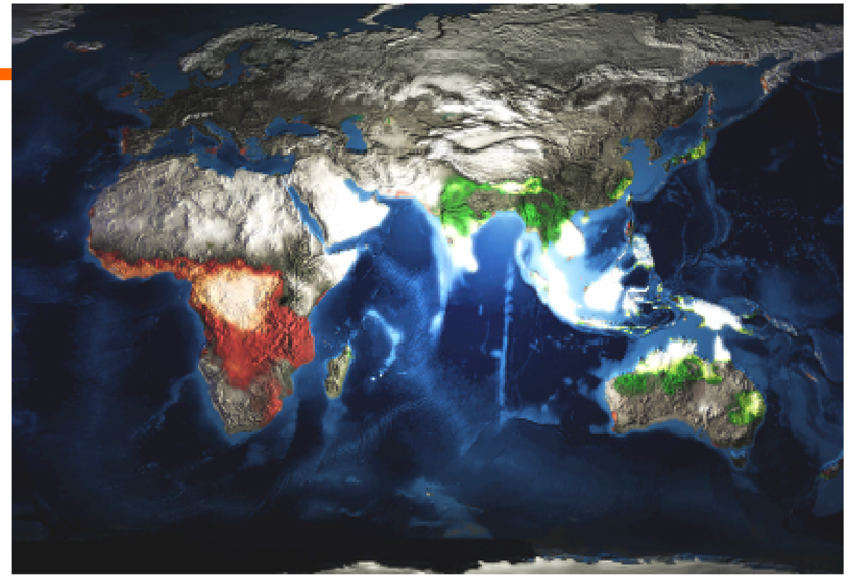
- **First-ever control runs of CCSM 3.5 at groundbreaking speed**

  ***"[On Jaguar,] we got 100-year runs in three days. This was a significant upgrade of how we do science with this model. 40 years per day was out of our dreams."***

  Peter Gent of NCAR, Chairman of CCSM Scientific Steering Committee, during keynote at CCSM Workshop, June 19, 2007

- **Major improvements in CCSM 3.5**
  - Arctic and Antarctic sea ice: Will the Arctic be ice free in summer of 2050?
  - Surface hydrology of land, critical for predictions of drought

- **Positioned to test full carbon-nitrogen cycle**



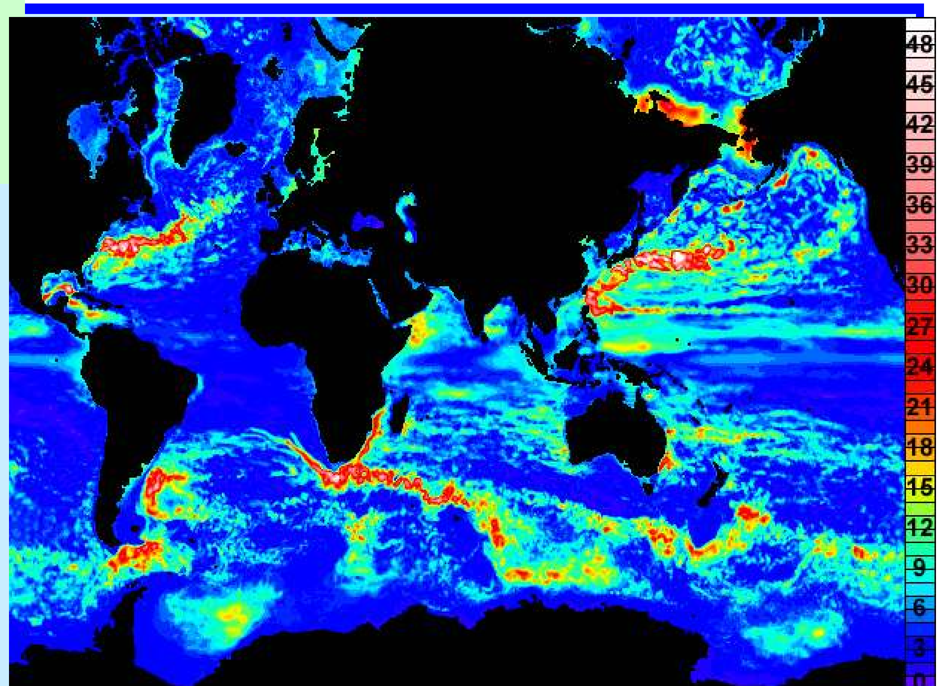
**Instantaneous net ecosystem exchange (NEE): eastern half is in sunlight and the terrestrial ecosystems are taking up carbon (negative NEE, shown in green to bright white). Meanwhile, the sun has not yet risen in the western half of the image where the ecosystems are only respiring (positive NEE, shown in red)**

# Understanding the Ocean's Role in Trapping Carbon Dioxide

*"…half of the carbon dioxide that has been emitted over the last 100 years or so currently resides in the atmosphere. The rest is in the ocean…"*

Synte Peacock, U. of Chicago, PI

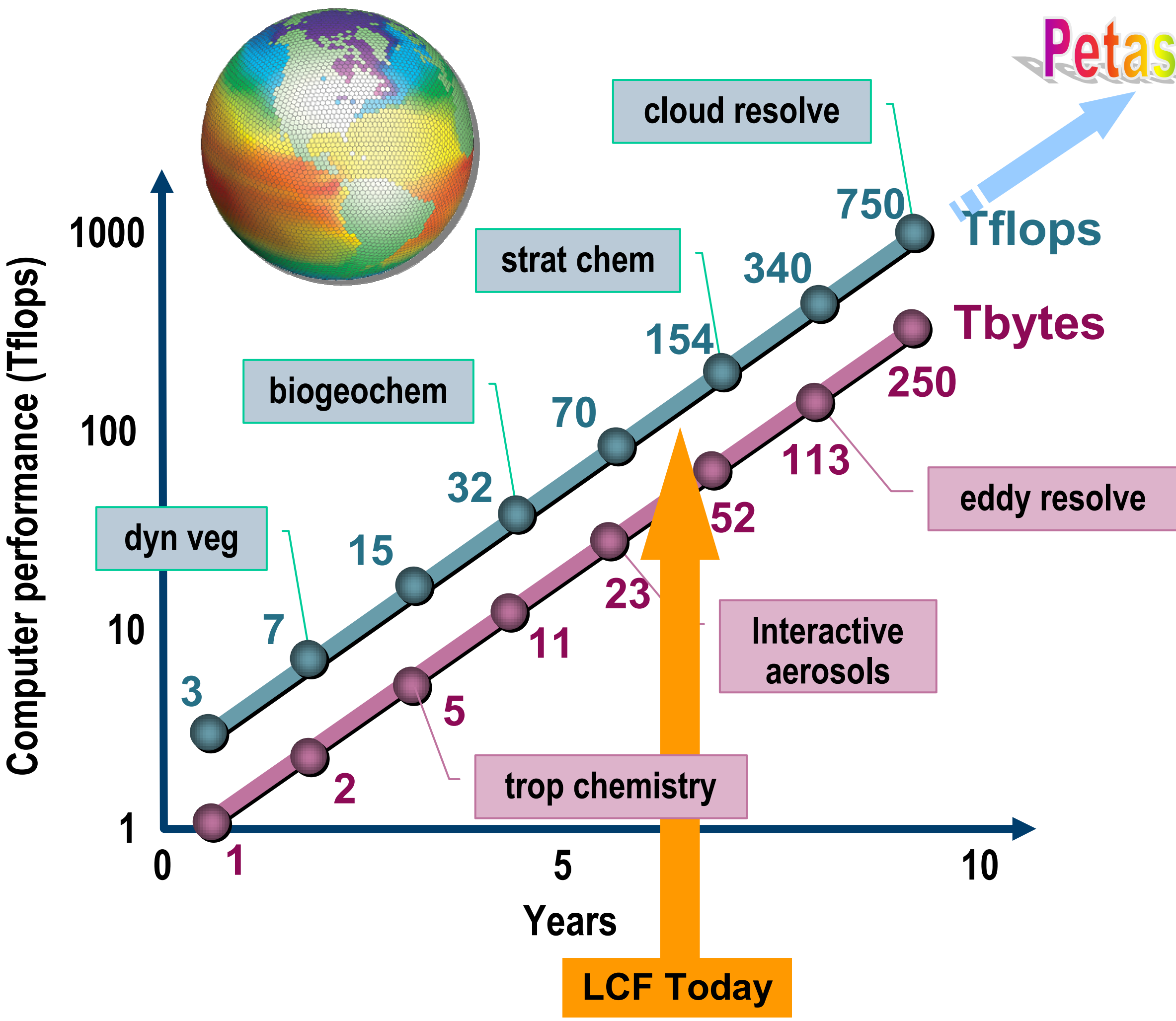
- Simulation promises to increase understanding of the ocean's role in regulating climate, as a repository for greenhouse gases
- The most fine-grained, global-scale simulations ever of how the oceans work
  - New knowledge of the currents and processes at work in the oceans
  - details about possible transport of gases and chemicals in the ocean




First-ever 100-year simulation of the ocean at a *fine enough scale to include the relatively small, circular currents known as eddies*. Until recently researchers lacked the computing power to simulate eddies directly on a global scale.

***Project looks into the fate of trapped heat and greenhouse gases***

# Climate Roadmap (2004 - 2014)




## Expected outcomes

### 5 years

- Fully coupled carbon-climate simulation
- Fully coupled sulfur-atmospheric chemistry simulation

### 10 years

- Cloud-resolving 30-km spatial resolution atmosphere climate simulation
- Fully coupled, physics, chemistry, biology earth system model

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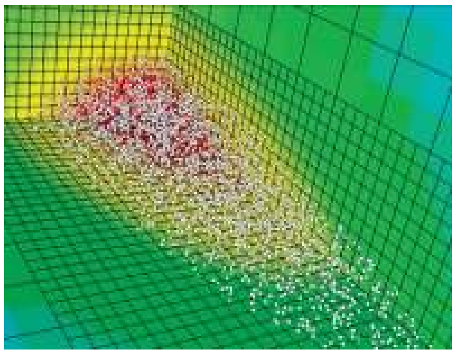
# Community Petascale Project for Accelerator Science and Simulation (COMPASS)

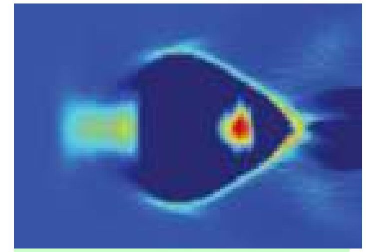
Advanced Scientific Computing Research Program



Terascale to the Petascale

Computational and Modeling Studies for Accelerator Design Research

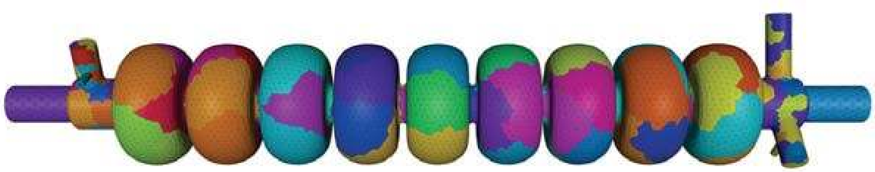
**Beam Dynamics, Electromagnetics, and Advanced Accelerator Concepts**

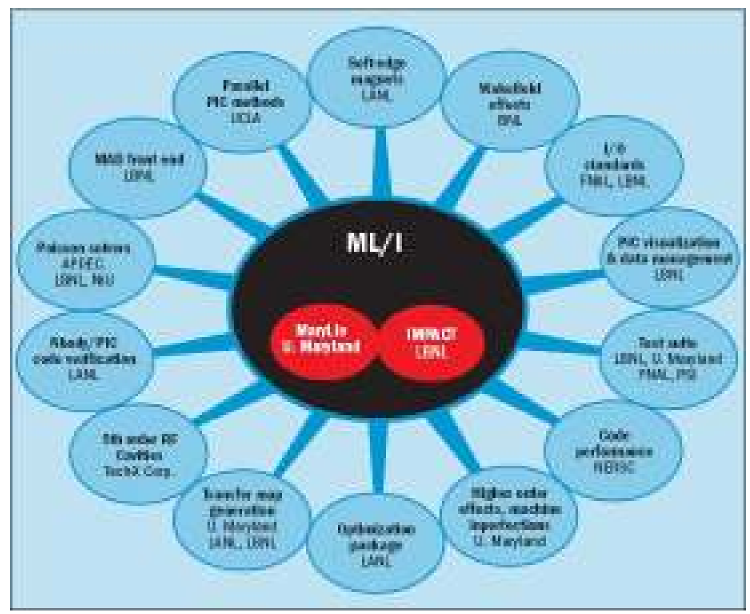


3 m annually for Five Years started April ’07

PI: Panagiotis Spentzouris

Collaborating Institutions: FNAL(lead), ANL, BNL, LBNL, LANL, ORNL, SLAC,Stonybrook U, TechX, TJNAL, U. Cal. Davis, U. Cal. LA, UMD.






**Applications for LHC, ILC, CeBAF, SNS….**

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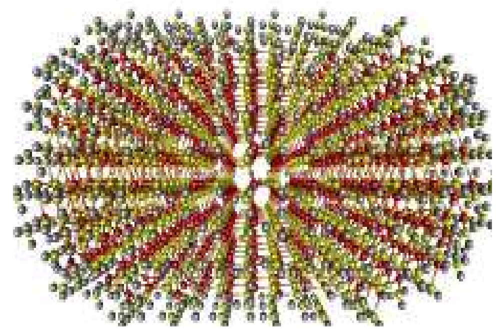
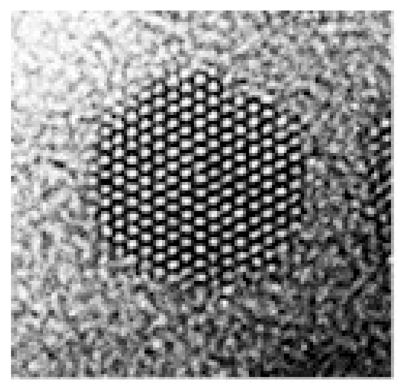
# Electronic Excitations and Optical Responses of Nanostructures

Advanced Scientific Computing Research Program

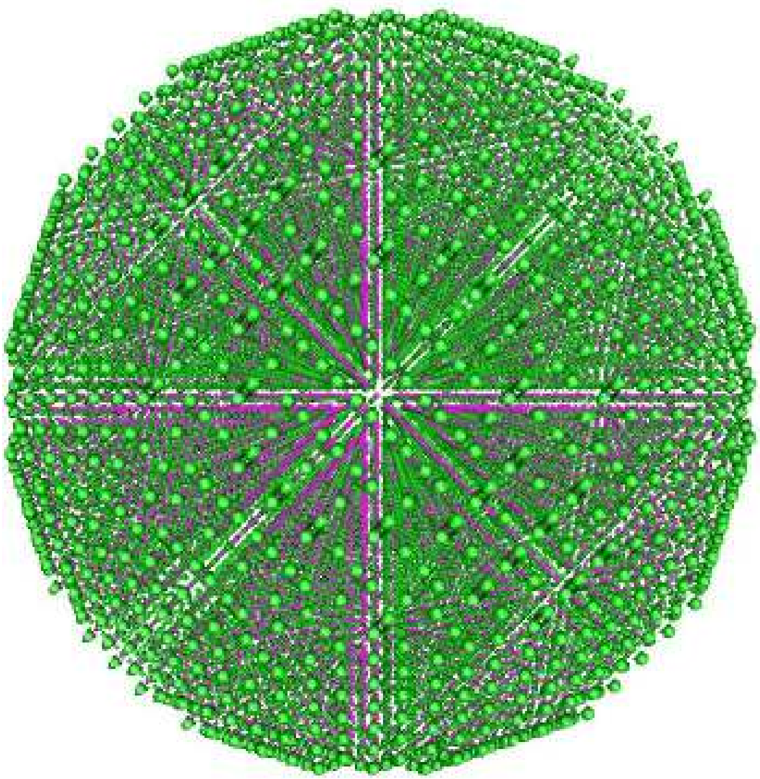

- Theory and modeling of the electronic excited-state and optical properties of various nanoscience structure
- Seek novel reformulations of the underlying physical theories by exploring new ideas in applied mathematics
- Scalable Methods





**P.I. s**
**Juan Meza and Martin Head-Gordon**

# Linear Scaling 3D Fragment (LS3DF) method



- Uses a novel divide and conquer approach to solve DFT
- Scales linearly with the number of atoms and has excellent parallel scaling
- Numerically equivalent to LDA
  - The total energy difference is 3meV/atom ~ 0.1 kcal/mol
  - Charge density difference: 0.2%
  - Atomic force difference: $10^{-5}$ a.u

**The charge density of a 15,000 atom quantum dot, $Si_{13607}H_{2236}$. Using 2048 processors at NERSC the calculation took about 5 hours, while a direct LDA calculation would have taken a few months.**

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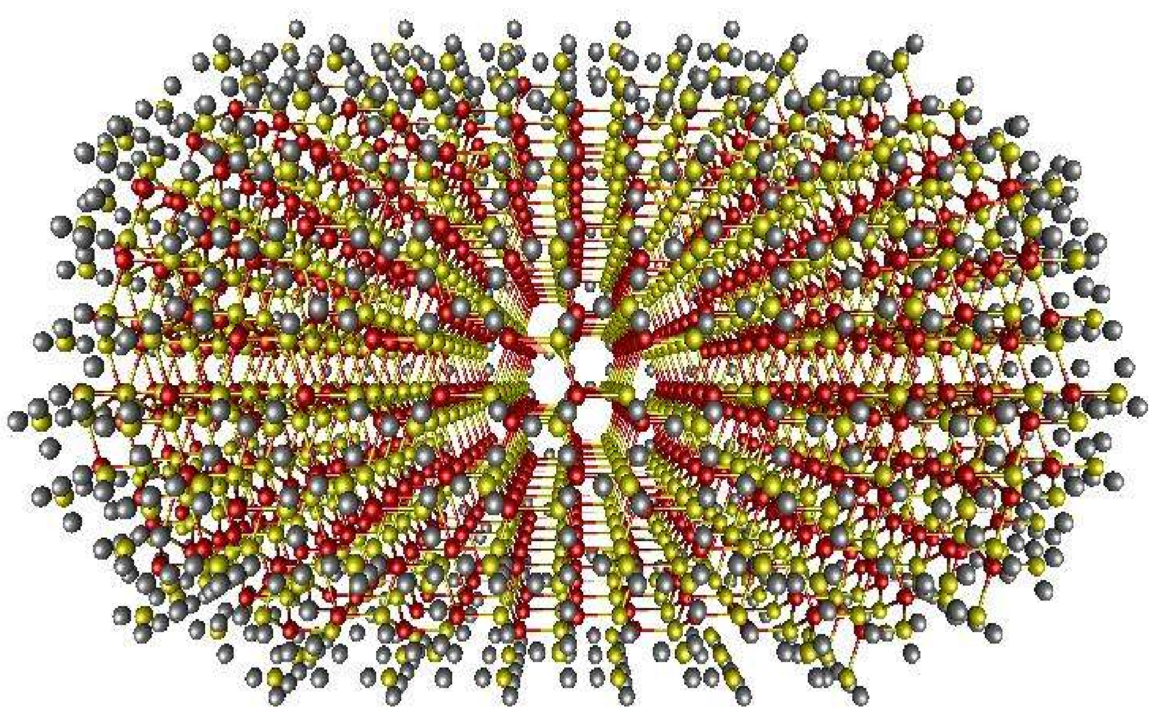
# Dipole Moment Calculation using LS3DF

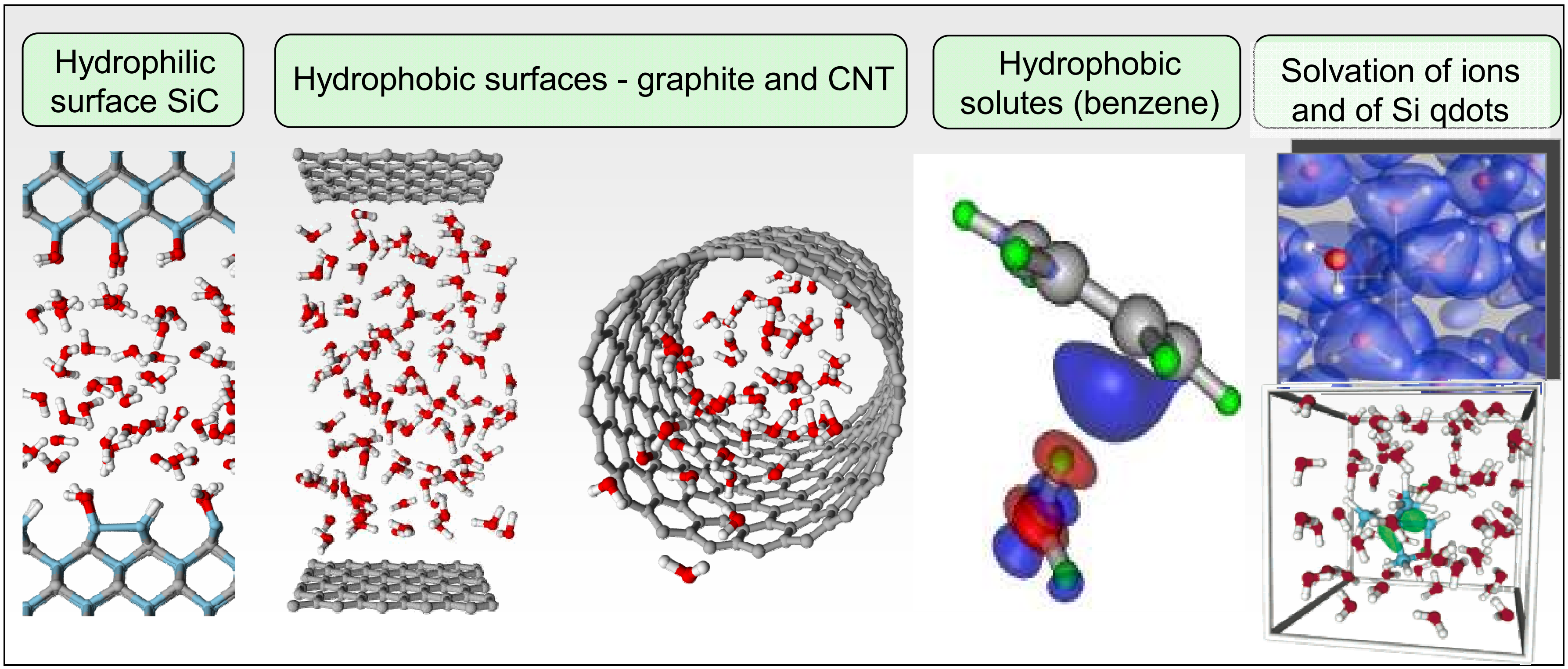
Advanced Scientific Computing Research Program



- The calculated dipole moment of a 2633 atom CdSe quantum rod, $Cd_{961}Se_{724}H_{948}$ .
- Using 2560 processors at NERSC the calculation took about 30 hours.

# Water at the interface

- Simulations address fundamental issues of interest to different disciplines, from chemistry and materials science (e.g. nanofluidic applications, and water in porous materials) to biology (e.g. water at interfaces with proteins, possibly influencing their folding). **P.I. Dr. Giulia Galli**



# ASCR efforts and SciDAC

- Funds SciDAC SAPs, CETs and Institutes
- Interfaces with Funding Partners
- Interfaces with SA Projects
- Managed by Research Division

- Facilities, ESnet, INCITE……

- Outreach Magazines:

SciDAC Review & ASCR Discovery

U.S. Department of Energy

Office of Science

# ASCR Facilities Update

Advanced Scientific Computing Research Program

- **LCF -- Argonne**
  - 5.7 Teraflop IBM Blue Gene/L (BGL) with 2,048 PPC processors
- **LCF -- Oak Ridge**
  - 119 teraflop Cray XT3/XT4 (Jaguar) with 11,708 dual core AMD Opteron processor nodes, 46 terabytes aggregate memory
  - 18.5 Teraflop Cray X1E (Phoenix) with 1,024 multi-streaming vector processors,

**NERSC**
  - 104 teraflop Cray XT4
  - 6.7 Teraflop IBM Power 5 (Bassi) with 888 processors, 3.5 terabytes aggregate memory
  - 3.1 Teraflop LinuxNetworx Opteron cluster (Jacquard) with 712 processors, 2.1 terabytes aggregate memory
- **ESnet**
  - Metropolitan Area Networks (MAN) in the San Francisco, Chicago and New York-Long Island Areas provide dual connectivity at 20 gigabits per second.

# Future Facility Upgrades

- ALCF
  - 100 teraflop IBM Blue Gene/P in transition to operations
  - 446 teraflop IBM Blue Gene/P upgrade in acceptance testing

- LCF – Oak Ridge
  - Cray XT4 250 TF upgrade completed and acceptance testing due to start
  - 1 Petaflop Cray Baker system to be delivered by end of 2008

**http://www.sc.doe.gov/ascr**

# INCITE: 2008 Awards

**The 2008 INCITE (Innovative and Novel Computational Impact on Theory and Experiment) awards provide the largest amount of supercomputing resource awards donated in DOE's history -- three times that of last year's award.**

- **265 million processor-hours**
- **55 scientific projects**

**Applications were chosen based on their potential breakthroughs in the science and engineering research and their suitability of the project for using supercomputers.**

# INCITE: 2008



Advanced Scientific Computing Research Program

## Organizations awarded include:

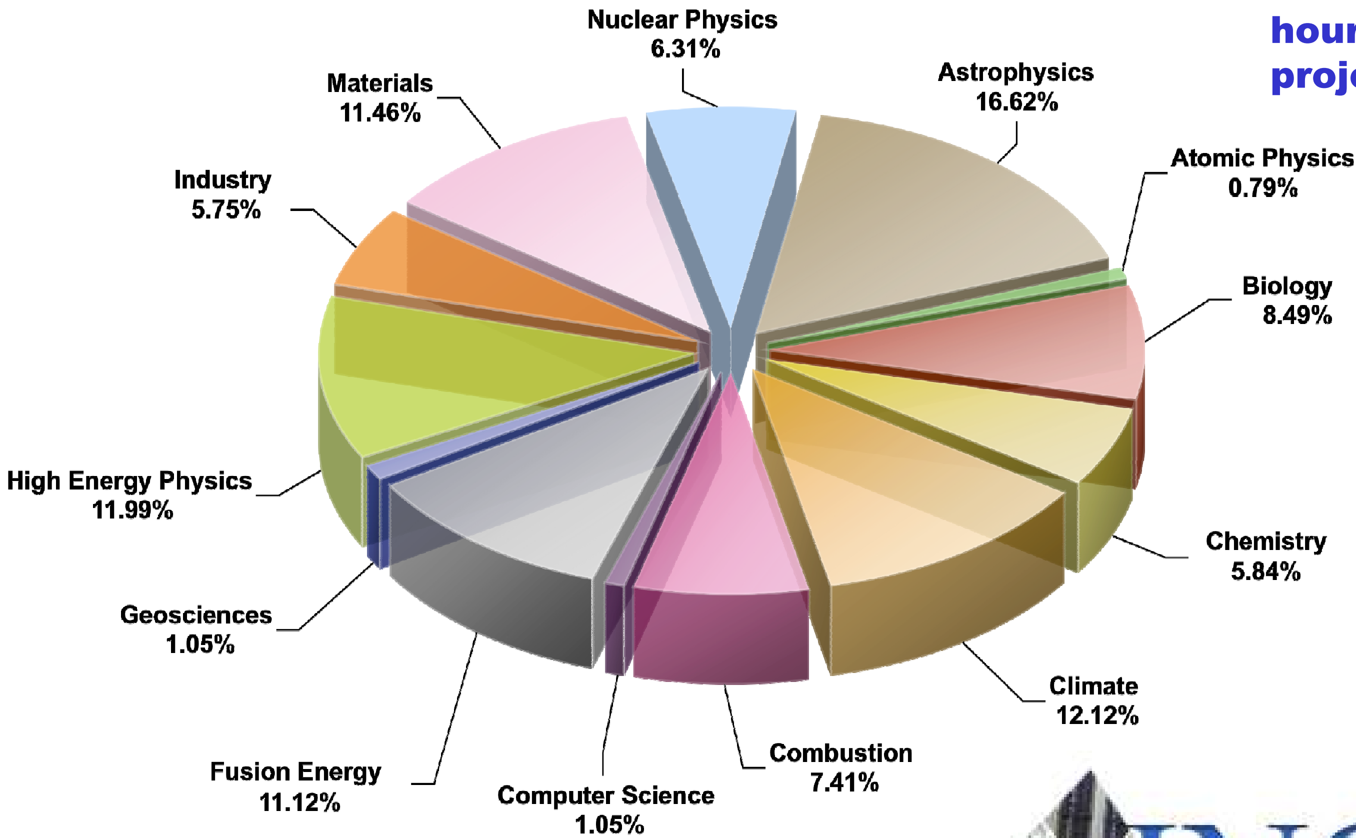
- **DOE Labs:** Argonne, Brookhaven, Fermi, Los Alamos, Lawrence Berkeley, Lawrence Livermore, NETL, Oak Ridge, Pacific Northwest, Princeton Plasma Physics, Sandia, Stanford Linear Accelerator
- **Other Agency Labs:** NASA, NASA/Goddard, NCAR, NIST, NOAA, NOAA/ESRL, SDSC, Woods Hole Oceanographic Institute
- **Non-U.S. Organizations:** CERFACS, **CRIEPI**, Max-Planck Gesellschaft, Universities of Strathclyde and Toronto, Weizmann Institute of Science
- **Industry:** Aeolus Research, Bell Labs, Boeing, Corning, Cray Europe, Gene Network Sciences, General Atomics, General Motors, GM R&D Center, IBM, IBM Research-Zurich, Pratt & Whitney, Proctor and Gamble, Vita Nuova

U.S. Department of Energy
Office of Science

# 2007 INCITE Allocations by Disciplines

Advanced Scientific Computing Research Program

**95 Million processor hours allocated to 45 projects in 2007**




Office of Science
U.S. DEPARTMENT OF ENERGY
INCITE
Advancing America's Science and Industrial Competitiveness

U.S. Department of Energy

Office of Science

Advanced Scientific Computing Research Program

# SciDAC

# Outreach

# Center

# SciDAC Outreach Center Mission

- Provide services that make SciDAC supported technologies more accessible both within and outside the SciDAC community
- Field inquires about SciDAC that range from general information to technical specifics
- Assist in deployment and bridge gaps between SciDAC stakeholders
- Provide a central orientation for all things SciDAC. Get interested parties to the right resources
- Foster awareness and education about HPC

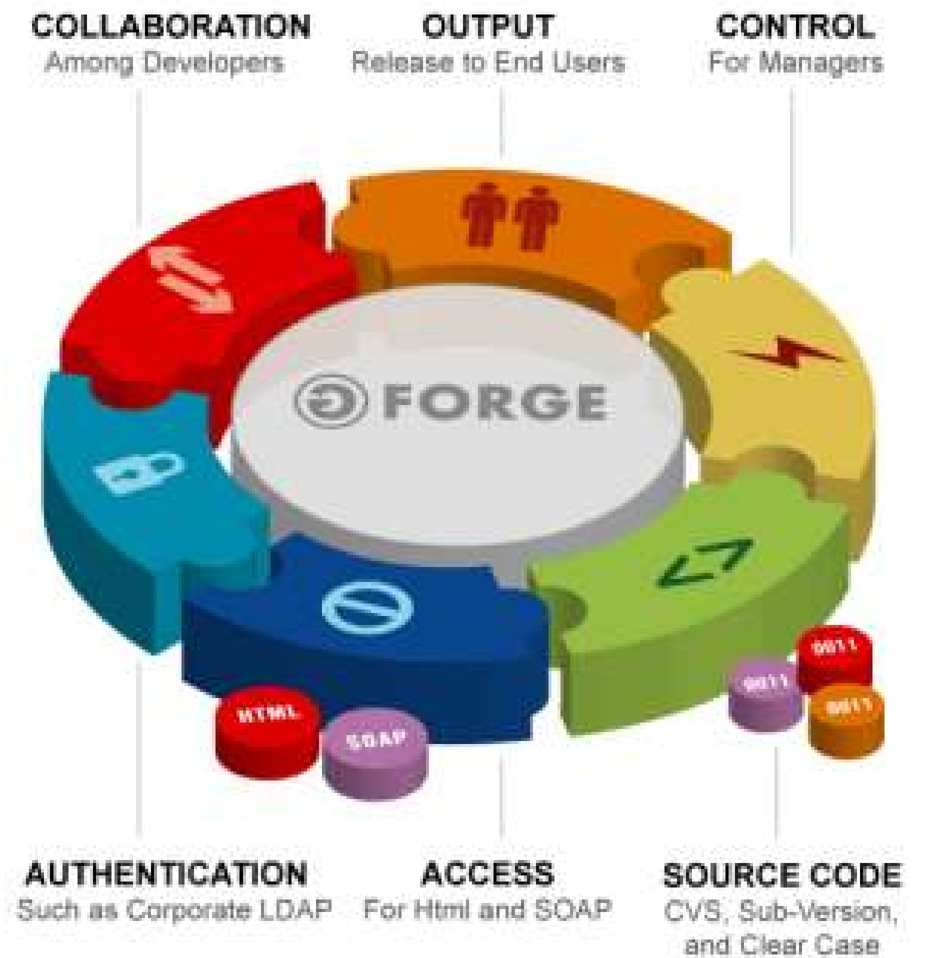
# Outreach can mean many things

We are currently focused on two approaches:

- Innovative web and software services
  - Tools which make SciDAC researchers more effective at delivering their technologies
  - Information services which provide an easy interface to SciDAC for all involved
- In person outreach
  - Workshops, trainings, and event coordination
  - Getting the right people to the right audiences

# Collaborative e-Services

- •Author Documents
- •Inform Collaborators
- •Inform the Public
- •Develop Software
- •Test Software
- •Package Software
- •Distribute Software




How?
http://outreach.scidac.gov/

# Computational Science Graduate Fellowship Program…

… provides up to 4-year doctoral fellowships to students performing computational science & engineering research

- Program of study in discipline area + computer science + applied mathematics
- Practicum at DOE lab for >12 weeks
- Currently supports 62 students at 29 universities in 17 states
- Pays for - Full tuition, Yearly stipend, Academic allowance, Workstation purchase, Fellows conference
- Nearly 225 students at more than 50 U.S. universities have trained as Fellows, and the demand is only growing – 395 applications received in 2007 – approximately 22 awards are made each year

**Nurturing the Computational Science, Math and Engineering communities and helping to train the next generation of leaders**

http://www.sc.doe.gov/ascr/CSGF/CSGF.html

U.S. Department of Energy

Office of Science

Advanced Scientific Computing Research Program

# Next issue…

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SciDAC Review - Home Page
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SciDAC
REVIEW
Scientific Discovery through Advanced Computing
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Welcome to the first issue of the SciDAC Review magazine, celebrating some of the successes and activities of the Scientific Discovery through Advanced Computing (SciDAC) program as it completes its first phase and embarks on SciDAC-2.
SciDAC is a specially designed program within the Office of Science of the US Department of Energy. It enables scientific discovery though advanced computing, and is driven by a spirit of collaboration. Discipline scientists, applied mathematicians, and computer scientists are working together to maximize use of the most sophisticated high-power computers for scientific discovery (www.scidac.org).
The SciDAC Review is a twice-yearly magazine that will showcase different SciDAC projects and share SciDAC-related news and science achievements through successive issues.
We wish to thank everyone who has kindly contributed time and effort to this issue.
Cover Story
IN THIS ISSUE
Our cover story is an interview with Dr Raymond Orbach, Director of the Office of Science, who talks to us about science, discovery, and SciDAC. We also showcase several projects - on accelerators, astrophysics, fusion and terascale solvers - that demonstrate the power of advanced computing as a discovery tool. And Dr Michael Strayer, Associate Director of the Office of Science and Director of the SciDAC program, looks to the future.
Table of Contents
The fall 2006 issue will discuss other SciDAC projects and science achievements.
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# SciDAC Review (cont.)

## THE ACCELERATOR SCIENCE AND TECHNOLOGY PROJECT

Fig. 17

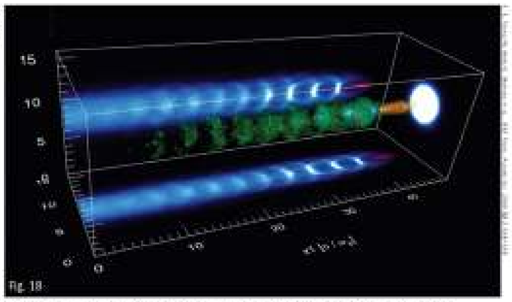

Fig. 18

**Fig. 17.** Partitioned mesh of the damped, detuned cell for the next linear collider (predecessor to the ILC). **Fig. 18.** Isosurface plots of the electron beam (orange) and electron plasma (green) density as the beam creates a wake in a self-ionized generated plasma. The projections on the walls are color contour plots of the electron plasma density.

"More advanced tools are needed to simulate the complicated cavity designs under consideration for future facilities, such as ILC and RIA, to accuracies in speed and problem size previously not possible."

Dr Kwok Ko
Co-Principal Investigator

millions of dollars or more in construction costs. Using simulation to predict and mitigate instabilities affects the maximum amount of current that can be transported; this ultimately affects how much science can be done at an accelerator facility. High-resolution simulations are crucial to predicting and minimizing the formation of beam halos and the loss of particles that strike the beam pipe. When too much charge is lost, the beam pipe and surrounding components become radioactive. This can hinder or prevent hands-on maintenance, which reduces the time for accelerator operation (and hence, reduces the science). For example, accelerators like the SNS linac or the proposed FNAL Proton Driver can lose about 1 W of power per meter of accelerator. When one considers that the beam power is now approaching 1 MW, the loss of 1 W/m represents a very tiny loss indeed. Beam halo is a key issue for future high-intensity accelerators, and high-resolution beam dynamics modeling is a critical tool for designing such ultra-low-loss accelerators.

### Electromagnetic modeling

Next-generation accelerators are planned with increasingly challenging specifications in beam energy, precision demands and machine current. As a result, the geometry of the accelerating cavity, for example, has become more complex and the design constraints more stringent. "While numerical modeling is already used extensively in the accelerator community," says Dr Kwok Ko, co-Principal Investigator on the AST project, "more advanced tools are needed to simulate the complicated cavity designs under consideration for future facilities, such as the ILC and the Rare Isotope Accelerator (RIA), to accuracies in speed and problem size previously not possible."

The Electromagnetic System Simulations (ESS) team, working within the AST project, is concerned with the design of the actual hardware of the accelerator, such as the accelerating cavity and the associated beam line sections. Simulating accelerator cavities prior to construction is a practice that has been in vogue for decades. Conventional electromagnetic software for modeling accelerating cavities include MAFIA, Microwave Studio and HFSS. Dr Ko says: "Most present codes are limited to small problem size as they only run on a single computer, while the latest supercomputers consist of thousands of processors with a significantly larger total memory." Evolution of massively parallel computer architecture providing extensive accessible memory invokes the need to develop scalable capability in software tools and computing techniques to harness this increase in compute power and memory. AST codes are filling this need to accelerate advances in accelerator design, including cavities with incredibly complex geometric shape and high accuracy requirements because of tight fabrication tolerances (see figures 15–17).

Scientists working on the AST project based at SLAC are developing parallel finite element electromagnetic codes that utilize the massive memory resources of the Department of Energy (DOE)'s Office of Science Supercomputers, e.g. the Cray/X1E (Phoenix) at NLCF and the IBM/SP (Seaborg) at NERSC. The suite of codes includes the eigensolver Omega3P, the S-matrix solver S3P, the time-domain solver T3P, and the particle tracking code Track3P, which can provide significant gains in accuracy, problem size and solution speed when run on the these flagship computers. In particular, Omega3P has proven invaluable in the application to the design of a new low-loss (LL) accelerating cavity for the ILC.

As in the case of the other SciDAC projects, the AST ESS team works in close collaboration with researchers in the Integrated Software Infrastructure Centers (ISICs) and Scientific Application Pilot Program (SAPP). This multi-disciplinary group of scientists is working together to improve a multi-step simulation process that starts with the geometry of the electromagnetic structure in the form of a drawing or base model. The systems are partitioned into meshes and studied on high-performance computers using solver codes. Visualization techniques are important aids for the analysis of the complex data sets resulting from the unstructured grid solutions. The major achievements include meshing, eigensolvers, visualization, refinement, and shape optimization of computational applications for accelerator design.



## New plasma acceleration methods

Conventional acceleration techniques, as described in the sidebar "Accelerating particles" on p16, are limited to the energies they can reach by their sizes. These techniques allow accelerating gradients of 20–100 MeV energies per meter traversed by the accelerated particles. In addition, the technology involved in maintaining strong fields across extended regions of space is formidable, and beams may become susceptible to break down conditions. To overcome these potential hurdles, the accelerator community is exploring novel methods to circumvent them for new generations of accelerators.

A promising answer lies in the use of the properties of plasmas to allow high-gradient acceleration when injected with a driver beam (see figures 18–23). As the driver beam cuts through the plasma it generates a wake that can trap plasma particles and carry them forward. This effect is able to accelerate the wake particles to high energies over extremely short length and time scales. The resulting accelerating gradients can be as high as 10–100 GeV per meter, resulting in a factor of 1000 magnification over conventional techniques. Just as nature eludes perfect symmetry, so also there is rarely a "perfect" solution to any problem. In the case of plasma acceleration, the difficulties lie in focusing and stabilizing the driver beams, which are usually lasers or particle beams.

Work in developing novel accelerator technology requires both simulation and experimental studies. AST researchers have designed the "QuickPIC" code – which allows a faster and more efficient use of the PIC method on HPC platforms. Recent experiments have shown significant energy gains by these methods and AST codes were used in the planning of these experiments.

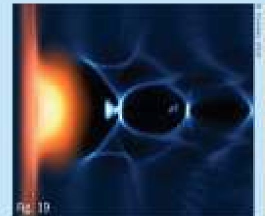

Fig. 19

Fig. 20

**Fig. 19.** *A 2D slice of a 3D-simulation showing the laser envelope (in orange) and the plasma density (in blue). As the laser moves from right to left it blows out the electrons, which rush back to the axis once the laser has passed. There, they feel a strong accelerating force and are self-injected in the laser's wakefield. They are accelerated until they outrun the wake.* **Fig. 20.** *Electron beam driven wakefield excitation. A 2D color contour plot of the beam and electron density is obtained from a 3D QuickPIC simulation. The beam is moving from right to left. The black line is the resulting accelerating electric field.*

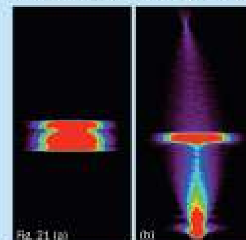

Fig. 21 (a) (b)

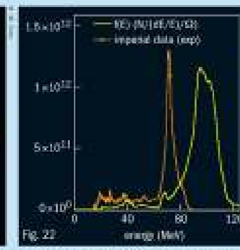


Fig. 22

**Fig. 21.** *3D QuickPIC simulations of the E-167 experiment at SLAC. Plots of the energy of the electron beam against one transverse coordinate.* **Fig. 21.(a)** *is the image without plasma, showing the energy chirp of the incident beam.* **Fig. 21.(b)** *is the image after the beam has propagated through the plasma, showing the acceleration of the tail and the deceleration of the head of the beam.* **Fig. 22.** *Comparison of the accelerated electron-beam energy spectra between experimental data and a 3D OSIRIS simulation.*

Just as nature eludes perfect symmetry, so also there is rarely a "perfect" solution to any problem.

# Acknowledgements


- from ASCR Office: Michael Strayer, Barbara Helland, Frederick Johnson, and Walt Polansky
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Giulia Galli (UC Davis)

Special thanks: Betsy Riley (OASCR and ORNL)

# Going Forward

High end computation and SciDAC are helping to transform basic scientific research and global science.

**Over the past five years, we have launched programs to**

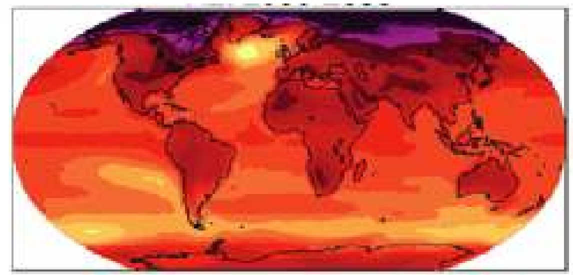
- **develop tools for increasingly detailed simulations**
- **extract the science from massive datasets** and
- **support the computing and networking demands of large-scale experimental facilities**

## Results

**Changes in the very fabric of scientific research and discovery**
**Substantial Reduction in U.S. Industry R&D costs and time to reach markets**

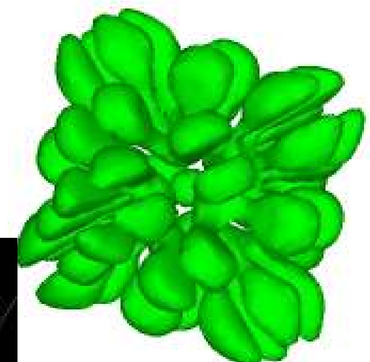
# Going Forward…

- Expanding SciDAC collaborations to new areas of basic and applied sciences –
- Includes environmental and global implications
- Facilities -> exa-scale
- Science at the exa-scale –
- Exciting possibilities – strengthening known successes and exploring new ones

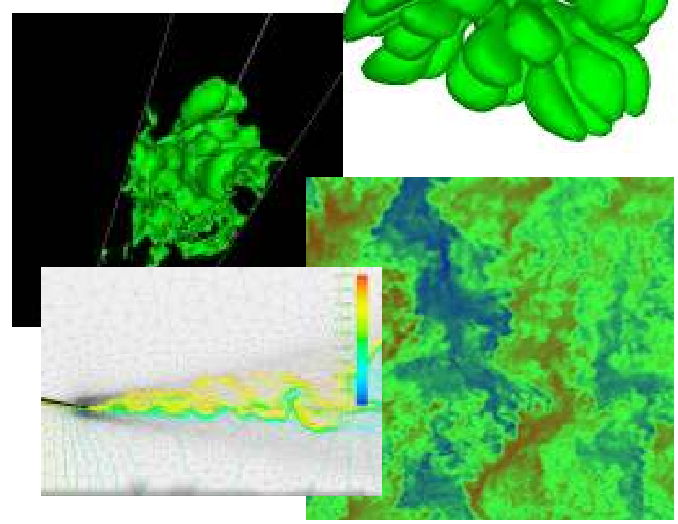



# SciDAC 2007 Conference

**Registered participants- over 300**
**Plenary talks- 36, Posters- 76, Panels- 2**



## SciDAC 2008, Seattle, Washington July ‘08

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