Update from the Office of Science

Advanced Scientific Computing Advisory committee

August 24, 2010

Dr. W. F. Brinkman
Director, Office of Science
U.S. Department of Energy
www.science.doe.gov

The Administration's S&T Priorities for the FY 2011 Budget

"When we fail to invest in research, we fail to invest in the future. Yet, since the peak of the space race in the 1960s, our national commitment to research and development has steadily fallen as a share of our national income. That's why I set a goal of putting a full 3 percent of our Gross Domestic Product, our national income, into research and development, surpassing the commitment we made when President Kennedy challenged this nation to send a man to the moon."

President Barack Obama
September 21, 2009

http://www.whitehouse.gov/the_press_office/Remarks-by-the-President-on-Innovation-and-Sustainable-Growth-at-Hudson-Valley-Community-College/

U.S. DEPARTMENT OF ENERGY

Energy R&D Organizations

- **Secretary** Steven Chu
  Deputy Secretary Daniel B. Poneman
  - **Under Secretary for Energy** Kristina Johnson
    - **Energy Efficiency & Renewable Energy** Cathy Zoi
    - **Fossil Energy** James Markowski
    - **Nuclear Energy** Pete Miller
    - **Electricity Delivery and Energy Reliability** Pat Hoffman (A)
  - **Under Secretary for Science** Steven E. Koonin
    - **Office of Science** William Brinkman, Patricia Dehmer
      - **Basic Energy Sciences** Harriet Kung
      - **High Energy Physics** Dennis Kovar
      - **Advanced Scientific Computing Research** Michael Strayer
      - **Nuclear Physics** Tim Hallman
      - **Biological & Environmental Research** Anna Palmisano
      - **Fusion Energy Sciences** Ed Synakowski
      - **Workforce Development for Teachers & Scientists** Bill Valdez
  - **Advanced Research Projects Agency – Energy** Arun Majumdar

Status of FY 2011 Budget Request and Appropriations

(dollars in thousands)

	FY 2010	Total Recovery Act	FY 2011						
	Current Approp.		FY 2011 Request to Congress	House Mark	House Mark vs. Request		Senate Mark	Senate Mark vs. Request	
Office of Science									
Advanced Scientific Computing Research	394,000	+161,795	426,000				418,000	-8,000	-1.9%
Basic Energy Sciences	1,636,500	+555,406	1,835,000				1,739,115	-95,885	-5.2%
Biological & Environmental Research	604,182	+165,653	626,900				614,500	-12,400	-2.0%
Fusion Energy Sciences	426,000	+91,023	380,000				384,000	+4,000	+1.1%
High Energy Physics	810,483	+232,390	829,000				820,085	-8,915	-1.1%
Nuclear Physics	535,000	+154,800	562,000				554,000	-8,000	-1.4%
Workforce Development for Teachers & Scientists	20,678	+12,500	35,600				21,000	-14,600	-41.0%
Science Laboratories Infrastructure	127,600	+199,114	126,000				126,000	——	——
Safeguards & Security	83,000	——	86,500				86,500	——	——
Science Program Direction	189,377	+4,600	214,437				208,000	-6,437	-3.0%
Small Business Innovation Research/Tech. Transfer (SC)	107,351	+18,719	——				——	——	——
Subtotal, Science	4,934,171	+1,596,000	5,121,437	4,881,650	-239,787	-4.7%	4,971,200	-150,237	-2.9%
Earmarks	76,890	——	——	18,350	+18,350	——	40,800	+40,800	——
Small Business Innovation Research/Tech. Transfer (DOE)	60,176	+72,775	——	——	——	——	——	——	——
Total, Science	5,071,237	+1,668,775	5,121,437	4,900,000	-221,437	-4.3%	5,012,000	-109,437	-2.1%

Office of Science – House Mark

(dollars in Thousands)

	FY 2010 Approp.	FY 2011 Request	House	House vs. FY 2010 Approp.		House vs. Request	
SC, Total	4,903,710	5,121,437	4,900,000	-3,710	-0.1%	-221,437	-4.3%

- No details are available, no vote on bill scheduled
- Includes $18,350 in Earmarks.
- Approximately the same as FY 2010.
- Ensures the United States' continued global leadership of basic science research and develops the fundamental knowledge necessary for the next generation of energy innovations.
- Investments in HEP pushes the edges of scientific knowledge and fosters our nation's world-leading scientists.
- Research in BES, FES, ASCR, NP, and BER build the foundation of knowledge that will enable us to transform our energy sector to be more secure and sustainable.

Office of Science – Senate Mark

(dollars in Thousands)

	FY 2010 Approp.	FY 2011 Request	Senate	Senate vs. FY 2010 Approp.		Senate vs. Request	
SC, Total	4,903,710	5,121,437	5,012,000	+108,290	+2.2%	-109,437	-2.1%

- Includes $40.8M in Earmarks, $11M for Artificial Retina, $15.4M for Nuclear Medicine research, $100M to support EFRCs, $16M for Fuels from Sunlight Energy Innovation Hub, $22M for a new Batteries and Energy Storage Energy Innovation Hub, $35M for EPSCoR, and $5M for Graduate Fellowship.
- NP is down $8M from request but has the nuclear medicine added
- Funding increase in FY 2011 will support initiatives to advance scientific understanding for new energy technologies.
- Concerned about LHC's planned shutdown; the Federal commitment to nuclear medicine research; cost increases and schedule delays related to the ITER project; and finding that the United States risks losing leadership and competitiveness in material science.

FY 2011 Senate Markup Details for ASCR

Advanced Scientific Computing Research

(in whole dollars)

	House	Senate	Conference
FY 2011 Request	$ 426,000,000	$ 426,000,000	$ 426,000,000
Committee Mark	424,800,000	418,000,000	—
Change to Request	-1,200,000	-8,000,000	
Congressional Direction:			
Mathematical, Computational, and Computer Sciences Research [a]	-1,200,000	—	—
Total Congressional Direction	-1,200,000	—	—
Net unspecified program impact	—	-8,000,000	

[a] The House subcommittee recommends $163,891,000 for Mathematical, Computational, and Computer Sciences Research, $1,200,000 below the request of $165,091,000.

DOE Office of Science Graduate Fellowships

The FY 2011 request doubles the number of graduate fellowships in basic science

$10 million is needed to FY 2011 to fund 150 additional fellowships

Purpose: To educate and train a skilled scientific and technical workforce in order to stay at the forefront of science and innovation and to meet our energy and environmental challenges and to couple the fellows into the Departments research

Eligibility:

- Candidates must be U.S. citizens and a senior undergraduate or first or second year graduate student to apply
- Candidates must be pursuing advanced degrees in areas of physics, chemistry, mathematics, biology, computational sciences, areas of climate and environmental sciences important to the Office of Science and DOE mission

Award Size:

- The three-year fellowship award, totaling $50,500 annually, provides support towards tuition, a stipend for living expenses, and support for expenses such as travel to conferences and to DOE user facilities.

FY 2010 Results:

- 150 awards were announced this summer using FY 2010 and American Recovery and Reinvestment Act funds.

FY 2011 Application Process:

- Funding Opportunity Announcement issued in Fall 2010
- Awards made in March 2011

Prospects for Solar Fuels Production

Two Limits

What We Can Do Today

$12/kg H_2 @ $3/pW PV

(BRN on SEU 2005)

PV cell

balance of system

current

electrolyzer

gas

fuel storage

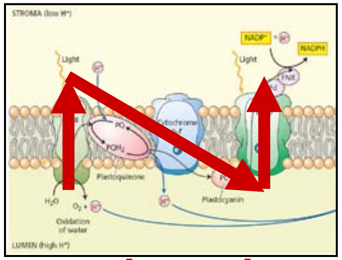
H_2 compression

High capital costs

We do not know how to produce solar fuels in a cost effective manner.

Ultimate Goal

solar microcatalytic energy conversion



liquid

fuel storage

gas

fuel storage

compression

Low capital costs

Chemists do not yet know how to photoproduce O_2, H_2, reduce CO_2, or oxidize H_2O on the scale we need.

Award of the "Fuel From Sunlight" Hub

- Winning team led by Cal Tech and LBNL
- Other institutions involved:
  - SLAC National Accelerator Laboratory
  - Stanford University
  - UC Berkeley
  - UC Santa Barbara
  - UC Irvine
  - UC San Diego
- Professor Nate Lewis leader
- Looking for a factor of 10 over nature
- Strong push to integrate processes to form a complete system

FY 2011 Energy Innovation Hub for Batteries and Energy Storage

Addressing science gaps for both grid and mobile energy storage applications

The Administration's Energy Plan has two goals that require improvements in the science and technology of energy storage:

- Solar and wind providing over 25% of electricity consumed in the U.S. by 2025
- 1 million all-electric/plug-in hybrid vehicles on the road by 2015

- Grid stability and distributed power require innovative energy storage devices
  - Grid integration of intermittent energy sources such as wind and solar
  - Storage of large amounts of power
  - Delivery of significant power rapidly
- Enabling widespread utilization of hybrid vehicles requires:
  - Substantially higher energy and power densities
  - Lower costs
  - Faster recharge times

World’s Most Powerful Computers for Open Science

#1

#9

WORLD’S FASTEST OPEN SCIENCE SUPERCOMPUTER
ALCF
ARGONNE LEADERSHIP COMPUTING FACILITY
JUNE 2008 • SOURCE: 31ST TOP500

#17

NERSC

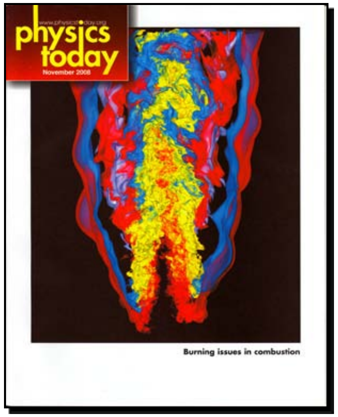
Rankings from June, 2010 Top 500 Supercomputing List

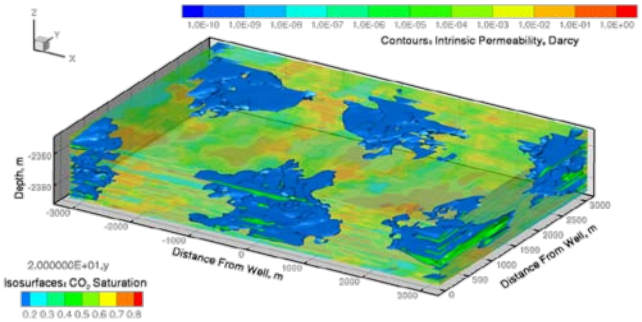
Exascale Initiative

The Goal: *“Provide the United States with the next generation of extreme scale computing capability to solve problems of National importance in Energy, the Environment, National Security, and Science”*

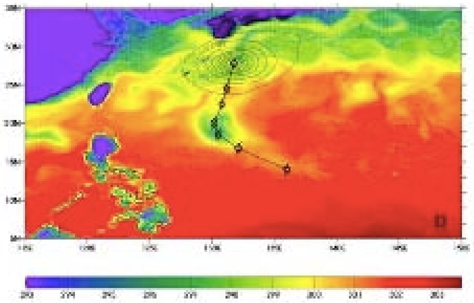
Why do Exascale?

- Environment
- Energy
- National Security
- Science and Innovation
- American Competitiveness



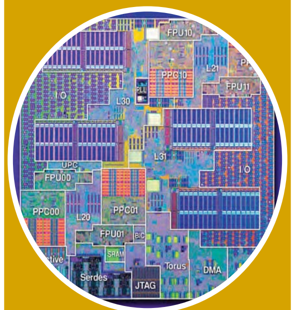


Geologic sequestration



Massive Earth System Model ensembles
(e.g. decadal forecasts, extreme weather)

Exascale Initiative Major Components



Platform R&D

2 Vendor Tracks

- Power
- Integration
- Risk Mitigation

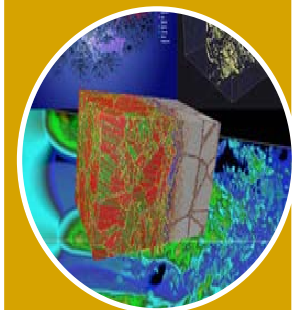
Critical Technologies

(everyone benefits)

- Memory
- Nonvolatile storage
- Optics

Software and Environments

- Operating environment
- Systems Software
- System reliability
- Programming model



Co-design

- Physics Models
- Applied Math
- Performance models
- Simulators
- Applications integration with vendors

Platforms

- Early prototypes to ensure component integration and usefulness
- Risk mitigation for vendors – Non recoverable engineering cost

Exascale Initiative

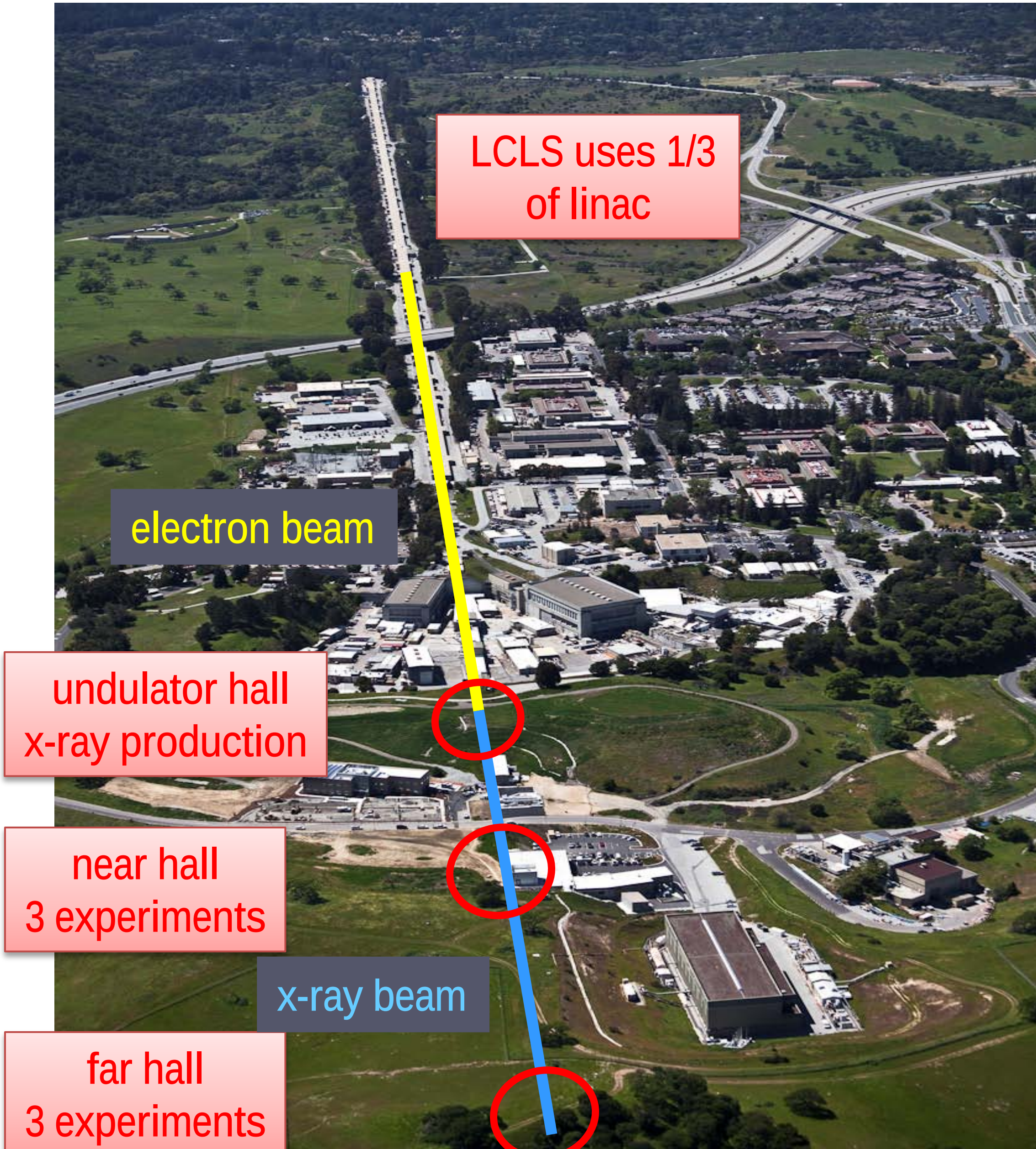
FY 2010: Focused on long lead time research for exascale:

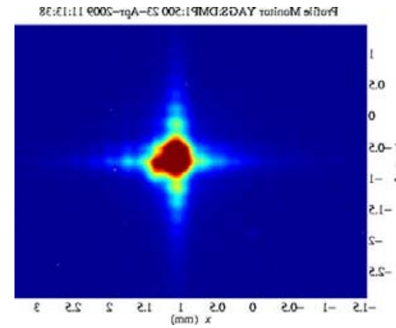
Underpins Exascale

- Applied Math
  - Complex mathematics with uncertainty quantification
    - Research that addresses the mathematical challenges involved in developing highly scalable approaches for uncertainty analysis in the modeling and simulation of complex natural and engineered systems.
- Computer Science
  - X-Stack Software Research
    - Emphasis on transformational computer science discoveries focused on the development of a scientific software stack that supports extreme scale scientific computing, from operating systems to development environments.
  - Advanced Architectures and Critical Technologies for Exascale Computing
    - Basic and applied research to address fundamental challenges in the design of energy-efficient, resilient hardware and software architectures and technology for high performance computing systems at exascale.
  - Scientific Data Management and Analysis at the Extreme
    - Innovative basic research in computer science for management and analysis of extreme-scale scientific data in the context of petascale computers and/or exascale computers with heterogeneous multi-core architectures.

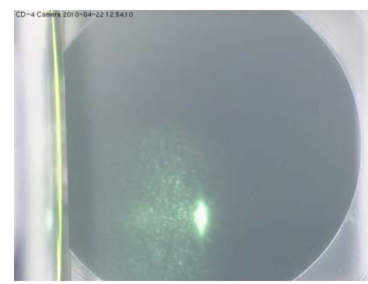
Linac Coherent Light Source or “LCLS” at SLAC

The World’s First X-ray Laser





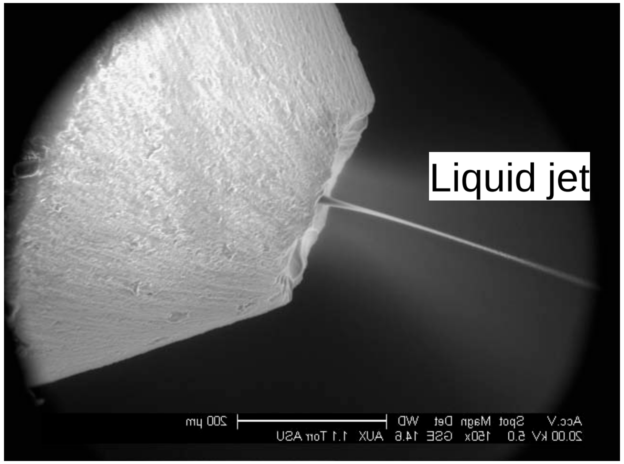
First X-rays: ~ 1 PM PDT 4/15/2009



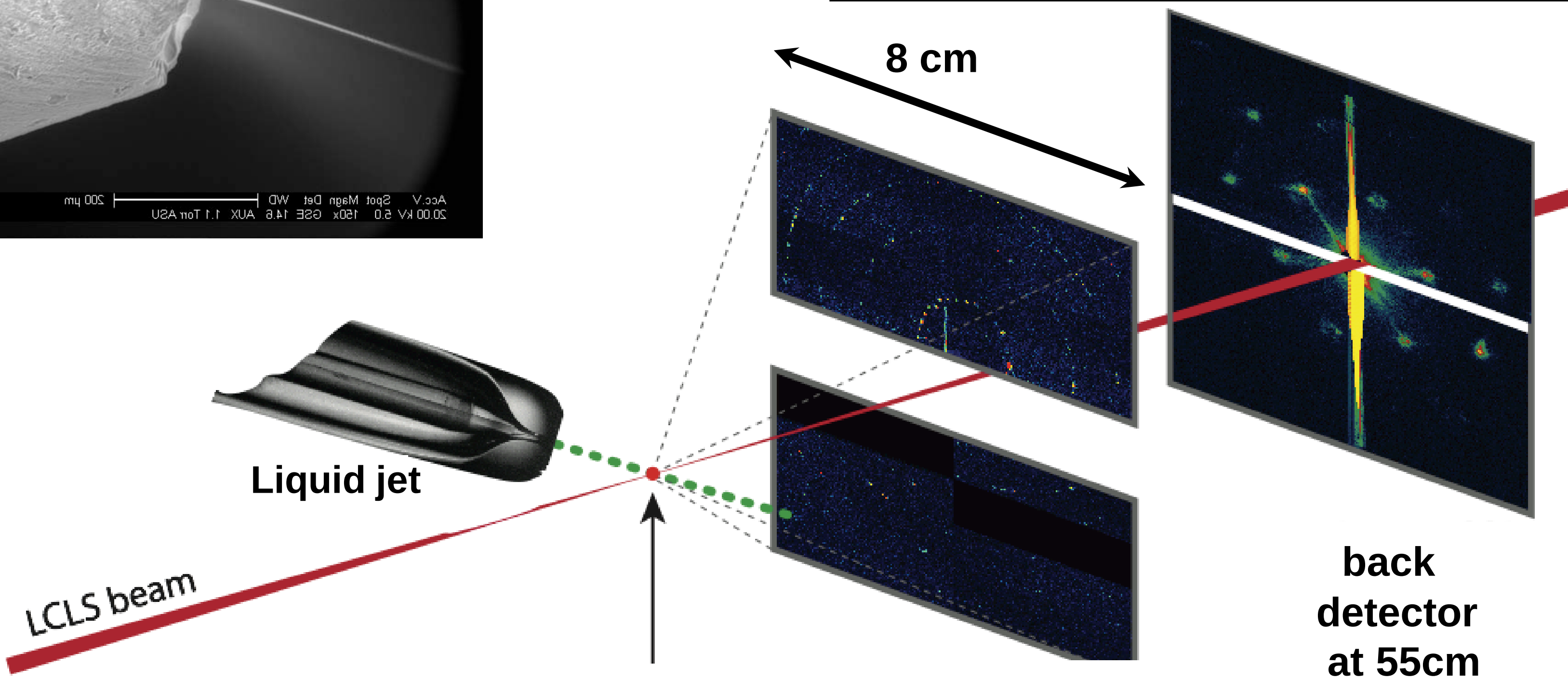
Detection of X-ray at Far Hall ~ 1 PM PDT 4/22/2010

Early Studies at LCLS: Nanocrystals in Water Microjet

John Spence et al. ASU



Spokesperson: **Henry Chapman** et al.
collaboration of
Center for Free Electron Laser Science DESY
Arizona State University, Max Planck CFEL
ASG, SLAC, LLNL, CBST, Uppsala University

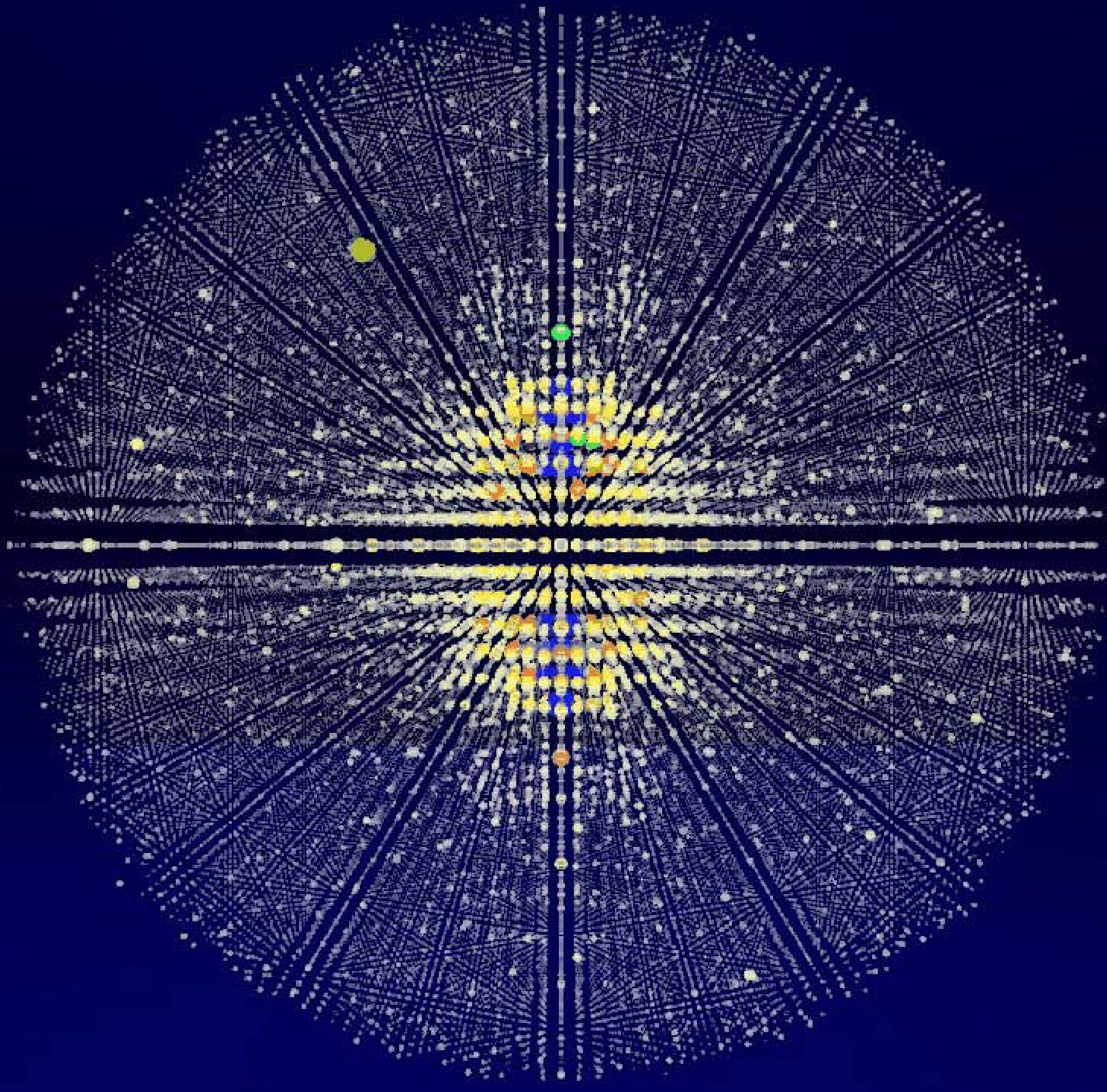


back detector at 55cm

1.8 keV
60 - 300 fs pulses
10^{13} photons / pulse

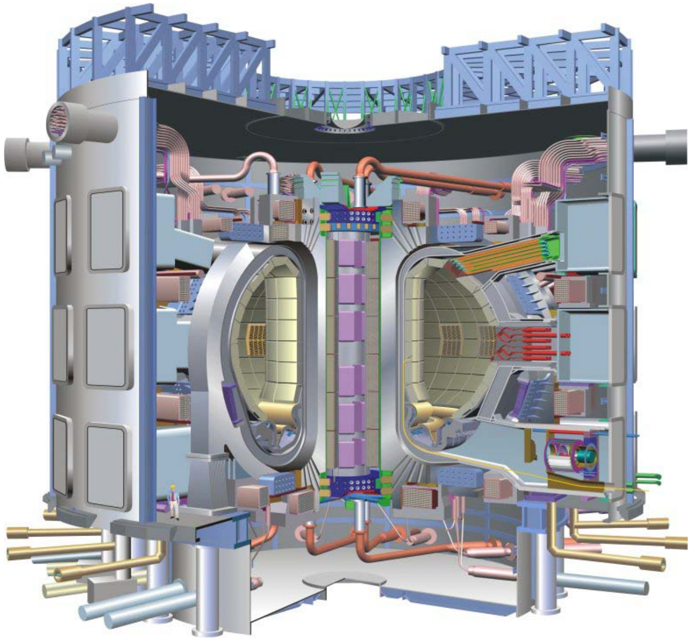
x-rays: 7 µm
liquid jet: 4 µm

front detector at 7cm



ITER

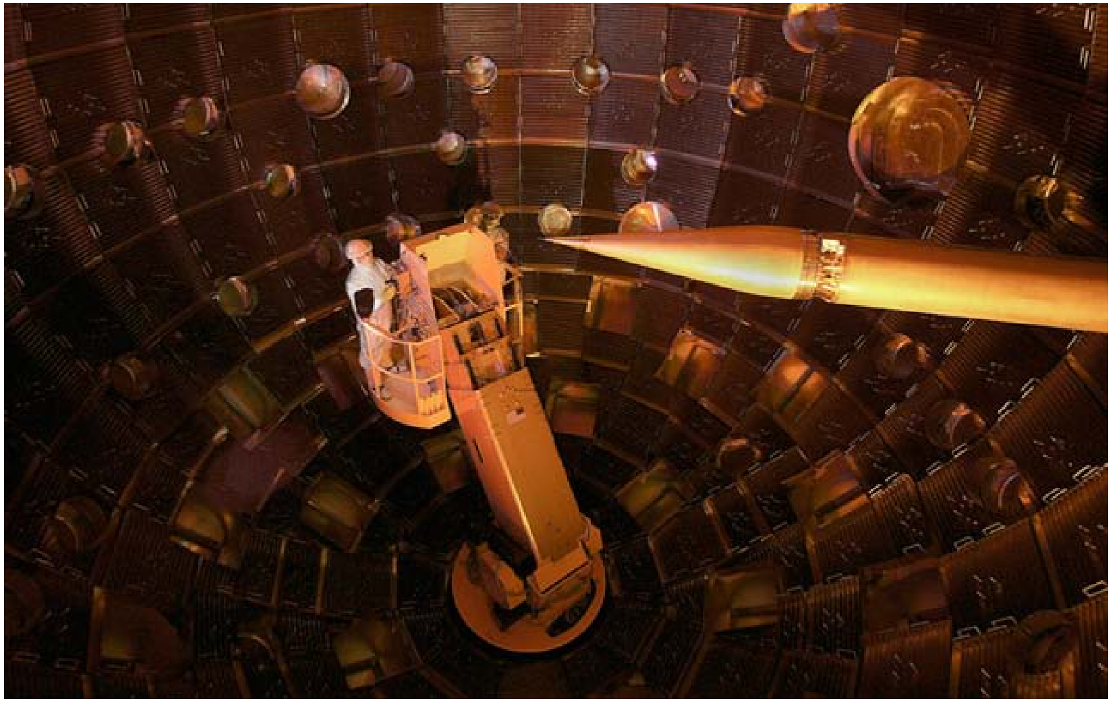
- ITER (Latin for “the way”) is a first of a kind major international research collaboration on fusion energy.
- U.S. is a 9.09% partner.
- ITER Goals
  - Designed to produce 500 MW of fusion power (Q $\geq$ 10) for at least 300-500 seconds
  - *Burning plasma* dynamics and control
    - U.S. emphasizes the value of ITER, its flexibility, and its diagnostics as a scientific instrument: develop a predictive capability of the burning plasma state
  - Will optimize physics and integrate many of key technologies needed for future fusion power plants
- The *Agreement on the Establishment of the ITER International Fusion Energy Organization for the Joint Implementation of the ITER Project*, entered into force in October 2007 for a period of 35 years.

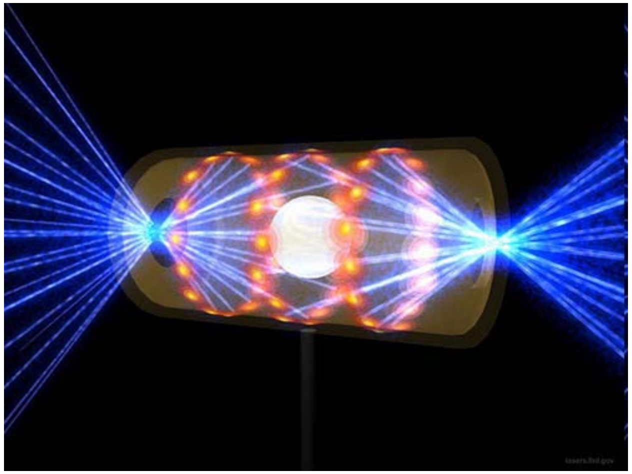


ITER Tokamak – Cross Sectional View

Inertial Fusion Energy: Nearing Ignition

- The newly completed National Ignition Facility – the world's most powerful laser system – recently began full operations
- NIF is on track to achieve the first laboratory demonstration of "ignition" or net energy gain

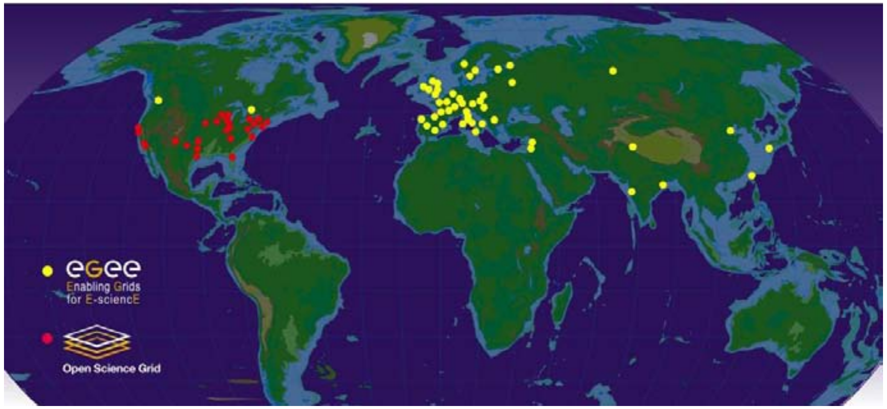




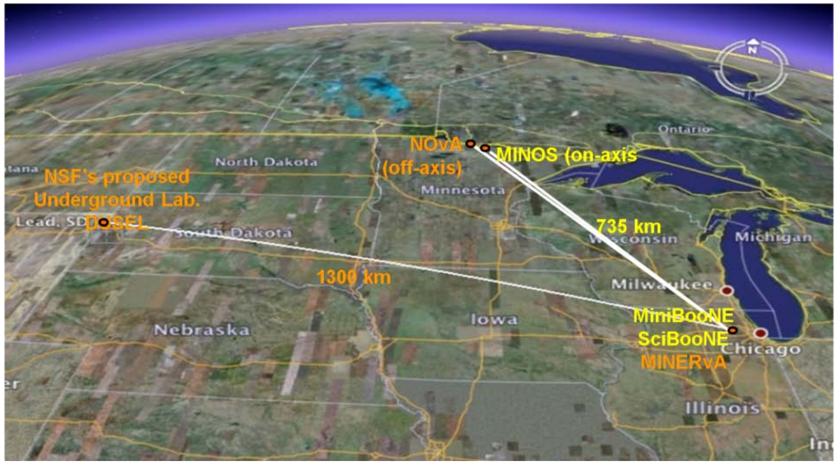
The U.S. High Energy Physics Program

The U.S. is uniquely positioned for a world-leading program in neutrino physics

The U.S. is a critical and strategic partner in global scientific collaborations that push the boundaries of High Energy Physics. The U.S. has developed components for the Large Hadron Collider at CERN and hosts centers for data analysis.



Network sites of the Open Science Grid and Enabling Grids for E-sciencE used for transmitting experimental data from the LHC to scientists worldwide.

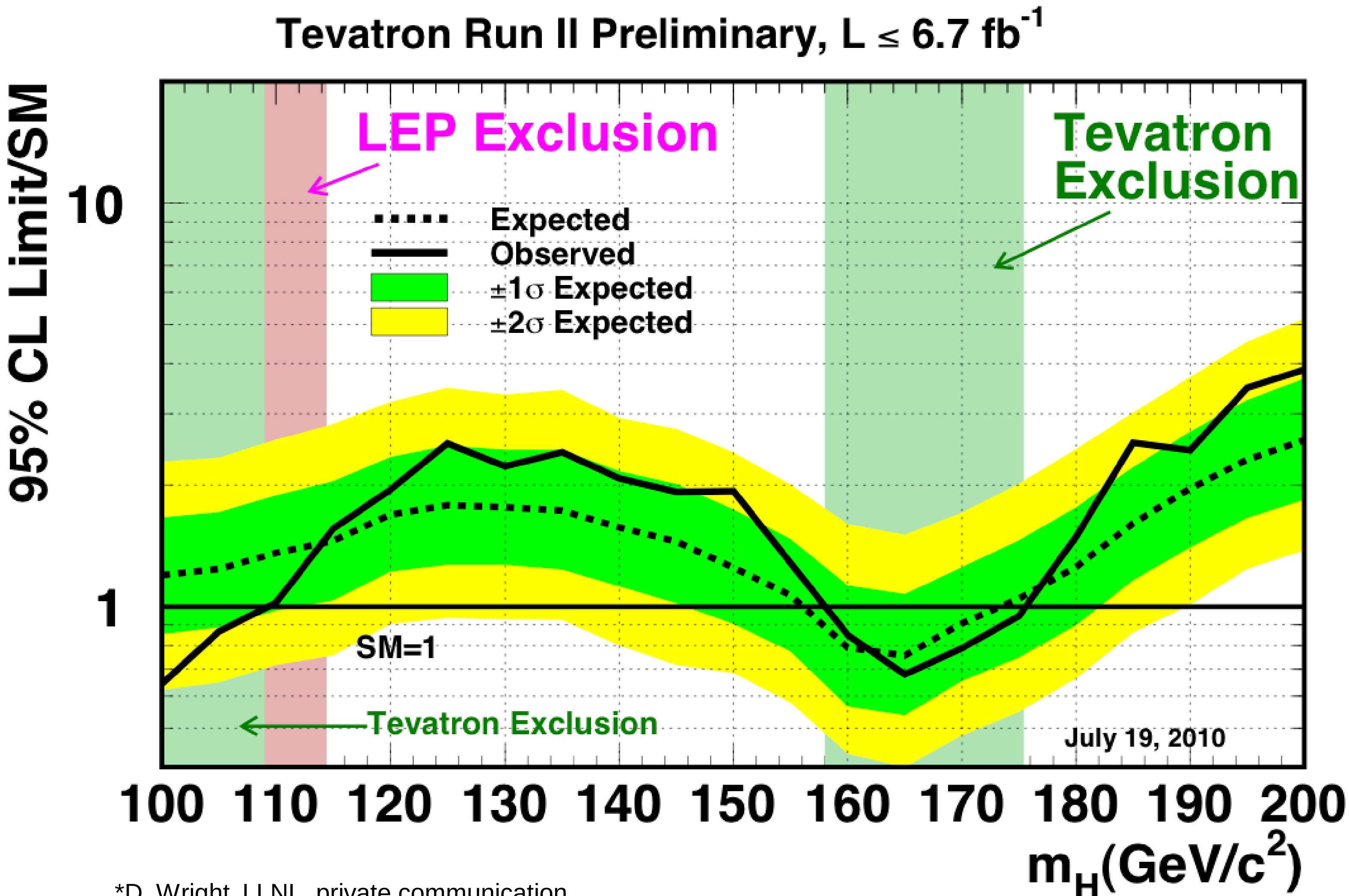


The NuMI beamline provides the world's most intense neutrino beam for the MINOS experiment and proposed NOvA and LBNE experiments

At home, HEP builds on its investments in tools and facilities to capture the unique opportunities of neutrino science. These opportunities are fundamental to the science of particle physics.

At the heart of the DOE HEP program is the world's most intense neutrino source at Fermilab, which serves MINERvA and MINOS and will support NOvA and the proposed LBNE (+$12,000K, HEP, initiated in FY 2011).

Progress Toward the Higgs Particle*



*D. Wright, LLNL, private communication

Accelerator Technology – Is it good enough?

- Long term waste storage needs dominated by actinides
- Fast Spectrum Reactors can burn actinides but require chemical processing
- Accelerator Driven Systems would allow the reduction of the actinides and burning of the spent fuel without chemical processing

Question is can accelerators be built with ~50MW of power in the beam and can associated targets be constructed

SBIR and STTR

- Continuous need for enhancing small businesses
- DOE-wide SBIR and STTR programs are managed by SC
- It is not a small program ~$150M/yr
- Steps are being taken to strengthen program

→ **Moved up to report to Deputy Director in SC**
→ **Enhancing office to make it more effective**
→ **Strengthening involvement of DOE executive management**

http://www.science.doe.gov/sbir/