Directing transformation: The science of fusion energy and striving towards a validated predictive capability

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Office of Science

For the Advanced Scientific Computing Advisory Committee December 9, 2015

We live in an unprecedented era of transformation: with benefit, burden, and promise





For the first time in history, we have an understanding of

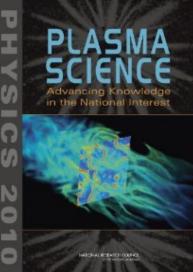
- the linkage between quality of life and energy availability
- our impacts on the globe of the drive to improve life quality
- that range of possibilities for our path forward

We have also come to understand that *fusion energy, in step* with high performance computing, can be a transformative clean energy source enabled by frontier science



Fusion has transformative potential: plentiful, carbon-free, base-load energy

Deuterium–Tritium Fusion Reaction Deuterium $E=mc^2$ Alpha Particle from SOHO (NASA) Neutron He **ENERGY MULTIPLICATION** About 450:1 PPPL#91X0410 BURNING PL



Create a star on earth. A hot plasma, or ionized gas, is the vehicle: isotopes of hydrogen collide hard and often to fuse into a helium nucleus and a neutron, with large net energy gain and self-heating the plasma ("burning plasma").

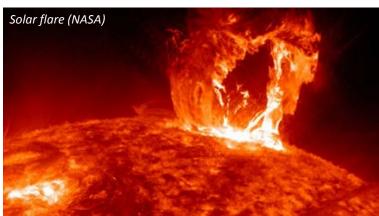
Fusion is ready for a major step - A National Academies assessment: fusion is ready and must advance to the major next step in demonstrating net fusion power. ITER represents that step

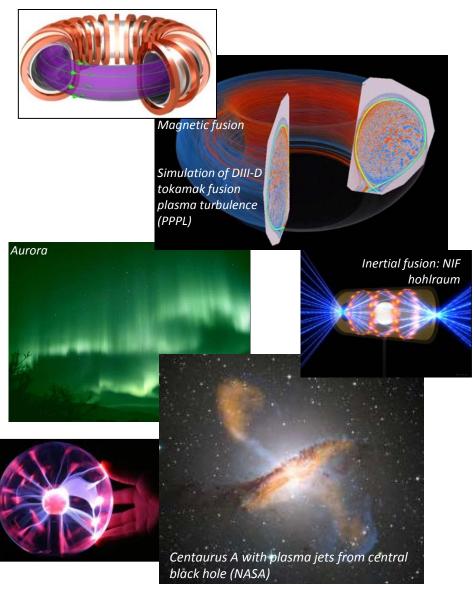
Fusion science is exciting and broad -The US has been a (or the) intellectual leader in creating a mature, exciting scientific endeavor that includes fusion and extends well beyond it



The fusion and plasma sciences are broad and tremendously rich

- A great intellectual framework has been developed, with rich and complex interplay. Energydirected research spawns great science
- Reminding ourselves of the evolution of the field can inspire regarding its potential





High power burning plasma science: fusion's leading frontier

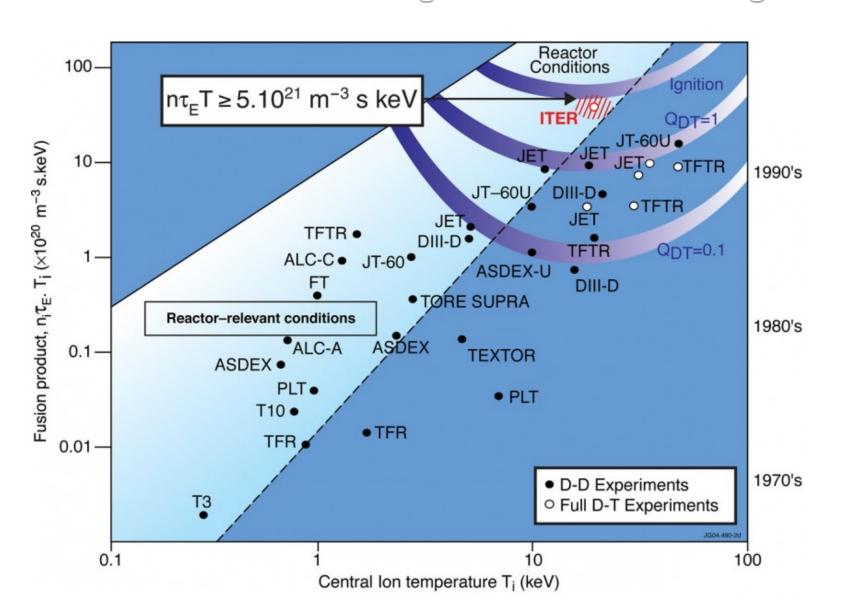
"All fusion reactors require a burning plasma. The key challenge is to confine the hot and dense plasma while it burns."

> Burning Plasma: Bringing a Star to Earth, p. 1 National Research Council

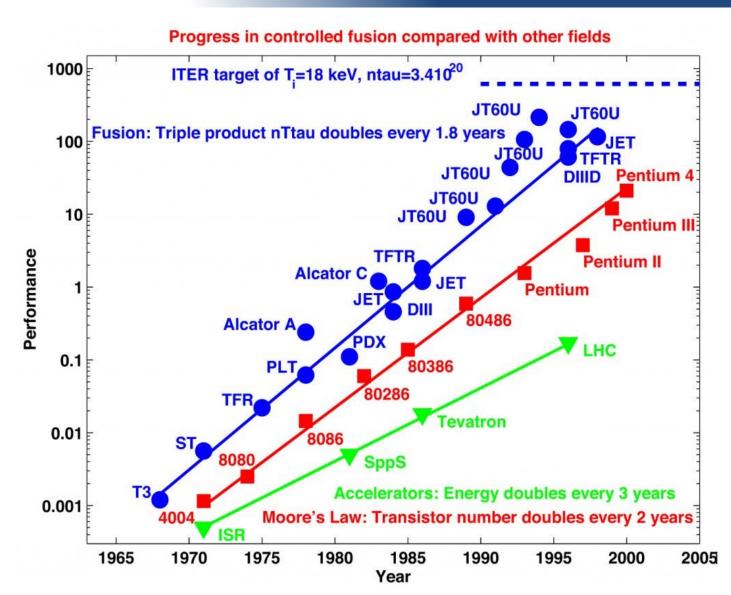


Scientific advance has made fusion an option: **the fusion reactor regime is within striking distance**

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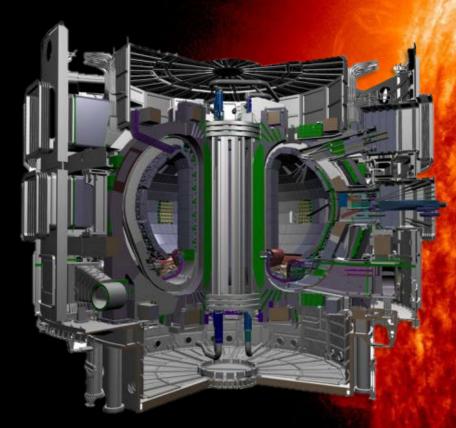






U.S. DEPARTMENT OF

ITER, together with a vigorous world program in fusion science, can be a truly transformative scientific instrument





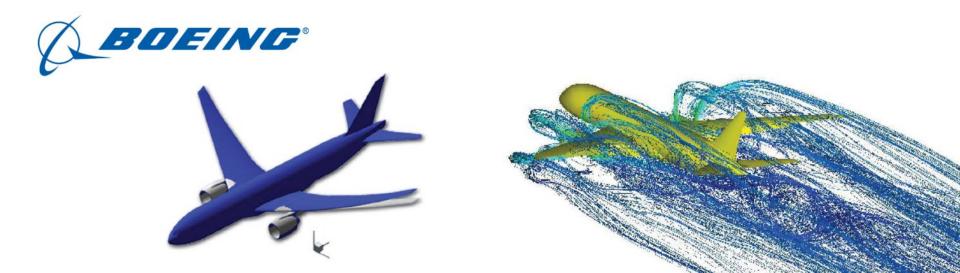
To reduce development costs, how fusion science relies on computing has to evolve

Consider the airline industry:

10-fold reduction in prototyping of wing designs

" By using supercomputers to simulate the properties of the wings on recent models such as the 787 and the 747-8, we only had to design seven wings, *a tremendous savings in time and cost*, especially since the price tag for wind tunnel testing has skyrocketed over the past 25 years."

- Doug Ball, Boeing (chief engineer for enabling technology and research)

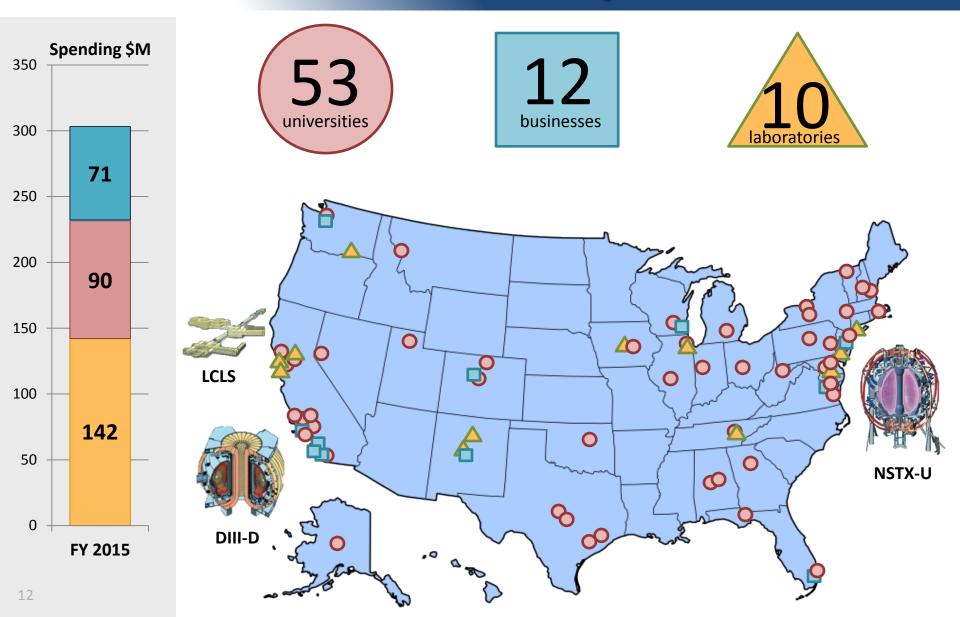




Some FES background



FES research is carried out at a diversity of US institutions



Burning Plasma Science in the U.S.: **Foundations**

Science that will drive economics of fusion:

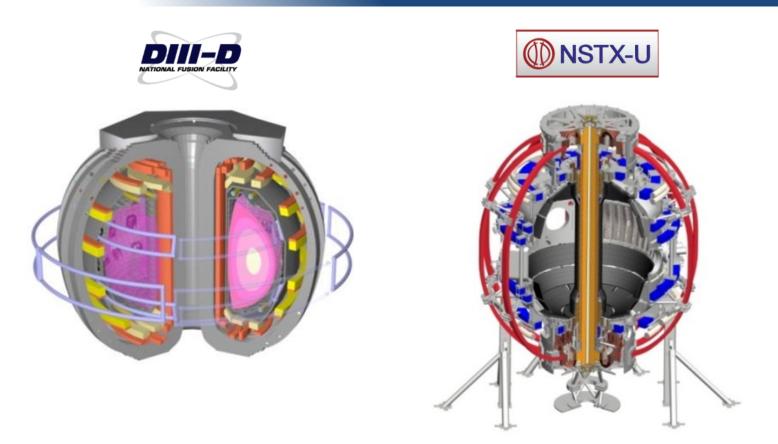
Heating efficiency and containment, maximum fuel pressure
 → confinement system size and complexity
 → attractiveness and cost





DIII-D and NSTX are flagships of a scientifically powerful combination

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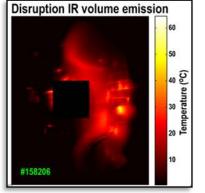
- The **aspect ratio** is central to much of toroidal confinement science
- It is also a driver in the ultimate cost and viability of a fusion power plant
- Smaller university scale facilities of varying magnitude support each
- V&V: increasingly the goal is detailed comparison of detailed measurement
 ¹⁴ with theory-based computation



DIII-D and NSTX-U are both highly flexible and world-leading in measurement capability and impact



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Comparative research between facilities, and in concert with overseas experiments, are hallmarks





Both have been highly impactful regarding burning plasma science fundamentals







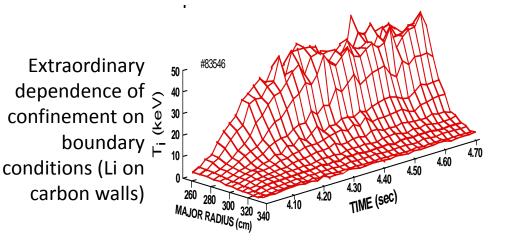
My own brush with computing as an experimentalist



A personal view of the evolution of a slice of fusion science...

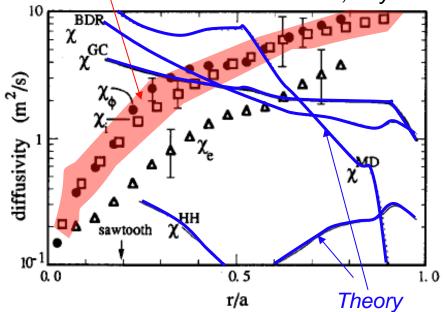
TFTR ('82 - '97)





Experimental χ_i, χ_{ϕ}

Scott et al., Phys. Fluids B 1990



... a taste of the early theoryexperiment comparisons in thermal conduction

17



Mid-90's example of a transformation: turbulence theory-based model challenges experimentalists

Mid 90's: IFS-PPPL model gets $T_i(r)$ in

very different confinement regimes about right

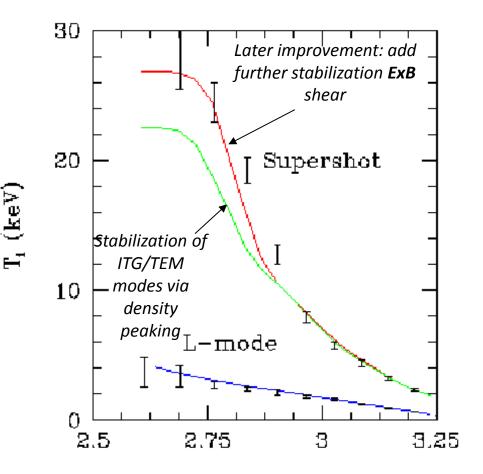
Linear gyrokinetics identify critical gradients.

Nonlinear gyrofluids map out parametric shape of χ_i .

I (spectroscopist) hear for first time from theorists: "We think your T_i data are incorrect in some cases - can you reanalyze these shots?"

→ Theorists were *right*. the measurement was *wrong*

→realization that simulation at the level of the turbulence had to be part of future predictions

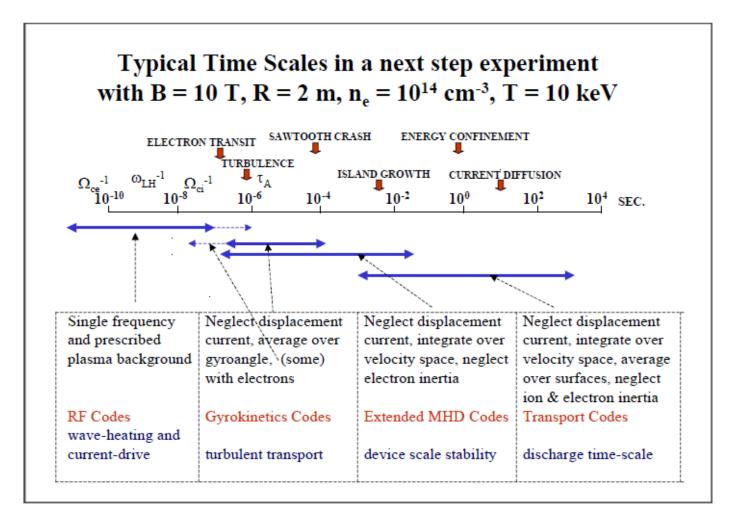


Kotschenreuther, Dorland, Hammett, Phys. Plasmas 2 (1995)



Physical processes in a tokamak discharge span multiple time and spatial scales

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2002 FESAC ISOFS Report



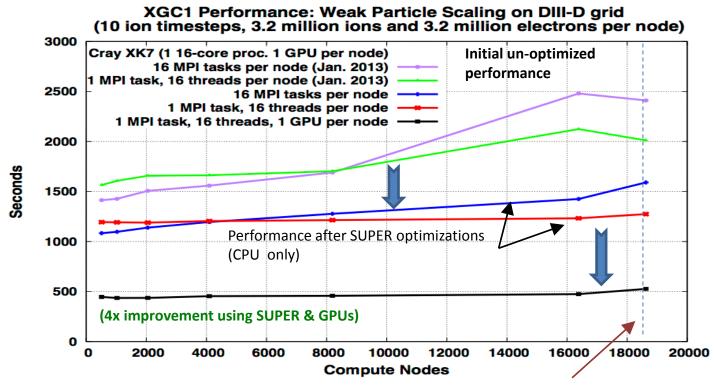
Meeting the challenge of validated predictive capability through partnership



FES – ASCR partnerships are impactful

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Partnerships between fusion scientists and computational scientists, under the auspices of SciDAC, have accelerated the rate of scientific discovery in fusion plasma science by improving the performance of fusion codes on leadership computing facilities and by addressing challenging data management and visualization issues associated with high-performance computing.



Maximum # of Titan cores



There has been significant progress in understand how the fusing plasma interacts with the material boundary

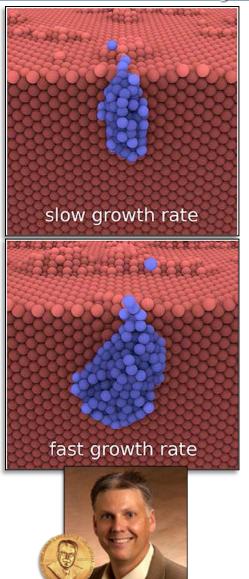
the Science:

Helium bubbles are detrimental to plasma-facing materials such as tungsten. Understanding how helium bubbles form and grow is important for predicting large-scale material response to the extreme fusion environment. The helium simulations find a qualitatively different growth mode when helium arrival rates approach experimental values.

When simulated helium bubbles grow quickly, the surrounding tungsten cannot respond, leading to over-pressurized bubbles that burst violently when they reach the surface. When the bubbles grow more slowly, the tungsten atoms pressed against the bubble's surface can diffuse around it, leading to a smaller bubble when it ultimately bursts.

the Impact:

These results highlight the importance of accounting for all relevant kinetic processes and how these kinetic processes enhance the interaction of, in this case, the helium bubble with the local microstructure. The results further have consequences for the nucleation of surface morphology on the tungsten, which is ultimately the source of fuzz, a nanostructured "steel wool"-like structure that causes significant degradation in performance of the material.



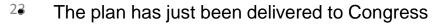


FES strategic plan places a strong emphasis on high performance computing

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Major themes of the FES strategic plan

- **Massively parallel computing** with the goal of validated whole-fusion-device modeling will enable a transformation in predictive power, which is required to minimize risk in future fusion energy development steps.
- Materials science as it relates to plasma and fusion sciences will provide the scientific foundations for greatly improved plasma confinement and heat exhaust.
- Research in the prediction and control of *transient events* that can be deleterious to toroidal fusion plasma confinement will provide greater confidence in machine designs and operation with stable plasmas.
- Continued stewardship of *discovery in plasma science* that is not expressly driven by the energy goal will address frontier science issues underpinning great mysteries of the visible universe and will help attract and retain a new generation of plasma/fusion science leaders.
- **FES user facilities** will be kept world-leading through robust operations support and regular upgrades.
- The strategic plan responds to several recent
 Congressional requests, viz., concerning a strategic plan (FY14), a fusion simulation program (FY14), and community workshops (FY15).





The Office of Science's Fusion Energy Sciences Program: A Ten-Year Perspective

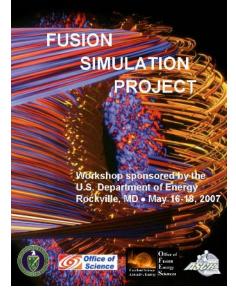
Report to Congress July 2015

> United States Department of Energy Washington, DC 20585



Recent efforts continue a strong tradition of planning and working together

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Our challenges are significant. Joint program review meetings and workshops shape future directions and provide unique opportunities to exchange information with all stakeholders.



Scientific Grand Challenges

FUSION ENERGY SCIENCES AND THE ROLE OF COMPUTING AT THE EXTREME SCALE



Large Scale Computing and Storage Requirements for Fusion Energy Sciences: Target 2017

Report of the NERSC Requirements Review Conducted March 19-20, 2013





Fusion Energy Sciences Network Requirements Review

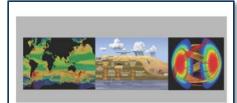
Final Report











Extreme-Scale Scientific Application Software Productivity: Harnessing the Full Capability of Extreme-Scale Computing

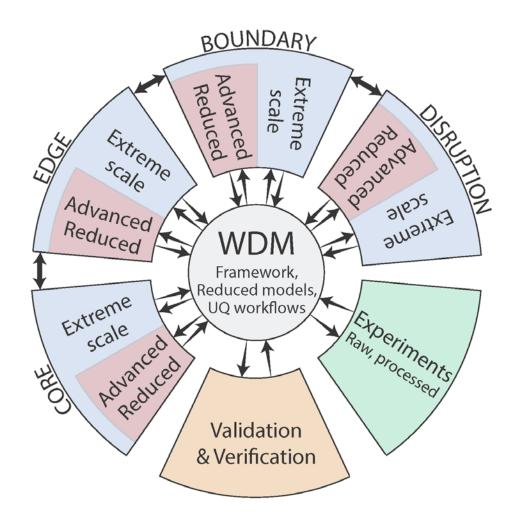
September 9, 2013



Michael Heroux (SNL), Robert Jacob (ANL), Phil Jones (LANL), Lois Curfman McInnes (ANL), J. David Moulton (LANL), Thomas Ndousse-Fetter (DOE/ASCR), Douglass Post (DOD), William Tang (PPPL)



Schematic overview envisioned for the WDM showing the interaction between topical areas

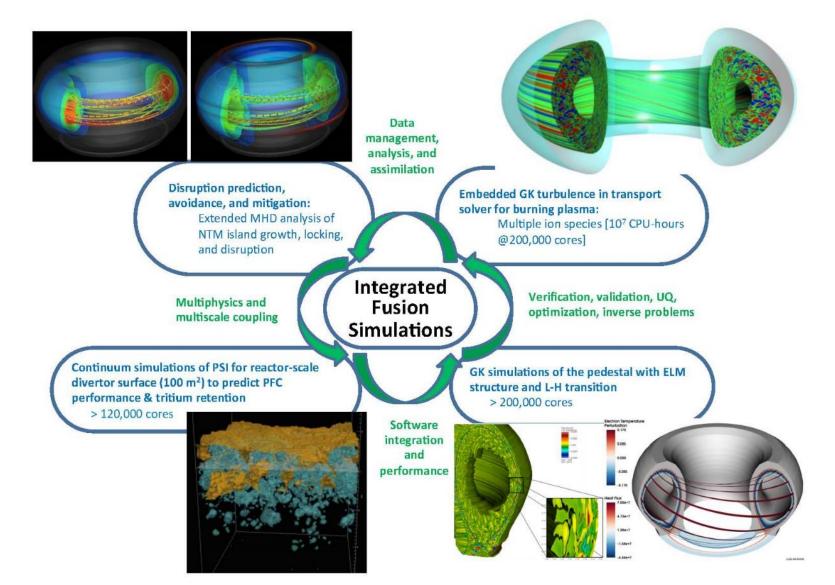


Flexibility envisioned for the WDM is embodied in the use of both Advanced Reduced models and Extreme Scale Simulations.

WDM framework provides verification and validation technology (UQ workflows) plus connection to experimental data (both raw and processed).

From WDM Workshop Summary, Bonoli and McInnis

Vision for integrated extreme-scale simulations

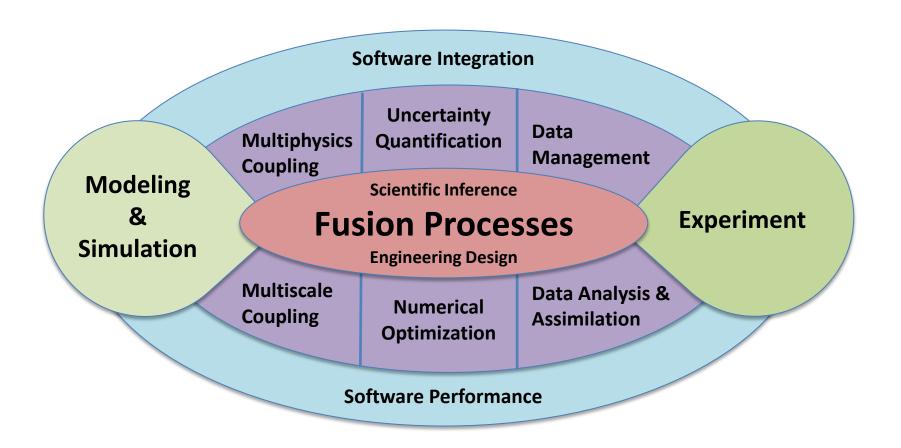


²⁶From WDM Workshop Summary, Bonoli and McInnis



Computational and enabling technologies in integrated fusion simulations

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Opportunity and challenge for computing and fusion: global cooperation

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EAST/DIII-D partnership: Joint teams execute research on both DIII-D & EAST

GA Remote Control Room:

Display hardware and software to provide control room experience remotely Accommodates 8 scientists & remote support staff Real-time audio/video, streaming of data during shot, display of real-time boundary/ signal traces

GA Science Collaboration Zone:

Dedicated network and cyberspace for between-shot transfer of data to GA DIII-D provides EAST data repository for all U.S. collaborators Data mirror at GA serves all US collaborators

First full 3rd shift remote operation July 22 and

Two 3rd shift periods (overnight in China) Executed vertical controllability experiments Enables US to use entire third shift (2016)

> General Atomics Remote Control Room supports 3rd shift operation of EAST by US scientists



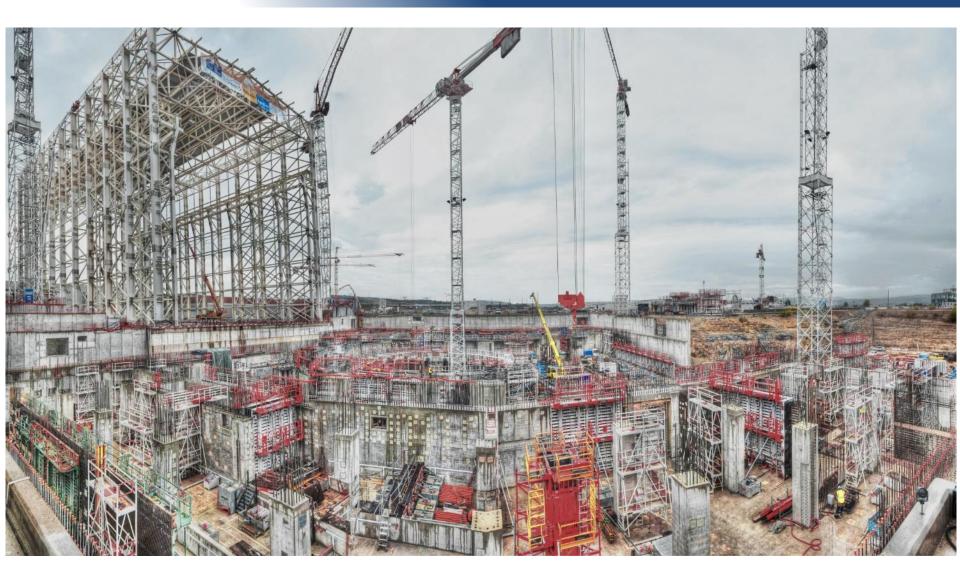


ITER construction site





ITER construction site



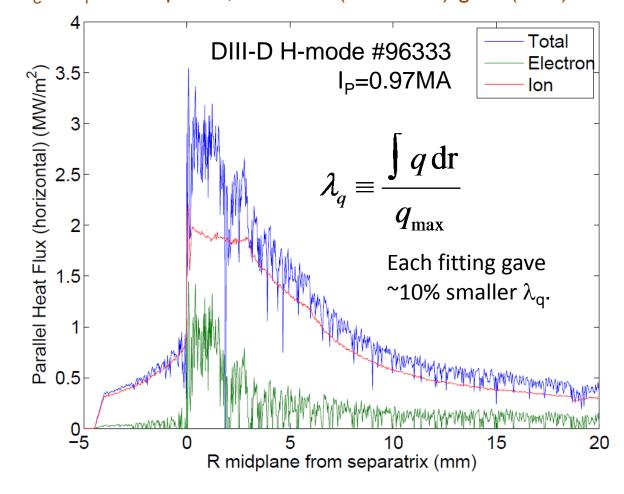
Thank you



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ENERGY dominated by ions in this DIII-D like edge plasma

 $K_e < K_i$ in scrape-off, and ions (electrons) gain (lose) kinet



$\lambda_q = 5.1 \text{ mm at}$ I_P=0.97MA

Enhancement by neutral particles is only ~10%

λ_q is closer to ion orbit spreading width than the radial blob size (≳1cm)

Heat-load spreading by **blobs** (represented by $\lambda_{qe} \sim 2mm$ in the figure) is masked by the ion orbital spreading.

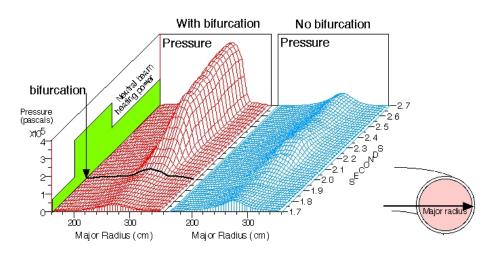


Transport barrier studies: exciting dynamics in the plasma drive important dynamics in the community

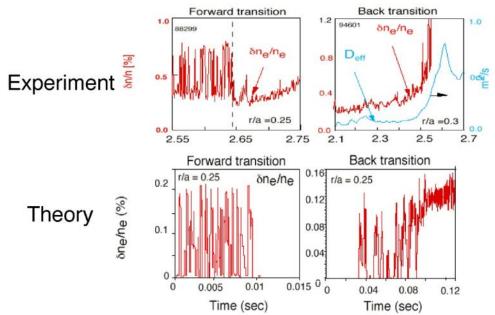
An exciting period scientifically and with respect to the community. The theoretical minimum in core transport can be realized

Scientific cross-connects: core and edge physics. ExB shear, a bifurcating core joins the bifurcating edge, the language of phase transitions enters the lexicon...

Institutional cross talk/stimulation/competition was vibrant

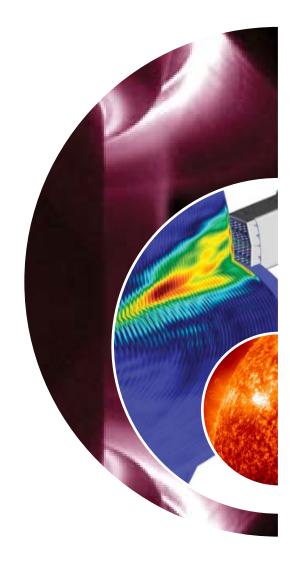


Density turbulence & confinement





U.S. Burning Plasma Science priorities:



Foundations

Focuses on U.S. capabilities targeting key scientific issues.

Long Pulse

Building on U.S. capabilities furthered by international partnership

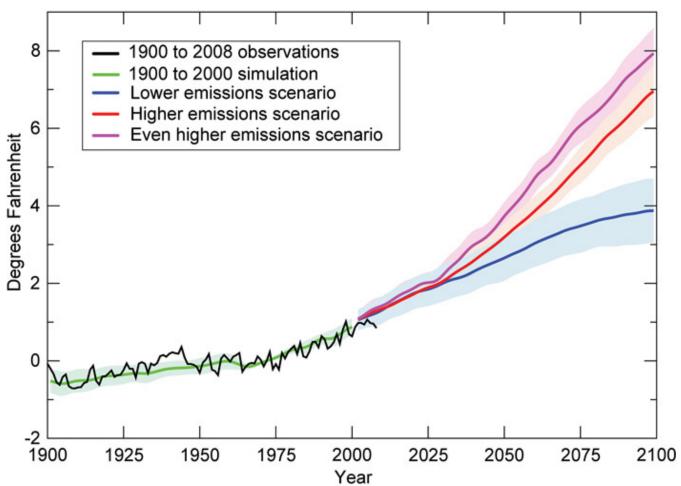
High Power

ITER is the keystone



This is an age of transformation: consequences are predictable

Global Average Temperature



http://www.epa.gov/climatechange/science/future.html



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ITER can be a vehicle for transforming international cooperation

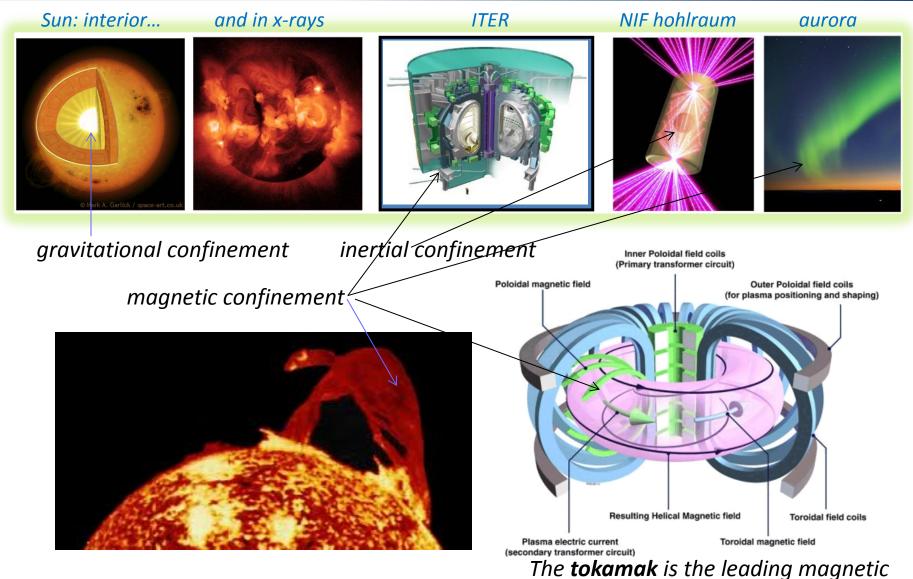
International partnership is essential



- Challenges are too big, too complex to go it alone; and major steps are expensive
- Grand challenge is optimizing the complex sociology of seven
 Members operating as a smartly functioning, directed whole



The science of fusion and plasmas extends from the laboratory to the stars and beyond



confinement concept for fusion

The FES magnetic fusion energy sciences program is organized along the following lines:

Foundations Long pulse High Power

Burning Plasma Science in the U.S.: Long pulse

Science that will drive economics:

Maintaining the magnetic cage:

External + internal B (tokamak) vs. externally imposed B (stellarator) Fusion materials:

Solid vs liquid, tritium breeding, closing the fuel cycle

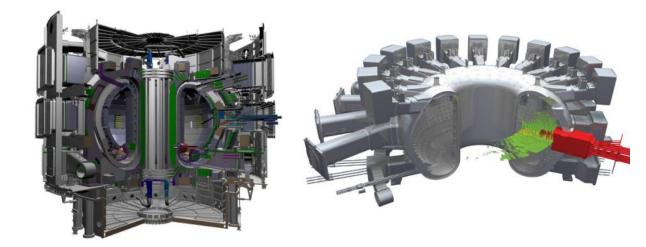


Burning Plasma Science in the U.S.: High Power

ITER is the scientific vehicle for the science of burning plasmas for the world

- ITER will establish the science of robustly and attractively controlling fusion plasmas that heat themselves
- Test the fundamentals and long pulse science at reactor scale







High power burning plasma science is essential for establishing fusion's science basis and thus its credibility

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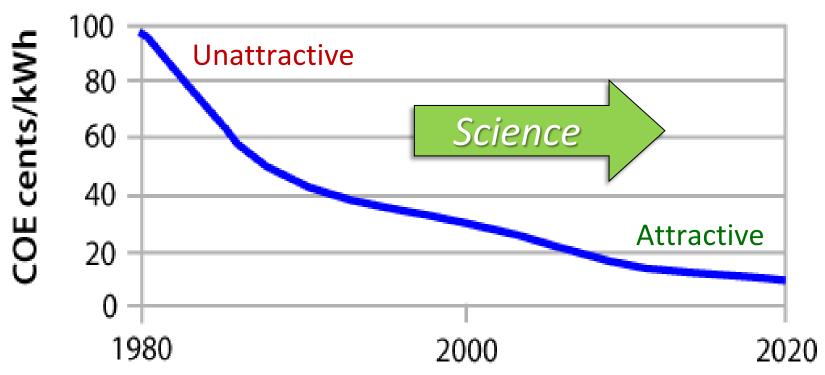
ITER:

The fundamental science of a burning plasma. ITER will establish the science of robustly and attractively controlling fusion plasmas that heat themselves



This is an age of transformation: energy science increases options

Photovoltaic Cost of Energy



http://www1.eere.energy.gov/tribalenergy/guide/costs_solar_photovoltaics.html



This is an age of transformation: science improves performance

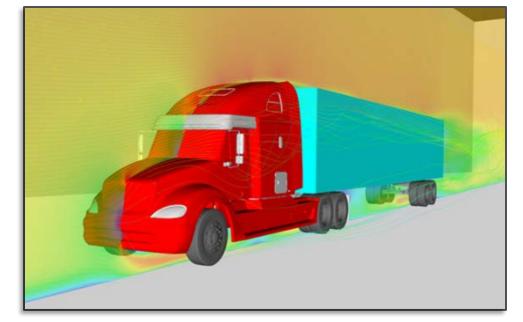
10% improvement in fuel efficiency has a powerful effect

2.5 million tons annual CO2 reduction

2.8 billion annual diesel fuel savings

\$8.3 billion annual fuel cost savings







NERSC roots in magnetic fusion research underline the deep connection between fusion research and high performance computing

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How a computer center dedicated to fusion research became the primary scientific computing facility for the Office of Science:

- **1974:** AEC establishes the Controlled Thermonuclear Research (**CTR**) center at LLNL (first computer: CDC 6600)
- **1976**: CTR is renamed the National Magnetic Fusion Energy Computer Center or NMFECC (first computers: CDC 7600; Cray-1)
 - Access to remote facilities is provided via the Magnetic Fusion Energy Network (MFEnet) which will evolve to today's ESnet
- **1983**: Access to NMFECC is extended to other ER (now SC) programs
- 1990: The center is renamed the National Energy Research Supercomputer Center (NERSC) to reflect its broader mission*

NERSC, along with the Oak Ridge and Argonne Leadership Computing Facilities, represent a critical resource for FES in its quest to develop a predictive capability for fusion plasmas.

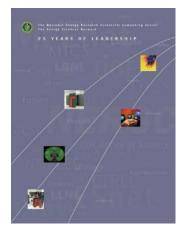
* Now known as the National Energy Research Scientific Computing Center





1976: CDC 7600 at MFECC







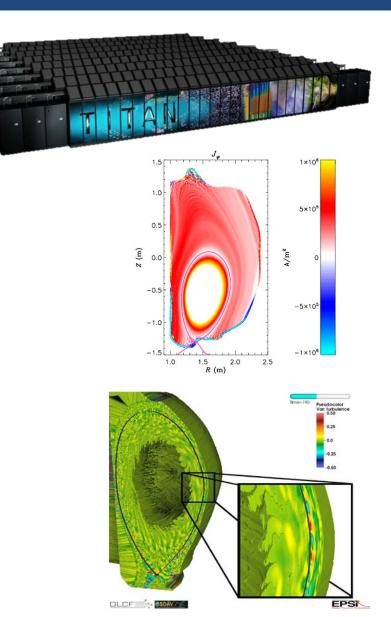
2013: Edison, CRAY XC30



Burning Plasma Foundations: SciDAC

The FES SciDAC program:

- The FES Scientific Discovery through Advanced Computing (SciDAC) program advances scientific discovery in fusion plasma science by exploiting SC leadership class computing resources and associated advances in computational science
- Addresses grand challenges in burning plasma science and materials science
- Highly collaborative program, leverages strengths of FES and ASCR





Disruptions

Boundary

Prioritization of multi-x topics in physics areas

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		Multi-X Topics								
	Near-termMid-termLong-term	U Models & multiscale analysis	C Scale-bridging R algorithms	Time advancement	 Meshing, geometry, & discretization 	C Solvers & C Preconditioners	90 Adaptivity	D Coupling errors & verification		
A.1.1	Integrated models: Two-fluid solver + discretization			D0	D4	D0				
A.1.2	Integrated models: Fluid-kinetic coupling (runaway e, energetic particles)									
A.1.3	Integrated models: Coupling with wall dynamics (melting, ionization, multiphase, radiation)									
A.2	Parameterized assessment: Model hierarchy to quantify errors in sampling of parameter space									
B.1	Pedestal characterization									
B.2.1	Detached divertor plasmas: Fast collisional algorithms (neutrals, plasma)									
B.2.2	Detached divertor plasmas: Plasma $+$ neutrals $+$ radiation coupling strategies									
B.2.3	Detached divertor plasmas: Kinetic + fluid coupling									



Prioritization of multi-x topics in physics areas

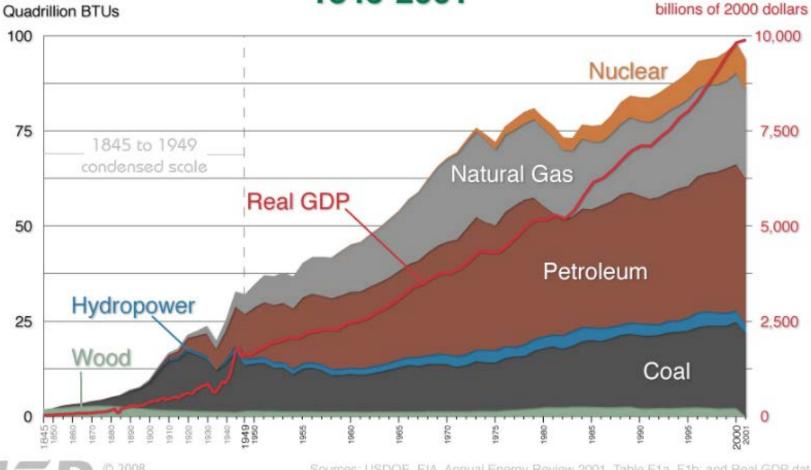
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U		Near-term Mid-term Long-term		Multi-X Topics							
			D	1	D2	D3	D4	D5	D6	D7	
	C.1.1	Time-dependent baseline: Coupling 1D + fast dynamics components									
	C.1.2	Time-dependent baseline: Coupling MHD + kinetics for NTM trigger									
	C.2.1	ELMs, sputtering, impurity transport: Effective impurity source at edge									
	C.2.2	ELMs, sputtering, impurity transport: Kinetic high-Z impurity transport									
	C.3.1	ITER core transport and ITBs: Coupling core models $+$ RF									
M	C.3.2	ITER core transport and ITBs: Coupling with ed (HMM, projective integration)	çe								
WDM	C.3.3	ITER core transport and ITBs: Reduced models in ITB triggers	or								
	C.3.4	ITER core transport and ITBs: Accelerate GK cosimulations	re								
	C.3.5	ITER core transport and ITBs: Sensitivity studies in high-D (> 20) space									
	C.4	Q=10 ITER scenario: Coupling MHD + EP + transport									
	C.5.1	Steady-state ST: Global GK simulations									
	C.5.2	Steady-state ST: Coupled ions-electrons, realistic mass ratios									
	C.5.3	Steady-state ST: EM effects (high- β)								48	

This is an age of transformation: energy transforms economies

Real GDP

US Consumption by Source v. Real GDP 1845-2001

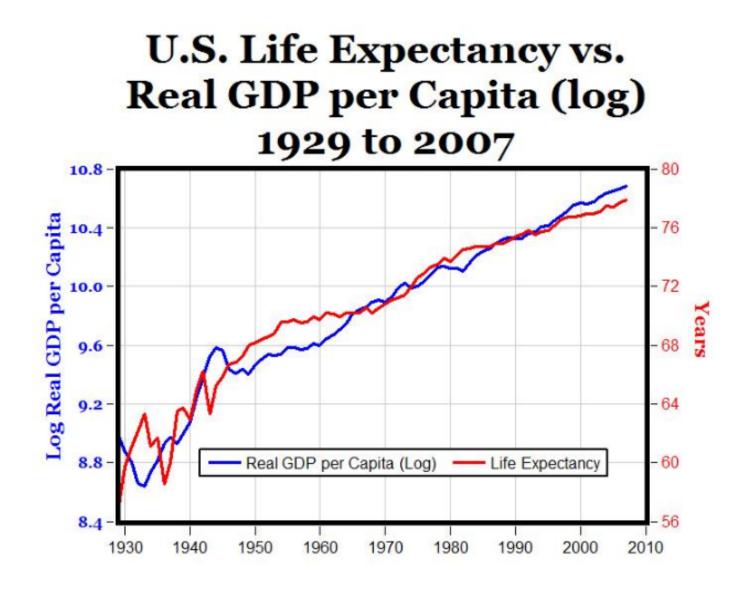


Sources: USDOE, EIA, Annual Energy Review 2001, Table F1a, F1b; and Real GDP data: Louis D. Johnston and Samuel H. Williamson, "The Annual Real and Nominal GDP for the United States, 1790-Present" Economic History Services, Oct. 2005, http://www.eh.net/hmit/gdp

RESEARCH

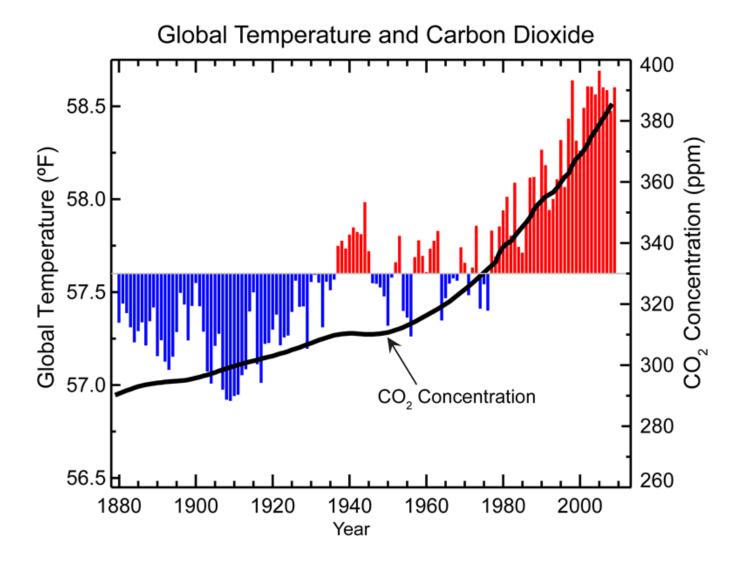


This is an age of transformation: energy transforms life quality





This is an age of transformation: global impacts are measurable



51 Figure from NOAA National Climate Data Center <u>http://www1.ncdc.noaa.gov/pub/data/cmb/images/indicators/</u>



<u>Foundations</u>: Fusion theory and computation are positioned to capture a computational revolution

The MFE **Theory** program:

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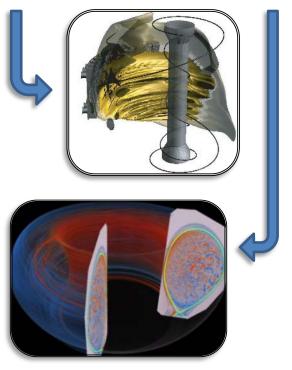
Focuses on fundamental plasma science of magnetic confinement with emphasis on burning plasma science

- Supported areas include macroscopic stability, confinement and transport, interaction of RF waves with plasmas, energetic particle physics, and plasma boundary physics
- Efforts range from small single-investigator grants, mainly at universities, to large coordinated teams at national laboratories, universities, and private industry
- Provides theoretical underpinning for advanced simulation codes (SciDAC) and Supports validation efforts at major experiments

The FES SciDAC program:

- The FES Scientific Discovery through Advanced Computing (SciDAC) program advances scientific discovery in fusion plasma science by exploiting SC leadership class computing resources and associated advances in computational science
- Addresses grand challenges in burning plasma science and materials science
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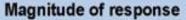


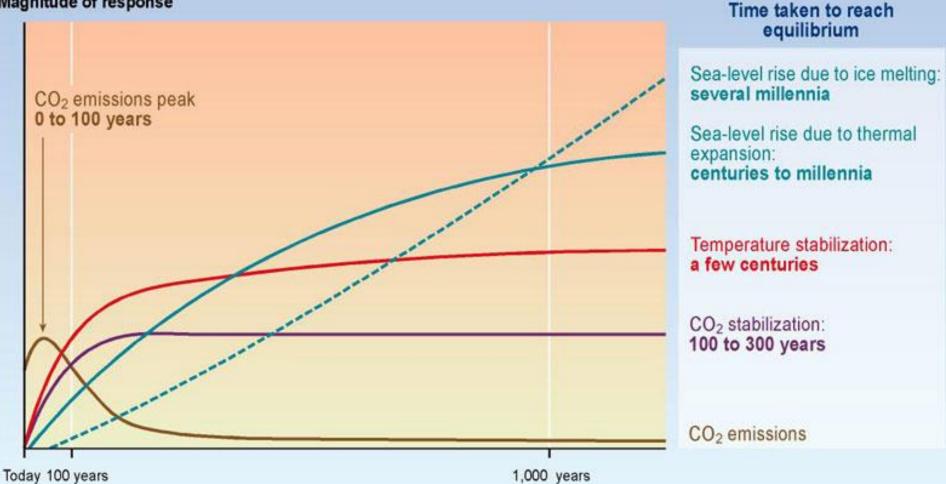


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This is an age of transformation: we now understand the scale of the solution to climate change that is required

CO₂ concentration, temperature, and sea level continue to rise long after emissions are reduced





INTERGOVERNMENTAL PANEL ON CLIMATE CHANGE