The FES Scientific Discovery through Advanced Computing (SciDAC) Program
Background and Future Plans

Presented at the VLT Teleconference

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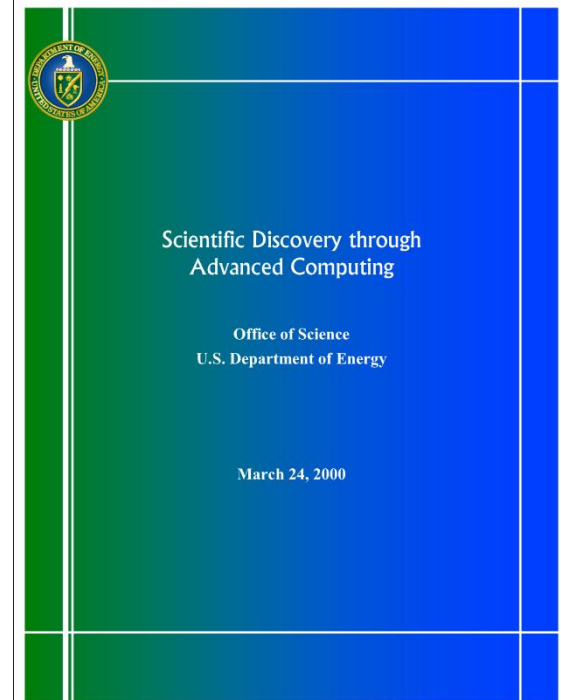**Office of Science**
U.S. Department of Energy

March 23, 2011

- **SciDAC Background**
- **SciDAC Characteristics**
- **SciDAC & FES**
- **Current FES SciDAC Portfolio**
- **FES SciDAC Contributions**
- **Future & Near Term Plans**
- **Additional Resources**

SciDAC Background

- The Scientific Discovery through Advanced Computing (SciDAC) program was initiated in **2001** as a partnership involving all of the Office of Science (SC) program offices

- Its goal was to dramatically accelerate progress in scientific computing that delivers breakthrough scientific results through partnerships comprised of applied mathematicians, computer scientists, and scientists from other disciplines
- Research funded under the SciDAC program must address the interdisciplinary problems inherent in ultrascale computing, problems that <u>cannot be addressed by a single investigator or small group of investigators</u>. The latter are typically funded by the core research programs
  - *Computation as the "third pillar" for scientific discovery, along with theory and experiment*
- SciDAC projects and researchers are expected to be leaders in the efficient and productive use of High Performance Computing resources, especially those at the SC Leadership Computing Facilities at ORNL and ANL

Scientific Discovery through
Advanced Computing

Office of Science
U.S. Department of Energy

March 24, 2000

SciDAC Characteristics

- Interdisciplinary and multi-institutional Centers
  - FES portfolio includes 19 Universities, 5 National Laboratories, and 5 Private Industry participants
- Centers are normally funded for 5 years, with a mid-term progress review during the third year
  - Some FES Centers were funded for 3 years → out of sync with the SC SciDAC program
- Non-Labs are managed as Cooperative Agreements rather than Grants, giving DOE a larger oversight role in directing their efforts and reprioritizing their deliverables to address emerging needs
- Computational resources are not provided automatically to SciDAC Centers; expected to compete for **INCITE** resources and also apply for **NERSC** resources
- SciDAC PIs and their collaborators are encouraged to attend the annual SciDAC Conference (2011 Conference: July 10-14, Denver, CO), which has emerged as a major conference for computational science
- The SciDAC paradigm (application scientists joining efforts with applied mathematicians and computer scientists to exploit HPC resources for scientific discovery) is unique in the world
  - The U.S. is also leading the world in making leadership class computational resources available for scientific discovery

Mission of FES SciDAC Program

- Advance scientific discovery in fusion plasma science and contribute to the FES goal of developing a validated predictive capability for magnetically confined plasmas by exploiting the emerging capabilities of petascale computing and beyond, and associated progress in software and algorithm development

- Current portfolio strongly focused on the needs of burning plasmas and ITER
  - Earlier portfolio (2001-2004) had a broader focus

- Critical for the success of large-scale integrated simulation efforts such as the FSP
  - SciDAC expected to provide the building blocks

FES SciDAC Funding History

FY'11 & FY'12: Request to Congress
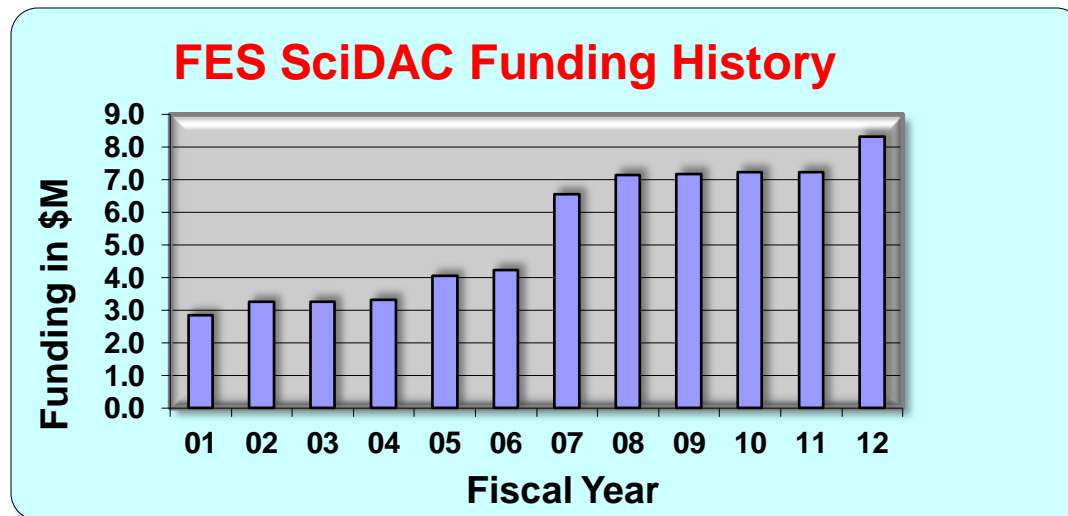
- **Single – physics ("out-of-cycle") projects**
  - Outside the normal 5-year cycle of the SC SciDAC program
  - Focused on "single-physics" (e.g., RF, turbulence, macroscopic stability, energetic particles, etc.)
  - Funded by FES only; applied math / CS support mainly via interaction with SciDAC Institutes and dedicated Science Application Partnership (SAP) support from ASCR
  - Last competition in 2010—five Centers were selected for funding
  - Funding levels range from $575K to $1,050K / year (total: $4.2M)

- **SciDAC-2 / Proto-FSPs**
  - Part of the regular 5-year cycle of the SC SciDAC program; eligible to re-compete in upcoming SciDAC competition
  - Focused on code integration and computational framework development, representing a first, small step towards the development of an integrated predictive capability for fusion burning plasmas, such as the one envisioned by the Fusion Simulation Program (FSP)
  - Integrated teams of application scientists and Applied Math / CS scientists
  - Current portfolio includes **three** large Centers, co-funded by FES and ASCR (each Center funded at $2M / year, $6M total, 50-50 split between ASCR and FES)

Current Portfolio – "single-physics" projects (2011-2015)

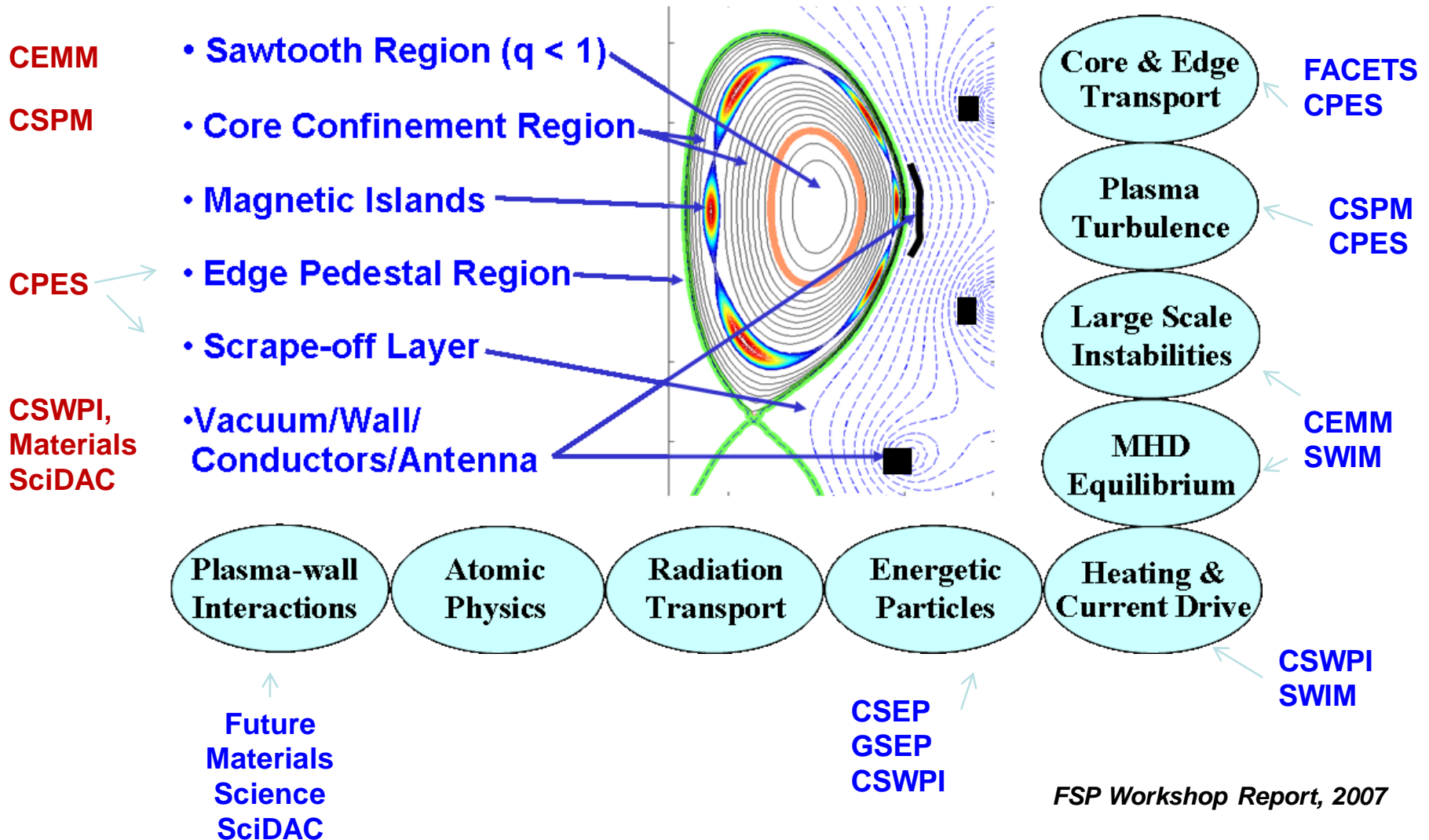| Project	PI	Collaborators
Center for Simulation of Wave-Plasma Interactions (CSWPI)	Paul Bonoli, MIT	CompX, Tech-X, Lodestar, General Atomics, PPPL, ORNL
Center for Extended MHD Modeling (CEMM)	Stephen Jardin, PPPL	General Atomics, HRS Fusion, Tech-X, MIT, U Colorado, Utah State U, RPI, U Washington, U Wisconsin
Center for the Study of Plasma Microturbulence (CSPM)	Jeff Candy, General Atomics	MIT, U Maryland, UCSD, LLNL, PPPL
Center for Simulation of Energetic Particles in Burning Plasmas (CSEP) - - *new*	Guoyong Fu, PPPL	U Colorado, U Texas, ORNL
Center for Gyrokinetic Simulation of Energetic Particle Turbulence & Transport (GSEP)	Zhihong Lin, UC Irvine	General Atomics, LLNL, ORNL

Integrated Efforts ("proto-FSPs") (2005-2011)

Project	PI	Collaborators
Center for Plasma Edge Simulation (CPES) *Focused on the physics of the edge pedestal*	CS Chang, NYU (*just moved to PPPL*)	NYU, Hinton Assoc., Caltech, UC Irvine, U Colorado, Columbia U, Lehigh U, MIT, Rutgers U, Georgia Tech, LBNL, PPPL, ORNL
Center for Simulation of Wave Interactions with MHD (SWIM) *Focused on employing RF methods to mitigate MHD instabilities*	Don Batchelor, ORNL	ORNL, CompX, General Atomics, Columbia U, Indiana U, MIT, Tech-X, PPPL, Lehigh U
Framework Application for Core-Edge Transport Simulations (FACETS) *Focused on developing a framework for coupling core-edge transport simulations*	John Cary, Tech-X	UCSD, LLNL, PPPL, ParaTools, ANL, Colorado State

All three Centers have developed computational frameworks (EFFIS, IPS, FACETS)

red: Applied Math / CS contributor

FES SciDAC contributions

Interacting physical processes within a tokamak discharge

CEMM

CSPM

CPES

CSWPI,
Materials
SciDAC

- Sawtooth Region (q < 1)
- Core Confinement Region
- Magnetic Islands
- Edge Pedestal Region
- Scrape-off Layer
- Vacuum/Wall/Conductors/Antenna

Core & Edge Transport — FACETS CPES

Plasma Turbulence — CSPM CPES

Large Scale Instabilities

MHD Equilibrium — CEMM SWIM

Plasma-wall Interactions

Atomic Physics

Radiation Transport

Energetic Particles

Heating & Current Drive — CSWPI SWIM

Future Materials Science SciDAC

CSEP GSEP CSWPI

FSP Workshop Report, 2007

- ASCR issued a **solicitation** for SciDAC Institutes (DE-FOA-0000505 & LAB 11-505)
  - ASCR-funded Centers to develop tools and resources addressing computational needs of science application areas, including fusion
- Will be followed by a series of <u>joint</u> solicitations with the SC program offices and NNSA focused on the domain science components of SciDAC
  - *Dates not fixed yet, but most likely in mid-2011*
- For the FES component, areas of focus have not been fully decided yet, but will allow the existing SciDAC-2 / proto-FSP Centers to compete
- Solicitation will include call for a new materials science SciDAC Center that will address the interactions of different materials located in and around the fusion chamber with the plasma (*full scope not decided yet*)

Additional Resources

- **SC SciDAC site:**
  http://www.science.doe.gov/ascr/Research/SciDAC.html

- **Report from the 2009 workshop on Fusion Energy Sciences and the Role of Computing at the Extreme Scale**

  - 2010 FES / NERSC / ASCR Workshop *on Large Scale Computing and Storage Requirements for Fusion Energy Sciences*

  - **2010 FES SciDAC Solicitation**

  - **Breakthroughs 2008**: *Panel on Recent Significant Advances in Computational Science*