

SciDAC, FSP & High Performance Computing Updates

CEMM Meeting at Sherwood Boulder, CO



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John Mandrekas

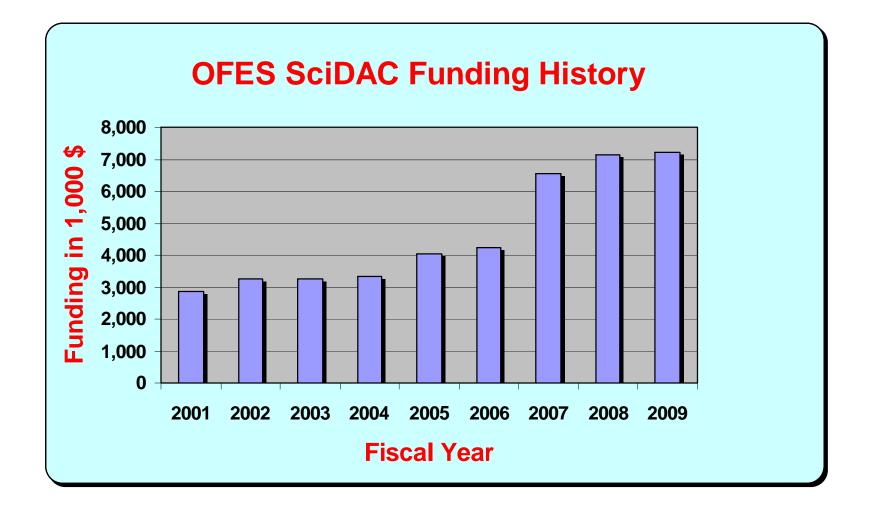
OFES March 30, 2008

Status of FES Scientific Discovery through Advanced Computing (SciDAC) Projects

| | <u>FY 2007</u> | <u>FY 2008</u> | FY 2009 (CONG) |
|-------------------------------------|----------------|----------------|----------------|
| Funding (\$ Millions) (FES only) | 6.5 | 7.1 | 7.2 |

- The current FES SciDAC portfolio includes eight projects
 - Five are focused on topical science areas (RF, MHD, Turbulence & Transport, Energetic Particles) and are funded entirely by OFES
 - Three are focused on integration (RF + MHD, plasma edge region, core + edge + wall) and are often referred to as *Fusion Simulation Prototype Centers* or "proto-FSPs". They are co-funded equally by OFES and OASCR
 - Together, the FES SciDAC projects address <u>9</u> out of the <u>15</u> topical scientific questions (T1-T6, T10-T12) and <u>4</u> out of the <u>6</u> campaigns of our 2005 FESAC Priorities Panel Report
- The FES SciDAC projects are set up as strong collaborations among 29 institutions. The institutional funding distribution is:
 - National Labs: 44%
 - Universities: 38%
 - Private Industry: 18%

SciDAC Funding History



Projects focused on topical science areas Funded or renewed in FY08 through FY10

| Project | Lead PI & Institution | Collaborating Institutions | |
|---|--------------------------|---|---|
| Center for Simulation of Wave- Plasma Interactions (<i>CSWPI</i>) | P. Bonoli MIT | CompX GA Lodestar | ORNL PPPL Tech-X |
| Center for Extended MHD Modeling (<i>CEMM</i>) | S. Jardin PPPL | GA LANL MIT NYU | Tech-X U Colorado Utah State U U Wisconsin |
| Gyrokinetic Particle Simulation of Turbulent Transport in Burning Plasmas (<i>GPS-TTBP</i>) | P. Diamond UCSD | Columbia U ORNL PPPL UC Irvine | UCLA UC Davis USC U Texas |
| Center for Simulation of Plasma Microturbulence (<i>CSPM</i>) | W. Nevins LLNL | GA MIT PPPL | U Maryland U Colorado |
| Gyrokinetic Simulation of Energetic Particle Turbulence and Transport (GSEP) | Z. Lin UC Irvine | GA LLNL | ORNL UCSD |

Projects focused on integration (proto-FSPs)

| Project | Lead PI & Institution | Collaborating Institutions | |
|--|--------------------------|--|---|
| Center for Simulation of Wave Interactions with MHD (SWIM) | D. Batchelor ORNL | Columbia U CompX GA Indiana U Lehigh U | MIT PPPL Tech-X U Wisconsin |
| Center for Plasma Edge Simulation (<i>CPES</i>) | C-S Chang NYU | Caltech Columbia U Hinton Assoc. LBNL Lehigh U MIT ORNL | PPPL Rutgers U U Colorado U Tennessee U Utah UC Irvine |
| Framework Application for Core- Edge Transport Simulations (<i>FACETS</i>) | J. Cary Tech-X | LLNL PPPL UCSD | ANL Colorado State U ORNL ParaTools, Inc. |

CPES & SWIM: FY06-FY10, 3rd year progress review in 2008
 FACETS: FY07-FY11 (SciDAC-2)

Important Dates

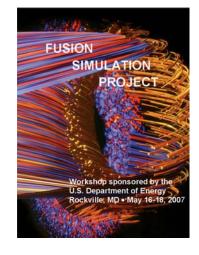
- June 5-6:
- June 23-24:
- July 13-17:
 July 18:
- Summer, 2008:

PSACI-PAC meeting (PPPL) 3rd year review for **CPES** & **SWIM** (Washington, DC) SciDAC Conference (Seattle, WA) Tutorials (Redmond, WA) INCITE Call for proposals

Status of the Fusion Simulation Project (FSP)

Progress since the May '07 workshop

- FESAC evaluated the FSP Workshop report and recommended to move forward to a *Project Definition* phase
- ASCAC has been charged to consider what is being proposed and to recommend an appropriate and mutually beneficial role for ASCR in the FSP (*final* report due: August 2008)
- The FES FY2009 CONG budget request includes \$1,976K to start the FSP Project Definition Phase
 - A solicitation for selecting a national team to carry out this work will be issued later in 2008





October 200

U.S. Department of Ener Office of Science

OFES High Performance Computing Resources 2008 Allocation Year (AY)

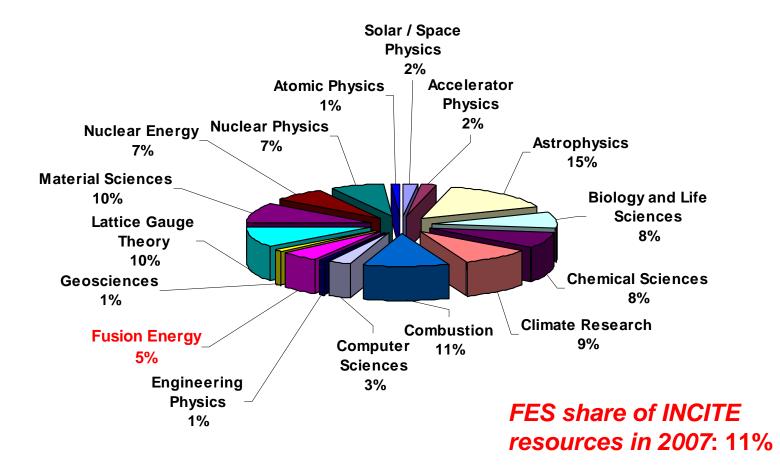
NERSC (Franklin, Bassi, & Jacquard)

- Significant increase in NERSC resources in 2008
- The 19,320 processor 101.5 TFlop/s Cray XT4 Franklin replaced Seaborg as NERSC's flagship system
- **53** FES repositories
 - 12 SciDAC
 - 1 INCITE
- OFES AY 08 allocation: 69.1 M hours
 - Compared to 16.7 M hours in AY07
- No additional resources are expected in 2008

2008 INCITE Program

- The Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program provides resources to large scale computationally intensive projects that can make high-impact scientific advances
- Now in its *fifth* year, INCITE includes HPC resources at ORNL, LBNL (NERSC), ANL, PNNL
- In 2008, 55 projects (31 new, 24 renewals) received 265 million processor-hours:
 - DOE Labs: 20
 - Universities: 17
 - Industry: 8
 - Other: 10
- Largest award: **26,700,000** hours (*Lattice QCD*), ORNL & ANL
- Largest award on XT4 @ ORNL: **18,000,000** hours (*Combustion*)
- Seven FES projects were selected for INCITE awards in 2008 (3 new, 4 renewals)
- Largest FES award: **8,000,000** on XT4 @ ORNL

2008 INCITE Awards *Allocations by Discipline*



FES INCITE Projects

New for 2008

Verification and validation of petascale simulation of turbulent transport in fusion plasmas

- PI: Patrick Diamond (UCSD)
- Cray XT4 (ORNL), 8,000,000 hours
- SciDAC: GPS-TTBP, GSEP, CPES

Fluctuation Spectra and Anomalous Heating in Magnetized Plasma Turbulence

- PI: William Dorland (U Maryland)
- Cray XT4 (ORNL), 4,000,000 hours
- Fusion Science Center for Multiscale Plasma Dynamics

High Resolution Global Simulation of Plasma Microturbulence

- PI: William Tang (PPPL)
- IBM Blue Gene / P (ANL), 2,000,000 hours
- SciDAC: -

Renewals

- Computational Atomic and Molecular Physics for Advances in Astrophysics, Chemical Sciences and Fusion Energy Sciences
- PI: Mitch Pindzola (Auburn U)
- Cray X1E (ORNL), 2,000,000 hours
- SciDAC: -

Gyrokinetic Steady State Transport Simulations

- PI: Jeff Candy (GA)
- Cray XT4 (ORNL), 1,500,000 hours
- SciDAC: SSGKT (FACETS SAP)

High Power Electromagnetic Wave Heating in the ITER Burning Plasma

- PI: E. Fred Jaeger (ORNL)
- Cray XT4 (ORNL), 1,000,000 hours
- SciDAC: CSWPI

Three-Dimensional Particle-in-Cell Simulations for Fast Ignition

- PI: Chuang Ren (U Rochester)
- NERSC (LBNL), 2,000,000 hours
- Fusion Science Center for Extreme States of Matter

2009 INCITE Program

- Expansion of the DOE Office of Science's computational capabilities should approximately *quadruple* the 2009 INCITE award allocations to close to a *billion* processor hours.
- FES SciDAC PIs are strongly encouraged to apply for INCITE resources—expect an announcement this summer
- INCITE projects are expected to be *computationally intensive* and their use of the resources should reflect this fact:
 - A computationally intensive research project will utilize a majority of the processors and multiple cores, if applicable, in the proposed research. A project that involves a large number of small independent jobs is not considered computationally intense (from the INCITE FAQ)
- Avoid submitting unfocused proposals combining several projects or with overlapping scope of work
 - Emphasize scientific discovery and ability to use HPC resources
- A community discussion on INCITE will be held at the PSACI-PAC meeting in June