PLASMA SCIENCE ADVANCED COMPUTING INTITUTE

PROGRAM ADVISORY COMMITTEE MEETING

W. M. TANG and V. S. CHAN

2-3 June 2005

PSACI Program Advisory Committee

William Kruer, *PAC Chairman*, Adjunct Professor of Applied Science, UC Davis
James Callen, Professor of Engineering Physics, U. of Wisconsin
Ronald Davidson, Professor of Astrophysical Sciences, Princeton U.
Patrick Diamond, Professor of Physics, UCSD
James Drake, Professor of Physics & Astronomy, U. of Maryland
*Brian Gross, Deputy Director and Head of Computing, Geophysical Fluid Dynamics Laboratory
*Robert Harrison, Chief Scientist for Computational Chemistry, ORNL
Russell Hulse, Nobel Laureatte and Distinguished Laboratory Fellow, PPPL
*Kai Li, Professor of Computer Sciences, Princeton U.
*William McCurdy, Senior Faculty Scientist, LBNL
*Steven Orszag, Professor of Mathematics and Chairman, Applied Math Department, Yale U.
*Malcolm Stocks, Corporate Fellow & Co-Director of Computational Science
& Materials Research Institute, ORNL

GENERAL CONSIDERATIONS

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(1) *Challenge* **is for Fusion SciDAC projects to effectively utilize terascale computing to produce significant** *new scientific insights/conceptual breakthroughs* **that are well appreciated by the FES as well as the general scientific community**

(2) Need to clearly demonstrate how the partnerships with OASCR (e.g.,SciDAC ISICs and SAPP) are helping to deliver _new_ capabilities -- *collaboratively building the necessary software, visualization, networking, etc. to enable effective use of hardware to accelerate scientific progress*

(3) Fusion SciDAC Program should demonstrate how it can enable for the US -- *a meaningful scientific leadership role and cost-effective participation on expensive new facilities located abroad such as ITER*
> **-- impact real decision-making in the large "scientific options space"**
> **-- harvest knowledge from major US investment abroad**

SPECIFIC CONSIDERATIONS IN
ASSESSING ACCOMPLISHMENTS OF FES SCIDAC CENTERS

- How well has each project made tangible progress toward achieving its scientific targets with respect to clear deliverables in the past year?

- What were the major impediments to more timely progress in each center/project?

- How have high-end computing resources been effectively utilized to accelerate progress toward achieving these goals?

- Are productive collaborative activities evident within each project and with other SciDAC activities (including relation between projects and enabling resource centers such as the SciDAC Integrated Software Infrastructure Centers (ISICs) and OASCR Scientific Application Pilot Programs (SAPPs)?

- What are some future topics with great potential for significant SciDAC achievements over the next five years?

  - Where are the associated computational science opportunities?

Present Fusion SciDAC Projects
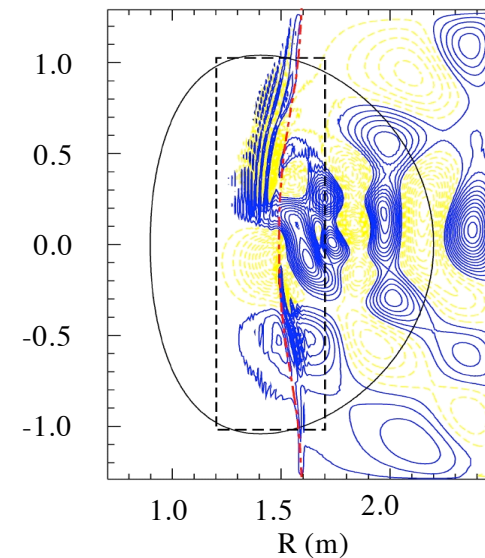
Extended MHD Modeling
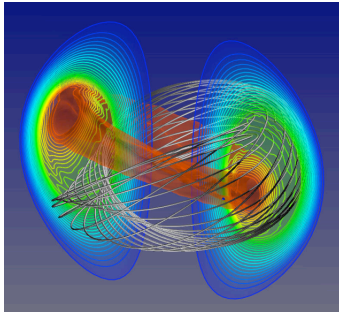
N=1 Plasma Instability

*PPPL, NYU
U. Wisconsin, SAIC,
U. Colorado, MIT,
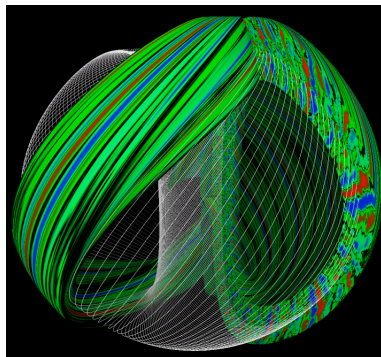General Atomics,
LANL*

Wave Plasma Interactions

*ORNL, PPPL, MIT,
Lodestar, CompX*

Wave Field

R (m)

Plasma Microturbulence

*PPPL, UC Irvine,
U. Colorado, UCLA*

Turbulent Eddies in Plasmas

THE NATIONAL FUSION ENERGY SCIENCES COLLABORATORY

(_involves 40 US sites in 37 states_)

Fusion Collaboratory

- Fusion Research Center
★ Large Fusion Experiment
▲ CSET Partner

- **Collaboratory Goals:**

-- enable more efficient use of experimental facilities by developing more powerful _between pulse data analysis_

-- enable _better access by researchers_ to analysis & simulation codes, data, and visualization tools

-- create _standard tool set_ for remote data access, security, and visualization

- **Collaboratory Partners:**

-- _3 large fusion experiments_*

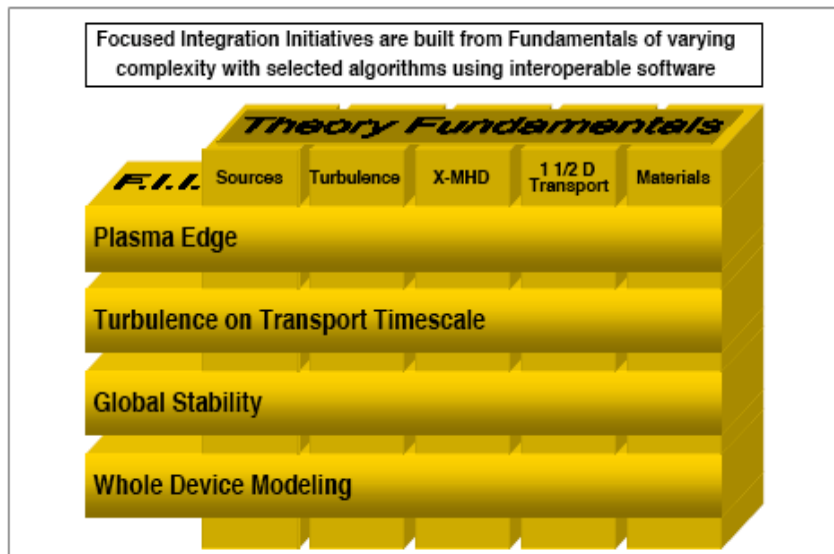   * C-MOD, DIII-D, NSTX

-- _4 computer science centers_ **

   ** ANL, LBNL, Princeton U., U. of Utah

FES SciDAC ACCOMPLISHMENTS

- **Advanced computation in tandem with theory and experiment has proven to be a powerful** *new tool for scientific understanding and innovation* **in FES research**

- **Plasma Science is** *effectively utilizing* **the exciting advances in Information Technology and Scientific Computing**
    - *References***:** *Advanced Computations in Plasma Physics* **Physics of Plasmas** <u>9</u> **(May, 2002) and** *Advances and Challenges in Computational Plasma Science* **Plasma Physics & Controlled Fusion** <u>47</u> **(February, 2005)**

- **Tangible progress toward more reliable predictions of complex properties of high temperature plasmas**
    - **Acquisition of** *scientific understanding* **needed for predictive models** <u>***superior to empirical scaling***</u>

INTEGRATED MODELING CHALLENGE:
"Fusion Simulation Project" (FSP)

- **Proposed $20M/yr with start-up "prototype" activity in FY '05 [$2M jointly from OFES & OASCR within SciDAC Program]**

Focused Integration Initiatives are built from Fundamentals of varying complexity with selected algorithms using interoperable software

- **Plan to leverage results from *SciDAC Program* for fundamental physics foundations and on Applied Math/Computer Science communities for needed algorithms**
- *Fusion Simulation Project is a potentially valuable US contribution to ITER*
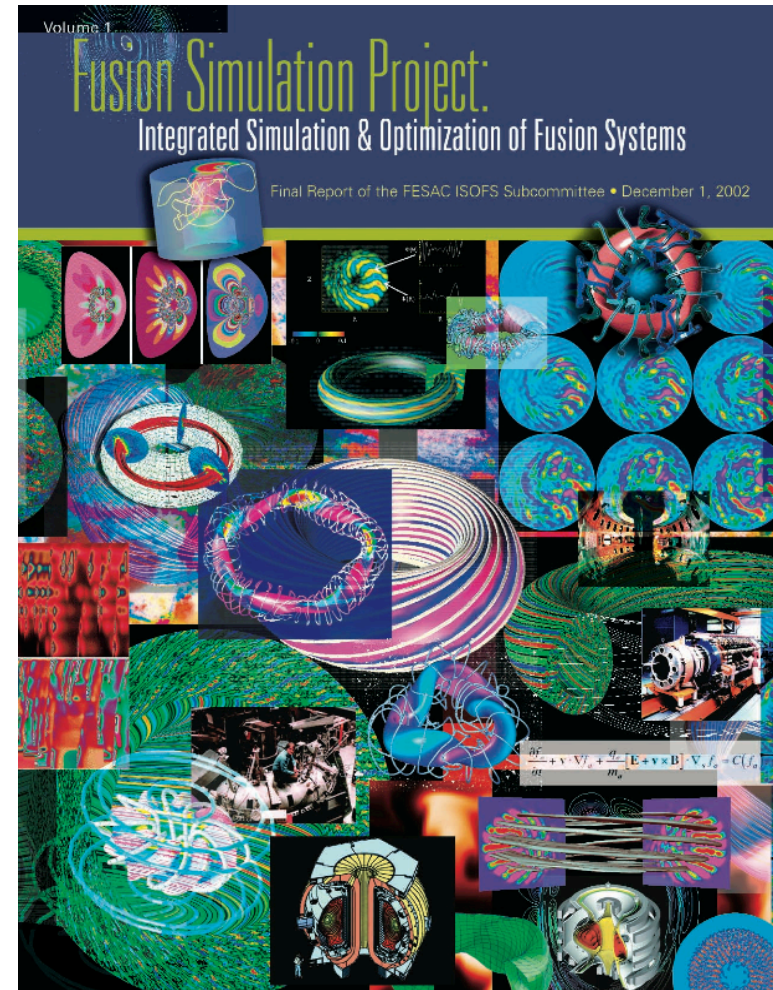
CHARGE FOR PSACI PAC MEETING

- **Evaluate substantive progress made by each project toward the scientific/computational goals and deliverables targeted by the Fusion SciDAC Centers in the first of a new 3-year funding period with respect to:**
  - **New scientific insights/conceptual breakthroughs enabled by the FES SciDAC Program**
  - **Demonstrated utilization of terascale computing capability**
  - **Likelihood of timely delivery of reliable computational modeling capabilities addressing burning plasma physics issues relevant to ITER**

- **Provide initial impressions of new $2M FSP (Fusion Simulation Project) Pilot components of the the FES SciDAC Program**

PLASMA SCIENCE ADVANCED COMPUTING INSTITUTE (PSACI)
PROGRAM ADVISORY COMMITTEE
AGENDA

THURSDAY, JUNE 2

9:00 AM -- 10:00 AM
Welcome from Rob Goldston followed by
CLOSED SESSION:
PAC discussions of charge, updates on the latest developments/issues at DOE and for PSACI involving the PSACI PAC, DOE Management, R. Goldston, W. Tang, and V. Chan
10:00 AM -- 10:15 AM
Coffee Break

10:15 AM -- 12:15 PM
OPEN SESSION
Presentations from Fusion SciDAC PI's

*Extended MHD Modeling (S. Jardin)
30 minutes presentation; 30 minutes discussion

*Simulation of Wave-Particle Interactions (D. Batchelor)
30 minutes presentation; 30 minutes discussion

12:15 PM -- 1:15 PM
LUNCH

1:15 PM -- 3:15 PM
OPEN SESSION
Presentations from Fusion SciDAC PI's (continued)

*Gyrokinetic Simulation of Turbulent Transport (W. Lee)
30 minutes presentation; 30 minutes discussion

*Fusion SciDAC Collaboratory (D. Schissel)
30 minutes presentation; 30 minutes discussion

3:15 PM -- 3:30 PM
Coffee Break

3:30 PM -- 5:00 PM

CLOSED SESSION
PAC begins formulation of recommendations and poses additional questions to SciDAC PI's

5:00 PM -- 6:00 PM
OPEN SESSION
Additional questions and requests for clarifications from PAC to PI's

7:00 PM
Dinner for Meeting Attendees

FRIDAY, JUNE 3

9:00 AM -- 10:15 AM
OPEN SESSION
Responses from Fusion SciDAC PI's to PAC questions & associated discussions

10:15 AM -- 10:30 AM
Coffee Break

10:30 AM -- 12:30 PM
Presentations of Executive Summary and Plans for the new FES SciDAC FSP Proto-type/Pilot
Centers by PI's and associated discussions with PSACI PAC

12:30 PM -- 3:00 PM
CLOSED SESSION (extending over lunch)
PAC drafts report with comments/recommendations

3:00 PM -- 3:30 PM
CLOSED DEBRIEF SESSION & ADJOURNMENT