PLASMA SCIENCE ADVANCED COMPUTING INSTITUTE

PROGRAM ADVISORY COMMITTEE MEETING

W. M. TANG and V. S. CHAN

7-8 June 2007

PSACI Program Advisory Committee

William Kruer, *PAC Chairman*, Adjunct Professor of Applied Science, UC Davis
James Callen, Professor Emeritus of Engineering Physics, U. of Wisconsin
John W. Connor, Head of Theory and Modeling, Culham Science Center, UKAEA
Ronald Davidson, Professor of Astrophysical Sciences, Princeton U.
James Drake, Professor of Physics & Astronomy, U. of Maryland
*Brian Gross, Deputy Director, Geophysical Fluid Dynamics Laboratory
*Robert Harrison, Chief Scientist for Computational Chemistry, ORNL
Russell Hulse, Nobel Laureatte, Professor of Science & Math Education, U. of Texas @ Dallas
Bruce Langdon, Plasma Theory Group Leader, AX Division, LLNL
*Kai Li, Fitzmorris Professor of Computer Sciences, Princeton U.
* **Daniel Meiron, Fletcher Jones Professor of Applied & Computational Mathematics and Computer Science, Cal Tech**
*Michael Norman, Professor of Physics and Center for Astrophysics and Space Sciences, UCSD
*Steven Orszag, Professor of Mathematics and Chairman, Applied Math Department, Yale U.
Miklos Porkolab, Professor of Physics and Director of PSFC, MIT
*Malcolm Stocks, Corporate Fellow & Co-Director of Computational Science & Materials Research Institute, ORNL

* *Non-Plasma Science Members*
New Members

GENERAL CONSIDERATIONS

(1) *Challenge* is for Fusion SciDAC projects to effectively utilize terascale (and soon petascale) computing resources to produce significant *new scientific insights/conceptual breakthroughs* that lead to validated predictive capabilities

(2) Need to clearly demonstrate how the partnerships with OASCR (e.g.,SciDAC CS & Applied Math Centers) are helping to deliver *new* capabilities -- *collaboratively building the necessary software, visualization, networking, etc. to enable effective use of hardware to accelerate scientific progress*

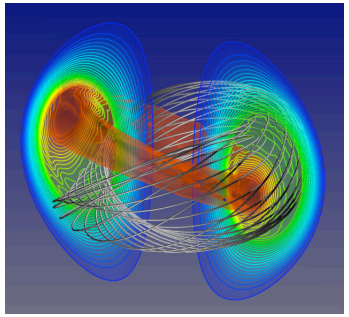
(3) Fusion SciDAC Program should demonstrate how it can enable for the US -- *a scientific leadership role and cost-effective participation on major new facilities located abroad such as EAST, JET, … leading to ITER*

- -- impact real decision-making in the large "scientific options space"
- -- harvest knowledge from major US investments abroad

Present Fusion SciDAC Projects

Extended MHD Modeling

PI: S. Jardin, PPPL



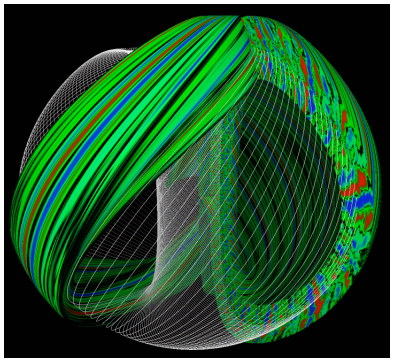
PPPL, NYU
U. Wisconsin, SAIC,
U. Colorado, MIT,
General Atomics,
LANL

N=1 Plasma Instability

Plasma Microturbulence

PI: W. Lee, PPPL

PPPL, UC Irvine,
U. Colorado, UCLA

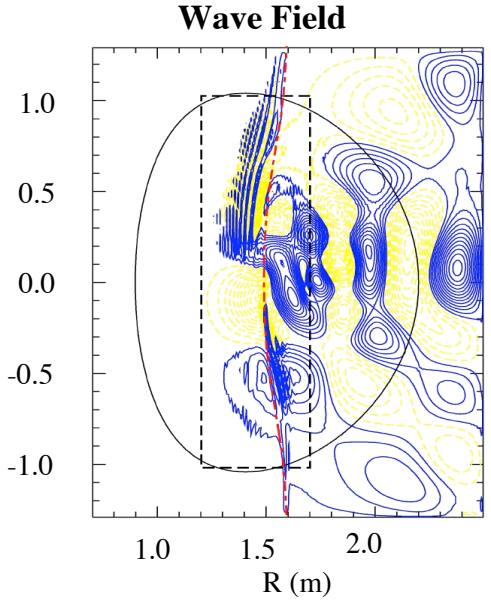


Turbulent Eddies in Plasmas

Wave Plasma Interactions

PI: P. Bonoli, MIT

ORNL, PPPL, MIT,
Lodestar, Tech-X



Integrated Modeling "Proto-FSP" SciDAC Projects:
"Fusion Simulation Project" (FSP)

- **Start-up SciDAC FSP "prototype" activity**
- **$2M per year provided jointly by OFES & OASCR within SciDAC Program for "Proto FSP's":**
  - **Center for Edge Simulations of Plasmas (PI: C. S. Chang, NYU)**
  - **Center for Simulations of Wave Interactions with MHD (PI: D. B. Batchelor, ORNL)**
- ***New Fusion Simulation Project being formulated -- targeting world leading US role in this area with impact on ITER & beyond***
  - *Presentation from A. Kritz, chair of recent major FSP Workshop*
- **Must leverage results from *SciDAC Program* for improved physics foundations and for needed algorithms & computational science infrastructure**

SPECIFIC CONSIDERATIONS IN ASSESSING ACCOMPLISHMENTS (Charges 1 & 2) OF FES SCIDAC CENTERS

With respect to both Charge 1 and Charge 2, the PSACI PAC is requested to respond with its evaluation of whether substantive progress has been made by each project toward the scientific/computational goals and deliverables targeted by the ***Fusion SciDAC centers at the end of a 3-year funding period*** and targeted by the ***Fusion SciDAC Proto-FSP centers in the second of a 3-year funding period*** with respect to:

(i) ***Scientific & Technical Merit*** ***with respect to improving predictive capabilities***

(ii) ***Utilization of Leadership-Class Computing*** ***for producing important new results and also demonstrating the scalability of the science with numbers of processors***

(iii) ***Potential for Impact on Burning Plasma Experiments*** ***such as progress on developing significantly improved predictive capabilities for dealing with prominent physics issues relevant to ITER***

CHARGE-1 FOR PSACI PAC MEETING

Charge 1: **Review and assess progress within CEMM (Jardin), CSWPI (Bonoli), & CGPS (Lee) with respect to:**

(i) results produced over the course of the past year

(ii) plans for the concluding phase of these 3-year projects this year

(iii) progress to date against the original plans

Associated PI Tasks: expected to describe

(1) how well each project has made progress toward achieving its scientific goals with respect to clear deliverables for the 3-year duration of the project

(2) what role have collaborative interactions within each project and also with other SciDAC activities played -- especially with respect to collaborations with the Computer Science and Math Centers for Enabling Technology (CET) and Science Applications Partnerships (SAPs)

(3) how leadership-class computing resources have enabled the achievement of the targeted scientific goals as well as demonstrated the scalability of the science with the number of processors on leadership class computing platforms

(4) what is the vision/scientific road-map for future research in this area, including quantifiable goals.

CHARGE-2 FOR PSACI PAC MEETING

Charge 2: Review and assess progress within the two SciDAC FSP (Fusion Simulation Project) Proto-type Centers which are in the second of a planned 3-years of funding with joint support from OFES and OASCR. These include: CPES (C. S. Chang) & SWIM (D. Batchelor)

Associated PI Tasks: expected to describe

(1) how well each project has made progress toward achieving its scientific targets with respect to clear deliverables during this second year of a 3-year project

(2) what role have collaborative interactions within each project and also with other SciDAC activities played -- especially with respect to collaborations with the Computer Science and Math Centers for Enabling Technology (CET) and Science Applications Partnerships (SAPs)

(3) how leadership-class computing resources have enabled the achievement of the targeted scientific goals as well as demonstrated the scalability of the science with the number of processors on leadership class computing platforms

(4) what are the plans (with targeted deliverables) for the next year to address the original 3-year goals of the project.

CHARGE-3 FOR PSACI PAC MEETING

Charge 3: **Review and assess initial progress and plans for a new SciDAC Proto-FSP Center (supported jointly by OFES & OASCR), its companion SciDAC SAPP (Science Applications Partnership Project) supported by OASCR, and the "Edge Simulation Laboratory" supported by OFES**

* SciDAC Proto-FSP Center for Framework Application for Core-Edge Transport Simulations **[FACETS] (J. Cary, Tech-X & U. Colorado)**

* SciDAC Science Application Partnership Program **(SAPP) on Steady State GK Transport Code Development [supporting FACETS Project] (M. Fahey, ORNL & J. Candy, GA)**

* OFES Edge Simulation Laboratory **[ESL] (R. Cohen, LLNL)**

- **Associated PI Tasks**:

  expected to make ***summary presentations*** which clearly highlight initial progress and plans for achieving the proposed goals of the project

CHARGE-4 FOR PSACI PAC MEETING

Charge 4: **Provide impressions of the new FSP initiative**

- featured presentation to PAC by Arnold Kritz who will ***summarize the results from the key May 16-18 "Fusion Simulation Project (FSP) Workshop"***
- FSP Workshop targets the ***updating/reformulation of the original FSP which was initially proposed 6 years ago***
- primary objective of new FSP is to produce a ***world-leading integrated predictive simulation capability*** that is important to ITER and relevant to major current and planned toroidal fusion devices
- involves development of ***advanced software designed to use leadership class computers*** for carrying out ***unprecedented multi-scale physics simulations*** to provide information vital to delivering a ***realistic integrated fusion simulation model with high physics fidelity***
- new FSP targeting approximate ***15 year timeline with funding at around $20M to $25M per year*** primarily by OFES with significant support from OASCR
- associated roadmap contains key deliverables targeted at end of 5, 10, and 15 years
  - time scale and scope dictated by ***need of ITER for reliable predictive tools***
  - ***opportunity for international leadership*** that US uniquely positioned to address
  - each phase of project to produce important new experimentally-validated scientific insights – the accelerated achievement of which ***will require the development of the necessary mathematical framework and algorithms***

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

THURSDAY, JUNE 6, '07

9:00 AM -- 9:45 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
9:45 AM -- 10:00 AM
Coffee Break

10:00 AM -- 12:30 PM
OPEN SESSION
Presentations from Fusion SciDAC PI's

*SciDAC Center for Extended MHD Modeling (S. Jardin, PPPL)
25 minutes presentation; 25 minutes discussion

*SciDAC Center for Simulation of Wave-Particle Interactions (P. Bonoli, MIT)
25 minutes presentation; 25 minutes discussion

*SciDAC Center for Gyrokinetic Particle Simulation of Turbulent Transport (W. Lee, PPPL)
25 minutes presentation; 25 minutes discussion

12:30 PM -- 1:15 PM
LUNCH

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

Integrated Modeling Presentations: Initial Progress & Plans for SciDAC Proto-FSP Integration Centers:

* SciDAC Integration Center for Simulation of Wave Interactions with MHD [SWIM] (D. Batchelor, ORNL)
30 minutes presentation; 30 minutes discussion

* SciDAC Integration Center for Plasma Edge Simulations [CPES] (C. S. Chang, NYU)
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 PI's

7:00 PM
Dinner for Meeting Attendees

FRIDAY, JUNE 7, '07

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

10:15 AM -- 11:15 AM
Report from FSP Workshop (A. Kritz, Lehigh U.)
30 minutes presentation; 30 minutes discussion

11:15 AM -- 12:15 PM
Progress & Plans for new SciDAC Proto-FSP Centers and for the OFES "Edge Simulation Laboratory"
* SciDAC Proto-FSP Center for Framework Application for Core-Edge Transport Simulations [FACETS]
(J. Cary, Tech-X & U. Colorado)
15 minutes presentation; 15 minutes discussion
*SciDAC Science Application Partnership Program (SAPP) on Steady State GK Transport Code Development (supporting FACETS Project)
(M. Fahey, ORNL & J. Candy, GA)
5 minutes presentation; 5 minutes discussion
* OFES Edge Simulation Laboratory (R. Cohen, LLNL)
15 minutes presentation; 15 minutes discussion

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

3:30 PM -- 4:00 PM
DEBRIEF SESSION & ADJOURN