PLASMA SCIENCE ADVANCED COMPUTING INSTITUTE

PROGRAM ADVISORY COMMITTEE MEETING

W. M. TANG and V. S. CHAN

5-6 June 2008

Plasma Science Advanced Computing Institute (PSACI)

W. M. Tang (Princeton U. & PPPL), Director, V. S. Chan (GA), Deputy Director,
Program Advisory Committee (PAC) chaired by W. Kruer (UC Davis)

CHARTER FROM OFES

- **Provide analyses and plans on how best to ensure timely progress toward scientific goals and deliverables targeted by FES advanced scientific computing programs, especially the FES SciDAC activities**
- **Convene PSACI meeting with PI's from existing Fusion SciDAC centers for annual progress assessments and to recommend priorities for future work**
- **Provide advice to prospective PI's from FES advanced scientific computing community on SciDAC goals and technical objectives**
- **Promote good communication and cross-fertilization/sharing of ideas among the fusion SciDAC centers**
- **Facilitate communication and promote collaborations between the Fusion centers and other SciDAC activities, especially in the Computer Science, Applied Mathematics, and Enabling Technology communities**
- **Assist with reporting to higher levels of DOE, OMB, OSTP, and Congress regarding advanced scientific computing progress, achievements, and goals in FES**

OFES PERSPECTIVE

J. Mandrekas and S. Eckstrand

- Proximity of this year's meeting to the OFES/OASCR review of the CPES and SWIM SciDAC Centers has naturally raised questions about the ***role of the PSACI and its relationship to regular DOE reviews.***

- While some overlap between the objectives of the PSACI-PAC meetings and DOE reviews is unavoidable and expected, ***the role of the PSACI-PAC is primarily advisory with goals of:***

  (1) ***providing "quality control" guidance*** for projects deemed worthy of funding by DOE via the regular peer review process

  (2) ***helping PI's to:***

  -- achieve objectives targeted in their funded proposals;

  -- plan for the future; and

  -- to ensure most efficient possible utilization of SC High-Performance Computing resources to achieve scientific discovery of critical importance to OFES

- Charges for present meeting are ***consistent with original PSACI Charter***

  -- possible changes in future if/when the Fusion Simulation Project (FSP) is fully operational

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 Laureate, 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 Member

GENERAL CONSIDERATIONS

(1) *FES-ASCR partnership enables* Fusion SciDAC projects to more effectively utilize terascale (and soon petascale) computing resources to produce significant *new scientific insights/conceptual breakthroughs* that lead to *validated predictive capabilities*

(2) FES SciDAC needs to show how partnerships with 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) FES SciDAC projects need to more clearly demonstrate their effectiveness in *utilizing experimental facilities and data* in *validating* simulation codes

(4) FES SciDAC 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, KSTAR, JET, … leading to ITER*

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

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

- **Fusion Simulation Project**

  - targeting world leading US role in this area with impact on ITER & beyond

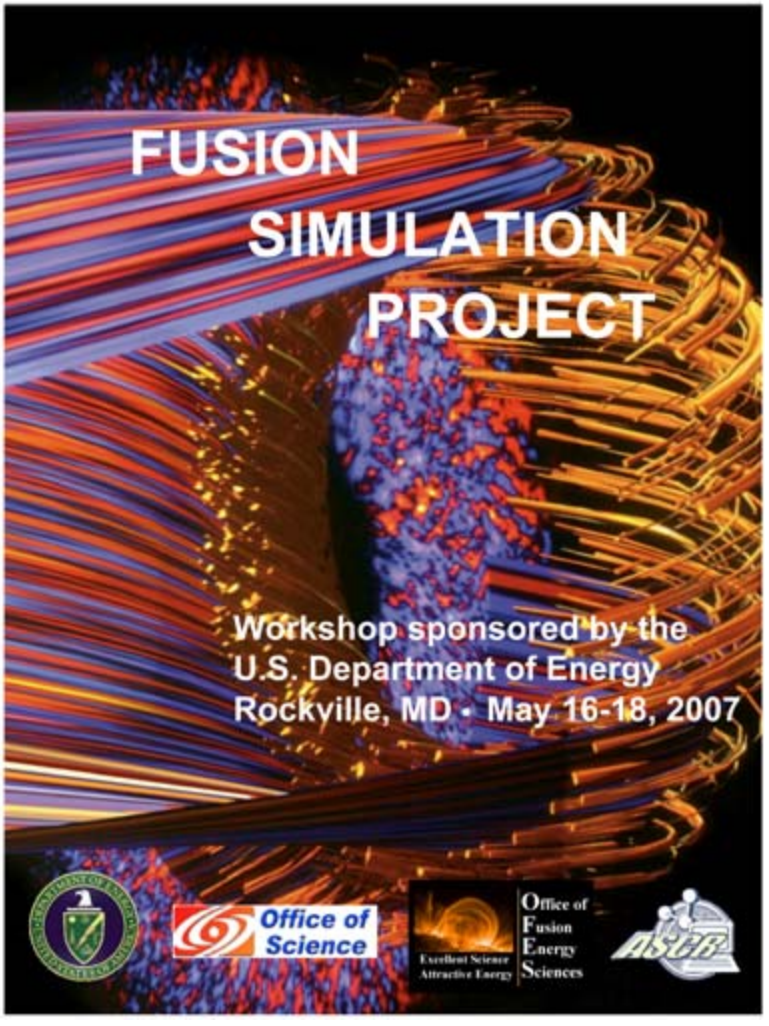
  - FSP Workshop Report: July '07

  - FESAC FSP Panel Report: October '07

  - OFES has accepted FESAC FSP Panel recommendation for "Project Definition Phase" -- commencing in FY'09

  - ASCAC FSP Panel Report due Aug. '08

- **$2M per year provided jointly by OFES & OASCR within SciDAC Program for "Proto FSP's":**
  - **Center for Plasma Edge Simulation (PI: C. S. Chang, NYU) - 3rd year**
  - **Center for Simulations of Wave Interactions with MHD (PI: D. B. Batchelor, ORNL) - 3rd year**
  - **Center for Framework Application for Core-Edge Transport Simulations FACETS (PI: J. Cary, Tech-X & U. Col.) - 2nd year**



FES ADVANCED COMPUTATIONAL PROJECTS

NEW:

- ***SciDAC Center for Gyrokinetic Particle Simulation of Turbulent Transport in Burning Plasmas (GPS-TTBP) (PI: P. Diamond, UCSD)***
- ***SciDAC Center for Extended Magnetohydrodynamic Modeling (CEMM) (PI: S. Jardin, PPPL)***
- ***SciDAC Center for Simulation of Wave-Plasma Interactions (CSWPI) (PI: P. Bonoli, MIT)***
- ***SciDAC Center for the Study of Plasma Microturbulence (CSPM) (PI: W. Nevins, LLNL)***
- ***SciDAC Center for Gyrokinetic Simulation of Energetic Particle Turbulence and Transport" (GSEP) (PI: Z. Lin, UCI)***
- ***Center for Gyrokinetic/MHD Hybrid Simulation of Energetic Particle Physics (CSEPP) (PI: G. Fu, PPPL)***

CONTINUING:

- ***OFES Edge Simulation Laboratory – completing third year with funding support from OFES and also OASCR (PI: R. Cohen, LLNL)***
- ***OASCR Multi-scale Gyrokinetics – completing third year of funding supported by OASCR's Multiscale Mathematics Research and Education Program (PI: W. Lee, PPPL)***

PI Task List

All PI's are expected to describe:

(1) ***progress toward achieving its scientific targets with respect to clear deliverables during this third year of a 3-year project***

(2) ***significant interactions with respect to collaborations with the Computer Science and Math communities, such as the SciDAC Centers for Enabling Technology (CET), SciDAC Institutes, and Scientific Applications Partnerships Projects (SAPP's)***

(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 these platforms -- including what new science is enabled at the terascale and also what might be expected at the petascale in the future***

(4) ***status of verification and validation efforts***

CHARGE-1 FOR PSACI PAC

Charge 1: **The PAC is requested to provide its views on the progress within the two SciDAC FSP Prototype Centers [CPES (C. S. Chang) & SWIM (D. Batchelor)] which are in the third of a planned 3-years of funding with joint support from OFES & OASCR -- with possibility of another 2-years extension pending upcoming OFES/OASCR Review (June 23-24, '08). It is asked to do so with regard to the scientific/computational goals and deliverables targeted at the end of this 3-year funding period with respect to:**

(i) ***Scientific & Technical Merit impacting improvement of 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 reliable modeling capabilities for dealing with recognized ITER-relevant physics issues***

* In addition to general PI Task List, the CPES & SWIM PI's are requested to describe plans (with targeted deliverables) for the next two years if the proposed renewal is approved by OFES/OASCR

CHARGE-2 FOR PSACI PAC

Charge 2: **The PSACI PAC is requested to comment on the progress, plans, and impact for:**

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

  -- completing second of planned five years of joint OFES/OASCR funding

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

  -- completing second of planned three years of OASCR funding

- OFES Edge Simulation Laboratory **(R. Cohen, LLNL)**

  -- completing third year with funding support from OFES and also OASCR

- OASCR Multi-scale Gyrokinetics **(W. Lee, PPPL)**

  -- completing third year of funding from OASCR's Multiscale Mathematics Research and Education Program

CHARGE-2 (continued)

Charge 2: The PAC is requested to comment on the progress, plans, and impact for these projects with respect to:

(i) ***Scientific & Technical Merit*** ***impacting improvement of 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 reliable modeling capabilities for dealing with recognized ITER-relevant physics issues***

CHARGE-3 FOR PSACI PAC

Charge 3: **Provide impressions of and advice on current situation regarding the adequacy of supercomputing cycles available to FES and the need for improved coordination between the INCITE and SciDAC Programs: "How can DOE-SC best move forward?"**

- ***Brief presentation of this issue to the PAC by John Mandrekas (OFES) who will lead the associated discussion***

CHARGE-4 FOR PSACI PAC

Charge 4: **The PSACI PAC is charged with providing its assessment of the first quarter (initial four months) progress within:**

- ***SciDAC Center for Gyrokinetic Particle Simulation of Turbulent Transport in Burning Plasmas (GPS-TTBP) (PI: P. Diamond, UCSD)***
- ***SciDAC Center for Extended Magnetohydrodynamic Modeling (CEMM) (PI: S. Jardin, PPPL)***
- ***SciDAC Center for Simulation of Wave-Plasma Interactions (CSWPI) (PI: P. Bonoli, MIT)***
- ***SciDAC Center for the Study of Plasma Microturbulence (CSPM) (PI: W. Nevins, LLNL)***
- ***SciDAC Center for Gyrokinetic Simulation of Energetic Particle Turbulence and Transport" (GSEP) (PI: Z. Lin, UCI)***
- ***Center for Gyrokinetic/MHD Hybrid Simulation of Energetic Particle Physics (CSEPP) (PI: G. Fu, PPPL)***

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

THURSDAY, JUNE 6, '07

9:00 AM -- 9:45 AM
CLOSED SESSION:

Welcome from Rob Goldston followed by 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 -- 12:00 PM
OPEN SESSION
Integrated Modeling Presentations: Progress & Plans for SciDAC Fusion Simulation Prototype 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 Simulation [CPES] (C. S. Chang, NYU)
30 minutes presentation; 30 minutes discussion
12:00 PM -- 12:45 PM LUNCH

12:45 PM -- 2:55 PM OPEN SESSION
* SciDAC Fusion Simulation Prototype Center for Framework Application for Core-Edge Transport Simulations [FACETS]
(J. Cary, Tech-X & U. Colorado)
20 minutes presentation; 20 minutes discussion
* SciDAC Scientific Application Partnership Program (SAPP) on Steady State GK Transport Code Development (supporting FACETS Project)
(M. Fahey, ORNL)
10 minutes presentation; 10 minutes discussion
* OFES Edge Simulation Laboratory (R. Cohen, LLNL)
20 minutes presentation; 20 minutes discussion
* OASCR Multiscale Gyrokinetics Project (W. Lee, PPPL)
15 minutes presentation; 15 minutes discussion

2:55 PM – 3:30 PM
* Supercomputing Cycles for FES (J. Mandrekas, OFES)
15 minutes presentation; 20 minutes discussion

3:30 PM – 3:45 PM Coffee Break

3:45 PM -- 5:30 PM CLOSED SESSION -- PAC begins formulation of recommendations and poses additional questions to the PI's

5:30 PM -- 6:00 PM OPEN SESSION -- Additional questions and requests for clarifications from PI's

7:00 PM Dinner for Meeting Attendees

FRIDAY, JUNE 6, '07

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

10:00 AM -- 1:00 PM
Progress & Plans for new Projects 15 minutes presentation; 15 minutes discussion

* SciDAC Center for Gyrokinetic Particle Simulation of Turbulent Transport in Burning Plasmas (GPS-TTBP) (P. Diamond, UCSD)

* SciDAC Center for Extended MHD Modeling (CEMM) (S. Jardin, PPPL)

* SciDAC Center for Simulation of Wave-Plasma Interactions (P. Bonoli, MIT)

* SciDAC Center for the Study of Plasma Microturbulence (CSPM) (W. Nevins, LLNL)

* SciDAC Center for Gyrokinetic Simulation of Energetic Particle Turbulence and Transport" (GSEP) (Z. Lin, UC-Irvine)

* Center for Gyrokinetic/MHD Hybrid Simulation of Energetic Particle Physics (CSEPP) (G. Fu, PPPL)

1:00 PM -- 3:30 PM CLOSED SESSION (extending over lunch)
PAC drafts report with comments/recommendations

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