June 21, 2005

Professor Robert J. Goldston, Director
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Dear Professor Goldston,

The Program Advisory Committee (PAC) of the Plasma Science Advanced Computing Institute (PSACI) met at the Princeton Plasma Physics Laboratory on June 2-3, 2005. The principal charge to the PAC was to assess the accomplishments of the three fusion energy science centers supported by the Scientific Discovery through Advanced Computing (SciDAC) program and the Fusion Collaboratory supported by the Office of Advanced Scientific Computing Research (OASCR). The three fusion science projects are virtual centers in Extended MHD, Plasma Microturbulence, and Wave-Plasma Interactions, and the National Fusion Energy Sciences Collaboratory is a partnership between the three major MFE experimental facilities (DIII-D, C-Mod, and NSTX) and key members from the CSET (Computer Science and Enabling Technology) community. An additional charge was to provide initial impressions of pilot components for the new $2M Fusion Simulation Project (FSP). To this end, we received presentations by the Principal Investigators (PIs) of each Center, including the Fusion Collaboratory. We were also given presentations by the PIs of two potential FSP projects on Edge Physics.

The presentations by the Fusion Energy Sciences SciDAC centers highlighted key accomplishments achieved during the first year of a new 3-year funding cycle. The PIs for the Fusion SciDAC centers (S. Jardin, W. Lee, and D. Batchelor) and the PI for the Fusion Collaboratory (D. Schissel) made oral presentations at the meeting and also provided two-page documents which highlighted significant accomplishments. The information provided by the PIs included a description of (1) how well each project has made progress toward achieving its scientific targets with respect to clear deliverables; (2) how super-computing resources have enabled the achievement of the targeted scientific goals in the timeliest manner; and (3) what role collaborative interactions have played within each project and also with other SciDAC activities. The PAC's role was to provide an evaluation/assessment of substantive progress made by each project toward the scientific/computational goals and deliverables targeted by the Fusion SciDAC centers (with respect to Scientific and Technical Merit, Readiness for Terascale Computing, and Potential for Impact on Other Scientific Disciplines).

The presentations are posted on the web (http://w3.theory/PSACI.html). These presentations demonstrate that the technical and computational advances have been quite substantial and have been detailed in numerous journal publications and invited papers at major meetings. The forefront advances in the modeling have also been prominently featured in presentations to other scientific communities and to the funding agencies. These advances make clear that advanced computation in tandem with theory and experiment is a powerful tool for scientific understanding and innovation in FES research. Plasma science is indeed effectively utilizing the exciting advances in information technology and scientific computing, and tangible progress is being made toward more reliable predictions of complex properties of high temperature plasmas. Very importantly, the FES SciDAC projects have brought together physicists, applied mathematicians, and computer scientists in close and productive working relationships, which provide a model for future research.

To illustrate the significant advances, let us briefly discuss some highlights in each area.

In partnership with the CSET community, the Center for Magnetohydrodynamic Modeling (CEMM) has continued to make advances in the development and application of improved MHD physics models. Significant progress was made this year in developing the computational algorithms required to efficiently advance the full two-fluid equations, including the dispersive whistler and kinetic Alfven waves that impact plasma dynamics at small spatial scales. New scientific results were obtained on many topics: such as the sawtooth cycle of a small tokamak, including the nonlinear role of the higher toroidal harmonics; early nonlinear evolution of edge localized mode (ELM) precursors; the saturation of the fishbone mode in a burning plasma, including mode chirping; and the saturation of the n=1 instability in the core of NSTX plasmas via two-fluid effects. The PAC commends the CEMM project for taking the lead and beginning to address its needs for closure relations to include relevant kinetic effects in the Extended MHD simulations. The PAC suggests that the CEMM explore the possibility of quantitative computational tests of the explosive instability theory of nonlinear ballooning recently proposed by Wilson, *et. al*. We also suggest that the CEMM include some consideration of subgrid scale type models of microturbulence effects on MHD as part of its program on kinetic closures. The PAC recommends that the nonlinear sawtooth benchmarking exercise between the M3D and NIMROD be brought to completion and appropriately documented. Since a major component of the CEMM interactions with the SciDAC Integrated Software Infrastructure Centers (ISICs) have come in the adaptive mesh refinement (AMR) area, the actual plans for integration of the AMR capability into the two major codes, M3D and NIMROD, need to be specified. Overall, progress was documented in about 15 publications, including 5 in Physics of Plasmas, 1 in Physical Review Letters, and 4 in Computer Physics Communications. Employment of terascale computing resources was exemplified by several million node-hours used on the IBM SP3 at NERSC. Future utilization by the CEMM of up to 1000 processors or more on leadership-class computing platforms will depend in large measure on the successful development and implementation of more efficient implicit schemes.

The new Center for Gyrokinetic Particle Simulation (GPS) of Turbulent Transport in Burning Plasmas has also made progress. The codes have been further developed, and a general geometry capability for shaped plasmas has been implemented with the goal of simulating ITER plasmas. The simulations have yielded thought-provoking results pertinent to ion-temperature-gradient (ITG) and electron-temperature-gradient (ETG) turbulence. For example, inclusion of the parallel acceleration nonlinearity of the nonlinear gyrokinetic equation was found to alter the evolution and approach to saturation in some cases. However, significantly improved understanding of the physics basis, generality, and consistency of this result is needed. Increasing attention is being given to delineating the role of collisions and noise in particle-in-cell simulation codes. The PAC recommends that collisional effects in the codes be intentionally varied in order to determine the levels at which such effects might dominate the instability saturation and the turbulent transport. We also recommend that the impact of collisional effects on the evolution and physics of both drift-ITG modes and zonal flows be explored. Particular emphasis should be placed on comparing and elucidating the physics of collisional and collisionless saturation of zonal flows. The role of possible tertiary instability should be studied, along with the effects collisions might have on it. The GPS group has also pursued interesting work on turbulence spreading and on the nonlinear evolution and saturation of ETG turbulence. The PAC notes that both these topics are important and merit further study with an increased emphasis on detailed diagnosis of the computational results and on comparison with theory. There have been extensive interactions with the CSET community on efficiently solving elliptic-type equations on MPP platforms, on data management, and on 3D interactive visualization software. Terascale computing is being aggressively used, and GTC, a gyrokinetic toroidal particle simulation code, which is the Fusion Energy Science representative in the NERSC benchmark suite for testing the most advanced computing platforms, provides the most impressive example of "leadership class" computing. The codes are well parallelized; the GTC code has recently achieved 3.7 teraflops sustained performance with 2048 processors using 6 billion particles and with 25% single-processor efficiency on the Earth Simulator Supercomputer in Japan. Over 12 journal articles have been either published or submitted, and 12 invited presentations have either been given or are scheduled to be given by this SciDAC Center.

The Center for Wave-Plasma Interactions is also developing new capability in a number of areas, including the treatment of the impact of energetic species on the RF wave-particle interaction processes as well as integrated launcher-edge simulations. As an example of the progress, preliminary full-wave/ Fokker-Planck calculations have been carried out and compared with ICRF beam acceleration experiments on DIII-D. The PAC commends these continuing productive interactions with the experimental community. The PAC recommends that a substantial effort be devoted to examining the origins of irreversibility and delineating the regimes of validity of the quasilinear calculations for evolving the distribution functions. For future integrated simulations of fusion devices, it is important to develop more sophisticated wave solvers using a multi-scale adaptive spectral representation of the fields. Much more work is needed on this topic. This project's utilization of terascale computing and associated productive interactions with the CSET community have focused on the dense-matrix solution of the complex linear wave equation. It is recommended that perhaps with increased funding support for CSET collaborations and reinstitution of support for the SAPP project, more rapid progress will be stimulated in the aforementioned challenge of developing and implementing advanced wave solvers. Terascale computing resources were aggressively used; a NERSC announcement in April highlighted the 68% of peak performance achieved on the IBM

SP3 by this project's wave-plasma calculations with a large linear dense matrix inversion. This SciDAC Center's progress was documented in approximately 6 journal articles and 5 invited papers at major meetings.

The National Fusion Collaboratory (NFC) has continued to be remarkably successful in providing vital infrastructure for national and international collaboration in experimental operation, data analysis, and simulation. FusionGrid services have enabled fusion scientists to use codes with less effort and better support. The code TRANSP, available as a FusionGrid service, has performed over 5800 simulations for ten different fusion devices throughout the world and is also being used for machine and experimental designs for both the Burning Plasma Experiment in the US and the International Thermonuclear Experimental Reactor. Recently the GATO ideal MHD plasma stability code was also released as a FusionGrid service. Shared display walls in Tokamak control rooms and significantly enhanced remote collaboration via Access Grid nodes are having a large impact on productivity. The NFC is enabling greater utilization of the existing US experiments by more scientists by facilitating real-time off-site interaction with the experiments. In addition, a unified FusionGrid security infrastructure has enabled more effective sharing of data and codes.

A number of recommendations for the FES PSACI Centers and the Fusion Collaboratory are summarized below:

1. The PAC notes that computational resources are significantly limiting progress in both code development and application (for example, 5 day turn around time on 1 hour code development runs). Attention needs to be given to effective capacity computing resources. This is an issue previously raised by the FES theory coordinating committee, and OFES has taken some steps to address this very important problem.

2. The PAC strongly emphasizes that more in-depth physics analysis of the simulation data and more extensive quantitative comparisons with theory and experiments would significantly increase the impact of the SciDAC centers on the fusion program. To this end, the PAC suggests that all the SciDAC projects give more attention to the development and implementation of diagnostics and analysis tools in addition to code development. More collaboration with fusion theorists and experimentalists which is focused on analysis of the simulation results would be beneficial to the SciDAC projects. To this end, OFES should consider making some modest financial resources available to facilitate such collaboration.

3. The PAC recommends that a continuing study group devoted to issues of noise, resolution, and artificial dissipation in microturbulence simulations be formed. Preferably, formation should occur via self-organization of interested parties. The study should not be limited to particle-in-cell codes, ETG models, or even to SciDAC projects, and international participation should be encouraged. In order to nucleate such a study, the PAC recommends that all interested parties participate in a code comparison for results on simulations of ETG turbulence. A

set of common problem should be identified which stress the performance of the codes with respect to noise, resolution, and artificial dissipation. A productive outcome of these comparisons would be a collection of papers by the investigators to be published in Physics of Plasmas. The data on these benchmarks would be made freely available to all interested parties within three months after acceptance for publication. It is our understanding that OFES will make computer time available for this important exercise.

4. The PAC recommends that the remarkably successful National Fusion Collaboratory continue to play a major leadership role in building collaborative infrastructure for future remote operation of experiments and in fostering collaborative development and use of simulation codes as well as data analysis codes. The NFC is encouraged to take a leadership role in establishing common data structures and protocols and a collaborative culture for integrating SciDAC and FSP project results into the broad fusion community, and in particular the large experimental communities.

5. The PAC notes that kinetic simulation of plasmas is not represented in the Princeton Plasma Physics graduate curriculum. It is suggested that a graduate course on this topic would make a very valuable contribution to attracting and training students in this important area of plasma science.

Finally, the PAC noted the quality of the two potential components of the new $2M FSP project. Both projects (Center for Plasma Edge Simulation, with C.S. Chang as PI and Fusion Simulation Prototype Center for Edge Plasmas, with R. H. Cohen as PI) are on the advanced modeling of edge physics. As we have previously pointed out, the modeling of edge plasmas is central to our ability to predict the performance of present and future fusion experiments, and the modeling of the critical edge region has lagged in comparison with efforts at modeling the plasma core. The PAC applauds OFES for confronting this issue by soliciting major proposals on code development and physics exploration of the edge plasma through FSP. The panel reviewing the major edge proposals was unable to make a decision on which proposal to fund and recommended that both proposals be funded for a period of up to three years before a final selection is made. If OFES makes the decision to fund both proposals for a limited time, the PAC emphasizes that it will be critical to make sure that the funding going to each team not be diffusely distributed, but rather focused on supporting a substantial fraction of a limited number of scientists who are committed to the goals of the project. Properly defining a reduced workscope with a limited number of team members will be essential to avoid spreading the available resources too thinly. For example, for the initial phase of Chang's team effort, we would recommend that the M3D effort on ELM modeling be reduced in priority.

The PAC was very pleased that Dr. Michael Strayer, head of the SciDAC program and acting head of the Mathematical, Information, and Computational Sciences (MICS) Division within OASCR, Dr. Mary Anne Scott, MICS program manager for collaboratories, and Drs. Steve Eckstrand, Curt Bolton, and John Mandrekas of the DOE

Office of Fusion Energy Sciences were able to attend the PAC meeting and productively participate. Their many valuable comments and insights were much appreciated by the PAC. We also thank you for your continued strong support. Finally, the PAC warmly applauds Dr. William Tang and Dr. Vincent Chan for their very effective leadership of the PSACI. Thanks to their vision and strong advocacy, the fusion science community is playing a highly visible and productive role in the national SciDAC program.

Respectfully for the PSACI-PAC,

William L. Kruer
Chair, PSACI-PAC