June 17, 2004

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 6-7, 2004. The principal charge to the PAC was to assess the accomplishments of the five fusion energy science projects supported by the Scientific Discovery through Advanced Computing (SciDAC) program and the Fusion Collaboratory supported by the Office of Advanced Scientific Computing Research (OASCR). An additional charge was to provide program guidance on the fusion energy science projects selected for the next three-year phase of the SciDAC program as well as on the Fusion Simulation Project (FSP) component of this program. To this end, we received presentations by the Principal Investigators (PIs) of each project, including the Fusion Collaboratory. We were also given presentations by the PIs of the newly-selected projects and on the initial plans for start-up of the FSP.

The final summary presentations from the Fusion Energy Sciences SciDAC centers highlighted key accomplishments achieved over the course of the past three years. These included the five plasma science projects (virtual centers in Plasma Microturbulence, Extended MHD, Plasma Waves, Magnetic Reconnection, and Atomic Physics) and the National Fusion Energy Sciences Collaboratory, which 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. The PIs for the Fusion SciDAC projects/centers (W. Nevins, S. Jardin, D. Batchelor, A. Bhattacharjee, and D. Schultz) 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 evaluation/assessment of substantive progress made by each project toward the scientific/computational goals and deliverables targeted by the Fusion SciDAC centers at the end of their three-year funding period (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.pppl.gov/theory/PSSACI04.html). These presentations demonstrate that the technical and computational advances have been very impressive 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 Fusion Energy Sciences (FES) continues to be at the very forefront in using high-end computing to successfully model complex multi-scale physics. Very importantly, the FES SciDAC projects have brought together physicists, applied mathematicians, and computer scientists in close and productive working relationships, which are a model for future research.

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

Through SciDAC-enabled collaborations, improved extended MHD physics models were developed, and significant advances in the algorithms were made. Many new scientific results were obtained on topics such as the dynamics of high-beta disruptions with detailed comparisons with experiments on the DIII-D tokamak and energetic particle-driven modes in spherical tokamaks with comparisons with NSTX experiments. Interactions with applied mathematicians and computer scientists resulted in significant algorithm improvements (such as optimized matrix solvers giving a factor of 4-5 reduction in computational time for real applications) as well as a code with adaptive mesh refinement for more efficient calculations. The task of cross-validation between the two principal codes, M3D and NIMROD, has begun with comparisons with the CDX-U experiment and is expected to continue. Scientific progress was marked by over twenty journal articles and many invited papers at major conferences which have resulted from the work in this area.

A suite of plasma microturbulence codes have been improved and validated by comparisons with one another and with experiments. Particularly impressive is the level of agreement reported for actual nonlinear benchmarks between major codes, such as the particle-in-cell code GTC and the continuum code GYRO. Key accomplishments include implementation of electromagnetic drift-wave turbulence algorithms in these codes and their applications to the modeling of the scaling of heat transport with machine size, which is a key issue for future large devices such as the ITER burning plasma experiment. High-end computing was aggressively used; for example, nearly 5M NERSC node-hours were used in FY'03 in addition to about 3.5M node-hours on the CCS at ORNL. In addition, the major codes in this project have been ported to "Leadership Class Supercomputers" such as implementation of the GTC code on the Earth Simulator Computer in Japan and implementation of both the GYRO and GTC codes on the CRAY X1 Computer at ORNL. As evident from seven invited papers at major conferences and over twenty journal publications, this project has been very productive in advancing scientific understanding.

There were many advances in the modeling of wave-plasma interactions. Through collaborations with the SciDAC science applications partnership program and the ORNL Center for Computational Science, great strides were made in increasing the speed,

resolution, and physics content of the wave solvers. As a result, it is now possible to model wave conversion processes in two dimensions for large scale fusion devices. For example, 2D ICRF mode conversion calculations led to a detailed understanding of experiments on Alcator C-Mod. Promising new approaches for addressing nonlinear physics challenges and for development of more efficient sparse matrix algorithms are being actively pursued. Over a dozen journal publications have resulted from the very productive work in this area.

State-of-the-art atomic and molecular collision codes were implemented on high-end computing facilities and used to study a wide range of atomic collision processes in fusion plasmas. The many advances include the first accurate electron-impact excitation cross sections for fusion species at intermediate energies using an MPP R-matrix code developed in this project. Collisional-radiative coefficients were obtained to support plasma transport studies in many fusion devices. High-end computing and implementation of advanced computational techniques were essential for these achievements, which resulted in the impressive publication of over ten Physical Review Letters during the course of this project.

In the magnetic reconnection studies, the first 2-fluid (Hall MHD) code with adaptive mesh refinement (AMR) was developed. A wide range of physics was studied, including "bursty" reconnection as well as sawtooth oscillations in tokamaks and in magnetotail substorms. However, the ambitious goal of applying the powerful AMR framework of the FLASH code to actual tokamak geometry did not lead to substantive results. Nevertheless, there were productive collaborations with the SciDAC TOPS group on development of fully implicit algorithms. In general, this project provided the fusion community with a valuable interface with the space plasma physics and ASCI scientific communities.

The National Fusion Collaboratory continues to enable more efficient use of experimental facilities and more effective integration of experiment, theory, and modeling. Many examples can be given. Worldwide data access on the FusionGrid is now available using the MDSplus data acquisition and management system. The code TRANSP, widely used for the time-dependent analysis and simulation of tokamak plasmas, is also presently available as a FusionGrid service. Recently, FusionGrid's remote collaboration services were used to lead a JET European fusion experiment. It is our understanding that OASCR will continue to fund the Collaboratory, which has been a remarkable success.

The PAC applauds the DOE for its timely execution of an excellent review process for the new SciDAC projects in the FES portfolio. Presentations were made to the PAC by the PIs of the two newly selected projects in Plasma Microturbulence (W. Lee) and MHD (S. Jardin). The presentations included a discussion of their goals as well as their vision/scientific road map for future research. These new centers for Extended Magnetohydrodynamic Modeling and for Gyrokinetic Particle Simulations of Plasma Turbulence and Kinetic MHD Physics are very high quality projects with focused and well-defined deliverables in the vital areas of extended MHD and plasma

microturbulence. Some technical feed back was provided by the PAC to the PIs at the conclusion of their presentations. We confidently look forward to the advances to come. The PAC notes that the excellent and very productive work on wave-plasma interactions and atomic physics modeling for fusion is presently unfunded. Since neither area receives significant funding from the base program and both have been aggressive and effective users of high-end computing resources, we encourage that some funding be found for work in these important areas. Further, we recommend that access to computer time and computer science resources be maintained for scientists who had funding under the previous SciDAC grant cycle but who will not receive further SciDAC funding. The PAC also continues to be very concerned that there is no SciDAC project on the vital topic of plasma edge modeling.

The PAC strongly supports the goal of integrated modeling and the proposed FSP, which has been endorsed by the US Fusion Energy Science Advisory Committee (FESAC) and by DOE. We were informed of the current plans to set aside $2M in FY'05 for FSP start-up planning. Of this, $1M would come from the SciDAC portfolio and $1M would be from OASCR. A planning committee has been recently formed. Dr. Douglass Post, chair of this committee, presented preliminary plans for use of the start-up funding and participated in discussions with the PAC. We note that the planning committee is an excellent one with broad expertise in areas ranging from ASCI and fusion codes to computer science. The PAC stresses the importance of a more detailed technical plan for the use of these significant start-up resources. We strongly recommend that the FSP planning activity:
(1) plan how to leverage the past and ongoing Fusion Energy Sciences SciDAC projects into the FSP and identify key missing scientific areas for the integrated modeling of a fusion burning plasma;
(2) propose an appropriate balance between the needed physics research and development and computational science developments during the early, middle and mature stages of the FSP project;
(3) make progress on some multi-scale (in both space and time) integrated modeling challenges by identifying and facilitating "prototype modeling" of a few key multi-scale scientific issues for burning fusion plasmas, such as sawtooth crash dynamics, ELMs, internal transport barrier formation and growth while maintaining MHD stability, and RF effects on plasma flows and in forming transport barriers;
(4) plan how to integrate relevant ISIC SciDAC projects into the FSP as a part of a broader plan to have the computer science and physics elements developed in parallel from the beginning and throughout the evolution of the FSP in order to establish an effective infrastructure for the efficient integrated modeling of burning plasmas; and
(5) identify key fusion burning plasma foci for the early, middle, and mature stages of the FSP.

The PAC was very pleased that Dr. Michael Strayer, head of the SciDAC program and acting head of the Mathematical, Information, and Computational Sciences Division within OASCR, and Drs. John Willis, Steve Eckstrand, Arnold Kritz, and Curt Bolton of the DOE Office of Fusion Energy Science were able to attend our meeting and productively participate. Their many valued comments and insights were much

appreciated by the PAC. We also thank you for your attendance and insightful comments. Finally, the PAC warmly applauds Dr. William Tang and Dr. Vincent Chan for their very effective leadership of the PSACI.

Respectfully for the PSACI-PAC,

William L. Kruer
Chair, PSACI-PAC