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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 5-6, 2008. There were several charges to the PSACI PAC. The first charge was to assess the progress of the two Scientific Discovery by Advanced Computing (SciDAC) Fusion Simulation Project (FSP) Prototype Centers which are in the third of a planned three-year funding cycle with joint support from the Office for Fusion Energy Sciences (OFES) and the Office for Advanced Scientific Computing Research (OASCR). These are the Center for Plasma Edge Simulation (CPES) led by C. S. Chang, and the Center for Simulation of Wave Interactions with MHD (SWIM) led by D. Batchelor. The second charge was to comment on the progress and plans for four additional computational projects. These are: a SciDAC Proto-FSP Center for Framework Application for Core-Edge Transport Simulations (FACETS) led by J. Cary, and funded jointly by OFES and OASCR; a SciDAC Science Application Partnership Program (SAPP) project on Steady-State Gyrokinetic Transport Code Development supporting the FACETS project led by M. Fahey and J. Candy, and funded by OASCR; an OFES and OASCR-funded Edge Simulation Laboratory led by R. Cohen; and an OASCR-funded Multi-scale Gyrokinetics project led by W. W. Lee. Additional charges were to provide comments on the adequacy of supercomputing cycles available to Fusion Energy Sciences (FES) and the need for improved coordination between the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) and SciDAC programs, as well as to provide initial feedback to six newly funded projects on their plans and progress. These new and/or renewed projects include: a SciDAC Center for Gyrokinetic Particle Simulation of Turbulent Transport in Burning Plasmas (GPS-TTBP) led by P. Diamond; a SciDAC Center for Extended Magnetohydrodynamic Modeling (CEMM) led by S. Jardin; a SciDAC Center for Simulation of Wave-Plasma Interactions (CSWPI) led by P. Bonoli; a SciDAC Center for the Study of Plasma Microturbulence (CSPM) led by W. Nevins; a SciDAC Center for Gyrokinetic Simulation of Energetic Particle Turbulence and Transport (GSEP) led by Z. Lin; and a Center for Gyrokinetic/MHD Hybrid Simulation of Energetic Particle Physics (CSEPP) led by G. Fu.

To respond to these charges, we received presentations by the Principal Investigators (PIs) or a representative of each project with particular attention given to scientific and technical merit impacting improved predictive capabilities, utilization of leadership-class computing for producing important new results, and demonstrating the scalability of the science with the number of processors, and potential for impact on burning plasma experiments. In each case , one-half of the time was allotted to presentation and one-half to questions and discussion, a procedure which proved to be especially fruitful. John Mandrekas (OFES) updated the PAC on the plans to achieve better coordination between the SciDAC and the INCITE programs.

The presentations to the PSACI PAC are posted on the PSACI website (http://w3.pppl.gov/theory/PSACI.html). These presentations relevant to Charges #1 and #2 demonstrate that substantial technical and computational advances continue to be made, and are detailed in numerous journal publications and invited papers at major meetings. Close interactions with the applied mathematics and computer science communities have played an essential role in these ongoing forefront advances. Of particular importance, impressive comparisons with and elucidations of experimental results have continued. To complement the detailed technical presentations and to focus attention on some key overarching issues, the PAC posed a number of questions to each of these projects. For example, the projects were requested to describe their research progress and plans for verifying the codes and algorithms. The projects developing and using framework tools (FACETS, CPES, and SWIM) were asked to discuss the utility of their framework tools, and the implications for FSP. The answers to the questions on the second day of the PAC meeting stimulated additional valuable discussions and feedback. One important outcome of this process is that the FACETS, CPES, and SWIM projects are strongly encouraged by the PSACI PAC to write a joint paper detailing why each chose their particular approach and the strengths and weaknesses of each approach. This would help to illustrate how the SciDAC Proto-FSP portfolio of projects collectively provide greater insights into this challenging area than each could on an individual basis. The replies from the PIs to all of the questions posed by the PAC are also posted on the website http://w3.pppl.gov/theory/PSACI.html.

In order to illustrate the significant advances and associated opportunities and challenges, let us briefly discuss some highlights in each area. We begin with the two projects in the first charge (CPES and SWIM).

The Center for Plasma Edge Simulation (CPES) is constructing the first edge gyrokinetic code in realistic tokamak edge geometry with diverted magnetic field. Accomplishments include development of a full-f gyrokinetic particle code (XGC1) with an electrostatic turbulence capability in edge geometry, as well as a kinetic equilibrium evolution code XGC0. The PAC applauds CPES for carrying out the first simulations of Ion Temperature Gradient (ITG) turbulence in the edge region of a toroidal plasma. The planned development of an electromagnetic capability is strongly encouraged. The PAC also recommends comparisons with other codes, such as the kinetic (continuum) simulations from the Edge Simulation Laboratory (ESL) project (when available), and with edge fluid code BOUT. There have been many close and productive interactions with computer science and applied mathematics teams – an excellent example being the End-to-end Framework for Fusion Integrated Simulation (EFFIS), which has been built and used to achieve multiple ELM cycle simulations using four different nonlocal codes.

Code performance has been improved with new algorithms implemented, and the full-f XGC1 code has demonstrated productive utilization of leadership-class computers. In general, there have been a limited number of physics studies carried out that have fully exercised the code capabilities because of the associated demand for large allocations of dedicated cycles. Specifically, in the last year approximately 2 million XT4 hours on Jaguar, and about 5 million hours on Franklin were used with the physics studies largely limited by availability of computing time. It is also noteworthy that 5 postdoctoral associates and 12 graduate students are being trained within CPES. This project appears to be on schedule to meet its 3-year milestones.

The Center for Simulation of Wave Interactions with MHD (SWIM) addresses the interaction of RF and particle sources on extended MHD phenomena. An Integrated Plasma Simulator (IPS) has been developed to allow efficient coupling of the full range of required fusion codes. The IPS has been used in a number of code benchmarking and ITER scenario studies. A noteworthy example is the time-dependent modeling of energetic minority ion tail formation in Alcator C-Mod using the codes AORSA, CQL3D, and TSC. A synthetic diagnostic was constructed, and detailed comparisons have been made with experiments. In other results, stabilization of resistive MHD magnetic islands by RF radiation has been successfully demonstrated by incorporating a phenomenological model of RF current drive into the NIMROD code. Significant progress has been made on the self-consistent treatment of the RF, including kinetic closures. The PAC strongly encourages continued verification studies, possibly using manufactured solutions. The PAC also noted that progressing beyond the Porcelli model to a full MHD model is an important goal in the sawtooth stabilization studies. The major codes being linked together in SWIM, such as M3D, NIMROD, and AORSA have productively utilized leadership-class computing facilities. However, it was reported that the requested computer time was not awarded to SWIM from the INCITE project this year. There have been productive interactions with other centers, such as CEMM and CSWPI, and with OASCR Centers for Enabling Technology, as well as international collaborations related to ITER. Students and postdoctoral associates are being trained at 4 different universities. The 3-year milestones for the SWIM project appear to be either completed, or on track for completion this year.

We now address the four computational projects in the second charge.

The Framework Application for Core-Edge Transport Simulations (FACETS) project aims to provide a coupled core-edge-wall computational capability to the fusion community with maximal re-use of existing software. Much progress has been made in the first year of funding. The framework was developed for composition of an arbitrary number of components connected through tight coupling. The UEDGE code was componentized and parallelized as the standard edge coupling component with respect to coupling to the core region of the plasma. Work began on inclusion of a wall model, and development of a visualization capability has commenced. The PAC applauds the particularly close interaction of the FACETS project with the computer science and applied mathematics communities. For example, PETSc solvers were installed in UEDGE for improved performance and restoration of parallelism. The project is not yet using leadership-class computing, but is planning to do so. Some efforts on verification are now underway, including comparisons of FACETS core transport with the ASTRA code. FACETS is clearly making important first strides towards developing a unified software framework for modeling fusion plasmas. The PAC appreciates the PI's perspective on the complementary strengths and weaknesses of the various approaches that are being used in the different projects. This was a significant factor in stimulating the aforementioned encouragement from the PAC for a joint paper on this topic involving FACETS, CPES, and SWIM.

The Steady-State Gyrokinetic Transport (SSGKT) project aims to develop an algorithmic strategy to employ local and global gyrokinetic turbulence simulations in steady-state transport calculations. This project is a Scientific Application Partnership with the FACETS project and is funded by OASCR. The SSGKT project involves a close and productive partnership between a computational fusion scientist and a computer scientist. The computer science focus is on coupling multiple instances of GYRO to a transport driver in an efficient way. The physics focus is on developing an iteration scheme that works for intermittent, time-dependent gyrokinetic data. A working prototype code (TGYRO) has been developed and is being tested with the goal of transferring TGYRO technology to the FACETS project. Leadership-class computing resources have been utilized to run the multiply-coupled GYRO.

The Edge Simulation Laboratory (ESL) project aims to model edge physics issues by development of a 5D Eulerian gyrokinetic code which evolves the full distribution function and includes divertor geometry and appropriate collision operators. The applied mathematics team funded by OASCR has now developed a solver and the infrastructure for the electrostatic full-f gyrokinetic equations in 4D and 5D mapped-grid structures. The PAC was informed that a delay in the funding of the applied math team has slowed this progress. The first version of the new ESL code (core only, 4D, electrostatic) will become available this summer. The physics team funded by OFES will then begin verification tests. The 5D code is expected within a few months thereafter, and a divertor capability in FY09. Meanwhile, the physics team has worked with prototype codes to explore various issues. A full-f, full-divertor-geometry code in energy and magnetic moment coordinates (TEMPEST) has been used to better understand the damping rate of geodesic acoustic modes. In addition, an efficient reduced neoclassical physics code (NEO) has been developed to model neoclassical dynamics. The physics team has also formulated a practical system of electromagnetic gyrokinetic equations for edge plasma simulations. This project clearly depends on close collaboration between the applied mathematics and physics components. It is expected that leadership-class computing resources will need to be utilized because the full distribution function will be evolved. In addition to moving forward on its physics goals, the ESL project can also provide valuable insights from enabling systematic comparisons between the PIC and continuum approaches.

The Multiscale Gyrokinetics for Fusion Plasma project aims to develop algorithms to better address the large range of time and space scales involved in simulating magnetized plasmas with massively parallel computers. Significant progress has been made in this project, which is entering its third year supported by OASCR. Algorithms have been developed to replace in gyrokinetic models the conventional rigid charged rings by time-varying so-called Kruskal rings. This can reduce the dimensionality of the phase-space dynamics from 6D to 5D. A new variational symplectic integrator for gyrocenter motion has been obtained, and a new iterative scheme has been developed to describe large-amplitude global zonal flows and small-amplitude mesoscale ITG modes in turbulence simulations. In addition, a sparse matrix iterative scheme using PETSc was implemented in GTS to resolve the multiscale problems associated with zonal flows and drift-wave perturbations. The results of this project have been well documented in a number of peer-reviewed publications. Finally, a graduate level course on Kinetic Theory and Modeling of Plasmas was developed by the PI and given at Columbia University. The course was very well received by the graduate students (approximately 17). The PAC applauds this important outreach to students, and recommends that this course be given more widely, including at Princeton University.

The third charge was to comment on the adequacy of supercomputing cycles available to FES and on the need for improved coordination between the INCITE and SCIDAC programs. John Mandrekas of OFES gave a clear overview of FES high-performance computing resources, and the INCITE program. There has been a significant increase in NERSC resources in 2008; i.e., the 19,320 processor 101.5 TFlops/s CrayXT4 Franklin replaced Seaborg as the flagship system. The allocations increased from 16.7 M hours in 2007 to 69.1 M hours in 2008, and these allocations are being actively utilized. The INCITE program provides high-performance computing resources to large computationally intensive projects that can make high-impact scientific advances. Now in its fifth year, INCITE includes high-performance computing resources at ORNL, LBNL, ANL, and PNNL, and is open to all scientific researchers and organizations. In 2008, 55 projects received 265 million processor hours. Seven FES projects were selected for INCITE awards in 2008, with the largest FES award being 8 million processor hours on the XT4 at ORNL. Over one-half billion hours are available in the 2009 INCITE program, and the submission deadline for proposals is in August, 2008. It was stressed that the INCITE projects need to be computationally intensive; i.e., must utilize a major fraction of the processors in the proposed research. Since many FES projects need much greater access to such high-performance computing resources, it is very important that they aggressively pursue this opportunity. There is also a need for additional resources for capacity computing which involves a large number of small independent jobs. OFES continues to make available additional resources for this computing. The PAC notes that there is also a need for providing significant funding support to maintain the facilities for capacity computing.

Relevant to Charge #4, the PAC received short presentations from the PIs (or a representative) of each of the six new projects, or newly renewed projects, and provided feedback for each project. These are a diverse set of projects addressing key ingredients for the comprehensive modeling of fusion plasma, including extended MHD, wave-plasma interactions, plasma microturbulence, and energetic particle turbulence and transport. The PAC was impressed with the high quality of the scientists involved and of the proposed work-scopes targeted. The PAC strongly encourages strong collaborative benchmarking activities whenever possible among the various projects, and emphasizes that attention be given to code verification and validation with experiments. We look forward to hearing about the exciting progress at our next meeting.

Given its importance, a final recommendation given last year is repeated below:

> The PAC continues to emphasize from a verification and validation perspective that more in-depth physics analysis of the simulation data and more extensive quantitative comparisons with analytic theories and with experimental observations would significantly increase the impact of the advanced computing projects on the fusion program. To this end, the PAC recommends that all of these projects give more attention to the development and implementation of modern diagnostics and analysis tools in addition to code development. It is also clear that more collaborations with fusion theorists and experimentalists which are focused on verification and validation of the simulation results would be very beneficial to the projects. To this end, OFES should consider making dedicated resources available to facilitate such collaborations. In other major computational science programs (such as the prominent DOE NNSA-sponsored ASCI Program), substantial verification and validation efforts demand significant commitments from key experimental projects to provide the associated run time as well as the enabling infrastructure costs.

The PAC notes that the number of projects for its consideration continues to significantly increase. In order to preserve adequate time for formulating a set of recommendations, either the number of projects that the committee considers should be reduced or the time available for this meeting should be expanded. Since a longer meeting is viewed as undesireable by most of the PAC, other options should be seriously considered. For example, the number of projects could be reduced by instituting a size (*i.e.*, budget) threshold for a project to be considered by the PAC. Another worthwhile guiding principle might be to focus primarily on those projects which include significant software architecture efforts and are expected to help form the basis of the FSP.

In summary, the ongoing achievements of the advanced computing projects make clear that advanced computations, in combination with theory and experiment, provide a powerful tool for scientific understanding and innovation in OFES research. Plasma science is indeed effectively utilizing the exciting advances in information technology and scientific computing, and tangible progress continues to be made toward more reliable predictions of complex properties of high temperature plasmas. Very importantly, these projects continue to bring together physicists, applied mathematicians, and computer scientists in close and productive working relationships, which provides an excellent model for future research.

Finally, the PAC is grateful to Dr. John Mandrekas of OFES, and to Dr. Lali Chatterjee of OASCR, for their expert participation in this year's meeting, and for their valuable input. We also thank you for your continued strong interest and support of these important activities. The PAC continues to be grateful to Dr. William Tang and Dr. Vincent Chan for their ongoing 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