CEMM Response to PAC Questions (06-06-03)

I. General Questions Posed by Bill McCurdy

1. **Have we demonstrated with substantive scientific results that we are effectively using terascale computing with successes that are well publicized?**
    a. We presented 8 new scientific results that all made use of high-end computing have all been presented at conferences, and have been or are in the process of being published.
    b. It was shown at the 2003 Sherwood meeting that by using 1000 processors, Eric Held could evaluate integral parallel heat flow closures that led to qualitatively and quantitively different physics compared to the diffusive form with a large conductivity coefficient.

2. **Is the partnership with the math ISIC centers actually building what's needed by FES?**
    a. We have a very good relation with the 3 ISIC centers, TOPS, TSTT, and APDEC.
    b. The TOPS center has given us access to an Algebraic Multigrid solver in M3D and a very fast direct sparse matrix solver for NIMROD. We have identified a number of additional areas that we will continue to collaborate in.
    c. The TSTT center is involved in evaluating and implementing high-order finite elements into M3D. We have taken some steps to ensure that this proceeds in a timely maner.
    d. The interaction with the APDEC center has been excellent. This has led to the joint development of an adaptive mesh refinement MHD code, AMRMHD, that has already led to discovery. We have several important applications in mind for this during the next year, including 3D toroidal pellet injection into a tokamak and high accuracy Hall reconnection.

3. **How are we playing a key role in helping to make the case for future experimental facilities such as ITER? How will we impact real decision-making in the large "scientific options space"?**
    a. Hybrid MHD simulations, now operational, allow us to study alpha particle effects on MHD modes (sawtooth, fishbone, hign-n, TAEs) in ITER. The results will impact reactor design and operation.
    b. We are in a unique position to calculate the nonlinear evolution of MHD activity in ITER, including sawtooth phenomena, neoclassical tearing modes, and resistive wall modes. The current Big Splash calculations involving NIMROD at NERSC will use the integral forms for both the electron parallel heat flow and viscous stress to get the NTM physics right, even in complicated magnetic geometry. The next phase will start looking at ways to actively control these modes through external sources such as RF and beams.

c. We are using the M3D code to calculate the effects of disruptions in ITER, in particular the 3D vessel currents due to VDE. The NIMROD code could also be used to calculate the heat load to the divertor during the disruption, as it is being used to do so in DIII.
d. The AMR MHD code should lead to a predictive model for pellet injection that could be used to design the ITER pellet injection system.

II. CEMM Specific Questions:

1. **How would you go about coupling MHD and microturbulence in the next round of SciDAC proposals?**
    a. One possible way of coupling MHD and microturbulence is using gyrokinetic closure on bulk ions and treating electrons as a fluid. This capability is in the M3D code, but has not been used extensively yet. This is described in Park, et al, Phys. Fluids (1999). A method to include nonlinear electron wave-particle resonances has not yet been formulated.
    b. The integral closures that Eric Held has been working on match onto the gyrofluid closures in the nearly collisionless limit. Particle trapping is presently being added, at which point they will have more physics than previous gyrofluid turbulence calculations. There is a close correspondence between this technique and the 3 + 1 gyrofluid moment model of Hammett and Perkins.
    c. This entire area needs more input, and we suggest more community involvement in developing ideas, possibly through the auspices of the Fusion Simulation Project.

2. **When will 2-fluid MHD start being used routinely?**
    a. For NIMROD, this will be in June of 2004. There was some setback when R. Nebel became disengaged from the project. Work is proceeding both on the formulation and the linear solver capability, both of which are needed.
    b. For M3D, a relatively simple 2 fluid description is being used routinely now in the stellarator studies. (There is a APS 2003 invited talk nomination on this topic). There is now active work on understanding the differences and limitations in different 2-fluid implementations that have been implemented, and in extending these to more complete descriptions, including neoclassical effects.
    c. For AMRMHD, work is progressing on implementing the Hall-term in the Ohm's law for the reconnection physics. We expect this to be completed during the next year.

3. **What diagnostics are needed to better understand the nonlinear results?**
    a. Possible ways to understand nonlinear saturation mechanisms of energetic particle-driven modes:

i. Compare single mode results with milti-mode results to check whether fluid nonlinearity is important
ii. Compare mode saturation level scaling with known analytic theories to determine saturation mechanism;
iii. Plot resonant particle phase-space diagram to see if there is island overlap and its role on nonlinear dynamics.

b. A powerful way to compare simulations with experiments is to add numerical "diagnostics" that mockup experimental raw data, such as soft-X ray and ECE signals. Some of this is already in place, and more will be as is useful.
c. We plan to do a systematic study of the approach to stochasticity being observed in the non-linear sawtooth test problems. Tools available include separately studying the effects of aspect ratio, non-circularity, and profile modification on mode growth and coupling.

4. How will you go about reaching closure on the non-linear sawtooth test problem?

a. We will continue our process of periodically meeting, comparing results in detail, and discussing the details of what needs to be done differently, and doing it.
b. This has the support of the Senior PIs, and it will lead to a publication with several of the junior members as lead authors.