GPSC's answers to PSACI PAC

1). Most important scientific findings by GPSC: enabled by MPP

a. The need for global simulation for turbulence transport

- Importance of velocity space nonlinearity is related to the size of a plasma
- Nonlocal effects and shaping: finite orbit effects in neoclassical transport, and turbulence spreading in the radial direction and energy cascade to low (m,n) modes in anomalous transport are important

c. Discrete particle noise does not affect nonlinear simulations of turbulence.

d. Resetting scheme resolves the issue of growing weights for delta f scheme.

e. Validation against the experimental results is the first step toward predictive capability and we need

- Multi species ions - need new solver
- Toroidal and poloidal rotations
- Electromagnetic effects

2). Contributions to GPSC by CSET, SAPP and others

a. Optimization and parallelization: PPPL (Ethier), PERI

b. Multiple domain decomposition: PPPL (Ethier), Adams (TOPS)

c. Solver: Adams (TOPS), Nishimura (UCI)

d. Visualization: IUV (Ma), ORNL (Klasky)

3). Maximum number of processors used to obtain scientific results
ETG simulation using GTC by Lin: 40 billion particles with 6400 cores (XT3 at ORNL)

4). e-i collisions for TEM -- we are ready

5) GPSC's path to petascale computing

- Burning plasmas: electromagnetic (Alfven) physics for ITER-size high-temperature plasmas

- For a simulation with 1 trillion particles on a 10,000x10,000x100 grid (100 particles/cell) for ITER-type plasmas with a grid size of the order of the electron skin depth, we need a 1 PF/s Jaguar at ORNLwith 50,000 XT3 quad-core processors, assuming half the memory for storing particle data and the other half for grid data.

- The solver will have 10^8 elements per plane and we need help from TOPS.

- 2D particle decomposition is in place, and 2D grid decomposition is in progress.

- The necessary algorithms are now under development for multiscale global simulations, including heating, turbulence and MHD.

- We have already carried out production runs on IBM BlueGene/L at T. J. Watson Center using 32,768 processors (peak performance is rated as 90 TeraFlop/sec).

- GTC has been selected for Joule applications at ORNL - a front runner for 250TF/1PF campaign, and we need help from math/computer SciDAC institutions.

5). Deliverable that has not been able to carry out in GTS -- electromagnetic effects for gyrokinetic PIC

- Fluctuation Dissipation Theorem indicates thermal fluctuations don't reside in shear-Alfven waves for a finite-β plasma. First time in PIC simulation history

- Split-weight scheme has been devised to solve this problem [Lee et al., PoP 2001]:

$$F = F_o + \delta f \rightarrow \delta f = \psi F_o + \delta h$$

- However, in the presence of inhomogeneity, we need the double split-weight scheme [Startsev, Lee and Wang, Sherwood 07]

$$F_e = (1+\psi)F_{0e} + F_{0e}\int dx_{||}\boldsymbol{\kappa}_e \cdot (\nabla A_{||} \times \hat{\mathbf{b}}_0) + \delta g_e \qquad F_i = F_{0i} + F_{0i}\int dx_{||}\boldsymbol{\kappa}_i \cdot (\nabla A_{||} \times \hat{\mathbf{b}}_0) + \delta g_i$$