Center for Gyrokinetic Particle Simulation of Turbulent Transport in Burning Plasmas

[http://w3.pppl.gov/theory/GPSC.html

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For the past year, the Center has carried out activities in areas of code development, code validation and physics investigations, and other critical code issues related to the core turbulence simulations. The goal of is to develop the capabilities with increasing fidelity for simulating the present-day tokamak experiments, such as NSTX as well as the ITER-scale burning plasmas in the future. The main activities have been centered around two basic versions of global gyrokinetic Particle-in-Cell codes, i.e., GTC-S (a.k.a GTS) for shaped plasmas and GTC for circular plasmas, as well as the wedge code, GEM for shaped plasmas. A companion code, GTC-Neo, has also been used for studying neoclassical transport.

1) Code Development: The activities for the past year include the implementation of the interface for GTS and GEM, both with general geometry capability, by directly using experimental plasma profiles through TRANSP and the MHD equilibria via JSOLVER and ESC. Electron dynamics has also been implemented in GTS (using the split-weight scheme) and GTC (using the hybrid scheme) for studying ITG/TEM modes. The fluid electron version in GTC has also been developed for comparison studies with low-n MHD modes. Furthermore, GEM now has finite-beta physics based on the Miller equilibrium with multi-ion species. With its interface with TRANSP and JSOLVER, it is also ready for validation work. The interface of GTC-Neo with the actual experimental data has also been completed.

2) Code Validation and Physics Investigations: One of the main activities of the Center for the past year has been the use of GTC-Neo and GTS for long time steady state simulations and comparisons of their results with the actual NSTX discharges. Good agreement has been obtained. For example, it is found that the steady state neoclassical ion thermal diffusivities calculated by GTC-Neo are much closer to the experimental data than those obtained by NCLASS, a commonly used code in the fusion community. The difference lies in the fact that GTC-Neo takes into account the finite orbit physics and, consequently, the non-local effects. Furthermore, we have found that, when ITG turbulence is present in the discharge, it tends to be dominant in the outer region of the NSTX plasma, whereas neoclassical transport tends to dominate in the inner region. Non-local features of the ITG turbulence have also been observed in these simulations in terms of turbulence spreading in the radial direction, as well as energy cascade from the high (local) poloidal and toroidal modes to the lower (global) ones. The significance of these simulations is that the mesoscale physics associated with microturbulence may actually be global in nature. The comparisons between GTS and GEM should be a priority in the near future to resolve this critical issue. In addition, recent validation studies using GEM have shown some qualitative agreements with the NSTX experimental data in the outer region of the discharges. In the area of physics investigations of ion temperature gradient (ITG) drift instabilities using GTC with adiabatic electrons, we have found that the velocity-space nonlinearity related to the parallel acceleration of the particles, which provides the necessary damping for the nonlinearly generated (m=0, n=0) zonal flows in the steady state stage of the turbulence, is important for large size tokamaks, e.g., a (minor radius) / ρ_i (ion gyroradius) > 400. The effects of nonadiabatic electrons on the ITG turbulence using GTC based on the split-weight scheme have also been found to enhance the ion thermal diffusivity and the zonal flow components have been observed to have a shorter wavelength. However, the corresponding electron thermal transport is small. These observations have been confirmed by another version of GTC based on the hybrid scheme as well as the GEM code using the split-weight scheme. In the area of collisionless trapped electron modes (CTEM) using GTC with the hybrid scheme, it is found that these modes, which are small scale in nature, can drive significant electron thermal transport in regions such as the internal transport barrier (ITB), where ion thermal transport is small. These modes have also been studied using the GEM code with the split-weight scheme. It is found that the suppression effect of zonal flows on the nonlinear CTEM transport is dependent on both electron temperature gradient and the electron to ion temperature ratio, which explains the previous contradictory conclusions. A linearized electromagnetic version of GTC in global geometry using the fluid electrons has successfully reproduced toroidal Alfven waves and demonstrated the finite-beta effects on ITG modes. In the theoretical front, a new momentum pinch mechanism, arising from the magnetic curvature when the ExB shear effects are small, has been investigated and the numerical verification campaign is underway.

3) Particle Noise and Growing Weights: With our recent articles in the journal Physics of Plasmas (PoP) dealing with the effects of discrete particle noise on turbulent transport, we believe that we have finally answered the question of "numerical pollution" of PIC simulations. Since the issue was first raised by Nevins et al. in a paper that appeared in PoP in 2005 using an analysis which didn't properly take into account the self-consistent plasma response, we have remedied this problem by carrying out a calculation based on the extension of the Fluctuation-Dissipation Theorem (FDT) to a nonlinearly saturated system and shown that intrinsic particle noise is orders of magnitude lower than the drift wave signal when the normal simulation parameters are used. Moreover, the problem of discrete particle noise has been studied based on the direct fluctuation measurements from gyrokinetic particle-in-cell simulations of stable plasmas. These measured values are in good agreement with the theoretical predictions based on the quasilinear analysis. One can then conclude that the noise-driven transport, which depends linearly on the entropy of the system, is negligibly small for the realistic turbulence simulations. The physics associated with the growing weights in δf simulations has been studied using the particle-continuum method. It is found that, by periodically coarse-graining the particle weights on a phase-space mesh, one can actually prevent the growing weights for the particles. However, numerically enhanced flux can result when a velocity space grid used in this process is not fine enough.

4) Code Optimization, Applied Mathematics and Computer Sciences: The version of GTC with adiabatic electrons has also been ported to various MPP platforms including the Cray X1E (Phoenix) and XT3 (Jaguar) at ORNL, and the IBM BG/L at Watson with excellent scalability. For example, it has achieved the performance of 20 teraflops/sec on 22,976 processors on Jaguar using 74 billion particles. Recently, our GTS code has been chosen as one of the three DoE codes (the only one from fusion) to be a part of the Joule Applications – a software effectiveness exercise for OMB. GTS has also been designated as one of the six early applications on the 250 TeraFlop Cray at ORNL. In preparation for these exercises, we have ported GTS to Jaguar (XT3) at ORNL and implemented the two-level parallel scheme that makes the code highly scalable in terms of the particles. Presently, scientists from the Performance Engineering Research Institute are helping us to optimize the code. In order to carry out ITER-size simulations in the future, we have also implemented a 2D grid domain decomposition in GTC and will eventually move this capability to GTS in and make the code fully parallelized. In the solver area, we have developed the interface between the gyrokinetic Poisson's equation in the original integral form and PETSc. We have also worked on high performance I/O, and data streaming/sharing mechanisms, and have shown that we can stream data from NERSC/ORNL to remote locations. Finally, our team has created world-class visualizations, which have led to new physics insights from these simulations.

5). Publications, invited talks and others: GPSC has over thirty journal publications for the past year, one invited talk at the SciDAC 2006 Conference and two invited talks at the 2007 IAEA Fusion Conference. Our work was also featured in the SciDAC Review Vol. 1 (2006) and a 3D visualization of a twisted mesh structure used in the GTS simulations was featured on the cover of the Battelle Annual Report – 2006.