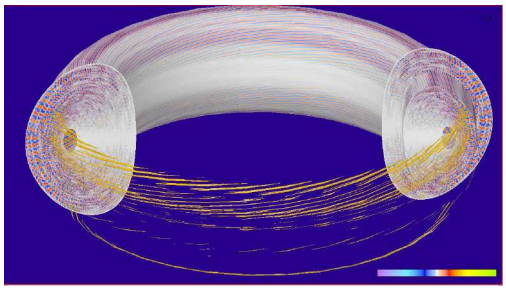

Center for Gyrokinetic Particle Simulation of Turbulent Transport in Burning Plasmas

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The goal of this newly formed Center is to study turbulent transport in toroidal plasmas and to develop the capabilities for simulating ITER-scale burning plasma experiments on massively parallel computers. Ultimately, our aim is to be able to effectively carry out multi-scale integrated simulations (both in time and in space) of fusion plasmas using the gyrokinetic particle approach. The first year activities are as follows:

1) Physics: based on GTC (a global code) and GEM (a wedge code).

Investigations of the electron temperature gradient (ETG) microinstabilities using our GTC code have led to the physics findings that (i) the toroidal mode coupling to longer wavelength modes is responsible for low-level nonlinear saturation of these instabilities; and (ii) the associated steady-state electron thermal diffusivity is much smaller than previously believed. The effects of nonlinear parallel acceleration on the collisionless ion temperature gradient (ITG) turbulence have also been studied, and it is found that the resulting thermal diffusivity settles into the steady state at a lower level and at a much faster rate when this additional nonlinear channel is introduced.

Electron dynamics and finite plasma pressure (finite-β) effects in GTC have been incorporated using split-weight/hybrid schemes and associated benchmarking exercises are currently in progress with GEM. General geometry capabilities in GTC for shaped plasmas by directly using experimental plasma profiles and the corresponding numerical equilibria have been developed (see the figure above). Progress has been made in advancing the physics understanding of turbulence spreading, core-edge coupling, energy cascade (to longer wavelength modes), global scale zonal flow formation and steady state transport in the presence of nonlinear parallel acceleration in DIIID-type plasmas.

GTC-Neo, a subset of GTC aimed at simulating neoclassical transport, has now been applied to realistic L-mode and H-mode cases for the NSTX spherical torus experiments. The calculated ion heat flux and radial electric field from GTC-Neo are now routinely compared to experiments. GEM has been used to study the effects of elongation and Shafranov shift on microturbulence and the effects on equilibrium shear flows. Code verification/comparison studies are in progress between GEM and other microturbulence codes such as GYRO (General Atomics) and GS2 (Maryland). For low-β circular equilibria with fully kinetic electrons, our GEM code is found to benchmark well with GYRO in terms of ion and electron energy flux. GEM has also been used for investigating collisionless and semi-collisional tearing modes for a successful Ph.D. thesis.

2) Applied Mathematics:

We have completed the finite-element interface between GTC and the DoE software

tool-kits, PETSc, HYPRE, Prometheus and SuperLU, for solving the field equations on MPP platforms. This is a crucial step for us in order to incorporate more realistic physics modules in GTC by solving the associated Poisson and Helmholtz problems. This work is the result of close collaborations with the Terascale Optimal PDE Simulations (TOPS) of the Integrated Software Infrastructure Centers (ISICs). It will also prepare us for simulating ITER-type of plasmas by solving a system of equations with up to 10 million unknowns.

3) Computer Sciences:

The GTC code, running mostly on Seaborg, the 6080-processor IBM SP P3 at NERSC for productions, has also been ported and benchmarked on a large number of platforms, including the Earth Simulator, the CRAY X1, and the IBM Blue Gene/L. In order to increase the concurrency of GTC, a new MPI-based particle decomposition was implemented in the code. The code was also vectorized and optimized for the new parallel-vector architectures. GTC fulfilled the very strict performance and scaling requirements of the Earth Simulator supercomputer (Japan) and achieved an unprecedented 3.7 Teraflops sustained on 2,048 processors. Some of the other platforms in the study were Phoenix at ORNL, Ram at ORNL, Thunder at LLNL, and a number of others. These exercises demonstrate the portability and scalability of PIC-based codes such as GTC on modern MPP architectures.

Building on an Object-Oriented version of GTC in Fortran90, an effort has been initiated to facilitate future team programming. The strategy is to provide an upper layer, which sits on top of GTC. The upper layer consists of classes (derived types and methods), which call the original GTC code under the hood. The derived types point to the original GTC data and the methods call the original GTC subroutines. The original GTC code is modified only very slightly. The end result will be a set of classes, which provide a stable interface to future modifications and isolates the various components from one another.

In the data management area, we have collaborated with the Scientific Data Management (SDM) ISIC and have successfully streamed data recently from NERSC/ORNL to PPPL. Our techniques now have a fail-safe mechanism and can stream data from a variety of platforms, such as Linux-X86, IBM SP, Cray-X1, and SGI Altix, to our cluster. Using the logistic networks (U. Tennessee) to store netcdf and hdf5 files allows us a very scalable/flexible way to share data among the SciDAC GPS Center collaborators. In conjunction with UC-Davis, we are developing a hardware accelerated volume visualization method, which will allow us to visualize GTC 3D data in real-time.

4) Collaborations:

The collaborations between members of our Center have been very active. For example, we have had a Center-wide meeting at the most recent APS/DPP conference in Savannah, GA last November and a dedicated Workshop on Plasma Turbulence at UC-Irvine last February with over fifty attendees including a dozen students from the U. S. and abroad. We have also had at least 10 video-conferences and 4 exchange visits.

5) Invited talks and Publications:

Prominent presentations include an invited talk given at the 2004 IAEA conference in Vilamoura, Portugal, two invited talks given at the 2004 APS/DPP Conference in Savannah, GA, and an invited talk presented at the 2004 IEEE ICOPS Meeting. Four more invited presentations were given at the 2005 SciDAC Conference in San Francisco, CA in June. Recent publications include a paper on ETG in Physics of Plasmas (PoP), two papers published in the supercomputing journals, and one in a visualization journal. In addition, a paper on edge-core coupling was recently submitted to PoP, two more to the Journal of Computational Physics (JCP) and one to Computer Physics Communications (CPC).

In summary, it has been a very productive year for us. However, our allocation at NERSC is smaller than requested and we need help to secure more computing cycles