Center for Gyrokinetic Particle Simulation of Turbulent Transport in Burning Plasmas -W.W. Lee

(1) Progress toward achieving Center's scientific targets with respect to clear deliverables;

• Physics: Studying ITG and ETG turbulence using GTC and introducing electron dynamics and implementing general geometry capabilities in GTC and GEM for shaped plasmas with the goal of simulating ITER plasmas.

• Mathematics: completing the finite-element interface between GTC and PETSc, HYPRE and Prometheus for solving elliptic-type equations on MPP platforms efficiently.

• Computer Sciences: modularizing, parallelizing and optimizing GTC for both cache-based and vector-parallel computers as well as interfacing with modern data management techniques (networking, storage, and processing) and 3D interactive visualization software. Team programming is also one of our main objectives.

(2) How super-computing/tera-scale computing resources have enabled the achievement of the targeted scientific goals in the timeliest manner;

• GTC has shown to be very efficient and scalable on Seaborg at NERSC, Cray X1 and Cheetah at ORNL, and the Earth Simulator in Japan. We've also ported GTC to Thunder at LLNL and BlueGene at Argonne.

• On the Earth Simulator, GTC recently achieved 3.7 Teraflop with 2048 processors using 6 billion particles with 25% single processor efficiency, which is about 10 times faster than the same run on Seaborg at NERSC.

• Allocated resources at NERSC has been used to study both ITG and ETG turbulence and the results were reported at the APS/DPP conference as invited talks. Researches on ITG with adiabatic electrons and in general geometry have been reported in Sherwood meeting.

(3) What role have collaborative interactions within each project and also with other SciDAC activities played;

• The collaboration between members of our Center has been very active: 1) a Center-wide meeting at the last APS/DPP conference at Savannah, GA last November and 2) a Workshop on Plasma Turbulence at UC-Irvine last February with over fifty attendants. We have also had at least 10 video-conferences and 4 exchange visits between the members.

• Some members of our Center will be involved with the "Center for Plasma Edge Simulation" (C. S. Chang, PI) for an integrated fusion simulation of the edge/boundary region under the sponsorship of SciDAC, OFES and OASCR.

• Collaborations with the TOPS (Terascale Optimal PDE Simulations) ISIC (PI: David Keyes, Columbia) for using PETSc (a key TOPS solver technology) and its interface with our GTC code. The SDM (Scientific Data Management) ISIC (PI: Ari Shoshani, LBNL) has also interacted with us on the issues of managing the GTC data. In addition, our visualization effort is greatly enhanced by the close contact with our SAPP collaborator, K. L. Ma at UC-Davis.

• As we march into more realistic simulations of fusion plasmas in the future, the requirements for the code become more demanding and we need more help from our ISIC's and SAPP's partners.

(4) What is the vision/scientific road-map for future research -- with special emphasis on how this could be influenced by the growth of the SciDAC Program.

• The growth of the SciDAC program, especially in terms of computing resources, will enable us to carry out realistic simulations of burning plasmas in ITER plasmas with sufficient spatial resolution and time duration.

• The code integration of core-edge capability from GPSC and the PESC will be challenging. This type of integration is the future for the fusion research and its feasibility depends on the availability of the terascale/petacale capabilities.

• As the SciDAC program broadens its scope, we plan to tackle the spatio-temporal integration in simulating fusion plasmas using gyrokinetic particle codes . A proposal related to this subject entitled "Multiscale Gyrokinetic Particle Simulation of Magnetized Plasmas" (W. W. Lee, PI) has already been submitted to OASCR for the Multiscale Mathematics and Education project. The proposal calls for the development of a set of multiresolution methods to resolve multiple spatio-temporal scales within a single mathematical model by adjusting resolution and scope as a function of space, time and data. It is aimed at simulating the high-frequency short-wavelength wave-heating physics, the mesoscale physics of microturbulence, and the large-scale low-frequency MHD physics for tokamak plasmas - all based on the particle simulation methodology and, preferably, in one code.

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(5) What are the major impediments for progress at present?

• Lack of computational resources - 2.4 million processor-hour for FY05 on Seaborg at NERSC.
• Need help to obtain machine time on Cheetah at ORNL
• Need more computational physicists for developing codes, running codes and extracting physics from the codes
• Need goodwill among colleagues

(6) Data analysis - GTC's own diagnostics, GKV, visualization

• Plans for the coming year- data format, data storage and post processing capabilities
• Needs theoretical and experimental input

(7) Ideal computational infrastructure -

• size, time, resource, architecture (high bandwidth and low latency -AMD Opteron),
• video game programming strategy to achieve 70% single processor efficiency.
• ITER-size plasma on Seaborg: 72 wallclock hours 1 billion particles on 1024 processors for 7000 timesteps for 1 μsec discharge.
• concept of steady state transport is important to achieve transport time scale simulation.

(8) Physics issues: low noise, growing weight, smoothing, nonlinear velocity space effects, turbulence spreading

- Phase space smoothing to reduce filamentation noise (Denavit JCP '72. Parker et al. '05) -- letting particles forgetting the past
- Velocity space nonlinearity is important also for energy conservation. Need theoretical understanding for the increase in zonal flow level also input for diagnostics.
- Turbulence spreading has been observed with and without zonal flow. Need theoretical support, diagnostics and etc.
- So-called growing weight problem:

Entropy Production - ITG modes

- δf-formulation: $F_i = F_{0i} + \delta f_i$, ν is the collison freqeuncy, and Q_{ix} is the radial ion enrgy flux

$$\frac{\partial}{\partial t}\langle \int \frac{\delta f_i^2}{F_{0i}} dv_\parallel + \tau\phi^2 + \tau|\nabla_\perp\phi|^2\rangle + \langle \tau\frac{\partial\phi}{\partial x_\parallel}\int v_\parallel \frac{\delta f_i^2}{F_{0i}} dv_\parallel + 2\tau\nu\int\frac{dv_\parallel}{F_{0i}}\left(\frac{\partial\delta f_i}{\partial(v_\parallel/v_{ti})} + \frac{v_\parallel}{v_{ti}}\delta f_i\right)^2\rangle = \kappa_{Ti}\langle Q_{ix}\rangle$$

$$\tau \equiv T_e/T_i, \quad \kappa_{Ti} \equiv -dlnT_{0i}/dx, \quad \langle\ldots\rangle \equiv \frac{1}{V}\int d\mathbf{x},$$

- Let $w \equiv \delta f_i/F_{0i}$, $E_\parallel \equiv -\partial\phi/\partial x_\parallel$, $\partial\delta f_i/\partial(v_\parallel/v_{ti}) \approx -\beta\delta f_i$, $\beta \ll 1$, N is the particle number,

$$\frac{\partial}{\partial t}\sum_{j=1}^{N}\frac{w_j^2}{1-w_j} + \tau\frac{\partial}{\partial t}\langle\phi^2 + |\nabla_\perp\phi|^2\rangle + \sum_{j=1}^{N}\left[-\tau E_{\parallel j}v_{\parallel j} + 2\nu\tau(1-\beta)^2(\frac{v_{\parallel j}}{v_{ti}})^2\right]\frac{w_j^2}{1-w_j} = \kappa_{Ti}\langle Q_{ix}\rangle$$

- Energy balance:

$$\sum_{j=1}^{N} E_{\parallel j}v_{\parallel j}w_j = \frac{1}{2}\frac{\partial}{\partial t}\sum_{j=1}^{N} v_{\parallel j}^2 w_j \approx \frac{1}{2}\frac{\partial}{\partial t}\sum_{j=1}^{N}\alpha v_{ti}^2 w_j, \quad \alpha \approx 1$$

- In the steady state $(\partial/\partial t\langle\phi^2 + |\nabla\phi|^2\rangle = 0)$, with $w \ll 1$:

$$\frac{\partial}{\partial t}\sum_{j=1}^{N}(1-\frac{\alpha}{4})w_j^2 + 2\nu\tau(1-\beta^2)\alpha\sum_{j=1}^{N} w_j^2 = \kappa_{Ti}\langle Q_{ix}\rangle$$

Velocity-Space nonlinearity reduces ion energy flux, but collisons enhance it.

PPPL PRINCETON PLASMA