Long Time Simulations of Microturbulence in Fusion Plasmas*

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Abstract. Recent long time microturbulence simulations of fusion plasmas using gyrokinetic particle codes on massively parallel computers with billions of particles have contributed to fundamental physics understanding, but have also attracted concern about the numerical convergence issue, i.e., whether these codes suffer from discrete particle noise due to the use of a large, but finite, number of particles. Here, we will show, both numerically and analytically, that numerical noise is not a cause for concern in long time simulations.

1. Introduction

Remarkable success has been achieved in the area of kinetic simulations of turbulence transport in tokamaks using massively parallel computers with gyrokinetic particle codes [1]. For example, the δf global toroidal gyrokinetic particle simulation code (GTC) [2] has recently been used for studying the long time behavior of microturbulence for fusion plasmas and the underlying transport physics [3, 4]. Since GTC has exhibited excellent scaling with thousands of processors and with a relatively high single processor efficiency on prominent supercomputers such as Seaborg (IBM SP3) at NERSC, Phoenix (Cray X1E) and Jaguar (Cray XT3) at ORNL, the BlueGene/L at IBM-Watson, the Earth Simulator in Japan, and many others [5], as shown in Fig. 1, we are able to utilize these resources to study the turbulence and transport physics in tokamaks with tens of billions of particles. The latest results give the peak performance of GTC at around 8.5 TeraFlops/Sec on some of the world's fastest machines. This type of capability is essential if one wants to make meaningful comparisons between the simulation observations and the actual experimental measurements as well as to use the simulation as a predictive tool. Recently, improvements in terms of the physics fidelity in GTC [6–8] have made us a step closer to these goals by enabling us to tackle problems associated with the realistic tokamak discharges, such as those in D3D
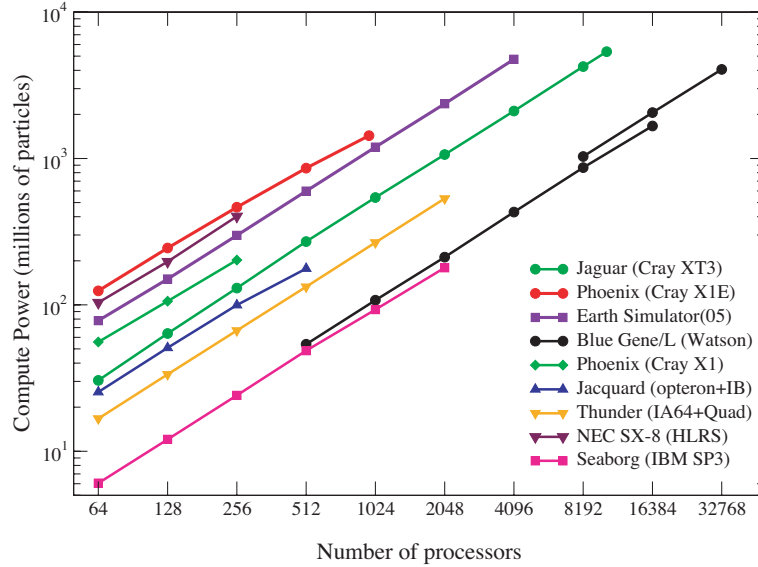
FIG. 1: *GTC performance on various MPP platforms expressed in terms of the number of particles (in millions) that one can push in one second in a time step.*

and NSTX. In addition, our GEM code, with the kinetic electron dynamics and electromagnetic perturbation capabilities based on the general toroidal equilibrium magnetic field configurations is also ready [9, 10]. Our ultimate goal is to simulate ITER plasmas using these codes on the DoE's leadership computing facilities. However, we are also compelled by the recent controversy in the fusion community to answer one important question, i.e., what about the discrete particle noise? In the present paper, we will show, by using the full power of modern computational resources and a new analytical approach, that discrete particle noise can easily be detected and minimized in gyrokinetic particle codes, and it should not be a concern.

Before we proceed, let us discuss our recent studies involving the often-neglected velocity space nonlinearity associated with the parallel acceleration of the particles. In global GTC simulations, it has shown a significant influence on the production of zonal flows and the temporal evolution of the ITG turbulence [3]. Specifically, the results with the inclusion of this additional nonlinear channel in the simulation exhibits a much faster evolution towards the steady state accompanied by a somewhat lower ion thermal diffusivity, χ_i, when compared against those where only the usual ExB nonlinearity is kept and this difference in χ_i increases with the simulation volume. This type of collisionless dissipation appears to affect the steady state transport differently than the collisional dissipation, which has been observed to increase the transport through the interplay between collisions and the zonal flows [11]. On the other hand, recent study on this subject using

the flux-tube version of GEM has found that this nonlinearity has no effect on the steady state ion thermal diffusivity, χ_i [12]. A possible explanation may come from our recent study showing that the velocity space nonlinearity has negligible effect on the steady state χ_i when the zonal flows are turned off. Namely, the velocity space nonlinearity is closely related to the zonal flow physics. Since the zonal flow patterns are more global in GTC than those in the flux-tube GEM, it may explain the difference between the two codes. More studies are needed.

Let us now turn to the noise issue. The long time simulations of microturbulence using gyrokinetic PIC codes for studying electron temperature gradient (ETG) drift instabilities [13] has lately been called into question with the claim that the discrete particle noise can dominate plasma transport at the late times in these simulations [14]. It also mentioned the possibility of noise pollution in the ITG simulations using GTC. To clarify the ITG noise issue, we have carried out systematic convergence studies with GTC to address the long time behavior of the ITG microturbulence by using unprecedented large number of particles per cell (from 10 to 800) on the leadership class supercomputer, the Cray X1E and XT3 at ORNL, and the IBM SP3 at NERSC. The high-resolution runs from these studies clearly indicate that the resulting χ_i's remain low and numerical noise plays a very insignificant role in the observed steady state thermal transport. The discrete particle noise, if it exists, tends to enhance the steady state flux rather than to suppress it as claimed by the paper [14]. In addition, results from investigations of the influence of non-adiabatic electrons [7] and of shaped-cross-section geometry [6] on global ITG simulations have confirmed this trend. In the area of ETG simulation, we have carried out gyrokinetic particle simulations using the flux-tube version of GEM. (A separate paper on ETG using GTC will be reported in this conference [4].) The suppression of turbulence due to zonal flows have been observed giving rise to low levels of electron thermal diffusivity, χ_e. These conclusions are also based on convergence studies by using particle numbers ranging from 10 to 512 per cell. To further understand the noise issue, we have used the Fluctuation-Dissipation Theorem for a nonlinearly saturated system arising from drift instabilities [17]. Based on this first principles approach using a system which deviates minimally from a Maxwellian and contains only damped and marginal stable modes, we have calculated the level for the discrete particle noise and found that the noise resides mostly in the high frequency modes and the the level of noise in the low drift frequency modes is orders of magnitude smaller than the nonlinear saturation level. These findings have also been verified numerically. It is therefore most informative if the discussions on particle noise can go hand in hand with the knowledge of nonlinear saturation. Unfortunately, that was not the case for the recent

paper on ETG noise [14], since the question of nonlinear saturation was not addressed, nor were adequate convergence studies on the ETG modes in terms of particle number scans performed.

2. ITG convergence studies

For the convergence studies on ITG, simulations using the GTC code [2] have been carried out with the usual adiabatic electron approximation. This global toroidal code uses field-line-aligned magnetic coordinates for a plasma with circular cross section. Particle pushing and field solve are carried out in the configuration space. There are 64 toroidal grid with $a/\rho_i = 125$ on each poloidal plane. The code uses an unstructured grid of the size ρ_s, i.e., the ion thermal radius measured with the electron temperature. Thus, the shortest wavelength modes that can be resolved in the code is $k_\perp \rho_s \approx 1$. The numbers of particles per cell used in the simulation are 10, 100, 400 and 800. The relevant (Cyclone-based) parameters are: $R/L_T = 6.9$, $R/a = 2.79$, $L_n/L_{Ti} = 3.13$, $\Omega_i \Delta t = 15$ and $T_e/T_i = 1$. The radial profile of the inhomogeneity is given by $(1/L)e^{-[(r-r_c)/r_w]^6}$, where L represents either the temperaure scale length L_{Ti} or the density scale length L_n with $r_c/a = 0.5$ and $r_w/a = 0.35$.

The simulation results are shown in Fig. 2, where all the runs are with the parallel velocity space nonlinearity and the nonlinear $\mathbf{E} \times \mathbf{B}$ generated zonal flows. Here, (a) the ion thermal diffusivity is measured in the GyroBohm unit of $c_s \rho_s^2/a$, (b) the rate of change of particle weights gives us another way to obtain χ_i which we will explain later, (c) the field energy is measured in terms of $e\phi/T_e$, and (d) the zonal flow amplitude is in term of v_{ExB}/c_s. As we can see, all the runs are well converged asides from the 10 particle per cell case. For this case, the signature of discrete particle noise is apparent, i.e., the steady state flux is higher than the converged value and the field energy is also higher. The fact that the zonal flow amplitude is lower with less particles is very interesting. It should be noted that the high frequency numerical noise associated with the case with 10 particle per cell is evident in Fig. 2(a) and its amplitude can be estimated by $\sqrt{\langle w_j^2 \rangle / N}$ [15], where N is the total number of simulation particles. We will discuss this later.

Let us remark briefly here that the time derivatives of the spatial averaged weight square $\langle w^2 \rangle$, as shown in Fig 2(a), is related to the entropy production as first pointed out in Ref. [16], where $w(\equiv \delta f/F)$ is the weight associated with the δf scheme and F is the usual total particle distribution. With the presence of the velocity space nonlinearity, it can be written as $\frac{\partial}{\partial t} \sum_{j=1}^{N} (1 - \alpha/4)w_j^2 = \kappa_{Ti}\langle Q_{ir} \rangle$, where $\alpha \approx 1$ is related to the velocity space nonlinearity and κ_{Ti} denotes ion temperature inhomogeneity and $\langle Q_{ir} \rangle \equiv \frac{1}{N} \sum_{j=1}^{N} w_j v_j^2 \mathbf{v}_{ExB} \cdot \hat{\mathbf{r}}$ is the ion thermal flux and $\chi_i = \langle Q_{ir} \rangle / (\kappa_{Ti} + \kappa_n)$. As we can see, the average weight of the particle is around 0.3
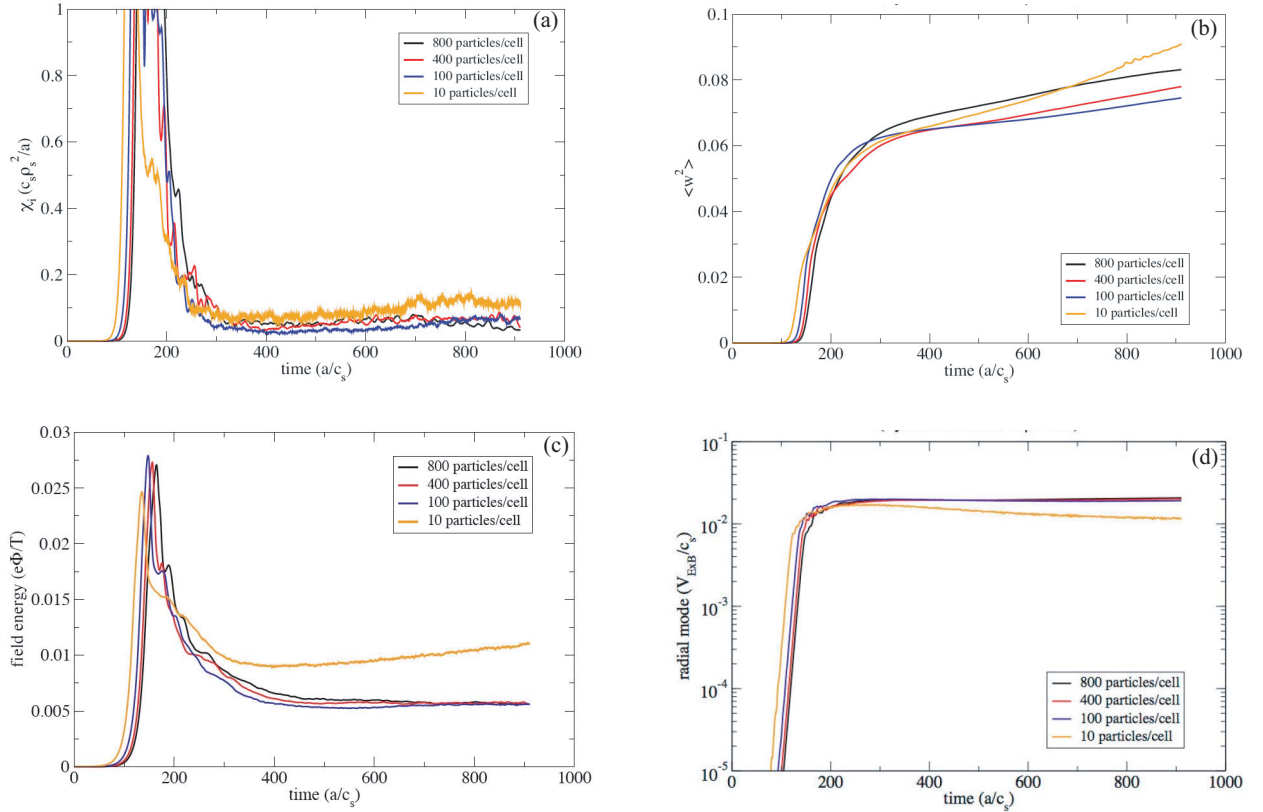
FIG. 2: *Particle number convergence studies for the ITG simulations: time evolution for (a) ion thermal diffusivity, (b) particle weights, (c) field energy, and (d) zonal flow amplitude for cases with 10 (yellow), 100 (blue), 400 (orange), and 800 (black) particles per cell.*

at the end of the run. The enhanced fluctuation of $\Phi(n = 0, m = 1)$ mode has also been also observed and the detail will be reported elsewhere. We believe these high resolution particle simulations of ITG modes have given us the concrete proof that discrete particle noise can easily be minimized through the use of the state-of-art supercomputers.

3. ETG convergence studies

The noise issue started with the ETG simulation [14]. Here, we will present some of our latest ETG simulations using the flux-tube version of GEM [18]. Again, a very large number of particles has been used to carry out the convergence studies. The code pushes electrons only by assuming that the ion response is adiabatic. The parameters are also the so-called "Cyclone base case." Except for $R/L_T = 5.3$, they are: $q = 4$, $\hat{s} = 0.8$, $R/L_n = 2.2$, $T_e = T_i$, $r/R = 0.18$, $\Delta t = 0.1 v_{te}/L_T$, $\Delta x = \Delta y = 2\rho_e$, $L_x = 256\rho_e$, $L_y = 128\rho_e$, and the grid is $128 \times 64 \times 32$. The reduction of the drive for 30% from the original $R/L_T = 6.9$ for the present case is because of
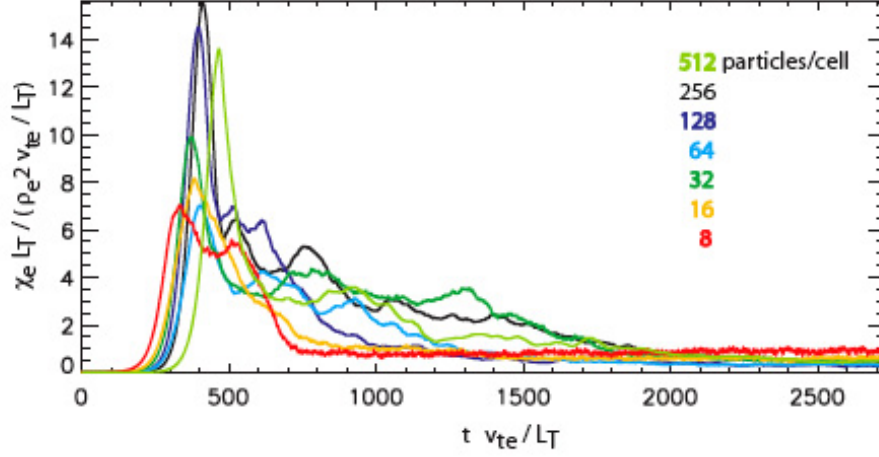
FIG. 3: Convergence studies of ETG modes using GEM.

the box size non-convergence issue for the stronger drive. As shown in Fig. 3, converged results in terms of particle scan with 8, 16, 32, 64, 128, 256, and 512 particles per cell have indeed been obtained. Again, the high frequency noise associated the case with 8 particles per cell is more noticeable, resulting in a slightly higher steady state χ_e.

4. Generalized fluctuation-dissipation theorem

To understand the issue of discrete particle noise, we have also resorted to re-visit the well-known Fluctuation-Dissipation Theorem (FDT). Following Kadomtsev [19], we have also applied FDT to a nonlinearly saturated system. The arguments for using FDT, which is based on a system in thermal equilibrium, for a nonequilibrium state are: 1) the nonlinearly saturated system has only damped and marginally stable modes since the saturation is caused by the $\mathbf{E} \times \mathbf{B}$ trapping of the resonant particles for our case, and 2) the deviation of the distribution in the nonlinear state from the initial distribution is negligibly small, i.e., $|\langle \delta f \rangle| \ll |F_0|$, where F_0 is the initial Maxwellain distribution and $\langle \delta f \rangle (\equiv \sum_{j=1}^{N} w_j / N)$ is the spatially averaged deviation of the distribution. Under these assumptions, the latest study has shown that fluctuation properties remain the same as those for the quiescent plasmas [17]. Specifically, the levels for the discrete particle noise for the high-frequency (HF) ω_H mode [20] and the low frequency (LF) ion acoustic (or drift) mode remain as $|e\Phi|/T_e|^2_{HF-noise} = 1/N k_\perp^2 \rho_s^2$, $|e\Phi/T_e|^2_{LF-noise} = 1/N(1 + k_\perp^2 \rho_s^2)$, respectively, where the latter is related to the instability and N is the number of simulation particles in the wave. One the other hand, the nonlinear saturation (NL) level for the simulation system can be calculated [17] as $|\delta\Phi|^2_{NL} = \gamma_l/\Omega_i/2k_x k_y \rho_s^2$, where γ_L is the linear growth rate, $k_\perp^2 \equiv k_x^2 + k_y^2$ and Ω_i is the ion cyclotron frequency.
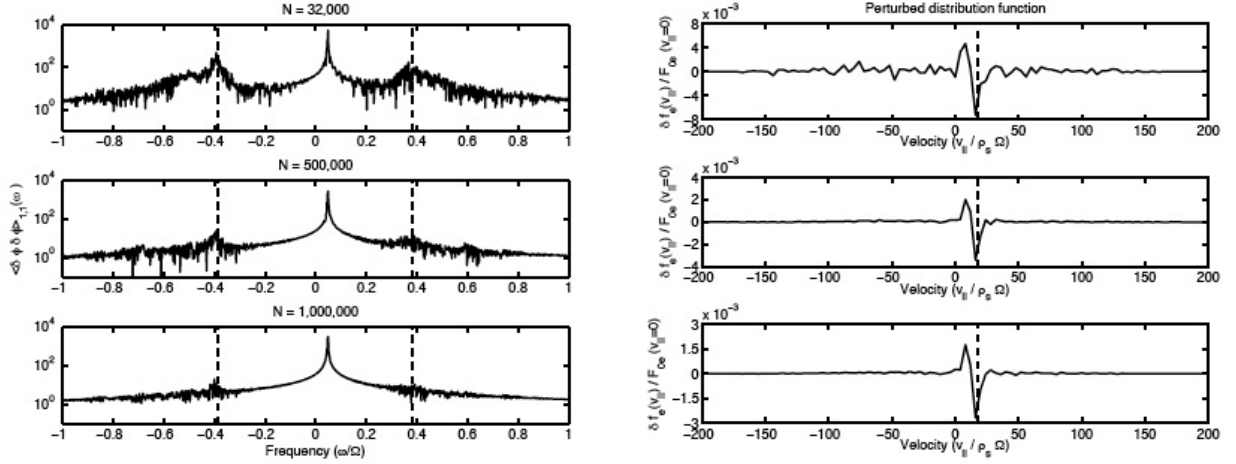
FIG. 4: *Particle scans for drift waves simulations in slab for the frequency spectra (left) and the background distribution change (right).*

To verify these predictions, we have carried out gyrokinetic particle simulation using a simple slab code with $L_x = 23\rho_s$. $L_y = 23\rho_s$, $L_z = 2300\rho_s$, $T_e/T_i = 1$, $m_i/m_e = 1837$, $\kappa_n\rho_s = 0.2$, $2k_xk_y\rho_s^2 = k_\perp^2\rho_s^2 = 0.149$ and $\gamma_L/\Omega_i = 0.003$. The total number of simulation particles are $N = 32,000, 500,000$ and $1,000,000$ for the three cases. As shown in Fig. 4, the high frequency noise decreases as N increases and the low frequency saturation amplitude is independent of N. Furthermore, the background change is negligibly small and its magnitude decreases for the larger N. For comparison, the theoretical saturation amplitude is about 2% (which is actually a factor of 2 lower than the simulation amplitude [17]), while the amplitude for the low frequency noise is about 0.003% for the most noisy case of $N = 32,000$. Thus, the signals at low frequencies are all from drift waves. These results are consistent with Kadomtsev's argument [19].

5. Conclusions

In this paper, we believe that we have presented enough evidence to alleviate the concern about the particle noise. We are now looking forward to using the improved GTC [6–8] and GEM. The latter has been recently extended to handle general toroidal equilibrium magnetic field configurations to enable realistic applications to actual experimental scenarios [21], for the simulation of ITER plasmas on the petascale leadership computing facilities provided by the U. S. DoE.

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