*33rd EPS Conference on Plasma Phys. Rome, 19 - 23 June 2006 ECA Vol.**30I**, O-3.004 (2006)*

Conservative gyrokinetic Vlasov simulation using Morinishi scheme

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1. Introduction

Long time micro-turbulence simulations with non-conservative effects such as heat and particle sources and particle collisions are desirable to address future issues, for example, the formation of transport barriers in advanced tokamaks. Compared with δf particle-in-cell (PIC) simulations, Vlasov simulations based on mesh approaches are more flexible in treating these non-conservative effects. In our previous work [1], a slab gyrokinetic Vlasov code was developed using the constrained-interpolation-profile (CIP) method, and it was successfully benchmarked against a gyrokinetic δf PIC code. However, the quality of the energy and particle number conservation in the Vlasov CIP code was almost the same level as the δf PIC code, and the breakdown of the conservation properties was still problematic in a long time simulation. To resolve this issue, we need a conservative Vlasov code that is numerically stable and robust in a long time simulation. Although a conventional finite volume method (FVM) conserves the guiding centre distribution function f, the scheme often becomes unstable. It was pointed out that such a numerical instability may be avoided by conserving the square quantity f^2, which bounds the amplitude of numerical oscillations [2]. In this work, we develop a conservative Gyrokinetic 5D Vlasov code (G5D) using Morinishi's Finite Difference operator (MFD) [3], which conserves both f and f^2. We discuss its numerical properties by comparing simulations with MFD and with FVM. We then show benchmarks of ion temperature gradient driven (ITG) turbulence simulations between the new Vlasov code and a conventional δf PIC code, and discuss the possibility of a long time micro-turbulence simulation. By taking the advantages of exact conservation properties in the new Vlasov code, we clarify roles of the $v_{||}$ nonlinearity. In the gyrokinetic simulation, the $v_{||}$ nonlinearity is often ignored as one of higher order effects. In Ref. [4], it was reported that in cylindrical simulations of ITG turbulence, neglecting the $v_{||}$ nonlinearity affects the error on the particle number conservation, leading to erroneous zonal flow structures and thereby potentially affecting the heat transport. However, in slab or cylindrical models, the $v_{||}$ nonlinearity itself does not violate the particle number conservation, and it is not clear whether the effect is numerical or physical. In the present study, we validate physical effects of the $v_{||}$ nonlinearity from the entropy balance relation, and then discuss its numerical effects on the Vlasov and PIC simulations.

2. Conservative Gyrokinetic 5D Vlasov code G5D

The physical model used in this study is kinetic ions and adiabatic electrons in a periodic slab configuration with a uniform magnetic field $\mathbf{B} = B_0 \nabla z$. The basic equations are the gyrokinetic Vlasov-Poisson system in the gyrocenter coordinates, $\mathbf{Z} = (t; \mathbf{R}, v_\parallel, v_\perp, \alpha)$,

$$\frac{Df}{Dt} \equiv \frac{\partial f}{\partial t} - \frac{c}{B_0}\frac{\partial \langle\phi\rangle_\alpha}{\partial y}\frac{\partial f}{\partial x} + \frac{c}{B_0}\frac{\partial \langle\phi\rangle_\alpha}{\partial x}\frac{\partial f}{\partial y} + v_\parallel \frac{\partial f}{\partial z} - \frac{e}{m_i}\frac{\partial \langle\phi\rangle_\alpha}{\partial z}\frac{\partial f}{\partial v_\parallel} = 0, \tag{1}$$

$$-\left(\nabla^2 + \frac{\rho_{ti}^2}{\lambda_{Di}^2}\nabla_\perp^2\right)\phi + \frac{1}{\lambda_{De}^2}(\phi - \langle\phi\rangle_{yz}) = 4\pi e\left[\int f\delta([\mathbf{R}+\rho]-\mathbf{x})d\mathbf{Z} - n_0\right], \tag{2}$$

where $\mathbf{R}$ is the guiding centre position, $\mathbf{R}+\rho$ is the particle position, $v_\parallel$ and $v_\perp$ are the velocities parallel and perpendicular to the field, α is the gyro-phase angle, c is the velocity of light, m_i and e are the mass and charge of ions, ρ_{ti} is the ion Larmor radius, λ_{Di} and λ_{De} are the ion and electron Debye lengths, n_0 is the equilibrium density, ϕ is the electrostatic potential, $\langle\cdot\rangle_\alpha$ is the gyro-averaging operator, and $\langle\cdot\rangle_{yz}$ denotes average over the y-z plane. Eq.(1) is solved using MFD and a fourth-order adaptive Runge-Kutta method (RKM) which keeps a constant Courant-Friedrichs-Lewy (CFL) number τ. Eq.(2) is solved using a Fast Fourier Transform (FFT) technique. The code is parallelised using a 3D domain decomposition technique (x-y-$v_\perp$) with the MPI, and processing efficiency with $\sim 25\%$ is sustained up to 1536 processors on the JAEA Altix3700Bx2 system. The gyrokinetic equation conserves any arbitrary function of f. From the viewpoint of the numerical simulation, conservations of f and f^2 are of particular importance. MFD conserves both f and f^2, while FVM conserves only f. In Fig.1, the simulation with FVM breaks down in the nonlinear phase, where f^2 increases with conserving f, leading to the growth of numerical oscillations. On the other hand, the simulation with MFD shows an exact conservation of f and an approximate conservation of f^2. Although a small error of f^2 comes from numerical dissipation in RKM, MFD is numerically stable in the nonlinear phase.

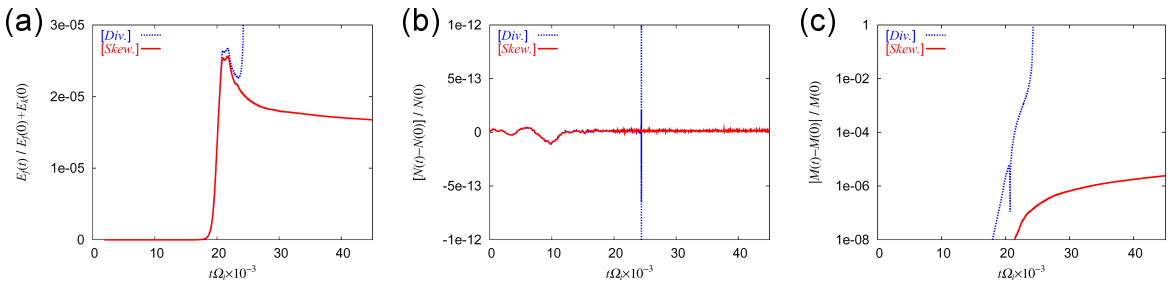

Figure 1: The time histories of (a) the field energy, and the relative errors of (b) the $L1$ norm, $N = \int f d\mathbf{Z}$, and (c) the $L2$ norm, $M = \int f^2 d\mathbf{Z}$, observed in 4D ITG simulations with FVM (blue) and with MFD (red). Numerical parameters are $(N_x, N_y, N_z, N_{v_\parallel}) = (128, 64, 32, 128)$, $\tau = 0.4$.

3. Comparisons of gyrokinetic Vlasov and f PIC codes

In the benchmark tests, we compare the new conservative Vlasov code G5D with a δf PIC code G3D [5]. G3D has been developed based on a finite element δf PIC method, where Eq.(1) is solved using the δf method, and in Eq.(2), ϕ is approximated using 2D (x-y) finite elements and a Fourier mode expansion (z). Firstly, we discuss long time behaviours of the Vlasov and PIC simulations in a reduced 4D model without gyro-averaging, and then, show comparisons in the 5D gyrokinetic model. We consider a hydrogen plasma in a periodic slab configuration with $L_z \sim 8000\rho_{ti}$, $v_{\parallel} = -5v_{ti} \sim 5v_{ti}$, $|v_{\perp}| = 0 \sim 3.5v_{ti}$, and flat n_0 and T_{e0} profiles, where v_{ti} is the ion thermal velocity and T_{e0} is the electron temperature. The 4D cases use a small system ($L_x = 2L_y \sim 31\rho_{ti}$) with periodic boundaries in x, where the ion temperature T_{i0} is given as $T_{i0} = T_{e0}(1/L_x - 1/2\pi L_{ti}\cos[2\pi x/L_x])$ with $L_{ti} \sim 37\rho_{ti}$. In the 4D simulation, two ITG modes, which propagate in opposite directions, are excited in the positive and negative temperature gradient regions, respectively (see Fig.2 (a)). In the nonlinear phase, ITG modes saturate by self-generated zonal flows, which break up the linear mode structures. In Figs.2 (b) and (c), the time histories of variations of the field energy, the kinetic energy, and the total energy show excellent agreement in the linear and early nonlinear phases. However, G3D shows numerical heating due to collisions among marker particles and the error of the total energy is $\sim 40\%$ of the field energy after ~ 150 linear growth times. In contrast, G5D keeps a good energy conservation as well as an exact particle number conservation. The 5D cases simulate more realistic large system ($L_x = L_y \sim 124\rho_{ti}$) with fixed boundaries in x, where the T_{i0} profile is given as $T_{i0}(x) = C\exp(-\Delta r/L_{ti}\tanh[\{x-2/L_x\}/\Delta r])$ and C is chosen so that $T_{e0} = \int T_{i0}dx/L_x$. In the 5D simulation, the linearly unstable mode is localised at $x = 0.5L_x$ (see Fig.3 (a)), and the turbulent region spreads towards the boundaries with zonal flows produced by nonlinear evolution processes (see Fig.3 (b)). Although the results from G5D and G3D show reasonably good agreement, differences are enhanced by complicated turbulent spreading processes.

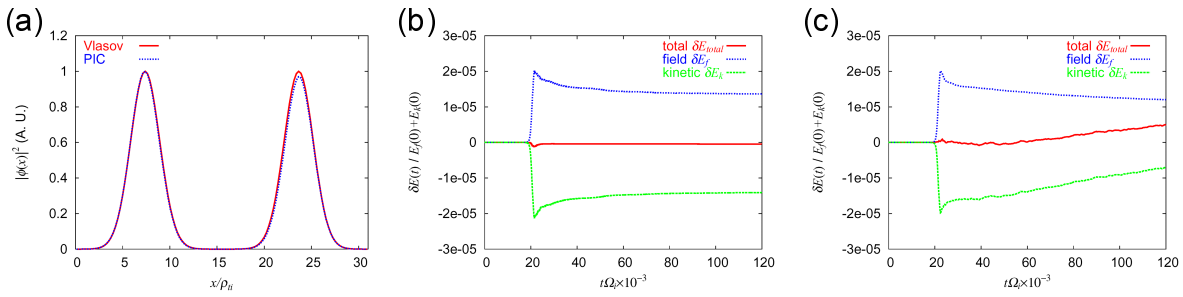

Figure 2: (a) the linear eigenfunction ($m = n = 2$) and the time histories of the field energy, the kinetic energy, and the total energy observed in 4D ITG simulations using (b) G5D ($(N_x, N_y, N_z, N_{v_{\parallel}}) = (128, 64, 32, 512), \tau = 0.4$) and (c) G3D ($N_p = 1.68 \times 10^7, \Delta t\Omega_i = 20$).

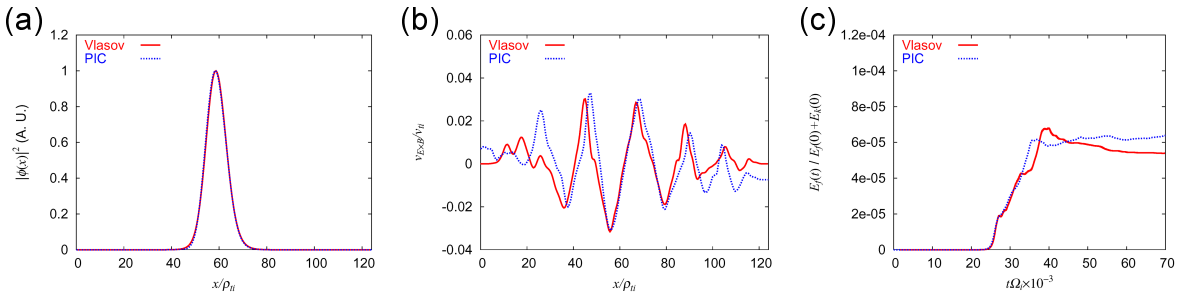

Figure 3: (a) the linear eigenfunction ($m = 3, n = 2$), (b) the nonlinear zonal flow structure, and (c) the time history of the field energy observed in 5D ITG simulations using G5D ($(N_x, N_y, N_z, N_{v_\parallel}, N_{v_\perp}) = (256, 64, 32, 192, 16), \tau = 0.4$) and G3D ($N_p = 6.7 \times 10^7, \Delta t \Omega_i = 20$).

4. Role of $v_\parallel$ nonlinearity

From the viewpoint of modern gyrokinetic theory, the gyrokinetic equation without the $v_\parallel$ nonlinearity is seen as a conservative gyrokinetic equation with a spurious source term, $Df/Dt = -e/m_i \partial_z \langle\phi\rangle_\alpha \partial_{v_\parallel} \delta f$, where δf is the nonlinear perturbation. The physical effect of the $v_\parallel$ nonlinearity can be validated from the entropy balance relation. In the 5D ITG simulation in Fig.3, it has been found that its contribution to the heat transport is negligible ($\sim 1\%$) compared with the entropy production. Then, we have checked its numerical effects by comparing the simulations with and without the $v_\parallel$ nonlinearity. The PIC simulation without the $v_\parallel$ nonlinearity uses partially linearised characteristics with $dv_\parallel/dt = 0$ and the δf equation derived from $Df/Dt = 0$. This inconsistent treatment leads to the error of δf. On the other hand, in the Vlasov simulation, the spurious source term does not affect the conservation of f but violates the conservation of f^2. As a result of accumulative errors on the conservation properties, the comparison has shown much larger differences than those expected from its physical effect. Therefore, a conservative gyrokinetic equation involving the $v_\parallel$ nonlinearity is essential for the gyrokinetic simulation.

5. Summary

A new conservative gyrokinetic Vlasov code has been developed. The code is numerically stable and robust in a long time micro-turbulence simulation. The code has been successfully benchmarked against the δf PIC code, and conservation properties are validated. From the conservation properties, the importance of the $v_\parallel$ nonlinearity has been demonstrated.

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