Comparisons of gyrokinetic PIC and CIP codes

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Introduction: A gyrokinetic simulation is an essential tool to study anomalous turbulent transport in tokamak plasmas. Although several gyrokinetic simulations have been developed based on particle and mesh approaches, most of full torus global simulations have adopted a particle approach because of limitations on computational resources. A δf Particle-In-Cell (PIC) method [1] enabled an accurate calculation of small amplitude ($\delta n/n \sim 1\%$) turbulent fluctuations in collisionless plasmas. However, it is difficult to apply the conventional δf PIC method to more realistic long time turbulence simulations where non-conservative effects such as heat and particle sources and collisions are important, because it was designed using conservation properties (Liouville's theorem) of a collisionless gyrokinetic equation. On the other hand, a mesh approach, which is much more flexible about treatments of these non-conservative effects, is likely to become another solution with recent advances in computational fluid dynamics (CFD) schemes and increasing computational resources. In order to asses a possibility of a mesh approach from a point of view of numerical properties and a computational cost, a new gyrokinetic Vlasov code has been developed using a Constrained-Interpolation-Profile (CIP) method [2], which is one of advanced CFD schemes based on a semi-Lagrangian approach. In the CIP method, a function f and its derivative $g = \partial f/\partial x$ are solved simultaneously, and a solution is expressed using a Hermite interpolation. In Ref. [3], a 2D Vlasov-Poisson system was solved using the CIP method and a semi-Lagrangian method with a spline interpolation, and it was shown that numerical oscillations are quite small in the CIP method compared with a spline interpolation. Since a generation of fine structures by phase mixing is universal phenomena, less numerical oscillation is a great advantage in a Vlasov simulation. In this work, the code is tested in 4-dimensional (4D) gyrokinetic simulations of the slab Ion Temperature Gradient driven (ITG) turbulence.

Gyrokinetic Vlasov CIP code: A 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 a 4D drift-kinetic/gyrokinetic-Poisson system,

$$\frac{\partial f}{\partial t} - \frac{c}{B_0}\frac{\partial \phi}{\partial y}\frac{\partial f}{\partial x} + \frac{c}{B_0}\frac{\partial \phi}{\partial x}\frac{\partial f}{\partial y} + v\frac{\partial f}{\partial z} - \frac{e}{m}\frac{\partial \phi}{\partial z}\frac{\partial f}{\partial v} = 0, \tag{1}$$

$$-\left(\nabla^2 + \nabla_\perp \cdot \frac{\rho_{ti}^2}{\lambda_{Di}^2}\nabla_\perp\right)\phi + \frac{1}{\lambda_{De}^2}\left(\phi - \langle\phi\rangle\right) = 4\pi e\left(\int f dv - n_0\right), \tag{2}$$

where $f(x,y,z,v)$ is a guiding-centre distribution function, v is a parallel velocity, c is the velocity of light, m and e are ion mass and charge, ρ_{ti} is the ion Larmor radius, λ_{De} and λ_{Di} are the ion and electron Debye lengths, n_0 is the equilibrium density, ϕ is the electrostatic potential, and $\langle\cdot\rangle$ is average on the y-z plane. In this model, the finite Larmor radius effect is kept only in the polarization density in Eq. (2). The drift-kinetic equation, Eq. (1), is integrated using a directional splitting method [4]. Here, a 2D CIP scheme is used on the x-y plane, and a 1D CIP scheme is used in the z- and v- directions, respectively. The boundary condition in the v-direction is f=0 at the boundaries. The order of integration is chosen as $xy/2$-$z/2$-v-$z/2$-$xy/2$, and in the steps $xy/2$ and v, Eq. (2) is solved using FFT. In the benchmark tests, a Fourier filter is used to emulate effects of a 2D spline base function (x-y) and a shape factor of finite size particles (z) in a finite element PIC method [5]. The code is parallelized using a 3D domain decomposition technique with MPI2 and OpenMP, and a processing efficiency with ~15% is sustained up to 512 processors on the JAERI Altix3900 system. In the preliminary ITG simulations, the nonlinear results have been converged with a CFL number, τ=0.1, and the grid size, $\Delta x=\Delta y=\rho_{ti}/4$. In the density spectrum, accumulation of the density in a short wavelength regime has not been observed. The positivity of f has been almost kept for whole simulation time, except for a small negative value, $f_{\min}/f_{\max} \sim -10^{-8}$, observed in the initial saturation phase. The code is stable and a numerical oscillation is quite small for a long time in the nonlinear phase.

Comparisons of gyrokinetic PIC and CIP codes: In the benchmark tests, ITG turbulence simulations using the CIP code and a δf PIC code, G3D [6], are compared. G3D has been developed based on a finite element δf PIC method, where Eq. (1) is solved using a nonlinear δf method, and in Eq. (2), ϕ is approximated using 2D (x-y) finite elements with quadratic splines and a Fourier mode expansion in the z-direction. In the present study, marker particles with the Maxwellian loading are used. The benchmark parameters are $L_x=2L_y=32\rho_{ti}$, $L_z=8000\rho_{ti}$, $L_v=\pm 5v_{ti}$, $L_n=\infty$, $L_{te}=\infty$, and $L_{ti}=38.4\rho_{ti}$. A periodic boundary condition is imposed in the x-direction by choosing a T_i profile with positive and negative gradient regions,

$$T_i = c_0\left[1 + c_1 \sin(\pi x / L_x)^2\right], \tag{3}$$

where c_0 and c_1 are given so that $T_e = \int T_i dx$. From a series of convergence tests, the standard numerical parameters are determined as $N_x \times N_y \times N_z \times N_v = 128\times 64\times 16\times 64$, $\tau=0.1$ in the CIP code, and $N_x\times N_y=32\times 16$, $n=k_zL_z/2\pi=\pm 0\sim 6$, $N_p=4\times 10^6$, $\Delta t=20\Omega_i^{-1}$ in the PIC code. In the present simulation, two ITG modes, which propagate in the opposite directions, are excited in positive and negative gradient regions. Both codes show almost the same linear mode structures with $m=k_yL_y/2\pi=2$. In the nonlinear phase, ITG modes saturate by self-generated zonal flows. Figure 1 shows contour plots of ϕ observed in the nonlinear quasi-steady phase. Zonal flows are almost symmetric between positive and negative gradient regions. The PIC and CIP codes show similar zonal flow patterns. In Fig. 2, the time histories of the field energy observed in the PIC and CIP codes are plotted. Here, in addition to the standard cases, higher resolution cases are also plotted in order to show their convergence. The linear growth rates observed in the PIC ($\gamma\sim 1.13\times 10^{-3}\ \Omega_i$) and CIP ($\gamma\sim 1.05\times 10^{-3}\ \Omega_i$) codes differ by ~7%. The saturation levels coincide with each other. In the standard cases, relative errors of the energy and particle conservations at $t\Omega_i=20$ are respectively $\sim 1.3\times 10^{-5}$ ($\sim 2.5\times 10^{-5}$) and $\sim 1.9\times 10^{-5}$ ($\sim 0.5\times 10^{-5}$) in the CIP (PIC) code. The present benchmark tests show that the results obtained from the PIC and CIP codes are almost equivalent.

Summary and discussions: In this work, a new gyrokinetic Vlasov code has been developed using the CIP method. The code is numerically stable and numerical oscillations are quite small. In the ITG simulations, the linear growth rates, the nonlinear saturation levels, the zonal flow structures, and the conservation properties were almost the same between the PIC and CIP codes. In the standard cases, memory usage and CPU time on the JAERI Origin3800 system were 1.7GB (27GB) and 120GFlops-h (35GFlops-h) in the CIP (PIC) code. Although these costs in a 4D slab problem are comparable between the two codes, a cost of the CIP code is expected to increase drastically in a 5D toroidal problem, where a mesh number increases ~100 times with the additional coordinate. In the future work, the code will be extended to a 5D toroidal code, and also non-conservative effects will be implemented.

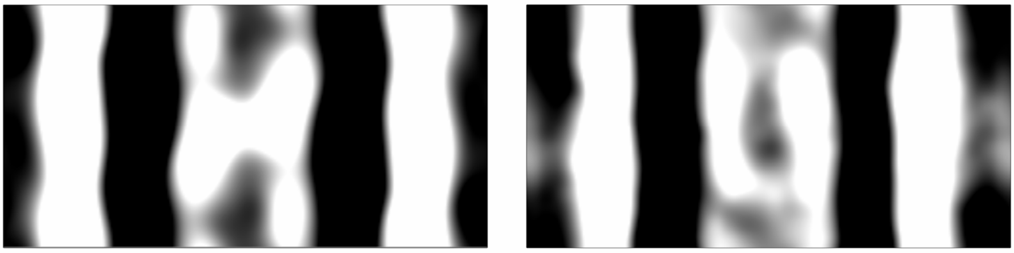

Figure 1: The *x*-*y* contour plots of ϕ observed in the nonlinear quasi-steady phase of the ITG turbulence simulations with CIP (left) and PIC (right) codes. Both results show similar zonal flow patterns.

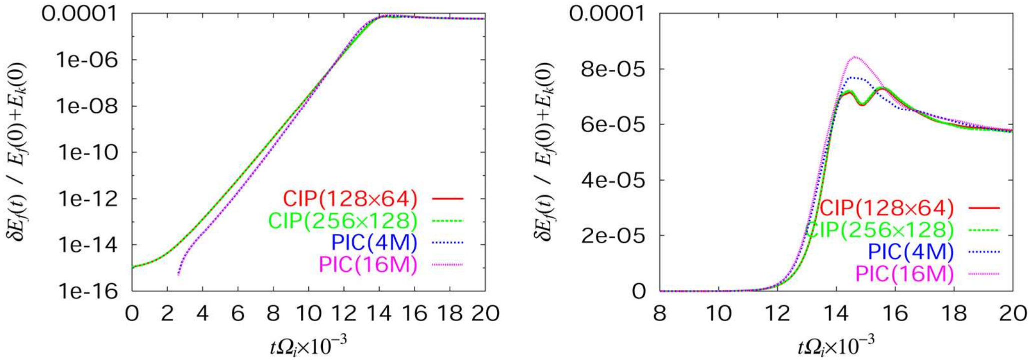

Figure 2: The time histories of the field energy observed in CIP ($N_x\times N_y\times N_z\times N_v$=128×64×16×64, 256×128×16×64) and PIC (N_p=4×10^6, 16×10^6) codes are plotted with logarithmic (left) and linear (right) scales. The linear growth rates and saturation amplitudes are converged and agree well between CIP and PIC codes.

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