

## Gyrokinetic Toroidal full- $f$ 5D Vlasov code GT5D

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### 1. Introduction

Conservative full- $f$  gyrokinetic simulations are desirable for studying long time behaviours of tokamak micro-turbulence such as the formation of transport barriers and the transition of turbulent transport. In our previous work, a conservative Gyrokinetic slab full- $f$  5D Vlasov code (G5D) was successfully developed based on a novel conservative and non-dissipative finite difference scheme proposed by Morinishi et al [1], and a possibility of robust and highly accurate long time micro-turbulence simulations was demonstrated [2]. In this work, we present a new conservative Gyrokinetic Toroidal full- $f$  5D Vlasov code (GT5D). To extend G5D to GT5D, Morinishi's Finite Difference operator (MFD) in general curvilinear coordinates is developed for the toroidal gyrokinetic equation. Here, one important requirement of MFD is that the Hamiltonian flows have to be discretised so that their incompressible condition is exactly satisfied. This is rather trivial for the slab gyrokinetic equation, in which Hamiltonian flows are decomposed to the  $E \times B$  drift, the parallel streaming, and the parallel acceleration. However, the toroidal gyrokinetic equation is given by a non-separable Hamiltonian, and its incompressible condition in 5D phase space is complicated. To resolve this issue, a new discrete expression of gyro-centre Hamilton's equation, which exactly satisfies the incompressible condition or the phase space conservation, is proposed by differentiating the vector potential and the gyro-centre Hamiltonian. The other techniques in GT5D are semi-implicit time integration for stiff linear terms based on an additive semi-implicit Runge-Kutta method (ASIRK) [3], a finite element gyrokinetic Poisson solver with an integral flux surface average operator [4], a full Finite Larmor Radius (FLR) operator with arbitrary large number sampling points, and a gyrokinetic Vlasov equilibrium defined with constants of motion [5]. GT5D is benchmarked against a Gyrokinetic Toroidal  $\delta f$  3D particle code (GT3D) [5]. In the benchmark, zonal flow damping tests and analyses of linear spectra of ion temperature gradient driven (ITG) modes are performed, and results obtained from GT3D and GT5D are compared quantitatively. In GT5D, first principles such as the particle number conservation and the total energy conservation are also examined.

### 2. Application of Morinishi scheme to toroidal gyrokinetic equation

The physical model used in this study is gyrokinetic ions and adiabatic electrons in a full torus geometry. In the modern gyrokinetic theory, the gyrokinetic Vlasov-Poisson system is

written in a conservative form using the gyro-centre Hamiltonian  $H = mv_{\parallel}^2/2 + \mu B + e\langle\phi\rangle_{\alpha}$  in the gyro-centre coordinates,  $\mathbf{Z} = (t; \mathbf{R}, v_{\parallel}, \mu, \alpha)$ ,

$$m^2 B_{\parallel}^* \dot{\mathbf{R}} = m \mathbf{B}^* \frac{\partial H}{\partial v_{\parallel}} + \frac{m^2 c}{e} \mathbf{b} \times \nabla H, \quad (1)$$

$$m^2 B_{\parallel}^* \dot{v}_{\parallel} = -m \mathbf{B}^* \cdot \nabla H, \quad (2)$$

$$\frac{Dm^2 B_{\parallel}^* f}{Dt} = \frac{\partial m^2 B_{\parallel}^* f}{\partial t} + \nabla \cdot (m^2 B_{\parallel}^* \dot{\mathbf{R}} f) + \frac{\partial}{\partial v_{\parallel}} (m^2 B_{\parallel}^* \dot{v}_{\parallel} f) = 0. \quad (3)$$

$$-\nabla_{\perp} \cdot \frac{\rho_{ti}^2}{\lambda_{Di}^2} \nabla_{\perp} \phi + \frac{1}{\lambda_{De}^2} [\phi - \langle\phi\rangle_f] = 4\pi e \left[ \int f \delta([\mathbf{R} + \boldsymbol{\rho}] - \mathbf{x}) m^2 B_{\parallel}^* d\mathbf{R} dv_{\parallel} d\mu - n_0 \right], \quad (4)$$

where  $\mathbf{R}$  is the guiding centre position,  $\mathbf{R} + \boldsymbol{\rho}$  is the particle position,  $v_{\parallel}$  is the parallel velocity,  $\mu$  is the magnetic moment,  $\alpha$  is the gyro-phase angle,  $\mathbf{B}$  is the equilibrium magnetic field,  $\mathbf{b} = \mathbf{B}/B$ ,  $m^2 B_{\parallel}^*$  is the Jacobian of gyro-centre coordinates,  $B_{\parallel}^* = \mathbf{b} \cdot \mathbf{B}^*$ ,  $\mathbf{B}^* = \mathbf{B} + (cm/e)\nabla \times \mathbf{b}v_{\parallel}$ ,  $c$  is the velocity of light,  $m$  and  $e$  are the mass and charge of ions,  $\rho_{ti}$  is the ion Larmor radius,  $\lambda_{Di}$  and  $\lambda_{De}$  are the ion and electron Debye lengths,  $n_0$  is the equilibrium density,  $\phi$  is the electrostatic potential,  $\langle\cdot\rangle_{\alpha}$  and  $\langle\cdot\rangle_f$  are the gyro-average and flux-surface-average operators, respectively. Hamilton's equation, (1) and (2), satisfies the phase space conservation,

$$\nabla \cdot (m^2 B_{\parallel}^* \dot{\mathbf{R}}) + \frac{\partial}{\partial v_{\parallel}} (m^2 B_{\parallel}^* \dot{v}_{\parallel}) = 0. \quad (5)$$

In general curvilinear coordinates, Eq. (3) is written as a continuity equation of  $f$  transported by incompressible flows satisfying  $\partial_{X_j}(\mathcal{J}V_j) = 0$ ,

$$\frac{\partial \mathcal{J}f}{\partial t} + \frac{\partial \mathcal{J}V_j f}{\partial X_j} = \frac{\partial \mathcal{J}f}{\partial t} + (\text{Conv.}) = 0, \quad (6)$$

where  $\mathcal{J}$  is the Jacobian and the index runs through  $j = 1 \sim 4$ . If we apply MFD for  $(\text{Conv.})$ , both  $(\text{Conv.})$  and  $f(\text{Conv.})$  are written in a conservative form or a flux balance form [2],

$$[\text{Conv.}] = [\delta_{2j}(\mathcal{J}V_j f) + \mathcal{J}V_j \delta_{2j}(f)]/2 = \delta_{1j}(\overline{\mathcal{J}V_j}^{1j} \widetilde{f}^{1j}) - f/2 \delta_{2j}(\mathcal{J}V_j), \quad (7)$$

$$f[\text{Conv.}] = \delta_{1j}(\overline{\mathcal{J}V_j}^{1j} \widetilde{f^2/2}^{1j}), \quad (8)$$

provided that discrete flows satisfy incompressible condition,  $\delta_{2j}(\mathcal{J}V_j) = 0$ . Here, the definitions of operators are  $\delta_{nj}A \equiv [A(X_j + n\Delta X_j/2) - A(X_j - n\Delta X_j/2)]/(n\Delta X_j)$ ,  $\overline{A}^{nj} \equiv [A(X_j + n\Delta X_j/2) + A(X_j - n\Delta X_j/2)]/2$ , and  $\widetilde{AB}^{nj} \equiv [A(X_j + n\Delta X_j/2)B(X_j - n\Delta X_j/2) + A(X_j - n\Delta X_j/2)B(X_j + n\Delta X_j/2)]/2$ . By conserving  $f$  and  $f^2$ , growth of numerical oscillations is suppressed, and robust simulation is enabled without numerical dissipation. A condition  $\delta_{2j}(\mathcal{J}V_j) = 0$  is equivalent to the phase space conservation (5). By differentiating the vector potential  $\mathbf{A}$  and

the gyro-centre Hamiltonian  $H$  in the cylindrical coordinates  $(R, \zeta, Z, v_{\parallel}, \mu, \alpha)$ , we find discrete forms of Eqs. (1) and (2) which satisfy the phase space conservation,

$$\left[ m^2 B_{\parallel}^* R \dot{\mathbf{R}} \right] \equiv m (\delta_{2\mathbf{R}} \times [\mathbf{A} + (cm/e) v_{\parallel} \mathbf{b}]) \delta_{2v_{\parallel}} H + (m^2 c/e) (H \delta_{2\mathbf{R}} \times \mathbf{b} - \delta_{2\mathbf{R}} \times [H \mathbf{b}]), \quad (9)$$

$$\left[ m^2 B_{\parallel}^* R \dot{v}_{\parallel} \right] \equiv -m \delta_{2\mathbf{R}} \times \mathbf{A} \cdot \delta_{2\mathbf{R}} H - (m^2 c/e) v_{\parallel} \delta_{2\mathbf{R}} \cdot (H \delta_{2\mathbf{R}} \times \mathbf{b}), \quad (10)$$

$$\delta_{2\mathbf{R}} \cdot \left[ m^2 B_{\parallel}^* R \dot{\mathbf{R}} \right] + \delta_{2v_{\parallel}} \left[ m^2 B_{\parallel}^* R \dot{v}_{\parallel} \right] = 0, \quad (11)$$

where  $\delta_{2\mathbf{R}} \cdot$  and  $\delta_{2\mathbf{R}} \times$  are divergence and rotation operators defined using centred finite difference. Although similar definitions can be found also for flux coordinates, we use the cylindrical coordinates to avoid difficulties in defining discrete operators at the magnetic axis. By using definitions (7), (9) and (10), conservative toroidal gyrokinetic simulations are enabled. In Eq. (4), flux coordinates are used, and  $f$  and  $\phi$  are transformed between two coordinate systems through a full FLR operator. In the time integration, ASIRK is applied by separating Hamilton's equation into stiff linear and non-stiff nonlinear operators.

### 3. Comparisons of GT5D and GT3D

In this work, we use a circular concentric tokamak configuration with  $R_0/a = 2.8$ ,  $a/\rho_{ti} = 150$ , and  $q(r) = 0.85 + 2.18(r/a)^2$ . Here,  $R_0$  is the major radius,  $a$  is the minor radius,  $r$  is a flux surface label, and  $q(r)$  is the safety factor. In both codes, a gyrokinetic Vlasov equilibrium  $f_0$  is defined using three constants of motion, the canonical toroidal angular momentum  $P_{\zeta}$ , the energy  $\varepsilon$ , and the magnetic moment  $\mu$  [5]. Numerical parameters in GT5D are determined from convergence tests as  $\Delta t = \Omega_i^{-1}$ ,  $\Delta R = \Delta Z \sim 2\rho_{ti}$ ,  $L_R = L_Z = 320\rho_{ti}$ ,  $L_{v_{\parallel}} = 10v_{ti}$  ( $v_{\parallel} = -5v_{ti} \sim 5v_{ti}$ ), and  $L_{v_{\perp}} = 5v_{ti}(\sqrt{2\mu B_0/m} = 0 \sim 5v_{ti})$ . Zonal flow damping tests with  $n = 0$  are performed in the 4D limit with  $N_{\zeta} = 1$ , while linear ITG simulations use a wedge torus configuration with  $N_{\zeta} = 16$  per a wavelength, where  $N_{\zeta}$  is a grid number in the toroidal angle  $\zeta$  direction.

Figure 1 shows zonal flow damping tests with flat background profiles ( $L_n = L_{ti} = \infty$ ) and the initial perturbation,  $\delta f(t=0) = 10^{-5}[1 + \cos(\pi r/a)]f_0$ . In Fig. 1(a), the time histories of zonal flow amplitudes observed in GT3D and GT5D coincide with each other, and in both results, the real frequency, the damping rate, and the residual flow level show good agreement with a theoretical prediction [6] with  $k_r \rho_{ti} \sim 0.04$ . In this test, the conservation properties are also checked in GT5D. In Fig. 1(b), the total particle number is exactly conserved. In Fig. 1(c), the total energy is conserved with the error of  $\delta E_{total} \sim 10^{-4} \delta E_f$ . Figure 2 shows linear ITG benchmark with  $R_0/L_n = 2.22$  and  $R_0/L_{ti} = 6.92$ . In Fig. 2(a), the frequency and growth rate spectra obtained from GT3D and GT5D show agreement within  $\sim 10\%$ . In Figs. 2 (b) and (c), linear eigenfunctions show ballooning structures with almost the same radial position and tilting angle. From these results, the physical validity of GT5D is confirmed.

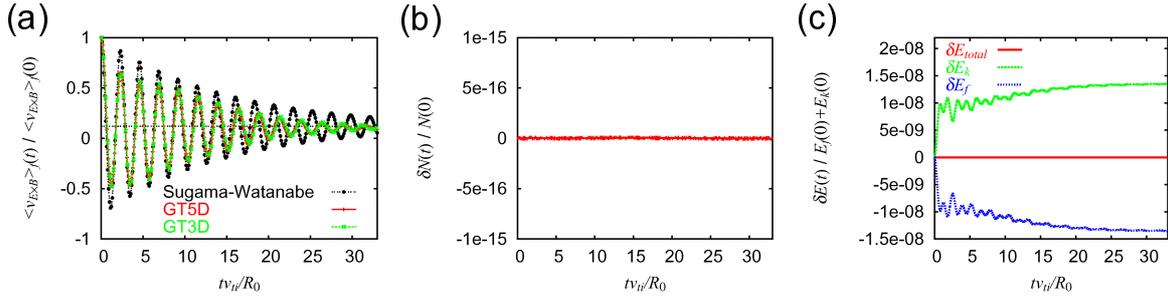


Figure 1: Zonal flow damping tests. (a) shows time histories of zonal flow amplitudes compared with a theory [6]. (b) shows the relative error of total particle number in GT5D. (c) shows time histories of the variations of total energy ( $\delta E_{total}$ ), kinetic energy ( $\delta E_k$ ), and field energy ( $\delta E_f$ ) in GT5D. Grid numbers used in GT5D are  $(N_R, N_\zeta, N_Z, N_{v_{\parallel}}, N_\mu) = (160, 1, 160, 128, 32)$ .

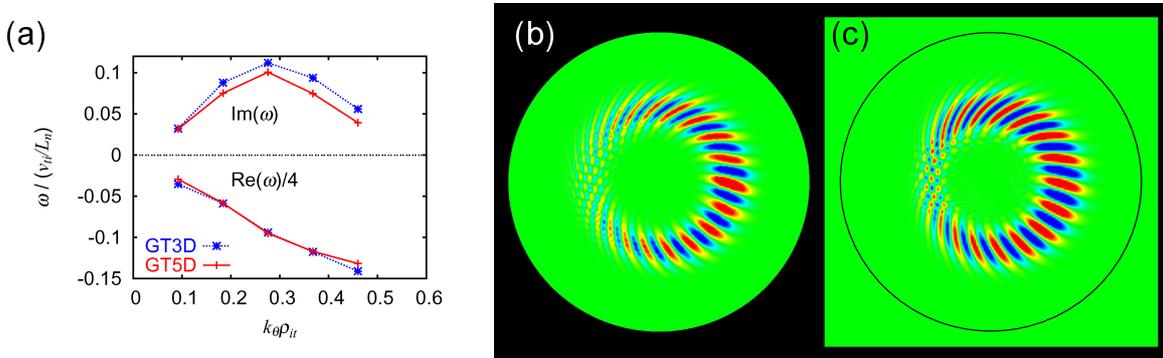


Figure 2: Linear ITG benchmark between GT5D and GT3D. (a) shows the frequency and growth rate spectra. (b) and (c) show linear eigenfunctions of  $n = 15$  mode ( $k_\theta \rho_{ii} \sim 0.28$ ) observed in GT3D and GT5D, respectively. Grid numbers used in GT5D are  $(N_R, N_\zeta, N_Z, N_{v_{\parallel}}, N_\mu) = (160, 16, 160, 64, 16)$  with wedge torus configuration.

## 5. Summary

A new conservative Gyrokinetic Toroidal full-*f* 5D Vlasov code (GT5D) has been developed. The code keeps relevant first principles, the phase space conservation, the particle number conservation, and the total energy conservation, which are essential for long time micro-turbulence simulations. GT5D has been successfully benchmarked against a gyrokinetic  $\delta f$  particle code GT3D through zonal flow damping tests and linear ITG benchmark calculations.

## References

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