

Gyrokinetic particle-in-cell turbulence simulations with an evolving background

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Abstract. Physics based control variates are widely used to reduce the numerical noise and, consequently, the computational cost, of global particle-in-cell simulations. Nevertheless, when plasma profiles change significantly during the nonlinear evolution of the system, control variates based on fixed background distribution functions become less and less effective. Recently, an adaptive scheme has been proposed for the code ORB5, based on an adaptive Maxwellian with time-evolving density and temperature profiles. In this work, we propose an alternative time-varying control variate to study deviation from Maxwellian equilibria based on the Phase-Space Zonal Structures (PSZS) transport theory. In particular, we show how the information provided by the finite element projection of the full distribution function can be used to adjust and update the control variate, i.e. the background distribution function, during the nonlinear evolution of the system for Maxwellian and non-Maxwellian plasma reference states.

Energetic particles (EPs) generated by fusion reactions play a pivotal role in the heating of magnetically confined plasmas during ignition. In present-day experiments EPs are produced by auxiliary heating mechanisms. In tokamaks, EP velocities typically reside between those of thermal bulk ions and thermal electrons. Consequently, the characteristic dynamical frequencies of EPs, associated with their guiding-center motions—namely transit, bounce, and precessional frequencies—are frequently comparable to the frequencies of shear Alfvén waves (SAWs). Accurate predictions of the interactions between SAW instabilities and EPs necessitate a kinetic approach because resonances with ions significantly alter magnetohydrodynamic (MHD) predictions. Nonlinear gyrokinetic (GK) theory offers a robust theoretical framework for evaluating such interactions between SAWs and EPs and their consequent implications on turbulent and collisional transport. Phase space structures, derived by averaging out the dependencies on angle-like variables in the EP distribution function, are not subject to rapid damping by collisionless processes such as Landau damping. These structures play a critical role in modulating EP transport induced by Alfvén instabilities in burning plasmas [1]. These phase space structures are commonly termed Phase Space Zonal Structures (PSZSs), by analogy with the meso-scale configuration space structures spontaneously generated by drift-wave turbulence, such as zonal flows and zonal fields. PSZSs serve as a slowly evolving nonlinear plasma

equilibrium. Recent advancements have led to the derivation of evolution equations for PSZSs from nonlinear GK theory [2]. These equations facilitate the formulation of reduced transport models, which describe the evolution of macroscopic plasma profiles over a prolonged duration akin to the energy confinement times in burning plasma experiments [3]. A direct calculation of the PSZS has been implemented in the ORB5 code [4], via a finite-element representation on 3D B-spline polynomials [5]. The particle-in-cell gyrokinetic code ORB5 relies on the use of physics based control variates (usually called *equilibrium distribution function*) to reduce the computational cost of the Monte-Carlo discretization (see [6] and references therein). This control variate is time independent. Nevertheless, plasma profiles can change significantly during the nonlinear evolution of the system or because of the effect of heat and particles sources or sinks. Therefore, a control variates based on fixed background distribution functions become less and less effective. Recently, an adaptive scheme has been proposed for the code ORB5, based on an adaptive Maxwellian with time-evolving density and temperature profiles [7] In this work, we propose an alternative time-varying control variate specifically devised to study deviation from Maxwellian equilibria.

Following the definitions of Ref. [2], the PSZS is defined as the angle average (orbit average) of the gyrocenter distribution function

$$\hat{F}_{0,sp}(P_\varphi, \mu, \epsilon) = \tau_b^{-1} \oint \frac{d\theta}{\dot{\theta}} F_{z,sp}, \quad \tau_b = \oint \frac{d\theta}{\dot{\theta}},$$

$$F_{z,sp} = \frac{1}{2\pi} \int_0^{2\pi} F_{sp}(P_\varphi, \mu, \epsilon, \theta, \varphi) d\varphi,$$

$$\dot{\theta} = -\frac{v_{\parallel}}{eB^*J} \frac{\partial P_\varphi}{\partial \psi}, \quad P_\varphi = m_{sp} v_{\parallel} \frac{T(\psi)}{q_{sp} B} + \psi, \quad \epsilon = \frac{1}{2} m_{sp} v_{\parallel}^2 + \mu B.$$

where ϵ is the kinetic energy, μ is the magnetic moment and P_φ is the canonical toroidal moment. Note that P_φ is a constant of motion for the unperturbed trajectories in axisymmetric systems (for $\mathbf{B} = T(\psi)\nabla\varphi + \nabla\varphi \times \nabla\psi$). The finite element (**B-splines**) representation is given in Ref. [5]

$$\hat{F}_{0,sp}(P_\varphi, \mu, \epsilon, t) = \sum_l F_l(t) \Lambda_l(P_\varphi, \mu, \epsilon), \quad (1)$$

$$\Lambda_l(P_\varphi, \mu, \epsilon) = \Lambda_i^d(P_\varphi) \Lambda_j^d(\epsilon) \Lambda_k^d(\mu),$$

where $\Lambda_l(P_\varphi, \mu, \epsilon)$ is the tensor product of 3 one dimensional B-splines of order d and $F_l(t)$ are the spline coefficients of the PIC discretized distribution function of the species sp . The spline coefficients are calculated by casting the problem in a mass-matrix form (Galerkin method) and solving for them using a direct method

$$\sum_l A_{l,m} F_l = \sum_{p=1}^N \int \hat{F}_{0,sp}(P_\varphi, \mu, \epsilon, t) \Lambda_\nu(P_{\varphi,p}, \epsilon_p, \mu_p) \tilde{J} dP_\varphi d\epsilon d\mu, \quad (2)$$

where $A_{l,m}$ are elements of a symmetric sparse band matrix of rank $(N_{P_\varphi} + d)(N_\epsilon + d)(N_\mu + d)$ and \tilde{J} is the Jacobian of the constant of motion phase-space. The right-hand-side (RHS) of eq. (2) is constructed by projecting the markers on the B-spline space. In the simplest electrostatic model implemented in ORB5 the Poisson equation has the form of quasi-neutrality equation written in the long wavelength approximation,

$$-\sum_{sp \neq e} \nabla_{\perp} \frac{n_{sp} m_{sp} c^2}{B^2} \nabla_{\perp} \phi = \sum_{sp} \int dW e_{sp} J_{0,sp} F_{sp}. \quad (3)$$

The statistical noise associated with the marker discretization of the charge density, corresponding to the RHS of eq. (3), is reduced by applying a static control variate $F_{cv,0}$

$$\sum_{sp} \int dW (e_{sp} J_{0,sp} F_{sp} - F_{cv,0,sp}) + \sum_{sp} \int dW F_{cv,0,sp} . \quad (4)$$

In most of the ORB5 simulations, $F_{cv,0}$ is set to be a (shifted) Maxwellian distribution function. The new adaptive control variate method proposed here consists of replacing $F_{cv,0,sp}$ with the time evolving function $\hat{F}_{0,sp}(t)$ of eq. (1),

$$\sum_{sp} \int dW (e_{sp} J_{0,sp} F_{sp} - \hat{F}_{0,sp}(t)) + \sum_{sp} \int dW \hat{F}_{0,sp}(t) . \quad (5)$$

The resulting code has been tested in electrostatic simulations in straight-tokamak geometry, also referred as periodic screw-pinch. The magnetic field is given by

$$\mathbf{B} = B_0 \left(-\frac{r}{Rq_s(r)} \boldsymbol{\theta} + \mathbf{z} \right) .$$

Simulations has been performed using the global full-f PIC code PICLS [8, 9]. The PICLS has been primarily developed to investigate the limits of the PIC methods and of the gyrokinetic models when applied to open field line regions. PICLS is based on a full-f gyrokinetic model for the ions, drift-kinetic electrons and uses logical sheath boundary conditions (not used in this work). Note that in a periodic screw-pinch the constant of motion variables used to construct $\hat{F}_{0,sp}(t)$ become

$$P_\varphi \rightarrow r, \quad \epsilon \rightarrow v_{\parallel}, \quad \mu \rightarrow v_{\perp} .$$

An example of $\hat{F}_{0,sp}(t)$ constructed on a (65, 65, 65) grid, for the numerical parameters of Tab. 1, is given in Fig. 1.

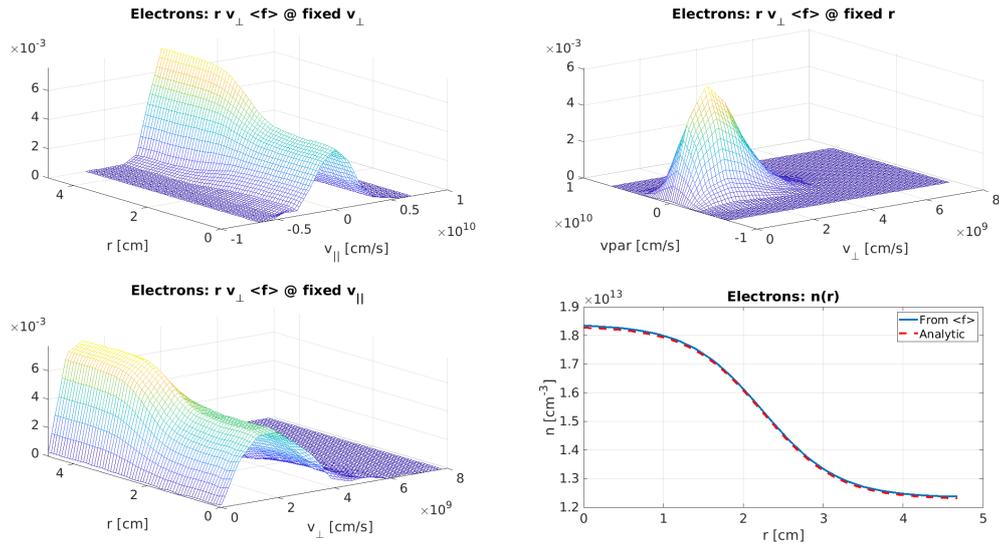


Figure 1: B-spline projection of the distribution function at $t = 0$ for the parameters of Tab. 1.

In particle-in-cell simulations the numerical noise is directly proportional to the variance of the weights and inversely proportional to the square-root of the number of markers. Therefore,

the time evolution of the reduced weight variance, σ^2 , can be used to evaluate the effectiveness of the control variate,

$$\sigma^2 = \frac{1}{N} \sum (\tilde{w}_p - \bar{\tilde{w}}_p)^2, \quad \bar{\tilde{w}}_p = \frac{1}{N} \sum \tilde{w}_p, \quad \tilde{w}_p \equiv \left(e_{sp} J_{0,sp} F_{sp} - \hat{F}_{0,sp}(t) \right).$$

Figure 2 compares the time evolution of the variance of the reduced weights \tilde{w}_p for the traditional and the time evolving control variate, showing that the new algorithm significantly reduces the statistical noise.

B_0	2 [T]	magnetic field
a	4.68 [cm]	minor radius
ρ_s	0.32 [cm]	sound Larmor radius
R	77.0 [cm]	major radius
m_i	3872 m_{elec}	ion mass (D)
n	[0,1,2]	toroidal modes
q	4	safety factor

Table 1: Parameters used for the ITG turbulence simulations in screw-pinch geometry.

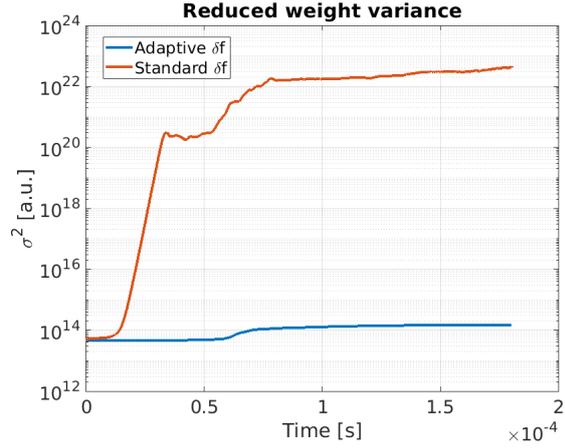


Figure 2: Time evolution of the reduced weight variance for the ITG turbulence simulations in screw-pinch geometry.

In conclusion, the B-spline solver of PICLS has been adapted to a 3D non periodic matrix problem. As a results, the numerically calculated PSZS can be used as a control variate for reducing the numerical noise in global gyrokinetic simulations. As a proof of principle, the algorithm has been tested in reduced geometry using the PICLS code showing that the reduced weight variance is significantly smaller than the standard control variate one.

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