Fluid moments and spectral diagnostics in global particle-in-cell simulations

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Abstract. The convergence properties of global electrostatic particle-in-cell gyrokinetic simulations have been studied by means of a set of new 3D diagnostics recently implemented in the code ORB5, allowing for measurements of electromagnetic potentials and relevant fluid quantities (density, temperature, vorticity) as well as turbulence spectral analysis. For all the quantities considered, non converged simulations show flatter spectra. However, not all the physically relevant quantities converge with the same rate: density fluctuation spectra can still show an unphysical flattening of the spectrum at high $k_{θρ_s}$, even when electrostatic potential and heat fluxes appear to be converged. A remarkable result is that resolution in terms of number of markers, required to correctly describe the turbulence density fluctuations, is found to be size-dependent: larger systems (ITER like) require less numerical particles per active mode than smaller systems.

1. Introduction
Global linear and nonlinear PIC codes are routinely used for solving the gyrokinetic equations, often in the limit of the electrostatic approximation. Most of the existing gyrokinetic PIC codes are based on the $δf$ method [1, 2, 3]. In the $δf$ method the distribution function $f$ of each plasma species is split into a time independent background distribution function $f_0$ and a time dependent perturbation $δf$, $f = f_0 + δf$. In the $δf$ method, the perturbed part only ($δf$) is discretized using numerical particles called markers. As long as the perturbation $δf$ remains small as compared to $f_0$, the $δf$ method reduces the statistical noise. The $δf$ method can be interpreted as a "control variate" algorithm [4, 5], a variance reduction technique widely used for Monte Carlo methods. In this paper we present a systematic study of the convergence properties of global electrostatic $δf$ PIC simulations when the number of markers is varied.

2. Simulation model
All the simulations presented in this work have been performed using the code ORB5 [6]. The ORB5 gyrokinetic model is based on the gyrokinetic Vlasov-Maxwell system of equations of Hahm and Brizard [7, 8, 9, 10]. The latter consists of a set of self-consistent and energy conserving nonlinear gyrokinetic equations for particles and fields. The code ORB5 solves the full-f Vlasov equation using a particle-in-cell $δf$ method: the fluctuating part of the distribution function, $δf$ is discretized using a population of numerical particles, called markers. Each marker
is characterized by a position in the 5D phase-space and by a weight, carrying the information of the average value of $\delta f$ in a small portion of the phase-space. The linearized field equations, the polarization equation and the parallel Ampère’s law [11], are discretized using finite elements. The code is based on straight-field-line coordinates and includes collision operators [12, 13]. In collisionless simulations, like the one performed in this paper, the dissipation necessary to assure entropy saturation and to reach a steady state is provided either by a zonal flow residual preserving Krook-operator [14] or by a coarse graining algorithm [15, 16]. The equations of the model, in the electrostatic limit, are:

$$\frac{Df}{Dt} = \frac{\partial f}{\partial \mathbf{R}} \cdot \dot{\mathbf{R}} + \frac{\partial f}{\partial p_z} p_z = C(f) + S$$  \hspace{1cm} (1)

$$\dot{\mathbf{R}} = \frac{p_z}{m B_\parallel} + \frac{1}{B_\parallel^2} \mathbf{b} \times \left[ \frac{\mu}{e} \nabla B + \nabla J_0 \Phi \right]$$

$$p_z = -\frac{m B^*}{B_\parallel} \left[ \mu \nabla B + \frac{e}{m} \nabla J_0 \Phi \right]: \dot{\mu} = 0$$  \hspace{1cm} (2)

$$\sum_{\text{species}} \delta n = -\nabla_\perp \left( \sum_{\text{species}} \frac{m_n}{e B^2} \right) \nabla_\perp \Phi$$  \hspace{1cm} (3)

where $\Phi$ is the electrostatic potential, $(\mathbf{R}, p_z, \mu)$ are the gyrocenter coordinates with $\mu \equiv v_\perp^2/2B$, magnetic moment per unit mass, and $p_z \equiv m v_\parallel$ is the canonical parallel momentum, $J_0$ is the gyroaverage operator; $\mathbf{b}$ is the unit vector for $\mathbf{B}$, $m$ and $e$ are the species mass and charge; $\delta n$ is the perturbed gyrocenter density $\delta n = \int dW \delta f(R + \rho - x)$, $\rho$ being the particle Larmor radius and $dW = 2\pi B_\parallel^* m^{-2} dq dp_z$, $B^*_\parallel$ is the variable part of the velocity space volume element.

For electromagnetic simulations, not considered in this paper, the system of equation is completed by the linearized gyrokinetic parallel Ampère’s law, which determines the evolution of the magnetic potential $A_\parallel$. In this case, the canonical parallel momentum becomes $p_z \equiv m v_\parallel + e J_0 A_\parallel$.

For $C(f) = 0$ and $S = 0$, this set of gyrokinetic equations is energy and momentum conserving. An elegant proof is given in Ref. [17].

In the absence of sources, $S = 0$, transport processes tend to relax the temperature profile. The heat source has the form of a Krook operator $S_H \propto -\gamma_H \delta f(\psi, v^2, t)$, modified to be particle conserving. The symbol $\sim$ stands for the operator which projects a general function $A(R, p_z, \mu, t)$ to a reduced space $\tilde{A}(\psi, \epsilon, t)$, where $\psi$ is the poloidal magnetic flux and $\epsilon$ is the kinetic energy. The complete definitions of the projection operator and of the heat source $S_H$ are given in Ref. [13]. This source term tends to readjust the temperature profile toward the background profile. Note that small profile variations are still allowed during the simulation. In this work, electrons have been modelled with a simple adiabatic fluid model $\delta n_e \propto (\Phi - \Phi_0)$, $\Phi$ being the axisymmetric component of the electrostatic potential $\Phi$. In the following, we will make use of the following definitions:

- **Radial heat flux** $Q_h \equiv \left\langle \frac{1}{\nabla \psi} \int dW \frac{1}{2} m v^2 \delta f \frac{d\psi}{dt} \right\rangle_{\nabla \mathbf{B}}$
- **Effective heat diffusivity** $\chi \equiv \frac{Q_h}{n \nabla T}$
- **Generalized vorticity** $\Omega \equiv -e \nabla_\perp \left( \sum_{\text{species}} \frac{m_n}{e B^2} \right) \nabla_\perp \Phi = \sum_{\text{species}} e \delta n$
- **Density fluctuation** $\delta n \equiv \int dW \delta f$
temperature fluctuations, \( \delta T \equiv \frac{1}{3} m \left[ \int \mu B dW \delta f + \int v_\parallel^2 dW \delta f - \left( \int v_\parallel dW \delta f \right)^2 \right] \)

where \( \psi \) is the poloidal magnetic flux. Moments are defined according to the prescriptions of the GEM gyrofluid model [18]. The generalized vorticity, expressed as a frequency, is \( \Omega \simeq eB/mD (n_e - n_i)/n_0 \) further details can be found in Ref.[19]. The work presented in this paper is based on a new set of 3D diagnostics implemented in ORB5, allowing for instantaneous measurements of electromagnetic potentials and relevant fluid quantities (density, temperature, vorticity) on a full resolution 3D spatial mesh, making a massive use of parallel I/O. The same set of diagnostics can be used for 3D data visualization.

3. Results

The nonlinear simulations described in this Section are based on parameters and profiles of the ITM Cyclone base case [20]. This is a standard benchmark case based on a circular low-\( \beta \) equilibrium, deuterium plasma, \( \rho^* \simeq 1/185 \) (mid radius), \( T_e = T_D \) and flat initial \( R/L_T \) profiles between \( 0.2 < s < 0.8, s \propto \sqrt{\psi} \). The \( q \) profile is parabolic, matching the local value of the local Cyclone case \( (q = 1.4) \) at mid-radius. A detailed description of the physical parameters and profiles can be found in [20]. Figure 1 shows the results of a scan on the initial temperature gradient, with all the other parameters kept fixed. Those simulations are equivalent in terms of physics and numerical parameters, to the standard ITM global case of Ref. [20], except for the presence of the heat source preventing profile relaxation. The ion heat diffusivity in gyro-Bohm units \( (\chi_{GB} \equiv \rho_c^2 c_s/a, \text{ with } c_s^2 \equiv T_e/mD \text{ and } \rho_c^2 \equiv T_e mD/(eB_0)^2) \) is plotted versus \( R/L_T \), both the quantities correspond to radial averages between \( 0.4 < r/a < 0.6 \). Here it is evident that the heat source prevents profile relaxation but still allows for local modifications of the gradient profile. The solid line represents the original Dimits fit for this curve, derived as a fit to the results of the LLNL gyrokinetic flux-tube PIC electrostatic turbulence code [21]. The ORB5 results follow the Dimits curve, although with lower diffusion coefficients, as expected by global simulations. They also correctly reproduce the linear \( R/L_T |_{\text{lin}} \simeq 4 \) and nonlinear critical thresholds \( R/L_T |_{\text{nonlin}} \simeq 6 \). This is particularly evident when considering the simulation with initial \( R/L_T \simeq 5 \) (dark green in Figure 1): after the initial linear phase, the heat flux drops rapidly to zero, showing that the mode was linearly unstable, but nonlinearly fully stabilized by zonal flow dynamics. The density, temperature, vorticity and potential spectra for a simulation

**Figure 1.** Radial averaged ion heat diffusivities in gyro-Bohm units versus \( R/L_T \) for the Cyclone base case with sources. During the saturation phase, \( \chi/\chi_{GB} \) lies close to the Dimits fit curve.

**Figure 2.** Different time averaged spectra for the initial \( R/L_T \simeq 10.3 \) simulations for the Cyclone base case with sources, calculated from 3D data.
with initial $R/L_T \simeq 10.3$ are presented in Figure 2. Time averaged spectra show evidence of the non-linear cascades to lower $k_\theta \rho_s$. Figure 3 shows, for the same simulation, poloidal cross-sections reconstructed from the 3D diagnostics data.

![Figure 3](image_url)

**Figure 3.** Poloidal cross-sections of different quantities for the initial $R/L_T \simeq 10.3$ simulations, reconstructed from 3D data.

### 3.1. Convergence in number of markers
The simulations with initial $R/L_T \simeq 10.3$ has been chosen for a systematic study of the convergence in number of markers for real space time traces and for the corresponding spectra. The quantities considered are: density fluctuations, electrostatic potential, temperature fluctuations and vorticity. Spectra have been obtained by performing a time average during the saturation phase of the simulation, while real space data correspond to radial averages between $0.5 < r/a < 0.7$. The convergence results are illustrated in Fig.4. For all the quantities considered, non converged time traces correspond to flat spectra at high $k_\theta \rho_s$. On the other hand, converged spectra always exhibit a clear power law down to the highest $k_\theta \rho_s$ values kept in the simulation. The most remarkable result is that not all the physically relevant quantities converge with the same rate. Figure 5 summarizes the results of Fig.4 by normalizing the time averaged quantities to the results of the simulations with the highest number of markers, plotted versus the number of markers per mode kept in the simulation. The number of markers per active mode has been already shown to be the relevant convergence quantity for the ORB5 code [22]. The electrostatic potential converges much faster than all the other quantities. The slowest converging field is the density fluctuation, $\delta n$. Remarkably, the ion heat flux diffusivities (and the heat fluxes) converge as fast as the potential, as it is illustrated in Fig.6. Although the heat flux, important for predicting turbulence induced transport in experiments, requires relatively few markers to converge (20M), comparisons with experimental measurements (for example, with
Figure 4. Time evolution of the radial averaged ($0.5 < r/a < 0.7$) signals (left) and time averaged spectra (right) for density, temperature, vorticity and nonzonal electrostatic potential for the initial $R/L_T \simeq 10.3$ simulations. Non converged time traces correspond to flatter spectra.

Joint Varenna-Lausanne International Workshop 2012 IOP Publishing
Journal of Physics: Conference Series 401 (2012) 012025 doi:10.1088/1742-6596/401/1/012025

Reflectometry data) rely on accurate description of the density fluctuation spectra. According to our results, the latter requires at least a factor of 10 more markers than what convergence studies based on potentials or fluxes suggest.
As a final test for the convergence in number of markers, we have reconstructed the total density, $n$, as the sum over markers of the contribution coming from the background Maxwellian, calculated at the marker position, plus the $\delta f$ contribution given by the marker weights. By binning the contributions of all the markers, it is possible to construct a projection of the total density on a 3D grid. The spectrum of this quantity is shown in red in Fig.7.

The spectrum of the total density is flat, with an amplitude 4 orders of magnitude smaller than the axisymmetric part, (not included in the figure). This level of “noise” is comparable with the amplitude of the density fluctuations described by the markers (in blue on Fig.7), even when 320M markers are used. Although this way of computing $n$ is generally not used by a $\delta f$ PIC code for computation, it is often used for diagnostics purposes. A better way of reconstructing the total density (and temperature) consists in using the analytical expression of the background.

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**Figure 5.** Radial and time averaged quantities of Fig.4, normalized to the 640M marker results, as a function of the number of markers per active mode.

**Figure 6.** Radial and time averaged ion heat diffusivity for the initial $R/L_T \simeq 10.3$ simulations. Dashed lines indicate values of $\pm 10\%$ of the 640M markers simulation.

**Figure 7.** Spectrum of the total density $n$ reconstructed by binning the marker weights ($\delta n$) and the background distribution calculated at the marker position ($n_0$), compared with the spectrum of the density fluctuation.

**Figure 8.** Spectrum of $\delta n$ before and after having filtered the physically irrelevant modes (noise).
distribution (not necessarily Maxwellian) in each bin and adding it to the $\delta f$ contribution coming from the marker weights.

3.2. $\rho^*$ scaling
The same convergence study has been performed for a set of simulations in which only the machine size has been varied, from small devices $\rho^* \sim 46$ to ITER like machines $\rho^* \sim 740$. Previous simulations [22] showed that the convergence in number of markers depends on the ratio of number of markers to the number of active modes included in the field equations. Note that in ORB5 the number of active modes does not correspond to the number of grid points, since in ORB5 field equations are solved on a non field aligned grid. All modes having $k_\parallel$ too large to contribute to the instability, are filter out from the simulation by applying a straight field line Fourier filtering on the right hand side of the field equations [6]. The same filtering procedure is applied to the 3D diagnostics. The effect of the Fourier filtering is shown in Fig.8. Filtering is required to get converged spectra since it reduces the amplitude of the noise (flat part of the unfiltered spectrum) of several orders of magnitude.

The $\rho^*$ scaling shows that the convergence in number of particles per mode is verified for all the values of $\rho^*$. However, the total number of markers also plays a role, due to the intrinsic Monte-Carlo nature of the PIC discretization. Since the number of active modes scale with $(1/\rho^*)^2$, smaller $\rho^*$ require more markers to keep the ratio markers over number of modes constant. On

![Figure 9](image_url)  
**Figure 9.** Top: convergence of $\delta n$ in number of markers per mode for different $\rho^*$ values. Bottom: noise/signal ratio, defined as the ratio of the average background noise to the average signal contained in the active modes.

![Figure 10](image_url)  
**Figure 10.** Different convergence criteria: results are considered converged when $\delta n$ is within $\pm 10\%$ (top) or $\pm 20\%$ (bottom) of the value of the best resolved simulation.
the other hand, more markers also imply a better discretization of the entire phase-space. In other words, the scaling in number of particles per mode holds, but the convergence depends on the machine size: the larger is the system the less particles per mode are needed for convergence. This is shown in Fig.9, top, where $\delta n$, averaged over time and radius, is plotted for different values of $\rho^*$. For each $\rho^*$ a number of simulations with different number of markers has been performed. As a result, ITER size plasma ($\rho^* \simeq 740$) require at least a factor of 2 less markers per mode than present day tokamaks ($\rho^* \simeq 185$). Therefore, the number of markers, and consequently the computational time does not scale with $(1/\rho^*)^2$, as it was predicted by dimensional arguments in the original analysis [23], but because of the statistical process of the PIC method it scales even better than this [24], making ITER size PIC simulations computationally affordable. The two graphs of Fig.9 show that this result holds even when different criteria for defining convergence are applied. Another remarkable result is that all the simulations seem to converge when the signal to noise ratio is around 1%, independent of $\rho^*$ (Fig.9 bottom). Here the signal to noise ratio ($s^2n$) is defined as the inverse of the ratio between the average signal contained in the modes actively contributing to the instability and the average amplitude of the modes having $k_\parallel$ too large to contribute to the instability.

Figure 11 shows radial (left) and time (right) averages of the ion heat diffusion coefficients. The heat diffusivities $\chi/\chi_{GB}$ are relatively small at large $\rho^*$ while they converge, as expected, toward similar values and profiles (at least for $s > 0.4$) for sufficiently small $\rho^*$. Figure 11 (right) also shows the time averaged $R/L_T$ profile. The heating operator prevented profile relaxation at small $\rho^*$. However, a significant relaxation is still present for simulations with larger $\rho^*$, this suggest that the chosen value for the relaxation coefficient, $\gamma_H$, was probably not adequate for those cases.

Figure 11. Spatial (left) and time (right) averages of the heat diffusion coefficients for different values of $\rho^*$. The heat source prevented temperature gradient relaxation only for small $\rho^*$, steady state values are influenced by the different $R/L_T$.

4. Conclusions
The convergence properties of global electrostatic particle-in-cell gyrokinetic simulations have been studied for the Cyclone base case by means of a set of 3D diagnostics originally introduced for visualization purposes. The new diagnostics allowed for high resolutions 3D measurements of electromagnetic potentials, density, temperature and vorticity as well as turbulence spectral analysis. For all the quantities considered, non converged simulations show flat spectra at high $k_\parallel \rho_s$. However, not all the physically relevant quantities converge with the same rate: density fluctuation spectra can still show an unphysical flattening, even when electrostatic potential and heat fluxes are converged. The main results of the $\rho^*$ scaling is that the resolution in terms of
number of markers, required to correctly describe the turbulence density fluctuations, is found to be size-dependent: larger systems (ITER like) require significantly less numerical particles per active mode than smaller systems. Therefore, the number of markers, and consequently the computational time does not scale with $(1/\rho_s)^2$, as it was predicted by dimensional arguments, but even better, making ITER size PIC simulations computationally affordable.

Acknowledgements: simulations were performed on the EFDA HPC-FF (project EMCONS) and IFERC-CSC (project EMFAST) supercomputers

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