Simulations of microturbulence in magnetised plasmas using a delta-f gyrokinetic approach with an evolving background Maxwellian

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Abstract. The gyrokinetic delta-f particle-in-cell (PIC) approach is known to be successful for simulating turbulence in the core of magnetic fusion plasmas, where fluctuations are relatively small and therefore the unperturbed particle distribution function, usually represented by a stationary Maxwellian $f_0$, remains a good choice of a control variate for reducing statistical sampling noise. However, towards the plasma edge, characterized by low density and temperature and strong gradients, relative deviation amplitudes typically become large, so that the essential assumption of $|\delta f/f_0| \ll 1$ underlying the delta-f PIC approach will not be valid, where $\delta f$ is the fluctuating part of distribution. This motivates the study of the limits of the delta-f approach in a simplified system mimicking the plasma edge. To this end, simulations are run using GK-engine, which is a delta-f PIC code that solves the nonlinear gyrokinetic equation in a sheared slab geometry, using B-spline finite elements to represent the self-consistent electrostatic field. Initial radial density and ion temperature profiles exhibiting high logarithmic gradients representing plasma edge conditions are used. In order to avoid practical problems of particles exiting the simulation domain as the ion temperature profile relaxes, all profiles are mirrored at domain-centre and periodic boundary conditions are imposed. The validity of the delta-f approach is measured by statistical noise estimates, while monitoring relative deviation levels of temperature via the kinetic energy. In particular, the effect of background profile gradients on these measures is investigated. As a first step towards reducing the amplitude of the deviation $\delta f$, an adaptive Maxwellian $f_0$ is implemented, whose time dependent temperature profiles are obtained by locally relaxing kinetic energy accumulating in $\delta f$ into $f_0$.

1. Introduction
The success of magnetic fusion energy research relies heavily in our understanding of plasma dynamics. In the most promising reactor concept, the tokamak, plasma is confined by magnetic fields in a toroidal vacuum chamber. A complete description of the plasma involves simulating both the core and the edge.

One of the approaches in simulating plasma is the gyrokinetic Particle-in-cell (PIC) method. The gyrokinetic formalism [1] reduces the number of phase space variables from five to six, representing the plasma as gyrocentres (see for example [10] and [11]), by assuming time and space scale separations. Using Monte Carlo sampling, the PIC method begins by representing an initial distribution function as a collection of numerical particles called ‘markers’, each having its respective weight. Each marker is then integrated along its characteristic through time.
Time-dependent profiles like the density and temperature can be derived by taking various velocity moments of $f$ and projecting them on a spline space. However, due to the statistical nature of this method, it is subjected to numerical sampling noise, which furthermore tends to accumulate over time and will inevitably corrupt moment calculations which are involved in the self-consistent field calculation.

An approach to reduce noise is to further separate the time evolution of $f$ into a stationary background $f_0$ and a time-dependent fluctuating component $\delta f$. This scheme is known as the delta-f scheme, as opposed to the full-f scheme in which $f$ is evolved as a whole. Then, the variance of the markers will be proportional to the relative deviation squared, $|\delta f/f_0|^2$. The interpretation of this method as a control-variate method is discussed in [2]. This scheme works particularly well at the plasma core as relative deviations are low.

However, the simulation of plasma at the edge involves high profile gradients and low density. This will often lead to cases with fluctuations as large as the background, which implies the loss of the delta-f scheme advantage. This would entail using a larger number of markers for reaching a similar noise level. One of the approaches to keep the relative deviations low is to evolve $f_0$ but on a lower time-scale than $\delta f$, where it has been suggested in [7], [8] and [9], for example. This work explores the implications of a specific instance of this approach. Namely, to have a time-evolving background by constraining $f_0$ to be a flux-surface-averaged (f.s.a) Maxwellian with a time-dependent temperature profile.

To that end, the source code used is the GK-engine [5], which models a collision-less electrostatic plasma consisting adiabatic electrons and a single ion species of equal and opposite charge represented by $f$, under a sheared-slab geometry. The self-consistent potential is presented by third-order B-splines. A review of such a scenario is given for example in [3]. All results follow from the application of this code to simulation of an Ion Temperature Gradient (ITG) instability.

This paper is organised as follows: section 2 describes the adaptive scheme used, section 3 the user-defined profiles used as input to all simulations, section 4 introduces measures to gauge the performance of the adaptive scheme, and section exhibits the results.

2. The adaptive scheme

All following definitions and notations are identical to that from [5], with relevant variables repeated here for completeness.

Let the phase space coordinates $\vec{Z} = (x, y, z, v_\parallel, \mu)$ represent the radial, poloidal, toroidal, parallel velocity and magnetic moment respectively. The flux-surfaces in this sheared-slab geometry are labeled by $x$, with the magnetic field pointing mainly in the $z$ direction, $B(x, y, z)\hat{b} = B_y(x)\hat{e}_y + B_z\hat{e}_z$, where $B_y$ is prescribed by the user-defined safety factor profile $q(x) = \frac{L_yB_z}{L_zB_y}$. Here, $L_i$ is the domain length of the $i^{th}$ dimension, a constant. Under the delta-f scheme, ion distribution is split into background and fluctuating parts:

$$f(t, \vec{Z}) = f_0(t, x, v_\parallel, \mu) + \delta f(t, \vec{Z}).$$

(1)

Here, the time variable $t$ is made explicit in the framework of the adaptive scheme. The $y$ and $z$ independence of $f_0$ is a constraint made in this work, and therefore the f.s.a $f_0$ takes the form of

$$f_0(t, x, v_\parallel, \mu) = \frac{n_{i0}(x)}{(2\pi T_{i0}(t, x)/m)^{3/2}} \exp \left(-\frac{mv_\parallel^2}{2 + \mu B(x)}\right),$$

2
where the user-defined f.s.a. profiles \( n_{i0}(x) \) and \( T_{i0}(0, x) \) represents the gyro-centre density and initial background ion temperature respectively.

The time evolution for \( T_{i0}(t, x) \) is given by a relaxation formula as follows,

\[
\frac{\partial}{\partial t} \left( \frac{3}{2} n_{i0}(x) T_{i0}(t, x) \right) = \alpha_E \left( \int \frac{2\pi B^*}{m} \left( \frac{1}{2} mv^2_{\parallel} + \mu B \right) \delta f \, dv_{\parallel} \, d\mu \right)_{f.s.a.},
\]

with \( m \) the ion mass, \( B^*(x) = B\left(1 + \frac{B'_y B'_z}{B^2} v_{\parallel}^2\right) \), \( B^2 = B_y^2 + B_z^2 \), \( e \) the electric charge, and \( <.>_{f.s.a} \) the flux-surface-averaging operator. Here, \( \alpha_E \) is a user-defined relaxation rate, and the left-hand side can be interpreted as the time derivative of the background f.s.a kinetic energy, given by

\[
E_{\text{kin}0}(t, x) = \frac{3}{2} n_{i0}(x) T_{i0}(t, x).
\]

Due to the time-independence of \( n_{i0}(x) \), \( E_{\text{kin}0} \) will be the variable instead of \( T_{i0} \), that will be used for the rest of this paper to study the effects of the adaptive scheme.

The fluctuation \( \delta f \) in eq. (1) is represented by a sample of \( N_p \) markers, with respective weights \( w_p \):

\[
\delta f(t, \vec{Z}) \approx \sum_{p=1}^{N_p} \frac{1}{J(x_p(t), v_{\parallel p}(t))} w_p(t) \delta(\vec{Z} - \vec{Z}_p(t)).
\]

where

\[
J(x, v_{\parallel}) = \frac{2\pi B^*(x, v_{\parallel}(t))}{m}
\]

is the jacobian of gyro-centre variables.

3. Initial flux-surface-averaged profiles

To simulate profiles with high gradients, the source code accepts user-defined f.s.a 3-parameter profiles for \( n_{i0}, T_{i0} \) and \( T_e \), with the latter corresponding to the electron temperature. The dimension-less parameters are \( A, \kappa \) and \( \Delta \), where \( A \) is the amplitude at slope centre, (see figures 1 and 2, ) \( \kappa \) is the maximum value of the absolute logarithm gradient of an arbitrary profile \( g \), expressed in normalised radial distance coordinate \( x/a = s \in [0, 1] \) as

\[
\kappa = \max_s \left| \frac{\partial \ln g(s)}{\partial s} \right|,
\]

and \( \delta \) measures the half-width of the slope, outside of which the profile has zero gradient. The explicit form of a profile \( g(s, \kappa, \Delta) \) is

\[
g(s, \kappa, \Delta) = \begin{cases} 
A \exp \left( \frac{2\kappa \Delta}{3} \right) & 0 \leq s < 0.5 - \Delta \\
A \exp \left( -\kappa(s - 0.5) + \frac{\kappa(s-0.5)^3}{3\Delta^2} \right) & |s - 0.5| \leq \Delta \\
A \exp \left( -\frac{2\kappa \Delta}{3} \right) & 0.5 + \Delta < s \leq 1
\end{cases}
\]

This particular profile is chosen to exhibit quadratic logarithmic gradients for smoothness, with highest absolute value, \( \kappa \), at \( s = 0.5 \). Also, \( g(0.5, \kappa, \Delta) = A \). Such a monotonically decreasing profile is used to mimick, for example, the density at the plasma edge.

However, it is observed that for long integration times, despite having a Dirichlet boundary conditions for the potential which is set to \( \phi = 0 \), markers tend to drift towards and accumulate
at the radial edge $s = 0$ and $s = 1$. Since the equation of motion for the guiding centre eq. (5),
with $< \cdot >$ being the gyro-averaging operator, should indeed result to a zero right-hand side, we
attribute this marker accumulation to numerical inaccuracies of the time integrator.

\[
\frac{d\vec{R}}{dt} = v_{||}\hat{b} + \frac{\mu}{B^*}\hat{b} \times \nabla B + \frac{1}{B^*}\hat{b} \times \nabla <\phi>
\] (5)

So as not to be concerned by how one should treat such accumulating markers, we have
decided on mirror-symmetrising the profile by duplicating the slope with reversed parity, and
impose periodic boundary conditions for the radial direction, which applies to both the potential
and markers. The periodicity of the potential, which does not necessarily equals to zero at the
edge, prevents marker accumulation. This mirroring operation also preserves all amplitudes,
gradients and widths of slopes of the original profile, so that measures like $\kappa$ and $\Delta$ remain
unchanged. Such a profile, before and after mirroring, is illustrated in figures 1 and 2.

![Figure 1. Initial 3-parameter profile.](image1)

For this case, amplitude is $A = 1$, peak absolute log-gradient $\kappa = 16$ at slope centre $s = 0.5$, and slope half-width $\Delta = 0.2$.

![Figure 2. Mirrored profile of figure 1, with values and gradients preserved.](image2)

Slope centres are now at $s = 0.25$ and $s = 0.75$. Only profiles of this form have
been used in simulations.

All radial profiles in this work have been mirrored. Since all fluctuation measures to be
discussed in the next section are generally symmetric about middle, $s = 0.5$, only the left halves
of profiles will be henceforth displayed.

4. Deviation measures

Since we are adapting $T_{i0}$, or equivalently, $E_{kin0}$, the effectiveness of the adaptive scheme will
be measured by the associated relative deviation. Let the f.s.a. $E_{kin}$ be decomposed into
background and deviation contributions respectively,

\[
E_{kin}(t, x) = E_{kin0}(t, x) + \delta E_{kin}(t, x),
\]

where

\[
E_{kin0}(t, x) = \frac{3}{2} n_0(x) T_{i0}(0, x) + \sum_j \xi_j(t) \Lambda_j(x),
\] (6)

\[
\delta E_{kin}(t, x) = \sum_{i,j} \left( \sum_p w_p(t) \left( \frac{mv_p^2}{2} + \mu_p B(x_p(t)) \right) M_{ij}^{-1} \Lambda_j(x_p(t)) \right) \Lambda_i(x).
\] (7)
Here, the background term $E_{\text{kin0}}$ has been split into a stationary and a time-dependent part represented by a B-spline expansion with time-dependent coefficients $\{\xi_j(t)\}_j$, with $\Lambda_j(x)$ the $j^{th}$ B-spline in the radial dimension. The $M_{ij}$ matrix element present in eq. (7) is its corresponding 'mass matrix', given by

$$M_{ij} = \int \Lambda_i(x)\Lambda_j(x) \, dx.$$  

Eq. 7 is acquired by projecting the appropriate velocity moments of eq. (3) onto a B-spline basis $\{\Lambda_i(x)\}_i$.

In order to measure the effect of the adaptive scheme, the kinetic energy relative deviation will be used, and it’s defined by

$$\tilde{E}_{\text{kin}} = \frac{\delta E_{\text{kin}}(t,x)}{E_{\text{kin0}}(t,x)}.$$  

This measures the relative contributions from the background and perturbed distributions respectively, in the calculation of the kinetic energy.

The relative deviation for the gyro-centre density $n(t, x)$ can be similarly defined, by replacing the term $\frac{m v_n^2}{2} + \mu_B B(x, t)$ in eq. (7) by the factor 1. Since the background density profile is not evolved here, it will not be shown in this paper.

Next, following [6], the measure of the mean of the squared weights over the markers, $<w^2>$, along with the weight standard deviation value, $\sigma_w = \sqrt{<w^4> - <w^2>^2}$, are used to estimate noise.

5. Simulation

The tokamak plasma modeled has aspect ratio $R_0/a = 3.667$. All length and time units are normalised to the minor radius $a$ and minor radius over ion sound speed $a/c_s$ respectively. The magnetic field on axis $B_z(s = 0)$ is set equal to $B_0 = 1$Tesla and the magnetic shear is set by the safety factor

$$q(s) = \begin{cases} 1.25 + 12 s^2 & 0.0 \leq s < 0.5 \\ 1.25 + 12(1 - s)^2 & 0.5 \leq s \leq 1.0 \end{cases}.$$  

The spatial resolution is $(N_x \times N_y \times N_z) = (256 \times 1024 \times 256)$ grid-points. Each simulation is initialised with 256M markers and a small $(m, n) = (-16, 8)$ mode density perturbation, where $m$ and $n$ is the poloidal and toroidal mode numbers respectively. The simulation is then evolved to a final time of $t_{\text{final}} = 150a/c_s$ with time-step $\Delta t = 0.15a/c_s$.

The initial radial profiles of $T_e(s)$, $T_i(s)$ and $n_{i0}(s)$ have the functional form of eq. (4), with all amplitudes such that $T_e = T_i = n_{i0}$ at slope centre $s = 0.5$. The slope widths are fixed at $\Delta T_e = 0.1$, $\Delta T_i = 0.2$ and $\Delta n = 0.3$ respectively. The electron temperature’s peak logarithmic gradient is fixed at $\kappa_{T_e} = 1.0$. As for the logarithmic gradients of $T_i$ and $n_{i0}$, their respective $\kappa$’s are set such that $\eta_h = \frac{\kappa_{T_i}}{\kappa_{n_{i0}}} = 2$ to ensure instability of the slab-like ITG mode, which requires $\eta_i > 1$.

Eq. (2) is evolved at every time-step $\Delta t_{\alpha} = K \Delta t$ for some integer $K$, with a given value of $\alpha_E$. The coefficients $\xi_j(t_i)$ from eq. (6) at time $t = t_i$ is updated to its new value at $t = t_i + \Delta t_{\alpha}$ with a forward Euler fashion according to

$$\xi_j(t_i + \Delta t_{\alpha}) = \xi_j(t_i) + \Delta t_{\alpha} \frac{1}{K} \sum_{k=1}^{K} \xi_j \left( t_i + k \frac{\Delta t}{\Delta t_{\alpha}} \right),$$  

where $\dot{\xi}_j$ is evaluated by inserting eq. (6) into eq. (2), and the increment to $\xi_j$ is done in a time-averaged manner to remove small time-scale fluctuations.
From the range of $\kappa_{Ti}$ chosen in this study, with the choice of $\Delta t_{\alpha} \sim a/c_s$ to match the relaxation rate of profiles, the fact that the relation

$$\alpha_E \Delta t_{\alpha} \leq 1$$

must always be satisfied to ensure numerical stability means that the relaxation rate must then be $\alpha_E \sim 10^{-1} c_s/a$.

Figure 3 shows the relative deviation of the kinetic energy without an adaptive scheme and thus will be used as reference. The assumption of $|\delta f|/|f_0| \sim$ small is violated here as the deviation component $\delta E_{kin}$ is of the same order of the background contribution $E_{kin0}$. This is due to the fact that the final ion temperature $T_i$ deviates the most from its initial value at around $s = 0.25$, as will be shown in figure 13.

It is observed in figure 4 that with less frequent update, $\tilde{E}_{kin}$ exhibits ‘saw-teeth’ like time evolution, with sharp decreases at times when the $\delta f$ part has been transferred to the $f_0$ part when taking the velocity moment to calculate the kinetic energy. However, by example of figure 9, the improvement for $\tilde{E}_{kin}$ is not sensitive to $\Delta t_{\alpha}$. The insensitivity to $\Delta t_{\alpha}$ also applies to noise measures of $<w^2>$ and $\sigma_w$, which are not shown in this paper. From figures 11 and 12, these noise measure cease to improve for values greater than $\alpha_E = 0.2 c_s/a$. This can be explained by the typical time scale of figure 8 (left), which is about $t \approx 30 a/c_s$. This corresponds a physical evolution time $t_{evol} \approx 30 a/c_s$ and a corresponding maximum of $\alpha_E \approx 0.3 c_s/a$, beyond which there is nothing to be gained from a higher relaxation rate. The same explanation applies to the case for $\sigma_w$.

**Figure 3.** Relative fluctuation of kinetic energy $\tilde{E}_{kin}$ without adaptive scheme.

**Figure 4.** $\tilde{E}_{kin}$ under adaptive scheme: $\Delta t_{\alpha} = 7.5 a/c_s$, $\alpha_E = 0.07 c_s/a$. 
Figure 5. $\tilde{E}_{\text{kin}}$ under adaptive scheme: $\Delta t_\alpha = 1.5a/c_s$, $\alpha_E = 0.07c_s/a$.

Figure 6. $\tilde{E}_{\text{kin}}$ under adaptive scheme: $\Delta t_\alpha = 1.5a/c_s$, $\alpha_E = 0.27c_s/a$.

Figure 7. Mean squared weights $< w^2 >$ binned in radial direction, without (left) and with (right) the adaptive scheme with parameters: $\Delta t_\alpha = 1.5a/c_s$, $\alpha_E = 0.07c_s/a$.

Figure 8. Weight standard deviation, $\sigma_w$ binned in radial direction, without (left) and with (right) the adaptive scheme with parameters: $\Delta t_\alpha = 1.5a/c_s$, $\alpha_E = 0.07c_s/a$. 
As verification, the final $T_i$ profiles of simulations with and without the adaptive scheme are shown in figure 13. The error bars are calculated from the standard deviation obtained from running around twenty simulations with different random sequences for the markers’ initial phase space coordinates. There, it is seen that all final $T_i$ profiles overlap within three standard deviations. As it can be seen in figure 13, the error bars for the adaptive scheme tend to be larger than the reference case in blue, apparently defeating the purpose of the introduction of the adaptive scheme to reduce noise.
Figure 13. Top: final $T_i$ profile averaged over a time window of $t \in [141.6, 150.6] a/c_s$. Middle: corresponding change of $T_i$ from the initial. Bottom: corresponding final negative logarithmic gradient. For each data point, the error bars represent 3 standard deviations evaluated at the same $s$ values with around 20 samples, but shifted slightly for illustration purposes.

As possible explanation of the large error bars could be due to the thus far neglected final term in the linearised quasi-neutrality equation, eq. 8.

$$\frac{e n_0}{T_e} (\phi - \phi_{00}) - \nabla_\perp \cdot \left( \frac{m n_0}{e B^2} \nabla_\perp \phi \right) = \frac{1}{2\pi} \int f(t, \vec{Z}) \delta(\vec{r} - (\vec{R} + \vec{p}_L(\mu, \alpha)))J d\mu dV || d\alpha - n_0$$

$$= \frac{1}{2\pi} \int \delta f \delta(\vec{r} - (\vec{R} + \vec{p}_L))J d\mu dV || d\alpha$$

$$= \frac{1}{2\pi} \int (f_0 - f_{00}) \delta(\vec{r} - (\vec{R} + \vec{p}_L(\mu, \alpha)))J d\mu dV || d\alpha$$

(8)
where $e$ is the electronic charge, $T_e$ the user-defined electron temperature profile, $\phi_{00}$ the f.s.a. function of the potential $\phi$, $\vec{r} = (x, y, z)$ the position vector, $\vec{\rho}_L$ the larmor radius vector, and $f_{00}(x, v_{||}, \mu) = f_0(0, x, v_{||}, \mu)$ the background distribution at initial time. The last term can be shown to be of order $O\left(\frac{\rho_L L}{L}\right)^2$, with $L$ the typical profile length scale. With high $\kappa_{Ti} = \frac{a}{T_i}$ values, this term is predicted to becoming more important. The inclusion of the former is nonetheless necessary in order to solve the equivalent mathematical problem like that of the non-adaptive case. Investigations in to the effects of this term’s inclusion will need to be conducted in a future work.

6. Conclusion

After mirror-symmetrising radial profiles to avoid markers accumulating at the radial domain edges, the mechanism of an adaptive ion temperature profile from a background local Maxwellian distribution is shown. This is indirectly done via the kinetic energy due to ease of separation between background and fluctuation components.

The adaptive scheme presented in this paper is parametrised by two user-defined parameters. The first is the relaxation rate which needs to be high enough to evolve the background fast enough to accommodate the physical evolution of the profiles ($\alpha E_{t_{\text{evol}}} > 1$). It is shown that the kinetic energy relative deviation decreases exponentially with increasing relaxation rate. The second parameter is the numerical frequency of update. It is shown that this frequency has a limited impact on the level of relative deviation provided that $\alpha E \Delta t_{\alpha} < 1$.

Noise, measured by variance in weights, is shown to be reduced only by a small value. This is due to the inherent long time-scales of the noise accumulation. Finally, the adaptive scheme is validated against the non-adapted ion temperature profile at a final time. As figure 13 shows, at 3-standard deviation errors, all curves overlap. The observation of the error bars of the adaptive cases being generally larger than that of the non-adapted case could be due the a neglected term of order $O\left(\frac{\rho_L L}{L}\right)^2$.

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