Development of a Grid-Based Gyro-Kinetic Simulation Code

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Abstract. The 4D Semi-Lagrangian code CYGNE for solving electrostatic drift-kinetic equations is presented. The code simulates well the linear phase. In the non-linear, phase development of negative value regions are investigated.

INTRODUCTION

Microturbulence is thought to play a key role in energy transport in thermonuclear fusion devices based on magnetic confinement. Its simulation in the frame of the 5 dimensional gyrokinetic equations represents a challenging numerical problem. As a first step toward the treatment of the 5D system in toroidal geometry, a 4D code, CYGNE [1], is being developed for solving the electrostatic drift-kinetic equations in cylindrical geometry. This code uses a semi-Lagrangian approach based on cubic spline interpolation. In this approach the distribution function f is computed on a fixed grid and is updated from time $t-\Delta t$ to time t using its invariance along particles trajectories. One of the main advantages of this method is that it provides a grid description of f, with no stability restriction on the time step such as the Courant Friedrichs Lewy condition. The code simulates well the linear phase. In the non-linear regime however, when fine scale structures start to appear, simulations exhibit development of negative value regions of the distribution function, as well as bad energy conservation, which are investigated in this paper.

PHYSICAL MODEL

A periodic cylindrical plasma of radius a and length L is considered. The plasma is confined by a uniform magnetic field of the form $\mathbf{B} = B_0\mathbf{e}_z$, where $\mathbf{e}_z$ is the unit vector along the z direction.
The equations of motion for the guiding centers of the ions in cylindrical coordinates (r,θ,z) are given by

$$\dot{\mathbf{R}} = v_{\|}\mathbf{e}_z + \frac{\mathbf{e}_z \wedge \nabla\phi}{B_0} = v_{\|}\mathbf{e}_z + \mathbf{v}_{GC} \quad (1)$$

$$\dot{v}_{\|} = -\frac{q_i}{m_i}\,\mathbf{e}_z \cdot \nabla\phi \quad (2)$$

where $q_i = Z_i e$ and m_i are the ion charge and mass, respectively, $\mathbf{v}_{GC}$ is the guiding center drift velocity, and ϕ is the electrostatic potential.

Neglecting finite Larmor radius effects, the time evolution of the ion guiding center distribution function $f(\mathbf{R}, v_\parallel)$ is governed by the drift-kinetic equation (DKE) :

$$\frac{\partial f}{\partial t} + \mathbf{v}_{GC} \cdot \nabla_\perp f + v_\parallel \frac{\partial f}{\partial z} + \dot{v}_\parallel \frac{\partial f}{\partial v_\parallel} = 0 \tag{3}$$

Assuming adiabatic electrons bound to the field lines, and including the linearised polarisation-drift term, the quasi-neutrality equation is given by:

$$-\nabla_\perp \cdot \left[\frac{n_0(r)}{B_0 \Omega_i} \nabla_\perp \phi(\mathbf{R},t) \right] + \frac{e n_0(r)}{T_e(r)} [\phi(\mathbf{R},t) - \bar{\phi}(\mathbf{R},t)] = \int f(\mathbf{R}, v_\parallel)\, dv_\parallel - n_0(r) \tag{4}$$

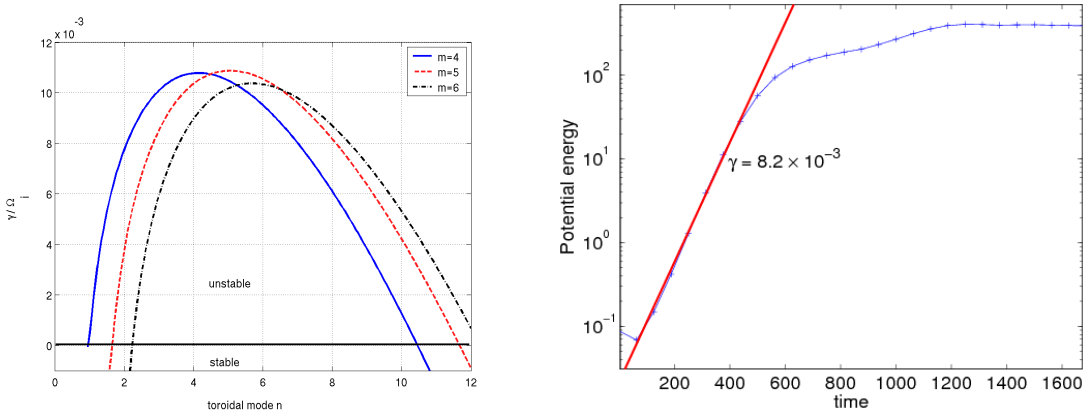
where $\Omega_i = q_i B_0 / m_i$ is the ion cyclotron frequency, n_0 and T_e are the initial density and electron temperature profiles, and $\bar{\phi}$ is the average of the electrostatic potential along the magnetic field lines given by $\bar{\phi}(r,\theta,t) = (1/L) \int_0^L \phi(r,\theta,z,t)\, dz$.
Equation (3) and (4) conserve the total energy, defined as $E_{tot} = E_{kin} + E_{pot}$ with

$$E_{kin} = \int \frac{1}{2} m_i v_\parallel^2 (f - f_{eq})\, d\mathbf{R}\, dv_\parallel \quad \text{and} \quad E_{pot} = \frac{1}{2} q_i \int (f - f_{eq}) \phi\, d\mathbf{R}\, dv_\parallel \tag{5}$$

where f_{eq} is the equilibrium part of f.

THE NUMERICAL SCHEME

A detailed description of the numerical scheme can be found in [1]. In summary, the code is based on the semi-Lagrangian approach, the 4D distribution function f is represented on a fixed grid in phase space. f is evaluated from time $t - \Delta t$ to time t by invoking its invariance along trajectories. More specifically, f is updated at grid point x_i using the relation : $f(x_i,t) = f(X(t-\Delta t, x_i, t), t - \Delta t)$, where $X(t-\Delta t, x_i, t)$ is the position at time $t - \Delta t$ of the trajectory that ends up on x_i at time t. This operation requires an interpolation of $f(t - \Delta t)$ which is performed with cubic splines.
A time-splitting technique is used to solve the DKE (3) with a sequence $S = (\hat{v}_\parallel/2)\ (\hat{z}/2)\ \hat{Q}\ \widehat{r\theta}\ (\hat{z}/2)\ \hat{Q}\ (\hat{v}_\parallel/2)$, where $\hat{v}_\parallel, \hat{z}, \widehat{r\theta}$ denote the advections in $v_\parallel$, z and r-θ plane, respectively, and $\hat{Q}$ denotes the solution of the quasi-neutrality equation (4). The advection in $\widehat{r\theta}$ must in fact be carried out simultaneously with the update of the self-consistent field ϕ and thus involves additional $\hat{Q}$ operations. This is achieved here with a predictor-corrector approach ensuring 2^{nd} order time accuracy, with the field ϕ being updated after the predictor step. The interpolations are performed using cubic splines.
The quasineutrality equation (4) is solved in Fourier space along θ and z, and using cubic spline finite elements method in the r direction.



(a) (b)

FIGURE 1. (a) linear growth rate from the local dispersion relation - (b) Potential energy growth, CYGNE

NUMERICAL RESULTS AND NEGATIVE VALUES STUDY

In the following, the system parameters are : $a = 14.5\rho_s$, $L_\theta = 2\pi$, $L_z = 1508\rho_s$ and $v_{\|max} = 6.1 v_{thi0}$, where $\rho_s = \sqrt{T_e(r_{peak})/m_i}/\Omega_i$, $T_{i0} = T_i(r_{peak})$ and $v_{thi0} = \sqrt{T_{i0}/m_i}$. The electron temperature is assumed uniform, while the ion temperature profile is defined by the functional form :

$$\frac{dlnT_i}{dr} = -\frac{\kappa_{T_i}}{a} cosh^{-2}\left(\frac{r - r_{peak}}{\Delta r_{T_i} a}\right) \tag{6}$$

with parameters $\kappa_{T_i} = 4$, $\Delta r_{T_i} = 0.1$, $r_{peak} = 0.5a$ and the ion density is initially constant. The time t is given in units of $\Omega_i = q_i B_0/m_i$. The grid is $N_r \times N_\theta \times N_z \times N_{v_\|} = 64 \times 64 \times 64 \times 64$ and $\Delta t = 2.5\ /\Omega_i$.
To validate the linear phase, we compare results from CYGNE with the numerical solution to a local dispersion relation computed using parmeters at $r = r_{peak}$. At this position the temperature gradient is the strongest, therefore the local growth rate is expected to be somewhat higher than the one found in the global simulation. With the local relation, the most unstable mode is found to be $(m = 4, n = 4)$, Fig. 1.a., with a growth rate of $\gamma = 10.3 \times 10^{-3}$, which is in good agreement with the result from CYGNE where we find a global growth rate for the potential energy of $\gamma = 8.2 \times 10^{-3}$ Fig. 1.b. In addition the code has been benchmarked against the linear code LORB5 [1].

In the non-linear regime negative values appear in the $(z, v_\|)$ plan, in the region $|\ v_\|\ | > 2v_{\text{th}}$, Fig.2, where $|f/f(v_\| = 0)| \ll 1$. The amplitudes of these negative values are largest in the region $2.2v_{\text{th}} \leq |\ v_\|\ | \leq 4v_{\text{th}}$, close to the position where the equilibrium gradients are strong.

The contributions of the negative part of the distribution function to the density is not very large : 0.1% at most in this case, Fig. 3.i.a.. However one can see that overshoot

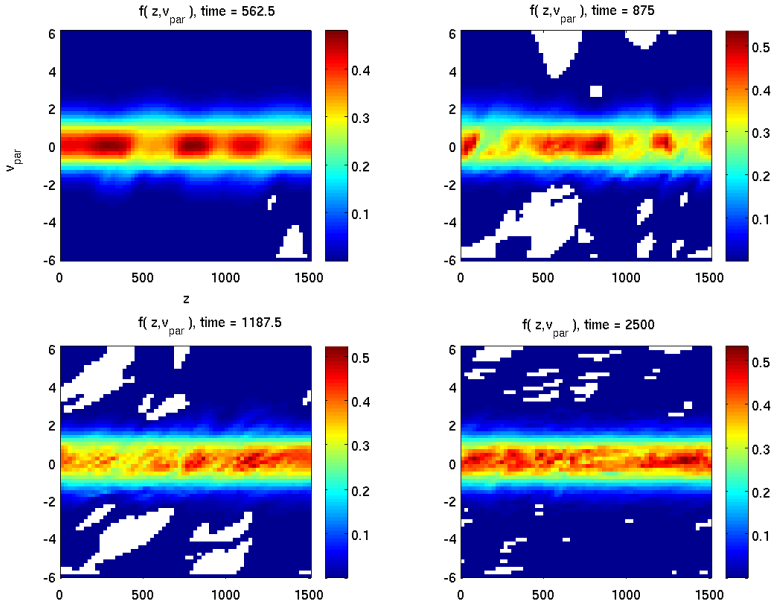
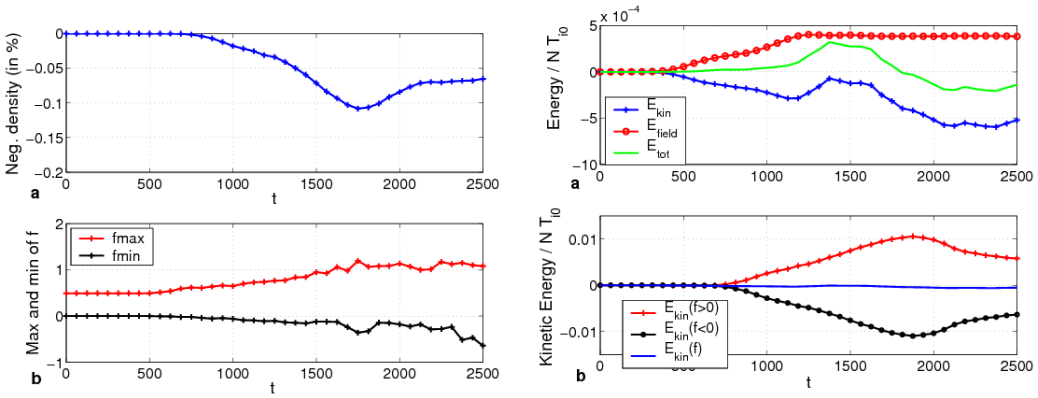


FIGURE 2. $(z, v_{\|})$ cross section of the distribution function at $(r = r_{peak}, \theta = 2\pi/3)$, negative values appears in white



(i) (ii)

FIGURE 3. (i.a.) Contribution of the negative part of f to the density, (i.b.) minimum and maximum of f - (ii.a.) Kinetic, potential and total energy,(ii.b) Contribution of the negative and positive part of f to the kinetic energy.

and undershoot are increasingly growing all over the run, Fig. 3.i.b.

In addition, since the kinetic energy is a second order moment of the parallel velocity and negative values concentrate in region of high $v_{\|}$, their contribution to this quantity rapidly become non negligible, Fig. 3 ii.b. - the contribution of the negative part of f to

the kinetic energy is defined as :

$$E_{kin}(f<0) = \int_{f<0} \frac{1}{2} m_i v_{\|}^2 (f - f_{eq})\, d\mathbf{R}\, dv_{\|} \tag{7}$$

After t=600, the total kinetic energy is the sum of a very large contribution from the positive part of f and from its negative part. For t=1000, the negative contribution to the kinetic energy is already one order of magnitude greater than the total kinetic energy. Note that the conservation of the total energy breaks down somewhat later at t=1200 Fig. 3 ii.a., showing that the simulation cannot be considered relevant from this point on.

The code CYGNE is based on a sequence of 1d advections, in z and in $v_{\|}$ directions, and 2d advections in (r,θ), which in the Semi-Lagrangian frame require an interpolation of f. These interpolations are performed using cubic splines which may introduce spurious oscillations through the Gibbs phenomena in regions where there is a discontinuity or a steep gradient. This happens in the non-linear regime when small scale structures develop , Fig. 4. In regions where $|f/f_{max}| \ll 1$ these oscillations lead to negative values.

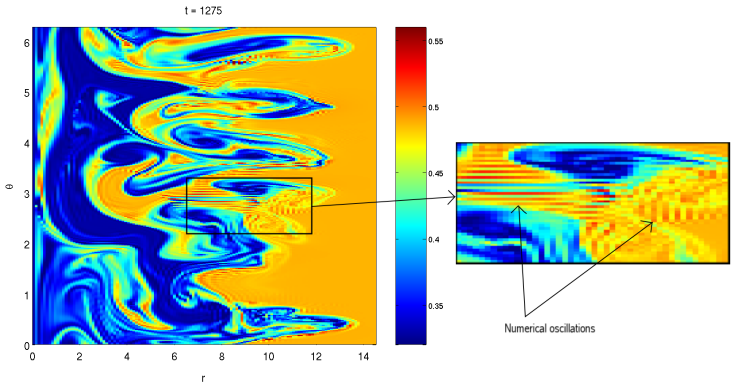


FIGURE 4. (r,θ) cross section, at $t = 1275$, grid : $128 \times 256 \times 128 \times 64$, $\Delta t = 0.5, z = 1/3L_z$

For the 1d advections it is possible to replace in the code the spline interpolation by a finite volume based scheme call Positive and Flux Conserving (PFC) method [2] which, using slope limiters, guarantees that the maximum and minimum values will not increase or decrease respectively. Fig. 5 a. shows the evolution of the negative values for the scheme with PFC method and cubic spline interpolation for the advection in z $v_{\|}$ direction. The PFC method reduces the development of negative values, as reflected by the decrease of the contribution of the negative part of f to the kinetic energy, however they still appear, which leads to the conclusion that the advection in (r,θ) is also a source for the negative values.

The phenomena is reduce when using more grid points Fig. 5. b. ii. Indeed with a finer grid the small scale structures are better resolved. On the contrary a smaller time step will increase the number of negative values, Fig. 5. b. i., since more interpolation steps are performed in this case to reach a given time.

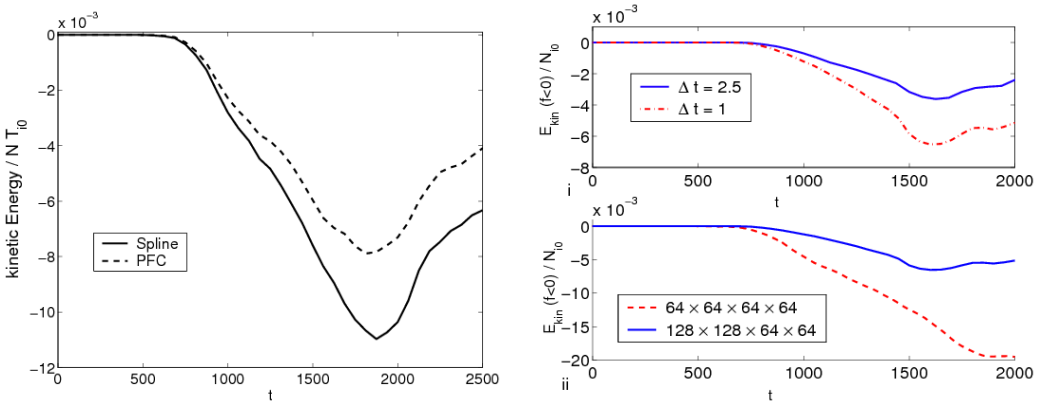


FIGURE 5. Contribution of the negative part of f to E_{kin} (a) PFC scheme and spline interpolation - (b) Convergence studies

CONCLUSION

The 4-D Semi-Lagrangian code CYGNE, solving the electrostatic drift-kinetic equations in cylindrical geometry, has been presented. It has shown a good description of the linear phase. In the non-linear regime, the development of negative value regions has been investigated. These negative values reflect a more general problem, namely the generation of spurious oscillations, which appear when fine scale structures develop. Such overshoots are inherent to the cubic spline interpolation step and results in the degradation of the simulation. The phenomena is reduced when using a finer grid but is increased with a smaller time step.

Some alternative scheme might be needed if one intends to carry out long time simulations. The Positive and Flux Conserving (PFC) method [2] has shown to be able to decrease the negative values, and some other scheme are under study such as the Essentially Non Oscillatory (ENO) scheme [3].

Finally, the physical case studied here corresponds to a strongly driven instability (large $\eta_i = dlnT_i/dlnN_i$) and some preliminary tests show that negative values are reduced for weaker driven cases (smaller η_i). further investigations are thus still to be done in that direction.

REFERENCES

1. M. Brunetti, V. Grangirard, O. Sauter, J. Vaclavik, and L. Villard. A semi-lagrangian code for nonlinear global simulations of electrostatic drift-kinetic itg modes. *Comput. Phys. Com.*, 163(1):1–21, 2004.
2. Francis Filbet, Eric SonnendrÃijcker, and Pierre Bertrand. Conservative numerical schemes for the vlasov equation. *J. Comput. Phys.*, 186(2):457–480, 2003.
3. C.W. Shu. Essentially non-oscillatory and weighted essentially non-oscillatory schemes for hyperbolic conservation laws. *Technical Report NASA CR-97-206253 ICASE Report No. 97-65*, 1997. Institute for Computer Applications in Science and Engineering.