EUROFUSION WP15ER-PR(16) 16767

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Preprint of Paper to be submitted for publication in
Physics of Plasmas

This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the Euratom research and training programme 2014-2018 under grant agreement No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

Mitigation of the cancellation problem in the gyrokinetic particle-in-cell simulations of global electromagnetic modes

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(Dated: November 18, 2016)

Abstract

Electromagnetic gyrokinetic particle-in-cell simulations have been inhibited for long time by numerical problems. This paper discusses the origin of these problems. It also gives an overview and summary of the mitigation techniques.

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I. INTRODUCTION

There is a large number of cases in fusion plasmas in which electromagnetic kinetic effects are of importance. These include Alfvén eigenmodes, reconnection, anomalous transport caused by electromagnetic drift microinstabilities etc. The characteristic frequencies of all these phenomena are smaller than the gyrofrequency. Therefore, gyrokinetic theory [1] can be applied. A potential benefit is a substantial reduction of the computational cost of the simulations.

In some cases a further reduction of the description is possible using, for example, local flux-tube simulations [2, 3], or the truncated fluid-electron scheme [4, 5], or the hybrid kinetic MHD (Magneto-Hydrodynamics) [6]. However, often it is necessary to assess the electron kinetics, such as trapped-electron effects, or non-adiabatic electron dynamics at resonant flux surfaces. This has to be done using fully gyrokinetic computations for all species. Global effects can also be of importance. For example, they are important in the interplay of global physics, e. g. MHD modes, and microturbulence, which is believed to affect the nonlinear evolution of the Alfvén Eigenmodes in toroidal geometry, sawtooth oscillations, neoclassical tearing modes, etc.

Unfortunately, global gyrokinetic electromagnetic simulations suffer from numerical problems. The $v_\parallel$-formulation of the electromagnetic gyrokinetic theory is difficult to implement using an explicit time solver. This was observed for the first time in 1992 by Reynders [7]. The $p_\parallel$-formulation does not have this problem. Therefore, it is nearly always used in electromagnetic gyrokinetic codes of all types (Eulerian, particle-in-cell, and semi-Lagrangian). However, there is a price to pay, the so-called cancellation problem [8]. This problem was first observed with a particle-in-cell code by Cummings [9] in 1995. As a consequence of the cancellation problem, electromagnetic gyrokinetic simulations have been limited to the very-low-beta cases $\beta < \sqrt{m_\mathrm{e}/m_\mathrm{i}}$, see Ref. [10]. The cancellation problem has been addressed within the particle-in-cell framework in Refs. [11–14] and using the Eulerian approach in Ref. [15]. Due to the progress made in understanding the numerical issues inhibiting the electromagnetic gyrokinetic codes, it has become possible to simulate Alfvénic physics using the global gyrokinetic particle-in-cell code GYGLES: Toroidal Alfvén Eigenmodes (TAE) [16–19], Global Alfvén Eigenmodes [16], the internal $m = 1, n = 1$ kink mode and $m = 1, n = 1$ reconnecting modes [20]. Later on, another approach to the mitigation of the cancellation

problem has been developed [21]. This approach is based on the so-called mixed-variable formulation [22] of the gyrokinetic theory. Further understanding of the mixed-variable mitigation has been achieved in Ref. [23]. The global particle-in-cell code EUTERPE [24] has been used in the papers [21–23]. Recently, a number of simulations have been performed addressing the Alfvénic physics, both in the linear and nonlinear regimes, using the gyrokinetic EUTERPE [25–27] and ORB5 [28, 29] codes. These simulations have become possible after the mitigation techniques have been employed to handle the cancellation problem.

The purpose of the present paper is to give an overview of the main numerical problems appearing in gyrokinetic electromagnetic simulations and give a summary of the mitigation techniques. The paper is organised as follows. In Sec. II, the $v_\parallel$- and $p_\parallel$-formulations of the electromagnetic gyrokinetic theory are discussed together with their numerical properties. In Sec. III, the cancellation problem and its mitigation techniques in the $p_\parallel$-formulation are described. Finally in Sec. IV, the mixed-variable formulation is addressed, completing the list of presently available mitigation techniques. The conclusions are discussed in Sec. V.

II. VARIOUS FORMULATIONS OF THE GYROKINETIC THEORY

The gyrokinetic theory is based on an expansion in small parameters defined by the so-called minimal gyrokinetic ordering [30]:

$$\epsilon_\mathrm{B} = \rho_\mathrm{g}/L_\mathrm{B} \ll 1 \ , \quad \epsilon = \omega/\omega_\mathrm{c} \sim k_\parallel/k_\perp \sim q\delta\phi/T \sim \delta B/B \ll 1 \ , \tag{1}$$

where $\rho_\mathrm{g} = \sqrt{mT}/(eB)$ is the particle gyroradius, L_B is the characteristic scale of the unperturbed magnetic field B, and T is the plasma temperature. This ordering implies that the fusion plasma is magnetized, the turbulence is low-frequency, flute-like and weak. Based on these small parameters, a perturbative elimination of the fast gyro-scale can be carried out. The gyrokinetic perturbative derivation starts from the perturbed Poincaré-Cartan form [1]:

$$\gamma = q\boldsymbol{A}^*(\boldsymbol{R}) \cdot \mathrm{d}\boldsymbol{R} + \frac{m}{q}\,\mu\,\mathrm{d}\theta - \left(\frac{mv_\parallel^2}{2} + \mu B\right)\mathrm{d}t \ + \ q\Big[A_\parallel(\boldsymbol{x})\,\boldsymbol{b}\cdot\mathrm{d}\boldsymbol{x} - \phi(\boldsymbol{x})\,\mathrm{d}t\Big] \tag{2}$$

where the perturbed electrostatic potential ϕ and the perturbed parallel magnetic potential $A_\parallel$ depend on the gyro-phase through $\boldsymbol{x} = \boldsymbol{R} + \boldsymbol{\rho}(\theta)$, which has subsequently to be eliminated. Here, $\boldsymbol{R}$ is the guiding-center position, $\boldsymbol{\rho}$ is the gyroradius, θ is the gyro-phase, m

is the particle mass, q is the particle charge, $v_\parallel$ is the parallel velocity, μ is the magnetic moment, B is the ambient magnetic field, $\boldsymbol{A}^* = \boldsymbol{A} + (mv_\parallel/q)\,\boldsymbol{b}$ is the so-called extended magnetic potential, $\boldsymbol{A}$ is the magnetic potential corresponding to the ambient magnetic field, and $\boldsymbol{b}$ is the unit vector in the direction of the ambient magnetic field.

The gyro-dependence is eliminated from the Poincaré-Cartan form using Lie transform techniques $\Gamma = \mathrm{e}^{\hat{G}}\gamma + \mathrm{d}S$, see Ref. [1]. This procedure allows a substantial amount of freedom. For example, the perturbed magnetic potential can be put into the Hamiltonian part of the Poincaré-Cartan form, leading to the so-called Hamiltonian, or $p_\parallel$-formulation:

$$\Gamma = q\boldsymbol{A}^* \cdot \mathrm{d}\boldsymbol{R} + \frac{B}{\Omega}\,\mu\,\mathrm{d}\theta - \left(\frac{mp_\parallel^2}{2} + \mu B + q\Big\langle \phi - p_\parallel A_\parallel \Big\rangle\right)\mathrm{d}t \tag{3}$$

Here, $p_\parallel$ denotes the parallel velocity coordinate in the $p_\parallel$-formulation. Here, we use this notation to stress the fact that the explicit expressions of the phase space gyrocenter coordinates through the guiding center coordinates depend on the formulation of the gyrokinetic theory chosen [1]. Ih the following, however, we will use for simplicity the same symbol $v_\parallel$ to denote the Lie transform of the parallel velocity in all the formulations considered.

Alternatively, the perturbed magnetic potential can be left in the symplectic part of the Poincaré-Cartan form, resulting in the symplectic, or $v_\parallel$-formulation:

$$\Gamma = q\boldsymbol{A}^* \cdot \mathrm{d}\boldsymbol{R} + \frac{B}{\Omega}\,\mu\,\mathrm{d}\theta + \langle A_\parallel\rangle \boldsymbol{b}\cdot\mathrm{d}\boldsymbol{R} - \left(\frac{mv_\parallel^2}{2} + \mu B + q\langle\phi\rangle\right)\mathrm{d}t \tag{4}$$

The gyrokinetic system of equations includes the gyrokinetic Vlasov equation, here written for the perturbed part of the distribution function $\bar{f}_{1s}$ with F_0 being the background distribution function, usually a Maxwellian:

$$\frac{\partial \bar{f}_{1s}}{\partial t} + \dot{\boldsymbol{R}}\cdot\frac{\partial \bar{f}_{1s}}{\partial \boldsymbol{R}} + \dot{v}_\parallel \frac{\partial \bar{f}_{1s}}{\partial v_\parallel} = -\dot{\boldsymbol{R}}^{(1)}\cdot\frac{\partial F_{0s}}{\partial \boldsymbol{R}} - \dot{v}_\parallel^{(1)}\frac{\partial F_{0s}}{\partial v_\parallel}\ , \tag{5}$$

the equations for the particle trajectories $(\dot{R}, \dot{v}_\parallel)$, and the field equations for the perturbed electrostatic and parallel magnetic potentials. These equations can straightforwardly be derived from the gyrokinetic Poincaré-Cartan form using the variational principle, see Ref. [1].

In the $v_\parallel$-formulation, the equations of motion are

$$\dot{\boldsymbol{R}} = v_\parallel \tilde{\boldsymbol{b}}^* + \frac{1}{q_s \tilde{B}_\parallel^*}\boldsymbol{b}\times\left[\mu\nabla B + q_s\left(\nabla\langle\phi\rangle + \frac{\partial\left\langle A_\parallel\right\rangle}{\partial t}\boldsymbol{b}\right)\right] \tag{6}$$

$$\dot{v}_\parallel = -\frac{1}{m_s}\tilde{\boldsymbol{b}}^*\cdot\mu\nabla B - \frac{q_s}{m_s}\left(\tilde{\boldsymbol{b}}^*\cdot\nabla\langle\phi\rangle + \frac{\partial\left\langle A_\parallel\right\rangle}{\partial t}\right) \tag{7}$$

$$\tilde{\boldsymbol{B}}^* = \boldsymbol{B} + \frac{m_s}{q_s}\,v_\parallel\,(\nabla\times\boldsymbol{b}) + \nabla\times\Big(\langle A_\parallel\rangle\,\boldsymbol{b}\Big)\ ,\quad \tilde{B}_\parallel^* = \boldsymbol{b}\cdot\tilde{\boldsymbol{B}}^*\ ,\quad \tilde{\boldsymbol{b}}^* = \tilde{\boldsymbol{B}}^*/\tilde{B}_\parallel^* \tag{8}$$

and the field equations, the quasineutrality condition and parallel Ampere's law, are

$$\sum_{s=\mathrm{i,f}} \int \frac{q_s^2 F_{0s}}{T_s} \left(\phi - \langle\phi\rangle\right) \delta_{\mathrm{gy}} \, \mathrm{d}^6 Z = \sum_{s=\mathrm{i,e,f}} q_s n_{1s} \ , \quad -\nabla_\perp^2 A_\parallel = \mu_0 \sum_{s=\mathrm{i,e,f}} j_{\parallel 1s} \tag{9}$$

Here, $\langle\phi\rangle$ is the gyro-average of the electrostatic potential, $\delta_{\mathrm{gy}} = \delta(\boldsymbol{R} + \boldsymbol{\rho} - \boldsymbol{x})$, $n_{1s} = \int \bar{f}_{1s} \, \delta_{\mathrm{gy}} \, \mathrm{d}^6 Z$ is the gyrocenter density, and $j_{\parallel 1s} = \int v_\parallel \, \bar{f}_{1s} \, \delta_{\mathrm{gy}} \, \mathrm{d}^6 Z$ is the gyrocenter current.

The problem with the $v_\parallel$-formulation is that the partial derivative $\partial\langle A_\parallel\rangle/\partial t$ appears on the right hand side of Eq. (7) for the parallel acceleration $\dot{v}_\parallel$. This equation can not be treated with an explicit time solver (such as the usual 4th order Runge Kutta method) in a numerical code, whereas implicit time solvers are usually very expensive in terms of the computation cost and therefore impractical.

In the $p_\parallel$-formulation, the gyrocenter trajectories are

$$\dot{\boldsymbol{R}} = \left(v_\parallel - \frac{q}{m}\langle A_\parallel\rangle\right) \boldsymbol{b}^* + \frac{1}{qB_\parallel^*} \boldsymbol{b} \times \left[\mu \nabla B + q\left(\nabla\langle\phi\rangle - v_\parallel \nabla\langle A_\parallel\rangle\right)\right] \tag{10}$$

$$\dot{v}_\parallel = -\frac{1}{m}\left[\mu \nabla B + q\left(\nabla\langle\phi\rangle - v_\parallel \nabla\langle A_\parallel\rangle\right)\right] \cdot \boldsymbol{b}^* \tag{11}$$

$$\boldsymbol{B^*} = \boldsymbol{B} + \frac{m_s}{q_s} v_\parallel \left(\nabla \times \boldsymbol{b}\right) \ , \quad B_\parallel^* = \boldsymbol{b} \cdot \boldsymbol{B^*} \ , \quad \boldsymbol{b^*} = \boldsymbol{B^*}/B_\parallel^* \tag{12}$$

Note that $\partial\langle A_\parallel\rangle/\partial t$ does not appear in this formulation, which opens a way for cheaper explicit time solvers to be used. The price for this is to be paid in the field equations:

$$\sum_{s=\mathrm{i,f}} \int \frac{q_s^2 F_{0s}}{T_s} \left(\phi - \langle\phi\rangle\right) \delta_{\mathrm{gy}} \, \mathrm{d}^6 Z = \sum_{s=\mathrm{i,e,f}} q_s n_{1s} \ , \quad \sum_{s=\mathrm{i,e,f}} \frac{\beta_s}{\rho_s^2} \langle \overline{A}_\parallel \rangle_s - \nabla_\perp^2 A_\parallel = \mu_0 \sum_{s=\mathrm{i,e,f}} j_{\parallel 1s} \tag{13}$$

Here, $n_0 \langle \overline{A}_\parallel \rangle_s = \int \langle A_\parallel \rangle F_{0s} \delta_{\mathrm{gy}} \, \mathrm{d}^6 Z$, $\rho_s = \sqrt{m_s T_s}/(q_s B)$, and $\beta_s = \mu_0 n_{0s} T_s / B^2$. Note that Ampere's law now contains the extra terms (the so-called skin terms) proportional to $\beta_\mathrm{i}/\rho_\mathrm{i}^2$ and $\beta_\mathrm{e}/\rho_\mathrm{e}^2$. This terms are induced by the choice of the coordinates in the $p_\parallel$-formulation. They have no physical meaning and must be cancelled with similar non-physical formulation-induced contributions in the parallel $p_\parallel$-current. Note that the terms to be cancelled, especially the electron skin term can be very large because of the small electron mass appearing in the denominator:

$$\frac{\beta_\mathrm{e}}{\rho_\mathrm{e}^2} A_\parallel = \frac{\mu_0 n_0 e^2}{m_\mathrm{e}} A_\parallel \tag{14}$$

This implies that the cancellation has to be performed very accurately.

III. CANCELLATION PROBLEM AND ITS MITIGATION

To understand which non-physical contributions are responsible for the cancellation in the parallel $p_\parallel$-current, let us define the Boltzmann-like adiabatic perturbation of the distribution function, corresponding to the perturbed $p_\parallel$-Hamiltonian:

$$\bar{H}_1 = q_s\Big\langle \phi - v_\parallel A_\parallel \Big\rangle \ , \quad F_{\rm e}^{\rm (ad)} = F_{0\rm e}\, {\rm e}^{-\bar{H}_1/T_{\rm e}} - F_{0\rm e} \approx -\frac{q_{\rm e}F_{0\rm e}}{T_{\rm e}}\Big\langle \phi - v_\parallel A_\parallel \Big\rangle \tag{15}$$

Note that this distribution generates a non-vanishing parallel adiabatic current. The adiabatic current appears due to the second term in the perturbed Hamiltonian, which is proportional to $v_\parallel$. This term appears in the $p_\parallel$-formulation, but not in the $v_\parallel$-formulation. Thus, the parallel adiabatic currents are "generated" by the $p_\parallel$-formulation and not by physics.

These currents coincide with the skin terms:

$$\mu_0 \bar{j}_{\parallel s}^{\rm (ad)} = \mu_0 q_s \int v_\parallel \, F_s^{\rm (ad)} {\rm d}^3 v = \frac{\mu_0 n_{0s} q_s^2}{m_s}\, A_\parallel = \frac{\beta_s}{\rho_s^2}\, A_\parallel \tag{16}$$

The non-physical formulation-induced contributions to the left hand side of Ampere's law and to the parallel current must cancel each other. This cancellation must be very accurate, since the non-physical terms are multiplied by a very large number. To understand what makes the accurate enough cancellation problematic, we need to recall the discretization scheme used in the particle-in-cell simulations.

The "Klimontovich" representation is used for the perturbed gyrokinetic distribution function, expressed in terms of its phase-space coordinates and weights w_ν:

$$\bar{f}_{1s}(\boldsymbol{R}, v_\parallel, \mu, t) = \sum_{\nu=1}^{N_p} w_{s\nu}(t)\delta(\boldsymbol{R} - \boldsymbol{R}_\nu)\delta(v_\parallel - v_{\nu\parallel})\delta(\mu - \mu_\nu) \tag{17}$$

The background distribution function is usually a Maxwellian:

$$F_{0s} = n_0 \left(\frac{m}{2\pi T_s}\right)^{3/2} \exp\left[-\frac{m_s v_\parallel^2}{2T_s}\right] \exp\left[-\frac{m_s v_\perp^2}{2T_s}\right] \tag{18}$$

Other choices are also possible, but they would lead to changes in the field equations since the pullback [1] depends explicitly on the ambient distribution function.

The fields can be represented on a spatial grid using, for example, finite elements, such as the B splines.

$$\phi(\boldsymbol{x}) = \sum_{l=1}^{N_s} \phi_l(t)\Lambda_l(\boldsymbol{x}), \quad A_\parallel(\boldsymbol{x}) = \sum_{l=1}^{N_s} a_l(t)\Lambda_l(\boldsymbol{x}) \tag{19}$$

The cancellation problem arises in particle-in-cell simulations since the current is computed with markers, discretising phase space, whereas the skin terms, known analytically, are discretised on the spatial grid using finite elements. This numerically different representation makes the cancellation inexact and leads to the *cancellation problem*. The terms to be cancelled are dominant and much larger than the terms describing the physical content.

$$\nabla_\perp^2 A_\parallel \ll \frac{\beta_\mathrm{e}}{\rho_\mathrm{e}^2} A_\parallel \;\Rightarrow\quad \bar{j}_{\parallel\mathrm{i}}^{(\mathrm{nonad})} + \bar{j}_{\parallel\mathrm{e}}^{(\mathrm{nonad})} \ll \bar{j}_{\parallel\mathrm{e}}^{(\mathrm{ad})} \tag{20}$$

The physics is described by the small rest:

$$-\nabla_\perp^2 A_\parallel = \mu_0 \left(\bar{j}_{\parallel\mathrm{i}}^{(\mathrm{nonad})} + \bar{j}_{\parallel\mathrm{e}}^{(\mathrm{nonad})} \right) \tag{21}$$

The error scales with $\delta A_\parallel \sim \beta/(k_\perp^2 \rho_\mathrm{e}^2)$ making the simulations of finite-beta global modes, characterised by small $k_\perp$, very challenging. This parameter regime is sometimes referred to as the MHD limit.

Mitigation strategies of the cancellation problem are based on the observation that the perturbed true-particle distribution function f_{1s} can be expressed through the gyrocenter distribution function $\bar{f}_{1s}$ by the $p_\parallel$-pullback transform [1]:

$$f_{1s} = \bar{f}_{1s} + \{S_1, F_{0s}\} + \frac{q_s \langle A_\parallel \rangle}{m_s} \frac{\partial F_{0s}}{\partial v_\parallel} \;, \quad \omega_{\mathrm{cs}} \frac{\partial S_1}{\partial \theta} = q_s(\psi - \langle \psi \rangle) \;, \;\; \psi = \phi - v_\parallel A_\parallel \tag{22}$$

This expression has to be used both in Ampere's law and in the quasineutrality condition.

In terms of this true-particle distribution function, Ampere's law becomes

$$-\nabla_\perp^2 A_\parallel = \mu_0 \int v_\parallel \left[\bar{f}_{1s} + \{S_1, F_{0s}\} + \frac{q_s \langle A_\parallel \rangle}{m_s} \frac{\partial F_{0s}}{\partial v_\parallel} \right] \delta(\boldsymbol{R} + \boldsymbol{\rho} - \boldsymbol{x}) \mathrm{d}^6 Z \tag{23}$$

Here, S_1 is the Lie-transform generating function. One can mitigate the cancellation problem if the entire true-particle distribution function is discretized using the same scheme, i. e. with the markers. This implies that both the background distribution function and its perturbation must be represented using the same Klimontovich representation written for the same set of markers:

$$\bar{f}_{1s}(Z) = \sum_{\nu=1}^{N_p} w_\nu \delta(Z - Z_\nu(t)) \;, \quad F_{0s}(Z) = \sum_{\nu=1}^{N_p} F_{0s}(Z_\nu)\, \zeta_\nu\, \delta(Z - Z_\nu(t)). \tag{24}$$

Here, ζ_ν denotes an elementary phase-space volume associated with a given marker and Z_ν are the phase-space coordinates of the marker. This marker discretization of the complete pullback transform of the gyrokinetic distribution function, i. e. the true-particle distribution

function, must be used both in Ampere's law and in the quasineutrality condition. Note that the second term on the right hand side of Eq. (23), proportional to $\{S_1, F_{0s}\}$, can be discretized on the grid since this term does not take part in the cancellation.

There is a technical problem with this approach, since Ampere's law is used to compute the parallel magnetic potential $A_\parallel$, but the true-particle distribution function, expressed through the gyrokinetic distribution function, depends on $A_\parallel$, which is unknown at this point of the computation. The solution of this problem is to introduce an easy-to-compute estimator for the $A_\parallel$-dependent part of the $p_\parallel$-pullback. In practice, one would simply use the skin term $(\beta_\mathrm{e}/\rho_\mathrm{e}^2)A_\parallel$ as the estimator. Formally, if we want to solve the equation $(s+L)\,a = j$, we can add a zero to the right hand side of this equation $(s+L)\,a = j+(\hat{s}-\hat{s})a$ with $\hat{s}$ being our arbitrary estimator, and reformulate the original equation as

$$(\hat{s}+L)\,a = j + (\hat{s}-s)\,a \tag{25}$$

If the estimator $\hat{s}$ has been chosen properly, then $\|\hat{s}-s\| = \mathcal{O}(\varepsilon)$. Therefore, we can use the small parameter ε to solve Ampere's law iteratively, expanding the vector potential in the series $a = a_0 + \varepsilon a_1 + \varepsilon^2 a_2 + \ldots$ and solving for the parallel magnetic potential order by order in ε:

$$(\hat{s}+L)\,a_0 = j\ ,\ (\hat{s}+L)\,a_1 = (\hat{s}-s)\,a_0\ , \ldots \tag{26}$$

Note that our estimator is given in the finite-element discretisation by the expression:

$$\hat{s}_{kl} = \int \frac{\beta_e}{\rho_e^2}\,\Lambda_k(\boldsymbol{x})\Lambda_l(\boldsymbol{x})\,\mathrm{d}^3x \tag{27}$$

and the marker-dependent part of the right hand side of the iterative scheme can conveniently be written through the control variate [14] as

$$j_k - s_{kl}a_l^{n-1} = \sum_{\nu=1}^{N_\mathrm{P}} v_{\parallel\nu}\left(w_\nu + \frac{q_s\langle A_\parallel^{(n-1)}\rangle}{m_s}\,\frac{\partial F_{0s}}{\partial v_\parallel}(Z_\nu)\,\zeta_\nu\right)\langle\Lambda_k\rangle_\nu \tag{28}$$

In practice, a straightforward and computationally cheap modification of the current assignment routine is sufficient to treat this contribution.

IV. MIXED-VARIABLE FORMULATION OF THE GYROKINETIC THEORY

The mitigation of the cancellation problem can further be facilitated by a proper choice of coordinates. Previously, we have mentioned that the perturbative derivation of gyrokinetic

theory leaves a lot of freedom in the choice of the variables. These alternative formulations may have very different numerical properties while still describing the same physics. As example, we have already discussed substantial numerical differences between the $v_\parallel$- and $p_\parallel$-formulations of the theory. Clearly, this freedom can be used to taylor the numerical properties of the equations to be solved by a code as desired. For electromagnetic particle-in-cell gyrokinetic codes, the mixed-variable formulation [21–23] is such a good choice reducing the numerical burden by proper coordinates. In this formulation, the $v_\parallel$- and the $p_\parallel$-gyrokinetics are "mixed" in such a way that the resulting equations have superior numerical properties compared to both original formulations without any significant computational penalty. Here, we briefly describe the mixed-variable formulation completing the list of the techniques presently available to mitigate the cancellation problem.

The derivation of the mixed-variable gyrokinetics starts with the splitting of the magnetic potential into the 'symplectic' and 'hamiltonian' parts:

$$A_\parallel = A_\parallel^{(\mathrm{s})} + A_\parallel^{(\mathrm{h})} \tag{29}$$

This splitting is completely arbitrary at this stage and will be specified further in a way which optimises the numerical properties of the equations solved.

After the splitting, the perturbed guiding-center phase-space Lagrangian takes the form:

$$\gamma = q\boldsymbol{A}^* \cdot \mathrm{d}\boldsymbol{R} + \frac{m}{q}\,\mu\,\mathrm{d}\theta + q\,A_\parallel^{(\mathrm{s})}\boldsymbol{b}\cdot\mathrm{d}\boldsymbol{x} + q\,A_\parallel^{(\mathrm{h})}\boldsymbol{b}\cdot\mathrm{d}\boldsymbol{x} - \left[\frac{mv_\parallel^2}{2} + \mu B + q\phi\right]\mathrm{d}t \tag{30}$$

Now, we apply a "mixed" Lie transform which moves $A_\parallel^{(\mathrm{h})}$ into the mixed-variable gyrokinetic Hamiltonian, whereas $A_\parallel^{(\mathrm{s})}$ remains in the gyrokinetic symplectic part of the Poincaré-Cartan form, which can be written as follows.

$$\Gamma = q\boldsymbol{A}^* \cdot \mathrm{d}\boldsymbol{R} + \frac{m}{q}\mu\,\mathrm{d}\theta + q\Big\langle A_\parallel^{(\mathrm{s})}\Big\rangle\boldsymbol{b}\cdot\mathrm{d}\boldsymbol{R} - \left[\frac{mv_\parallel^2}{2} + \mu B + q\Big\langle\phi - v_\parallel A_\parallel^{(\mathrm{h})}\Big\rangle\right]\mathrm{d}t \tag{31}$$

The equations of motion in the mixed-variable formulation can straightforwardly be derived from this Poincaré-Cartan form. The unperturbed equations of motion are not changed, the perturbed equations of motion are

$$\dot{\boldsymbol{R}}^{(1)} = \frac{\boldsymbol{b}}{B_\parallel^*} \times \nabla\Big\langle\phi - v_\parallel A_\parallel^{(\mathrm{s})} - v_\parallel A_\parallel^{(\mathrm{h})}\Big\rangle - \frac{q}{m}\,\langle A_\parallel^{(\mathrm{h})}\rangle\,\boldsymbol{b}^* \tag{32}$$

$$\dot{v}_\parallel^{(1)} = -\frac{q}{m}\left[\boldsymbol{b}^*\cdot\nabla\Big\langle\phi - v_\parallel A_\parallel^{(\mathrm{h})}\Big\rangle + \frac{\partial}{\partial t}\Big\langle A_\parallel^{(\mathrm{s})}\Big\rangle\right] - \frac{\mu}{m}\,\frac{\boldsymbol{b}\times\nabla B}{B_\parallel^*}\cdot\nabla\Big\langle A_\parallel^{(\mathrm{s})}\Big\rangle \tag{33}$$

Note that the time derivative of $A_\parallel^{(\mathrm{s})}$ appears on the right hand side of the parallel acceleration. Generally, this would require an implicit time solver, which would be computationally inpractical. However, since we have added a new degree of freedom by the splitting the magnetic potenital into two parts, we must introduce a constraint in order to remain on a physical hypersurface in the resulting extended phase space. This constraint is also arbitrary and can be specified to optimise numerical properties of our equations. We choose the ideal parallel Ohm's law as the constraint for the symplectic part of the magnetic potential:

$$\frac{\partial}{\partial t} A_\parallel^{(\mathrm{s})} + \boldsymbol{b} \cdot \nabla \phi = 0 \tag{34}$$

This constraint gives an explicit expression for $\partial A_\parallel^{(\mathrm{s})}/\partial t$ so that an explicit time solver, such as the usual 4th order Runge-Kutta method, is sufficient to treat the parallel acceleration $\dot{v}_\parallel^{(1)}$ in this mixed-variable formulation of the theory.

The quasineutrality equation has in the mixed variables the same form as in the $p_\parallel$-formulation. Ampere's law takes the form:

$$\sum_{s=\mathrm{i,e,f}} \frac{\beta_s}{\rho_s^2} \left\langle \overline{A}_\parallel^{(\mathrm{h})} \right\rangle_s - \nabla_\perp^2 A_\parallel^{(\mathrm{h})} = \mu_0 \sum_{s=\mathrm{i,e,f}} j_{\parallel 1 s} + \nabla_\perp^2 A_\parallel^{(\mathrm{s})} \tag{35}$$

Note that the skin terms appear in this equation but they envolve only the hamiltonian part of the magnetic potential $A_\parallel^{(\mathrm{h})}$.

Since the splitting of the magnetic potential into two parts is arbitrary, it can be performed at the beginning of each time step, keeping $A_\parallel^{(\mathrm{h})}$ small during the entire simulation. This leads to the following algorithm [21, 23].

1. At the end of each time step, redefine the magnetic potential splitting:

$$A_{\parallel(\mathrm{new})}^{(\mathrm{s})}(t_i) = A_\parallel(t_i) = A_{\parallel(\mathrm{old})}^{(\mathrm{s})}(t_i) + A_{\parallel(\mathrm{old})}^{(\mathrm{h})}(t_i) \tag{36}$$

2. As a consequence, redefine $A_{\parallel(\mathrm{new})}^{(\mathrm{h})}(t_i) = 0$

3. The new mixed-variable distribution function must coincide with its $v_\parallel$(symplectic)-formulation counterpart computed at the appropriate point of the symplectic phase space (a transformation of the original point in the mixed-variable space).

$$f_1^{(\mathrm{s})}(Z^{(\mathrm{s})}, A_\parallel) = f_1^{(\mathrm{m})}(Z^{(\mathrm{m})}, A_\parallel^{(s)}, A_\parallel^{(h)}) \tag{37}$$

This expression is completely general and can also be used in the nonlinear simulations [23], implying in practice that the marker weight is kept fixed during the transformation, but its position "jumps" according to the coordinate transformation

$$v_{\parallel}^{(\mathrm{s})} = v_{\parallel}^{(\mathrm{m})} - \frac{e}{m} \left\langle A_{\parallel}^{(\mathrm{h})} \right\rangle \tag{38}$$

In a linear case, one could use the approximation

$$f_{1s(\mathrm{new})}^{(\mathrm{m})}(t_i) = f_{1s}^{(\mathrm{s})}(t_i) = f_{1s(\mathrm{old})}^{(\mathrm{m})}(t_i) + \frac{q_s \left\langle A_{\parallel(\mathrm{old})}^{(\mathrm{h})}(t_i) \right\rangle}{m_s} \frac{\partial F_{0s}}{\partial v_{\parallel}} \tag{39}$$

In this case, we modify the marker weight while keeping its position fixed.

4. Proceed, explicitly solving the mixed-variable system of equations at the next time step $t_i + \Delta t$ in a usual way, but using the symplectic ($v_{\parallel}$-formulation) coordinates and symplectic distribution function as the initial conditions.

Note that some additional nonlinear terms may appear in the equations of motion, as discussed in Ref. [23]. These new terms reflect the fact that although the original $p_{\parallel}$-Lagrangian and the mixed-variable Lagrangian describe the same physics, this symmetry is broken by the truncation involved into the perturbative Lie transform. This symmetry breaking is however limited to higher orders. The truncated equations describe the same physics to the relevant order. Numerically, the difference between the truncated systems may be visible, although small.

V. CONCLUSIONS

The numerical difficulties inhibiting electromagnetic gyrokinetic simulations have been observed a long time ago. In the $v_{\parallel}$-formulation, the numerical problems were seen in 1992 by Reynders [7]. In the $p_{\parallel}$-formulation, the cancellation problem was noted by Cummings [9] in 1995. For a long time, the cancellation problem prevented any substantial effort on global gyrokinetic particle-in-cell simulations in realistic geometry. As a simplification, various reduced models, such as the hybrid kinetic-MHD or fluid-electron models, have been used to circumvent this problem. However, these reduced models have important limitations related to closure issues. One well-known example of such limitations is given by the difficulties in describing the micro-tearing physics with the fluid-electron model, described in Ref. [5].

In the last decade, a lot of work has been done to mitigate the cancellation problem. Approaches such as the control-variate mitigation and mixed-variable pullback scheme have been formulated and successfully tested in realistic tokamak and stellarator geometries. It has been shown that these mitigation schemes can be used both in linear and nonlinear regimes. The mitigation schemes have been validated on many examples, including an international ITPA benchmark [31]. Finally, we believe that the fully gyrokinetic electromagnetic PIC simulation schemes approach the mainstream of the simulation practice.

ACKNOWLEDGMENTS

We acknowledge J. Nührenberg, S. Günter, P. Helander, F. Zonca, E. Poli, and F. Jenko for their support. This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the Euratom research and training programme 2014-2018 under grant agreement No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission

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