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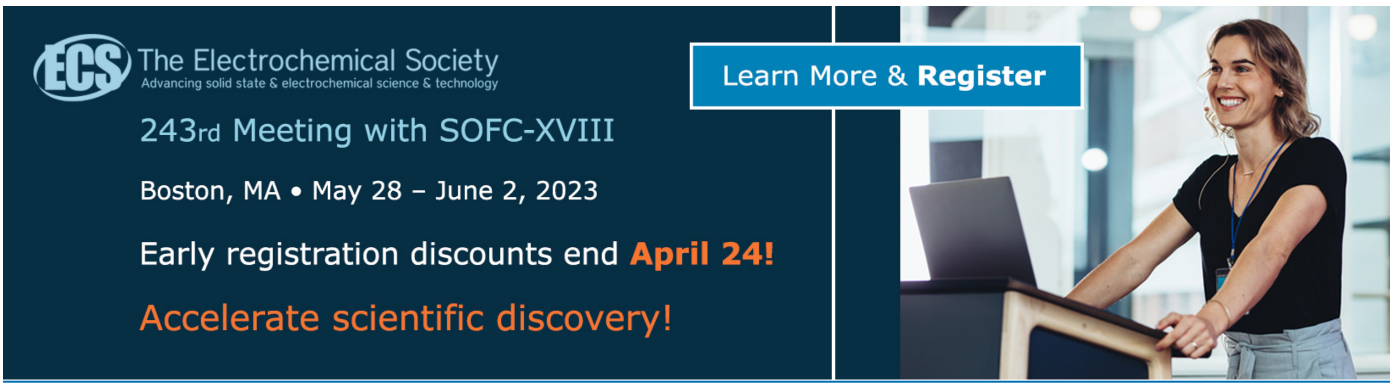

Long-wavelength closures for collisional and neutral interaction terms in gyro-fluid models

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Abstract. A collisional gyro-fluid model is presented. The goal of the model is edge and scrape-off layer turbulence. The emphasize in the model derivation heavily lies on "implementability" with today's numerical methods. This translates to an avoidance of infinite sums, strongly coupled equations in time and intricate elliptic operator functions. The resulting model contains the four moments density, parallel momentum, perpendicular pressure and parallel energy and is closed by a polarisation equation and parallel Ampere law. The central ingredient is a collisional long-wavelength closure that relies on a drift-fluid gyro-fluid correspondence principle. In this way the extensive literature on fluid collisions can be incorporated into the model including sources, plasma-neutral interactions and scattering collisions. Even though this disregards the characteristic finite Larmor radius terms in the collisional terms the resulting model is at least as accurate as the corresponding drift-fluid model in these terms. Furthermore, the model does enjoy the benefits of an underlying variational principle in an energy-momentum theorem and an inherent symmetry in moment equations with regards to multiple ion species. Consistent particle drifts as well as finite Larmor radius corrections and high amplitude effects in the advection and polarization terms are further characteristics of the model. Extensions and improvements like short-wavelength expressions, a trans-collisional closure scheme for the low-collisionality regime or zeroth order potential must be added at a later stage.

Keywords: gyro-fluid, collisions, long-wavelength limit

1. Introduction

Gyro-kinetic and in extension gyro-fluid models arguably have difficult and often impractical expressions for collisional inter-species interaction terms [1, 2, 3]. Furthermore, little to no work exists on plasma-neutral interaction terms in gyro-fluid models, as does work on external sources like heating or particle injection. The result is that practical implementations of gyro-fluid models largely ignore collisions and plasma neutral interactions altogether [4, 5, 6, 7]. Drift-fluid models are preferred for that purpose even though these models do not share many advantages of gyro-fluid models: finite Larmor radius corrections, consistent particle drifts, an energy and momentum theorem based on variational methods in the underlying gyro-kinetic model and an inherent symmetry in moment equations with regards to multiple ion species [8, 9, 10, 11].

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In this work we derive a collisional closure for gyro-fluid models that is both practical to implement numerically and easy to derive. It is known that drift-fluid models can be obtained in the long-wavelength limit of gyro-fluid models when the gyro-radius is small compared to the typical length-scales [12, 13, 14]. The central argument for a long-wavelength closure of gyro-fluid models is that this correspondence extends to the collisional (scattering and reacting) terms: they are such that their long-wavelength limit corresponds to the drift-fluid terms. In that way a gyro-fluid model can be built based on the extensive literature on fluid collisions [15, 16].

Our goal is to derive a practical four-moment, electromagnetic, multi-species model that in particular can be used in the Theory, Simulation, Verification and Validation (TSSV) task 3 for edge plasma fluid simulations. We will therefore focus on numerical "implementability" avoiding infinite sums, strongly coupled equations or intricate operator functions. We further highlight the impact of the derived collision terms on the conservation of currents "vorticity" equation [14] as well as the impact on rotation [13].

In section 2 we start our derivation from the basic Vlasov equation and show the generic gyro-fluid moment equation. In Section 3 we present our main closure scheme and present a possible choice of fluid collision terms for both plasma-neutral as well as Coulomb collisions. Finally, we present the complete model in Section 4 followed by a discussion of possible numerical realisations and boundary conditions in Section 5. We conclude in Section 6.

2. Elements of a gyro-fluid model

We formally start with the kinetic Vlasov equation in the form presented by [15]

$$\frac{\partial f_a}{\partial t} + \boldsymbol{v}\cdot\nabla f_a + \frac{q_a}{m_a}(\boldsymbol{E} + \boldsymbol{v}\times B)\frac{\partial f_a}{\partial \boldsymbol{v}} = C_a \tag{1}$$

Here, $f_a(\boldsymbol{x},\boldsymbol{v},t)$ is the particle distribution function of species a dependent on position $\boldsymbol{x}$, velocity $\boldsymbol{v}$ and time t. The Lorentz force mediates the interactions with the electric field $\boldsymbol{E}$ and magnetic field $\boldsymbol{B}$ with charge q_a and mass m_a. The main focus in this work lies on the collision and source term C_a that is presented as

$$C_a := \sum_{scatt.=ii,ie,ee} C_{a,scatt} + \sum_{react.=iz,rec,cx} C_{a,react} + \sum_{sources} C_{a,sources} \tag{2}$$

We formally distinguish between (i) scattering (Coulomb) collisions i.e. collisions between ions "ii", ions and electrons "ie" and electrons "ee", (ii) interactions between the plasma and neutrals in ionization "iz", recombination "rec" and charge exchange "cx" and (iii) external sources like for example plasma heating through microwave interaction or neutral beam and pellet injection.

Eq. (1) can be converted to gyro-kinetic coordinates [17] ($\boldsymbol{X}$, μ, $v_\parallel$, θ) with gyro-centre position $\boldsymbol{X}$, magnetic moment μ, parallel canonical velocity $mw_\parallel = mv_\parallel + qA_\parallel$ and gyro-angle θ. The parallel magnetic field potential $A_\parallel$ represents magnetic field fluctuations with $\tilde{\boldsymbol{B}} = \nabla\times A_\parallel \hat{\boldsymbol{b}}$. The resulting gyro-kinetic particle distribution function $F = F(\boldsymbol{X}, w_\parallel, \mu, t)$ is gyro-averaged by construction, while $B = B(\boldsymbol{X})$ is the magnetic field strength that acts as the volume form in the symplectic phase space. The gyro-kinetic collision operator $C = C(\boldsymbol{X}, w_\parallel, \mu, \theta, t)$ is left unspecified for now but needs to be averaged over the gyro-angle with the gyro-average $\langle\cdot\rangle$.

$$\frac{\partial(BF)}{\partial t} + \nabla\cdot\left(BF\dot{\boldsymbol{X}}\right) + \frac{\partial\left(BF\dot{w}_\parallel\right)}{\partial w_\parallel} = \langle BC\rangle \tag{3}$$

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where the equations of motion are given by [18, 13]

$$\begin{aligned}\dot{\boldsymbol{X}} =& \frac{1}{B}\Bigg(\boldsymbol{B}v_\parallel + \frac{mv_\parallel^2}{q}\nabla\times\hat{\boldsymbol{b}} + \frac{\mu B}{q}\hat{\boldsymbol{b}}\times\nabla\ln B \\ &+ v_\parallel\nabla\times A_\parallel\hat{\boldsymbol{b}} + \hat{\boldsymbol{b}}\times\nabla\Psi\Bigg) \qquad (4)\\ m\dot{w}_\parallel =& -\frac{1}{B}\left(\boldsymbol{B} + \frac{mv_\parallel}{q}\nabla\times\hat{\boldsymbol{b}} + \nabla\times A_\parallel\hat{\boldsymbol{b}}\right) \\ &\cdot(\mu B\nabla\ln B + q\nabla\Psi) + q\dot{\boldsymbol{X}}\cdot\nabla A_\parallel \qquad (5)\\ \dot{\mu} =& 0 \qquad (6)\\ \dot{\theta} =& \frac{qB}{m} + \frac{q^2}{m}\frac{\partial\Psi}{\partial\mu} \qquad (7)\end{aligned}$$

For brevity of notation we omit the species index a in the equations. In the velocity equation (4) we find the parallel velocity $v_\parallel$, the curvature and grad-B drifts as well as the magnetic field perturbation and $\boldsymbol{E}\times\boldsymbol{B}$ drifts. The latter two are given by the perturbed parallel magnetic potential $A_\parallel$, the background static magnetic field $\boldsymbol{B}$ with unit vector $\hat{\boldsymbol{b}} := \boldsymbol{B}/B$ and the gyro-centre potential $\Psi = \Psi_1 + \Psi_2 = \langle\phi\rangle - q\partial_\mu(\langle\phi^2\rangle - \langle\phi\rangle^2)/2B$ [18], where ϕ is the electric potential and $\langle\cdot\rangle$ the gyro-average. In the parallel acceleration (5) we find the generalized mirror and parallel electric forces. The magnetic moment is conserved by construction (6) while the gyro-angle is averaged out in the conservative gyro-kinetic Vlasov equation (3).

In order to derive the gyro-fluid equations we first define the velocity space moment operator

$$\|\zeta\| := \int m^2 BF\zeta \mathrm{d}w_\parallel \mathrm{d}\mu \mathrm{d}\theta \qquad (8)$$

where $\zeta(\boldsymbol{X}, w_\parallel, \mu, t)$ is any function defined on phase-space and the integration encompasses the entire velocity space where B acts as the volume form. Notice that we name the first few fluid moments $N := \|1\|$, $NU_\parallel := \|v_\parallel\|$, $P_\perp \equiv NT_\perp := \|\mu B\|$ and $E_\parallel \equiv (P_\parallel + mNU_\parallel^2)/2 := \|mv_\parallel^2/2\|$ with $P_\parallel \equiv NT_\parallel$. We also define the moment operator for the collision function C analogous to the velocity space moment operator for the gyro-kinetic distribution function F in Eq. (8)

$$\|\zeta\|_C := \int m^2 BC\zeta \mathrm{d}w_\parallel \mathrm{d}\mu \mathrm{d}\theta \qquad (9)$$

Analogous to the moments of F we name the source moments $\Lambda_N := \|1\|_C$, $\Lambda_{P_\perp} := \|\mu B\|_C$, etc. Using Eq. (3) together with the fact that $\partial/\partial t$ and ∇ commute with the velocity integral and F vanishes for $w_\parallel = \pm\infty$ we find the important identity

$$\frac{\partial}{\partial t}\|\zeta\| + \nabla\cdot\|\zeta\dot{\boldsymbol{X}}\| = \left\|\frac{\mathrm{d}\zeta}{\mathrm{d}t}\right\| + \|\zeta\|_C = \left\|\frac{\partial\zeta}{\partial t} + \dot{\boldsymbol{X}}\cdot\nabla\zeta + \dot{w}_\parallel\frac{\partial}{\partial w_\parallel}\zeta\right\| + \|\zeta\|_C \qquad (10)$$

From this we get (neglecting finite Larmor radius effects on the $A_\parallel$ terms) [18] with

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$$
\begin{aligned}
&k, l \in 1, 2, 3, \ldots \\
&\frac{\partial}{\partial t}\|(\mu B)^k v_\parallel^l\| \\
&+\nabla\cdot\left((\hat{\boldsymbol{b}}+\boldsymbol{b}_\perp)\|(\mu B)^k v_\parallel^{l+1}\| + \frac{m}{q}\|(\mu B)^k v_\parallel^{l+2}\|\boldsymbol{K}_{\nabla\times\hat{\boldsymbol{b}}} + \frac{1}{q}\|(\mu B)^{k+1} v_\parallel^l\|\boldsymbol{K}_{\nabla B} + \frac{\hat{\boldsymbol{b}}}{B}\times\|(\mu B)^k v_\parallel^l \nabla\cdot\Psi\|\right) \\
&= k\left((\hat{\boldsymbol{b}}+\boldsymbol{b}_\perp)\|(\mu B)^k v_\parallel^{l+1}\| + \frac{m}{q}\|(\mu B)^k v_\parallel^{l+2}\|\boldsymbol{K}_{\nabla\times\hat{\boldsymbol{b}}} + \frac{1}{q}\|(\mu B)^{k+1} v_\parallel^l\|\boldsymbol{K}_{\nabla B} + \frac{\hat{\boldsymbol{b}}}{B}\times\|(\mu B)^k v_\parallel^l \nabla\cdot\Psi\|\right) \\
&\quad \cdot\nabla\ln B \\
&\quad - l\left(\frac{1}{m}\|(\mu B)^{k+1} v_\parallel^{l-1}\|(\hat{\boldsymbol{b}}+\boldsymbol{b}_\perp) + \frac{1}{q}\|(\mu B)^{k+1} v_\parallel^l\|\boldsymbol{K}_{\nabla\times\hat{\boldsymbol{b}}}\right)\cdot\nabla\ln B \\
&\quad - l\left(\frac{q}{m}(\hat{\boldsymbol{b}}+\boldsymbol{b}_\perp)\cdot\|(\mu B)^k v_\parallel^{l-1}\nabla\Psi\| + \boldsymbol{K}_{\nabla\times\hat{\boldsymbol{b}}}\cdot\|(\mu B)^k v_\parallel^l \nabla\Psi\|\right) - l\frac{q}{m}\|(\mu B)^k v_\parallel^{l-1}\|\frac{\partial}{\partial t}A_\parallel \\
&\quad + \|(\mu B)^k v_\parallel^l\|_C
\end{aligned}
\tag{11}
$$

The definitions of the curvature operators $\boldsymbol{K}_{\nabla\times\hat{\boldsymbol{b}}}$ and $\boldsymbol{K}_{\nabla B}$ can be found in table A1. Note that

$$\boldsymbol{K}_{\nabla B}\cdot\nabla\ln B = 0 \tag{12}$$

and we have

$$\boldsymbol{b}_\perp := \frac{\nabla\times A_\parallel\hat{\boldsymbol{b}}}{B} = A_\parallel\boldsymbol{K}_{\nabla\times\hat{\boldsymbol{b}}} + \frac{\nabla A_\parallel\times\hat{\boldsymbol{b}}}{B} \tag{13}$$

Eq. (11) reveals already the structure of our equations as being a combination of a convection term on the left hand side as well as two generalized mirror force terms $\propto \nabla\ln B$ and the general parallel electric field force. The significance of Eq. (11) lies in the fact that we are able to write the gyro-fluid equation at any moment.

3. The long-wavelength collisional closure

As with any fluid model, the infinite hierarchy of moments given in Eq. (11) needs to be closed. Several approaches exist. First, we can assume that the distribution function follows a Maxwellian [4].

$$F = F_M = N\frac{1}{2\pi T_\perp m}\sqrt{\frac{1}{2\pi T_\parallel m}}\exp\left(-\frac{m(v_\parallel - U)^2}{2T_\parallel} - \frac{\mu B}{T_\perp}\right) \tag{14}$$

From equation (14) we can for example derive [18]

$$
\begin{aligned}
R_{\perp\parallel} = \|(\mu B)m(v_\parallel - U_\parallel)^2\| = NT_\perp T_\parallel \qquad R_{\perp\perp} &= \|(\mu B)^2\| = 2NT_\perp^2 \\
R_{\parallel\parallel} &= \|m^2(v_\parallel - U_\parallel)^4\| = 3NT_\parallel^2
\end{aligned}
\tag{15}
$$

However, the somewhat distinct feature of a gyro-fluid model is that it needs special attention in terms that involve the gyro-average (for example $\frac{\hat{\boldsymbol{b}}}{B}\times\|(\mu B)^k v_\parallel^l \nabla\cdot\Psi\|$, which lead to infinite sums in the gyro-fluid equations even if we assume the Maxwellian distribution function. These terms can be expressed via Pade approximations [18], which are numerically tractable and we will define explicitly in Section 4.

Finally, we have the somewhat inconspicuous term $\|(\mu B)^k v_\parallel^l\|_C$. In fact, this term hides the complicated coordinate transformation of the Coulomb collision operator. Expressions for this operator have so-far only been found for linearized models [1, 19] or if linearization is omitted, the expressions are highly impractical to implement numerically [2]. Furthermore, only Coulomb collisions were considered without taking plasma-neutral interactions into account.

3.1. The long wavelength collisional closure

We here propose a different approach from trying to explicitly work out the gyro-kinetic coordinate transformation. We know from previous work that gyro-fluid models coincide in drift-fluid models in the long-wavelength limit [12, 14]. Our main idea is to choose the collisional terms such that in the long wavelength limit the drift-fluid terms are recovered and quasi-neutrality in the gyro-fluid model is retained. In other words we first chose a closure of the fluid collisional terms that result by taking moments of the original Vlasov equation (1) and in a second step transform the fluid closure to gyro-centre coordinates.

It can be shown that gyro-fluid expressions can be transformed to their corresponding fluid expressions in the long-wavelength limit via [13]

$$
\begin{aligned}
n &= N + \Delta_\perp\left(\frac{mP_\perp}{2qB^2}\right) + \nabla\cdot\left(\frac{mN\nabla_\perp\phi}{B^2}\right) \qquad && nu_\parallel = NU_\parallel \\
p_\perp &= P_\perp + \Delta_\perp\left(\frac{mR_{\perp\perp}}{2qB^2}\right) + \nabla\cdot\left(\frac{mP_\perp\nabla_\perp\phi}{B^2}\right) \qquad && e_\parallel = E_\parallel
\end{aligned}
\tag{16}
$$

The omission of the correction terms in the parallel momentum and energy equations originates in the neglect of the corresponding terms in the Hamiltonian. This can possibly be extended later but is problematic because such an extension couples the parallel Ampere law to the polarization equation, which is numerically problematic [17, 13].

The main observation now is that the fluid moment transformation (16) holds just as well for the moments of any other function on phase space, including the collision operator. Furthermore in the long-wavelength limit the relations can easily be inverted

$$
\begin{aligned}
\Lambda_N &= s_n - \Delta_\perp\left(\frac{ms_{p_\perp}}{2qB^2}\right) - \nabla\cdot\left(\frac{ms_n\nabla_\perp\phi}{B^2}\right) \qquad && \Lambda_{mNU_\parallel} = s_{nu_\parallel} \\
\Lambda_{P_\perp} &= s_{p_\perp} - \Delta_\perp\left(\frac{ms_{r_\perp}}{2qB^2}\right) - \nabla\cdot\left(\frac{ms_{p_\perp}\nabla_\perp\phi}{B^2}\right) \qquad && \Lambda_{E_\parallel} = s_{e_\parallel}
\end{aligned}
\tag{17}
$$

All that remains to do is to find appropriate expressions for the fluid collision terms s_n, $s_{p_\perp}$, $s_{nu_\parallel}$ and $s_{e_\parallel}$ that we can plug into Eq. (17). In the following we will set $s_{r_\perp} = 0$. The only constraint that we have on the collisional terms is that they should conserve the electric charge

$$
\sum_{\text{sp}} qs_n = 0 \tag{18}
$$

where we sum over all species.

3.2. Fluid collision terms

For the following terms for plasma-neutral interactions and ellastic collisions we follow References [15, 16]. We have ionization

$$
\begin{aligned}
s_{n,i,iz} &:= n_e n_n K_{i,iz} \qquad && s_{mnu_\parallel,i,iz} := m_i u_{n,\parallel} s_{n,i,iz} \\
s_{p_\perp,i,iz} &:= \left(\frac{1}{2}m_i u_{n,\perp}^2 + T_n - \delta_{i,e}\phi_{iz}\right) s_{n,i,iz} \qquad && s_{E_\parallel,i,iz} := \left(\frac{1}{2}m_i u_{n,\parallel}^2 + \frac{1}{2}T_n - \delta_{i,e}\phi_{iz}\right) s_{n,i,iz}
\end{aligned}
\tag{19}
$$

where we used $m_i/m_n \approx 1$. Here, n_n is the neutral density, T_n the neutral temperature and $u_{n,\parallel}$ is the neutral parallel velocity. $K_{i,iz}$ is the ionization rate.

Further, we have recombination

$$
\begin{aligned}
s_{n,i,rec} &:= -n_e n_i K_{i,rec} \qquad && s_{mnu_\parallel,i,rec} := m_i u_{i,\parallel} s_{n,i,rec} \\
s_{p_\perp,i,rec} &:= t_{i,\perp} s_{n,i,rec} \qquad && s_{E_\parallel,i,rec} := \left(\frac{1}{2}m_i u_{i,\parallel}^2 + \frac{1}{2}t_{i,\parallel}\right) s_{n,i,rec}
\end{aligned}
\tag{20}
$$

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where we used $m_i/m_n \approx 1$ and neglect $u_{i,\perp}^2 < t_{i,\perp}$. Charge exchange reads

$$\begin{aligned}
s_{n,i,cx} :=& 0 \qquad s_{mnu_\parallel,i,cx} := (m_i u_{n,\parallel} - m_i u_{i,\parallel}) n_i n_n K_{cx} \\
s_{p_\perp,i,cx} :=& \left(\frac{1}{2} m_i u_{n,\perp}^2 + T_{n,\perp} - t_{i,\perp}\right) n_i n_n K_{cx} \\
s_{E_\parallel,i,cx} :=& \left(\frac{1}{2} m_i u_{n,\parallel}^2 + \frac{1}{2} T_n - \frac{1}{2} m_i u_{i,\parallel}^2 - \frac{1}{2} t_{i,\parallel}\right) n_i n_n K_{cx}
\end{aligned} \tag{21}$$

We follow here [16] and in the simplest case consider charge-exchange as an ionization followed by an immediate recombination. Finally, Coulomb collisions can be described by [15]

$$\begin{aligned}
s_{n,i,scatt} :=& 0 \qquad s_{mnu_\parallel,i,scatt} := -m_i n_i \sum_k \nu_{ik}^\parallel (u_{\parallel,i} - u_{\parallel,k}) \\
s_{p_\perp,i,scatt} :=& \sum_k \frac{3 n_i m_i \nu_{ik}^\perp (t_{\perp,i} - t_{\perp,k})}{m_i + m_k} \\
s_{E_\parallel,i,scatt} :=& u_{i,\parallel} s_{mnu_\parallel,i,scatt} + \sum_k \frac{3 n_i m_i \nu_{ik}^\parallel (t_{\parallel,i} - t_{\parallel,k})}{m_i + m_k}
\end{aligned} \tag{22}$$

which is essentially Spitzer resistivity and the collisional thermal energy exchange

4. The collisional gyro-fluid model

We now have all ingredients to finally note our full-F, collisional, multi-species gyro-fluid model. This section largely bases on the ground work by references [18, 4].

4.1. Density Equation: $k = l = 0$

$$\frac{\partial}{\partial t} N + \nabla \cdot \boldsymbol{J}_N = \Lambda_N \tag{23}$$

where we have the drift current

$$\begin{aligned}
\boldsymbol{J}_N :=& (\hat{\boldsymbol{b}} + \boldsymbol{b}_\perp) N U_\parallel \\
&+ N \frac{\hat{\boldsymbol{b}}}{B} \times (\nabla \Gamma_1(\phi) + \nabla \psi_2 + \Gamma_2(\phi) \nabla \ln(B/T_\perp)) \\
&+ \frac{P_\parallel + m N U_\parallel^2}{q} \boldsymbol{K}_{\nabla \times \hat{\boldsymbol{b}}} + \frac{P_\perp}{q} \boldsymbol{K}_{\nabla B}
\end{aligned} \tag{24}$$

We have

$$\psi_2 := -\frac{m}{2qB^2} |\nabla_\perp \phi|^2 \tag{25}$$

We use the Pade approximations [18]

$$\Gamma_1 := \left(1 - \frac{\rho^2}{2} \Delta_\perp\right)^{-1} \qquad \Gamma_2 := \frac{\rho}{2} \frac{\partial}{\partial \rho} \Gamma_1 \qquad \Gamma_3 := \left(1 + \frac{\rho}{2} \frac{\partial}{\partial \rho}\right) \Gamma_2 \tag{26}$$

$$\rho^2 := \frac{m T_\perp}{q^2 B^2} \tag{27}$$

These operators are involved with dynamic finite Larmor radius effects in the model [5, 6]. Expressions for Γ_2 and Γ_3 can be found in [18], which are essentially Helmholtz type operators.

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A possible improvement to the model is to follow [18] and relieve the long wavelength limit of the polarization term to yield $\psi_2 = -m|\nabla_\perp\sqrt{\Gamma_0}\phi|^2/2qB^2$ with $\Gamma_0 = (1-\rho^2\Delta_\perp)^{-1}$. However, this will lead to both additional terms in Γ_2 and Γ_3 and also leads to (yet unsolved numerical) problems in the polarisation equation (a matrix square root $\sqrt{\Gamma_0}$ needs to be computed). We have recently achieved a numerical realisation of the isothermal variant [20] but a solution for the thermal, multispecies variant is still ongoing work. In this first iteration of the model we thus keep the long wavelength approximation $\Gamma_0 = 1$.

4.2. Polarisation equation
The polarisation equation reads

$$\sum_{\text{sp}}\left[q\Gamma_1^\dagger N + \nabla\cdot\left(\frac{mN}{B^2}\nabla_\perp\phi\right)\right] = 0 \tag{28}$$

where we sum over all species and define

$$\Gamma_1^\dagger := (1-\Delta_\perp\rho^2/2)^{-1} \tag{29}$$

4.3. Parallel momentum equation $k = 0$, $l = 1$

$$\frac{\partial}{\partial t}\left(mNU_\parallel\right) + qN\frac{\partial}{\partial t}A_\parallel + \nabla\cdot\boldsymbol{J}_{mNU} = F_{mNU,\nabla B} + F_{mNU,E} + \Lambda_{mNU} \tag{30}$$

with the momentum currents

$$\begin{aligned}\boldsymbol{J}_{mNU} :=& (mNU_\parallel^2 + P_\parallel)(\hat{\boldsymbol{b}}+\boldsymbol{b}_\perp)\\ &+ m\frac{\hat{\boldsymbol{b}}}{B}\times\Big(NU_\parallel\left[\nabla\Gamma_1(\phi)+\nabla\psi_2+\Gamma_2(\phi)\nabla\ln(B/T_\perp)\right]+\\ &\frac{Q_{\perp\parallel}}{T_\perp}\left[\nabla\Gamma_2(\phi)+(\Gamma_3-\Gamma_2)(\phi)\nabla\ln(B/T_\perp)\right]\Big)\\ &+ m\frac{Q_{\parallel\parallel}+3U_\parallel P_\parallel + mNU_\parallel^3}{q}\boldsymbol{K}_{\nabla\times\hat{\boldsymbol{b}}}\\ &+ m\frac{U_\parallel P_\perp + Q_{\perp\parallel}}{q}\boldsymbol{K}_{\nabla B}\end{aligned} \tag{31}$$

and the electric and mirror force terms

$$\begin{aligned}F_{mNU,E} =& -mN(\hat{\boldsymbol{b}}+\boldsymbol{b}_\perp)\cdot(\nabla(\Gamma_1(\phi)+\psi_2)+\Gamma_2(\phi)\nabla\ln(B/T_\perp))\\ &- m\boldsymbol{K}_{\nabla\times\hat{\boldsymbol{b}}}\cdot\Big(NU_\parallel\left[\nabla(\Gamma_1(\phi)+\psi_2)+\Gamma_2(\phi)\nabla\ln(B/T_\perp)\right]\\ &+\frac{Q_{\perp\parallel}}{T_\perp}\left[\nabla\Gamma_2(\phi)+(\Gamma_3-\Gamma_2)(\phi)\nabla\ln(B/T_\perp)\right]\Big)\\ F_{mNU,\nabla B} =& -P_\perp(\hat{\boldsymbol{b}}+\boldsymbol{b}_\perp)\cdot\nabla\ln B - m\frac{U_\parallel P_\perp + Q_{\perp\parallel}}{q}\boldsymbol{K}_{\nabla\times\hat{\boldsymbol{b}}}\cdot\nabla\ln B\end{aligned} \tag{32}$$

4.4. Parallel Ampere law
Neglecting all finite Larmor radius effects on $A_\parallel$ we simply have

$$-\mu_0\Delta_\perp A_\parallel = \sum_{\text{sp}} qNU_\parallel \tag{33}$$

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4.5. Perpendicular pressure equation, $k = 1$, $l = 0$

$$\frac{\partial}{\partial t} P_\perp + \nabla\cdot \boldsymbol{J}_{P_\perp} = \boldsymbol{J}_{P_\perp}\cdot\nabla\ln B + \Lambda_{P_\perp} \tag{34}$$

with

$$\begin{aligned}\boldsymbol{J}_{P_\perp} :=&(\hat{\boldsymbol{b}}+\boldsymbol{b}_\perp)(U_\| P_\perp + Q_{\perp,\|})\\ &+\frac{1}{q}\left(mU_\|^2 P_\perp + 2mU_\| Q_{\|\perp} + R_{\perp\|}\right)\boldsymbol{K}_{\nabla\times\hat{\boldsymbol{b}}} + \frac{1}{q}R_{\perp\perp}\boldsymbol{K}_{\nabla B}\\ &+ P_\perp\frac{\hat{\boldsymbol{b}}}{B}\times\left(\nabla(\Gamma_1(\phi)+\psi_2) + \nabla\Gamma_2(\phi) + \Gamma_3(\phi)\nabla\ln(B/T_\perp)\right)\end{aligned} \tag{35}$$

Note the alternative formulation $\nabla\cdot\boldsymbol{J} - \boldsymbol{J}\cdot\nabla\ln B = B\nabla\cdot(\boldsymbol{J}/B)$ and the closure relation $R_{\perp\perp} = 2NT_\perp^2$

4.6. Parallel energy equation $k = 0$, $l = 2$

$$\frac{\partial}{\partial t}E_\| + qNU_\|\frac{\partial A_\|}{\partial t} + \nabla\cdot\boldsymbol{J}_{E_\|} = F_{E_\|,\nabla B} + F_{E_\|,E} + \Lambda_{E_\|} \tag{36}$$

with

$$E_\| := \frac{1}{2}(P_\| + mNU_\|^2) \tag{37}$$

$$\begin{aligned}\boldsymbol{J}_{E_\|} =& \frac{1}{2}(\hat{\boldsymbol{b}}+\boldsymbol{b}_\perp)\left(mNU_\|^3 + 3U_\| P_\| + Q_{\|\|\|}\right)\\ &+\frac{1}{2q}\left(m^2NU_\|^4 + 6mU_\|^2P_\| + 4mU_\|Q_{\|\|\|} + R_{\|\|\|}\right)\boldsymbol{K}_{\nabla\times\hat{\boldsymbol{b}}}\\ &+\frac{1}{2q}\left(mU_\|^2P_\perp + R_{\perp\|} + 2Q_{\perp\|}U_\|\right)\boldsymbol{K}_{\nabla B}\\ &+\frac{1}{2}\frac{\hat{\boldsymbol{b}}}{B}\times\left((P_\| + mNU_\|^2)\nabla(\Gamma_1(\phi)+\psi_2) + \frac{2mU_\|Q_{\perp\|}}{T_\perp}\nabla\Gamma_2(\phi)\right)\\ &+\frac{1}{2}\frac{\hat{\boldsymbol{b}}}{B}\times\left(\left(P_\| + mNU_\|^2 - \frac{2mU_\|Q_{\perp\|}}{T_\perp}\right)\Gamma_2(\phi)\nabla\ln(B/T_\perp) + \frac{2mU_\|Q_{\perp\|}}{T_\perp}\Gamma_3(\phi)\nabla\ln(B/T_\perp)\right)\end{aligned} \tag{38}$$

and the generalized mirror and electric forces / energy transfer

$$\begin{aligned}F_{E_\|,\nabla B} :=& (P_\perp U_\| + Q_{\perp\|})(\hat{\boldsymbol{b}}+\boldsymbol{b}_\perp)\cdot\nabla\ln B\\ &+\frac{1}{q}(mU_\|^2P_\perp + 2mU_\|Q_{\perp\|} + R_{\|\perp})\boldsymbol{K}_{\nabla\times\hat{\boldsymbol{b}}}\cdot\nabla\ln B\end{aligned} \tag{39}$$

$$\begin{aligned}F_{E_\|,E} :=& (\hat{\boldsymbol{b}}+\boldsymbol{b}_\perp)\cdot\left(NU_\|\left[\nabla(\Gamma_1(\phi)+\psi_2) + \Gamma_2(\phi)\nabla\ln(B/T_\perp)\right] + \right.\\ &\left.\frac{Q_{\perp\|}}{T_\perp}\left(\nabla\Gamma_2(\phi) + (\Gamma_3(\phi)-\Gamma_2(\phi))\nabla\ln(B/T_\perp)\right)\right)\\ &+\boldsymbol{K}_{\nabla\times\hat{\boldsymbol{b}}}\cdot\left[E_\|\left[\nabla(\Gamma_1(\phi)+\psi_2) + \Gamma_2(\phi)\nabla\ln(B/T_\perp)\right] + \right.\\ &\left.+\frac{2mU_\|Q_{\perp\|}}{T_\perp}\left(\nabla\Gamma_2(\phi) + (\Gamma_3(\phi)-\Gamma_2(\phi))\nabla\ln(B/T_\perp)\right)\right]\end{aligned} \tag{40}$$

As closure relation we propose for the parallel fluxes of perpendicular/parallel pressure

$$Q_{\perp\|} = -\kappa_{\perp\|}\hat{\boldsymbol{b}}\cdot\nabla T_\perp \qquad Q_{\|\|\|} = -\kappa_{\|\|\|}\hat{\boldsymbol{b}}\cdot\nabla T_\| \tag{41}$$

Alternatively we can use an expression for drift-kinetic models [21]

$$Q_{\perp\|} = -\eta_{\perp\|}P_\perp(U_{\|,e} - U_{\|,i}) - \kappa_{\perp\|}\hat{\boldsymbol{b}}\cdot\nabla T_\perp \qquad Q_{\|\|\|} = -\eta_{\|\|\|}P_\|(U_{\|,e} - U_{\|,i}) - \kappa_{\|\|\|}\hat{\boldsymbol{b}}\cdot\nabla T_\| \tag{42}$$

4.7. Energy conservation and conservation of currents
The model energy density equation reads [4, 18]

$$\frac{\partial}{\partial t}\mathcal{E} + \nabla\cdot \boldsymbol{J}_{\mathcal{E}} = \Lambda_{\mathcal{E}} \qquad \mathcal{E} := \sum_{\text{sp}}\left(P_\perp + E_\parallel - qN\psi_2\right) + \frac{(\nabla_\perp A_\parallel)^2}{2\mu_0} \tag{43}$$

with

$$\Lambda_{\mathcal{E}} := \sum_{\text{sp}}(q(\Gamma_1(\phi)+\psi_2) - \Gamma_2(\phi))\Lambda_N + \left(1 + \frac{q\Gamma_2(\phi)}{T_\perp}\right)\Lambda_{P_\perp} + \Lambda_{E_\parallel} \tag{44}$$

Due to size limitations we omit the expression for the energy current $\boldsymbol{J}_{\mathcal{E}}$.

In the recent Reference [14] the conservation of currents or "vorticity" equation for our model was explicitly derived in the long wavelength limit:

$$\partial_t\nabla\cdot\left[\sum_{\text{sp}}\frac{mn}{B^2}\left(\frac{\nabla_\perp p_\perp}{nq} + \nabla_\perp\phi\right)\right] = \ldots + \nabla\cdot\left[\sum_{\text{sp}}\frac{m}{B^2}\left(\frac{\nabla_\perp s_p}{q} + s_n\nabla_\perp\phi\right)\right] \tag{45}$$

We here only show the dependence on the fluid source terms. Under a flux-surface average this equation becomes an equation for angular momentum [13]. Eq. (45) is a consequence of the conservation of charge (18) and shows that sources of pressure (heating) as well as density can lead to poloidal rotation.

5. Aspects of a numerical implementation
In this section we sketch how a possible implementation of our equations could look like. Our goal here is to convince the reader of the possibility to implement the presented model with today's numerical methods.

First, we notice the general form of the equations that we derived in Section 4. Due to the time derivatives on $A_\parallel$ our system of equations is of the form

$$\begin{pmatrix} 1 & & & & \\ & 1 & & & qN \\ & & 1 & & \\ & & & 1 & qNU_\parallel \\ & q & & & -\mu_0\Delta_\perp \end{pmatrix}\frac{\partial}{\partial t}\begin{pmatrix} N \\ NU_\parallel \\ P_\perp \\ E_\parallel \\ A_\parallel\end{pmatrix} + \nabla\cdot\begin{pmatrix}\boldsymbol{J}_N \\ \boldsymbol{J}_{mNU} \\ \boldsymbol{J}_{P_\perp} \\ \boldsymbol{J}_{E_\parallel} \\ 0\end{pmatrix} = \begin{pmatrix} 0 \\ F_{mNU,\nabla B} + F_{mNU,E} \\ \boldsymbol{J}_{P_\perp}\cdot\nabla\ln B \\ F_{E_\parallel,\nabla B} + F_{E_\parallel,E} \\ 0\end{pmatrix} + \begin{pmatrix}\Lambda_N \\ \Lambda_{mNU} \\ \Lambda_{P_\perp} \\ \Lambda_{E_\parallel} \\ 0\end{pmatrix} \tag{46}$$

The last equation is obtained by deriving the parallel Ampere law (33) in time. In each step the polarisation equation Eq. (28) needs to be solved and the gyro-average operators (26) need to be applied.

We here emphasize that the equations (46) are completely symmetric with respect to several ion species. This is one of the advantages over existing drift-fluid models. Furthermore, the polarisation equation decouples from the dynamical system (i.e. there is no time-derivative in Eq. (28)). This contrasts to drift-fluid models where the potential is given by the vorticity equation, which leads to a strongly coupled system that is hard to solve numerically [11].

5.1. Timestepper and the mass matrix
The main difficulty when formulating a timestepper for Eq. (46) is the mass matrix. Writing Eq. (46) in the form $\boldsymbol{M}(\boldsymbol{y})\dot{\boldsymbol{y}} = \boldsymbol{G}(y,t)$ with $\boldsymbol{y} = (N, NU_\parallel, P_\perp, E_\parallel, A_\parallel)$ and $\boldsymbol{M}$ and $\boldsymbol{G}$ implicitly defined, we see that we have to invert $\boldsymbol{M}$ to yield the canonical form $\dot{\boldsymbol{y}} = \boldsymbol{f}(\boldsymbol{y},t) \equiv \boldsymbol{M}^{-1}\boldsymbol{G}$.

Inspecting the matrix $\boldsymbol{M}$ we see that only the $\dot{NU_\parallel}$ and $\dot{A}_\parallel$ equations are strongly coupled and lead to the equation

$$\left(-\sum_{\text{sp}} qN - \mu_0\Delta_\perp\right)\dot{A}_\parallel = \sum_{\text{sp}} G_{NU_\parallel} \tag{47}$$

Once $\dot{A}_\parallel$ is known the equations for $\dot{NU_\parallel}$ and $\dot{E}_\parallel$ can easily be inverted. The equations for $\dot{N}$ and $\dot{P}_\perp$ are entirely decoupled. With the right hand side $\boldsymbol{f} \equiv \boldsymbol{M}^{-1}\boldsymbol{G}$ reliably computable, the formulation of an adequate timestepper for the general form $\dot{\boldsymbol{y}} = \boldsymbol{f}(\boldsymbol{y}, t)$ poses no difficulty. An abundance of timesteppers like Runge-Kutta or multistep methods are available.

Note that in our model we ignore all gyro-averaging effects on $A_\parallel$. This is mainly because of the difficulty of integrating $\partial_t NU + N\partial_t\Gamma_1 A_\parallel$ in time (the Gamma operator does not commute with the time derivative). Further research is needed to show that it can be done at no significant computational cost. For now $\Gamma_1 A_\parallel \approx A_\parallel$ is kept at lowest order.

5.2. Spatial discretization: advection and diffusion

The difficulty for the spatial discretization is to construct an appropriate advection solver for the terms $\nabla\cdot\boldsymbol{J}$ that is both stable and conserves invariants (for example the mass). Here, we distinguish between the advection perpendicular and parallel to the magnetic field.

For the perpendicular direction, we recommend discontinuous Galerkin methods [22], which can be seen as generalizations of finite element and finite volume schemes and have excellent stability, parallelization and conservation properties. For the parallel direction (terms of the form $\nabla\cdot(\hat{\boldsymbol{b}}U_\parallel..)$) the flux-coordinate independent approach is the state of the art [23, 24] as flux-tube approaches don't generally work for geometries including X-points and direct discretizations have too much numerical diffusion and a too severe CFL condition. However, do note the "self-advection" parallel Burger terms in the $NU_\parallel$ and $E_\parallel$ equations (e.g. $mNU_\parallel^2$ and the factor $U_\parallel^3$ in the curvature drift), which without viscosity can lead to shocks. Additional artificial parallel diffusion may be necessary to stabilize the scheme.

The implementation of the force terms $F_{\nabla B}$ and F_E as well as the collisional and source terms suggested in Section 3.2 is straightforward.

5.3. Elliptic solvers

We need elliptic solvers to solve both the polarization equation (28) as well as the application of the gyro-averaging operators Γ_1, Γ_2 and Γ_3 (26) and (29) (which also involve inversion of an elliptic problem). The main difficulty here is that both the elliptic operator (28) as well as the Helmholtz-type operators (26) and (29) depend on a dynamic field (density respectively temperature), i.e. the discretization matrices change in each timestep. When inverting these numerically iterative schemes seem paramount and one should use preconditioners that are (i) easy and fast to compute and apply and/or (ii) reused from previous timesteps such that their re-computation is ammortized. The Γ_2 and Γ_3 operators can be applied by successively applying Γ_1. The inversion of the Ampere equation in the form (47) poses no principle difficulty compared to the polarisation and gyro-average operators.

5.4. Boundary conditions

Depending on the chosen simulation domain various boundary conditions must be considered. If the domain should not include the core region of the plasma, one must either fix the values of the four moments at the inner boundary (gradient driven simulation) or specify a constant influx of mass and energy (flux-driven simulation). There are two major issues when it comes to the outer boundary including the divertor: (i) when using structured spatial grids, the shape of the wall and divertor are generally not conforming to said grid and (ii) the formulation of sheath boundary conditions for the proposed fluid model has strong influence on the numerical stability of simulations.

The first problem can be solved by either using unstructured grids that are conforming to the wall or by using immersed boundary conditions as proposed in Ref. [25]. For the second problem we propose to start with insulating sheath boundary conditions that are shown to work in Reference [26]. More realistic boundary conditions that come closer to model kinetic effects as in [27] are subject to future extensions.

6. Conclusions

A 4-moment, multispecies, electromagnetic, full-F gyro-fluid model including sources as well as reacting (plasma-neutral interactions) and scattering collisions was derived. The numerical implementability with today's numerical methods (avoiding infinite sums, nested time and/or elliptic constructs) was discussed. The model includes finite Larmor radius effects wherever possible and takes other (collisional) terms in the long wavelength limit. This makes the model at least as accurate as drift-fluid models with regards to collisional terms. Consistent particle drifts as a result of gyro-kinetic equations of motion are retained and the explicit energy theorem and conservation of currents are shown.

Various improvements and future updates are possible. Firstly, it is known that the scrape-off layer may not entirely be in the high collisionality regime [27]. For this regime, a trans-collisional closure must be derived. Other shortcomings of the model include for example the absence of a zeroth order high amplitude electric potential [28]. Furthermore, closure schemes that take trapped particle dynamics into account should be considered. Finally, the "correct" derivation of a non-linear, short-wavelength collision operator may yield superior modelling capabilities in the future. However, the presented model is ready to be implemented today.

Appendix A. The magnetic field

We assume a three-dimensional flat space with arbitrary coordinate system $\boldsymbol{x} := \{x_0, x_1, x_2\}$, metric tensor g_{ij} and volume element $\sqrt{g} := \sqrt{\det g}$. Given a vector field $\boldsymbol{B}(\boldsymbol{x})$ with unit vector $\hat{\boldsymbol{b}}(\boldsymbol{x}) := (\boldsymbol{B}/B)(\boldsymbol{x})$ we can define various differential operations.

Table A1. Definitions of geometric operators with b^i the contra-variant components of $\hat{\boldsymbol{b}}$ and g^{ij} the contra-variant elements of the metric tensor. We assume $(\nabla\times\hat{\boldsymbol{b}})_\parallel = 0$.

Name	Symbol	Definition
Projection Tensor	h	$h^{ij} := g^{ij} - b^i b^j$ Note $h^2 = h$
Perpendicular Gradient	$\nabla_\perp$	$\nabla_\perp f := \hat{\boldsymbol{b}}\times(\nabla f\times\hat{\boldsymbol{b}}) = h\cdot\nabla f$
Perpendicular Laplacian	$\Delta_\perp$	$\Delta_\perp f := \nabla\cdot(\nabla_\perp f) = \nabla\cdot(h\cdot\nabla f) = -\nabla_\perp^\dagger\cdot\nabla_\perp$
Curl-b Curvature Operator	$\mathcal{K}_\kappa$	$\mathcal{K}_\kappa(f) := \boldsymbol{K}_{\boldsymbol{\kappa}}\cdot\nabla f = \frac{1}{B}(\hat{\boldsymbol{b}}\times\boldsymbol{\kappa})\cdot\nabla f$ with $\boldsymbol{\kappa} := \hat{\boldsymbol{b}}\cdot\nabla\hat{\boldsymbol{b}}$
Grad-B Curvature Operator	$\mathcal{K}_{\nabla B}$	$\mathcal{K}_{\nabla B}(f) := \boldsymbol{K}_{\nabla \boldsymbol{B}}\cdot\nabla f = \frac{1}{B}(\hat{\boldsymbol{b}}\times\nabla\ln B)\cdot\nabla f$
Curvature Operator	$\mathcal{K}$	$\mathcal{K}(f) := \boldsymbol{K}\cdot\nabla f = \nabla\cdot\left(\frac{\hat{\boldsymbol{b}}\times\nabla f}{B}\right) = \nabla\times\frac{\hat{\boldsymbol{b}}}{B}\cdot\nabla f,$
Parallel derivative	$\nabla_\parallel$	$\nabla_\parallel f := \boldsymbol{B}\cdot\nabla f/B$ Notice $\nabla\cdot\hat{\boldsymbol{b}} = -\nabla_\parallel \ln B$

Explicit expressions for the above expressions depend on the choice of the magnetic field and the underlying coordinate system. Note that we have

$$\begin{aligned} \boldsymbol{K} = \boldsymbol{K}_{\nabla\times\hat{\boldsymbol{b}}} + \boldsymbol{K}_{\nabla B} \qquad \nabla\cdot\boldsymbol{K}_{\nabla\times\hat{\boldsymbol{b}}} = -\nabla\cdot\boldsymbol{K}_{\nabla B} = -\boldsymbol{K}_{\nabla\times\hat{\boldsymbol{b}}}\cdot\nabla\ln B, \\ \nabla\cdot\boldsymbol{K} = 0, \qquad \boldsymbol{K}_{\nabla\times\hat{\boldsymbol{b}}} - \boldsymbol{K}_{\nabla B} = \frac{1}{B^2}(\nabla\times\boldsymbol{B}), \qquad \nabla_\parallel \ln B = -\nabla\cdot\hat{\boldsymbol{b}}. \end{aligned} \tag{A.1}$$

The last equality holds if $\nabla\cdot\boldsymbol{B} = 0$. In any arbitrary coordinate system we have

$$(\nabla f)^i = g^{ij}\partial_j f \ , \quad \nabla\cdot\boldsymbol{v} = \frac{1}{\sqrt{g}}\partial_i\left(\sqrt{g}v^i\right) \ , \quad (\boldsymbol{v}\times\boldsymbol{w})^i = \frac{1}{\sqrt{g}}\varepsilon^{ijk}v_j w_k \ . \tag{A.2}$$

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