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GEM-X Equations

Ion gyrokinetic equation

This is the ion gyrokinetic equation we are solving in the SOL. We will start with drift fluid electrons. The ion equations of motion are discussed later.

$$\frac{\partial f}{\partial t} + \dot{\mathbf{z}} \cdot \frac{\partial f}{\partial \mathbf{z}} = 0, \tag{1}$$

where $\mathbf{z} = \Big(\mathbf{R}, v_\parallel, \mu\Big)$, $f(\mathbf{z},t) = f_0(\mathbf{z}) + \delta f(\mathbf{z},t)$, $\dot{\mathbf{z}} = \dot{\mathbf{z}}^0 + \dot{\mathbf{z}}^1$, and $\dot{\mathbf{z}}^0 \cdot \partial_{\mathbf{z}} f_0(\mathbf{z}) = 0$.

$$\partial_t \delta f + \dot{\mathbf{z}} \cdot \partial_{\mathbf{z}} \delta f = -\dot{\mathbf{z}}^1 \cdot \partial_{\mathbf{z}} f_0 \tag{2}$$

Note that Eq. (2) is **fully nonlinear** assuming f_0 is an equilibrium. We will obtain f_0 assuming a Maxwellian distribution with profiles given by a steady-state SOLPS-ITER solution. We can allow for neoclassical axisymmetric evolution from this initial equilibrium by keeping ion collisions and the $\mathbf{v}_D \cdot \nabla f_0$ magnetic drift term. There is a major advantage formulating the problem this way, Eq. (2), because the calculation can be solved as an linear initial value problem when nonlinearities are dropped. The provides a way to benchmark codes and study what instabilities are present. A total-f formulation, starting with Eq. (1), does not allow for isolating the linear physics from the equilibrium evolution. Such codes will be difficult to validate, requiring fully nonlinear benchmarking between similar codes. The nonlinear δf method does require a well-defined marker particle equilibrium distribution function. However, recent marker particle control techniques developed in GEM can alleviate this issue[**?**].

Ion equations of motion

$\mathbf{R} = \mathbf{R}^0 + \mathbf{R}^1$, $v_\parallel = v_\parallel^0 + v_\parallel^1$, $\mu = \frac{m v_\perp^2}{2B} = \text{constant}$

$$\dot{\mathbf{R}}^0 = \frac{1}{B^*}\left\{ v_\parallel \mathbf{B}^{*0} + \frac{1}{e}\hat{\mathbf{b}} \times \mu \nabla B^0 \right\}, \tag{3}$$

$$\dot{v}_\parallel^0 = -\frac{1}{B^*}\left\{ \mathbf{B}^{*0} \cdot \frac{\mu}{m} \nabla B^0 \right\}, \tag{4}$$

$$\dot{\mathbf{R}}^1 = \frac{1}{B^*}\left\{ v_\parallel \delta\overline{\mathbf{B}}_\perp + \hat{\mathbf{b}} \times \nabla \delta\bar{\phi} \right\}, \tag{5}$$

$$\dot{v}_\parallel^1 = \frac{1}{B^*}\left\{ \mathbf{B}^{*0} \cdot \frac{e}{m} \bar{E}_\parallel \hat{\mathbf{b}} + \delta\overline{\mathbf{B}}_\perp \cdot \frac{\mu}{m} \nabla B^0 \right\}. \tag{6}$$

$$\mathbf{B}^* = \mathbf{B}^0 + \delta\overline{\mathbf{B}}_\perp + \frac{m}{e} v_\parallel \nabla \times \hat{\mathbf{b}}, \tag{7}$$

$$B^* = \hat{\mathbf{b}} \cdot \mathbf{B}^* \tag{8}$$

$$\mathbf{B}^{*0} = \mathbf{B}^0 + \frac{m}{e} v_\parallel \nabla \times \hat{\mathbf{b}}. \tag{9}$$

$$\delta\bar{\phi} = \frac{1}{2\pi} \int \delta\phi(\mathbf{R} + \rho) \mathrm{d}\theta \tag{10}$$

Field equations

$$\nabla_\perp^2 A_\parallel = -\mu_0 \left(\bar{J}_{\parallel \mathrm{i}} + J_{\parallel \mathrm{e}} \right) \tag{13}$$

We use a Pade approximation to the modified Bessel function Γ_0[**?**] to write the gyrokinetic Poisson equation in differential form[**?**]

$$\nabla_\perp \cdot \frac{n_0 m}{eB^2} \nabla_\perp \Phi = -\left(1 + \rho_i^2 \nabla_\perp^2\right) \left(\delta \bar{n}_i - \delta n_e\right) \tag{14}$$

$$\delta \mathbf{B}_\perp = \nabla A_\parallel \times \hat{\mathbf{b}} \tag{15}$$

$$E_\parallel = -\hat{\mathbf{b}} \cdot \nabla \phi - \partial_t A_\parallel \tag{16}$$

$$\delta \bar{n}_\mathrm{i} = \int \delta f \delta(\mathbf{R} + \rho - \mathbf{x}) \mathrm{d}\mathbf{R} \mathrm{d}^3 v \tag{17}$$

$$\bar{J}_{\parallel,\mathrm{i}} = q \int v_\parallel \delta f \delta(\mathbf{R} + \rho - \mathbf{x}) \mathrm{d}\mathbf{R} \mathrm{d}^3 v \tag{18}$$

Drift-fluid electron equations

$$\begin{aligned} &\partial_t \delta n_\mathrm{e} + \mathbf{v}_E \cdot \nabla \left(n_0 + \delta n_\mathrm{e}\right) + n_0 B \tilde{\mathbf{b}} \cdot \nabla \frac{u_{\parallel \mathrm{e}}}{B} \\ &+ \frac{1}{m_\mathrm{e} \Omega_\mathrm{e} B} \hat{\mathbf{b}} \times \nabla B \cdot \nabla \left(\delta P_{\perp,\mathrm{e}} + \delta P_{\parallel,\mathrm{e}} \right) + \frac{2 n_0}{B^2} \hat{\mathbf{b}} \times \nabla B \cdot \nabla \delta \phi = 0 \end{aligned} \tag{19}$$

$$e \left(n_0 + \delta n_\mathrm{e}\right) E_\parallel = -\left(\hat{\mathbf{b}} + \frac{\delta \mathbf{B}_\perp}{B} \right) \cdot \nabla \left(P_{\parallel 0\mathrm{e}} + \delta n_\mathrm{e} T_{\parallel,0\mathrm{e}} \right) + \eta \left(\bar{J}_{\parallel,\mathrm{i}} - J_{\parallel,e} \right) \tag{20}$$

Cylindrical coordinate system

Show coordinate system to make sure direction of $\hat{\phi}$ is correct.

Units

The Units section will need to be kept up to date. If we use SI units there are some very large and small numbers (m_e, n for example). I simply specify SI units here.

GEM-X uses SI units. Length in meters, time in seconds, velocity in m/s, energy in Joules, ϕ in Volts, B in Tesla, E v/m. Any use of temperature will be expressed in energy as kT. ϵ_0, μ_0, and k (Boltzmann's constant) will be input parameters to allow for simple dimensionless tests of the code. I.e. these constants can be set to one. Likewise for e, m_e, q_α, m_α, where the α is the species index. *f has SI units. What are they? $m^{-6}s^3$?? $\delta n = \int \delta f B d\mu dv_\parallel$ has units of m^{-3}. δn and δf are large numbers!*

$\nabla_\perp$ and $\nabla_\parallel$ finite difference scheme

Order of time-integration

Discuss the order of solution of the equations. Use an enumerated list with simplified equations for illustration. To begin with, we describe the sequence of a simple Euler advance of our system. Following this simplified conceptual advance, we discuss the actual predictor-corrector sequence.

1. Deposit ion charge and current.
2. Solve Ampere's law and GK Poisson equation, Eqs.(13) and (14).
3. Solve Ohm's law, Eq. (20) for the new $E_\parallel$.
4. Time advance Eq. (16) to obtain the new $A_\parallel$.
5. Time advance the electron continuity equation, Eq.(19), to obtain the new δn_e.
6. Push particles to the next time level.

Numerical integration of ion equations of motion

My preference is the predictor-corrector scheme[**?**]. Let us look at a general first-order equation $\dot{\mathbf{x}} = F(\mathbf{x}, \mathbf{t})$. This form can be generalized to solve

Eqs. (3-8) and Eqs. (16) and (19).

$$\tilde{\mathbf{x}}^{n+1} = \mathbf{x}^{n-1} + \Delta t F\left(\mathbf{x}^n, t^n\right), \tag{21}$$

$$\mathbf{x}^{n+1} = \mathbf{x}^n + \frac{\Delta t}{2}\left(F\left(\mathbf{x}^n, t^n\right) + F\left(\tilde{\mathbf{x}}^{n+1}, t^{n+1}\right)\right). \tag{22}$$

This is what is known as a multi-step, multi-value method[**?**]. With time levels $n-1$ and n, you advance to time level $n+1$. I have tested this scheme for long time integration of closed particle orbits in large aspect ratio circular tokamak geometry and it s very good at preserving the closed orbit. RK2 performs poorly by comparison.

What is used by GEM is RK2 (I have not verified this is really RK2)

$$\tilde{\mathbf{x}}^{n+\frac{1}{2}} = \mathbf{x}^{n-1} + \frac{1}{2}\Delta t F\left(\mathbf{x}^n, t^n\right), \tag{23}$$

$$\mathbf{x}^{n+1} = \mathbf{x}^n + \frac{\Delta t}{2}\left(F\left(\mathbf{x}^n, t^n\right) + F\left(\tilde{\mathbf{x}}^{n+1}, t^{n+\frac{1}{2}}\right)\right). \tag{24}$$

Another single-step scheme that would be worth a try is

$$\tilde{\mathbf{x}}^{n+1} = \mathbf{x}^n + \Delta t F\left(\mathbf{x}^n, t^n\right), \tag{25}$$

$$\mathbf{x}^{n+1} = \mathbf{x}^n + \frac{\Delta t}{2}\left(F\left(\mathbf{x}^n, t^n\right) + F\left(\tilde{\mathbf{x}}^{n+1}, t^{n+1}\right)\right). \tag{26}$$

I have tested these three schemes by tracing closed trapped and passing orbits in cylindrical geometry with large time step. Since the latter two schemes are more dissipative, they result in the orbit spiraling inwards. The damping rate can be calculated by formulating the simple harmonic oscillator problem $\ddot{x} = -\omega_0^2 x$ with an x and v variable. Then substitute the assumed solution $\exp(-in\Delta t\omega)$ in the particular numerical scheme, and solve for ω to obtain the imaginary part.

Numerical time advance for $A_\parallel$ and δn_e

Please write out the numerical method for $A_\parallel$. Currently, using simple predictor-corrector or RK2. My preference is the predictor-corrector scheme[**?**]. I am not sure if there is an earlier reference. It is a multi-step multi-value method that is both fast and weakly dissipative. RK4 is fine but will be slower. Also, it is nice to consistently use the same time advance for the electron fluid and the ions.

Guiding-center equations in cylindrical coordinates

Equation of motion for (R, Z, ζ) is derived from the (simplified) guiding center velocity

$$\mathbf{v}_G = v_\parallel \mathbf{b} + \frac{v_\parallel^2 + v_\perp^2/2}{\Omega B^2}\mathbf{B}\times\nabla B + \frac{\mathbf{E}\times\mathbf{b}}{B} + v_\parallel \frac{\delta\mathbf{B}_\perp}{B} \tag{27}$$

$$\begin{aligned}\frac{dR}{dt} &= \mathbf{v}_G\cdot\nabla R\\ \frac{dZ}{dt} &= \mathbf{v}_G\cdot\nabla Z\\ \frac{d\zeta}{dt} &= \mathbf{v}_G\cdot\nabla\zeta\end{aligned} \tag{28}$$

B-star effects will be added later.

$$\mathbf{B} = B_R\hat{R} + B_Z\hat{Z} + B_\zeta\hat{\zeta} \tag{29}$$

$$\nabla B = \frac{\partial B}{\partial R}\hat{R} + \frac{\partial B}{\partial Z}\hat{Z} \tag{30}$$

$$\mathbf{B}\times\nabla B = -B_\zeta\frac{\partial B}{\partial Z}\hat{R} + B_\zeta\frac{\partial B}{\partial R}\hat{Z} + \left(B_R\frac{\partial B}{\partial Z} - B_Z\frac{\partial B}{\partial R}\right)\hat{\zeta} \tag{31}$$

$$\mathbf{E} = E_R\hat{R} + E_Z\hat{Z} + E_\zeta\hat{\zeta} \tag{32}$$

$$\mathbf{E}\times\mathbf{B} = (E_Z B_\zeta - E_\zeta B_Z)\hat{R} - (E_R B_\zeta - E_\zeta B_R)\hat{Z} + (E_R B_Z - E_Z B_R)\hat{\zeta} \tag{33}$$

Using ζ as the field-line direction requires care in calculating $E_\zeta = -\partial\phi/\partial\zeta$ on the grids. And it is necessary to calculate perturbations at the particle location using the local field-aligned coordinates.

We will consider only perpendicular magnetic perturbations. Given $A_\parallel$, $\delta\mathbf{B}_\perp = \nabla\times A_\parallel\mathbf{b}$ has three components in (R, Z, ζ).

$$\delta\mathbf{B}_\perp = \delta B_R\hat{R} + \delta B_Z\hat{Z} + \delta B_\zeta\hat{\zeta} \tag{34}$$

All equilibrium quantities, B, $\partial B/\partial R$, etc. are 2D arrays on (R, Z) grids. Linear interpolation along the field line is used to obtain values at particle location.

The guiding center motion is given by,

$$\begin{aligned}v_\parallel\mathbf{b}\cdot\nabla R &= v_\parallel\frac{B_R}{B}\\ v_\parallel\mathbf{b}\cdot\nabla Z &= v_\parallel\frac{B_Z}{B}\\ v_\parallel\mathbf{b}\cdot\nabla\zeta &= v_\parallel\frac{B_\zeta}{RB}\\ \mathbf{v}_D\cdot\nabla R &= -\frac{e_B}{B^2}B_\zeta\frac{\partial B}{\partial Z}\end{aligned}$$

$$
\begin{aligned}
\mathbf{v}_D \cdot \nabla Z &= \frac{e_B}{B^2} B_\zeta \frac{\partial B}{\partial R} \\
\mathbf{v}_D \cdot \nabla \zeta &= \frac{e_B}{RB^2} \left(B_R \frac{\partial B}{\partial Z} - B_Z \frac{\partial B}{\partial R} \right) \\
\mathbf{v}_E \cdot \nabla R &= \frac{1}{B^2} (E_Z B_\zeta - E_\zeta B_Z) \\
\mathbf{v}_E \cdot \nabla Z &= -\frac{1}{B^2} (E_R B_\zeta - E_\zeta B_R) \\
\mathbf{v}_E \cdot \nabla \zeta &= \frac{1}{RB^2} (E_R B_Z - E_Z B_R) \\
v_\parallel \frac{\delta \mathbf{B}_\perp}{B} \cdot \nabla R &= \frac{v_\parallel}{B} \delta B_R \\
v_\parallel \frac{\delta \mathbf{B}_\perp}{B} \cdot \nabla Z &= \frac{v_\parallel}{B} \delta B_Z \\
v_\parallel \frac{\delta \mathbf{B}_\perp}{B} \cdot \nabla \zeta &= \frac{v_\parallel}{RB} \delta B_\zeta
\end{aligned} \tag{35}
$$

with $e_B = m(v_\parallel^2 + v_\perp^2/2)/qB$.

The mirror force is given by

$$
\dot{v}_\parallel = -\frac{\mu}{m} \mathbf{b} \cdot \nabla B = -\frac{\mu}{mB} \left(B_R \frac{\partial B}{\partial R} + B_Z \frac{\partial B}{\partial Z} \right) \tag{36}
$$

We will neglect FLR effect for now (5/22/2023).

Jacobian

$$
\begin{aligned}
x &= R \sin \zeta \\
y &= R \cos \zeta \\
z &= Z
\end{aligned} \tag{37}
$$

$$
dx\, dy\, dz = J\, dR\, dZ\, d\zeta \tag{38}
$$

$$
J = \left| \frac{\partial (x, y, z)}{\partial (R, Z, \zeta)} \right| = R \tag{39}
$$

Total volume of the simulation box is,

$$
\begin{aligned}
V &= 2\pi l_Z \frac{1}{2} ((x_0 + l_x/2)^2 - (x_0 - l_x/2)^2) \\
&= 2\pi x_0 l_x l_z
\end{aligned} \tag{40}
$$

Trace field lines

Imagine a particle moving along the field line with $v_\parallel = 1$, the equation of motion is

$$
\begin{aligned}
\frac{dR}{dt} &= \mathbf{b} \cdot \nabla R \\
\frac{dZ}{dt} &= \mathbf{b} \cdot \nabla Z \\
\frac{d\zeta}{dt} &= \mathbf{b} \cdot \nabla \zeta
\end{aligned}
$$

Along the field line,

$$\begin{aligned}\frac{dR}{d\zeta} &= \frac{\mathbf{b}\cdot\nabla R}{\mathbf{b}\cdot\nabla\zeta} = R\frac{B_R}{B_T}\\ \frac{dZ}{d\zeta} &= \frac{\mathbf{b}\cdot\nabla Z}{\mathbf{b}\cdot\nabla\zeta} = R\frac{B_Z}{B_T}\end{aligned}$$

Equilibrium profiles are 2D

$$-\frac{1}{B}\mathbf{E}\times\mathbf{b}\cdot\nabla n_0 \approx \frac{1}{B}\left(E_R\frac{\partial n_0}{\partial Z} - E_Z\frac{\partial n_0}{\partial R}\right) \tag{41}$$

The gyrokinetic Poisson solve in matrix form

We start by writing a Poisson equation that has a form like Eq. (14). The FLR effect LHS term can be easily be evaluated using the usual finite-difference operator, so we start with the following form

$$\nabla\cdot(\epsilon(x,y)\nabla\phi(x,y)) = -\rho(x,y). \tag{42}$$

This is the usual Poisson equation with a nonuniform dielectric $\epsilon(x,y)$. Comparing to Eq. (14) to Eq. (42), we can make the two equations equivalent by setting $\epsilon = \frac{n_0 m}{eB^2}$ and $\rho = \left(1+\rho_i^2\nabla_\perp^2\right)\left(\delta\bar{n}_i - \delta n_e\right)$. We can rewrite Eq. (42) as

$$\epsilon\nabla^2\phi + \nabla\epsilon\cdot\nabla\phi = -\rho. \tag{43}$$

We will work in 2D Cartesian coordinates to start with and simplify Eq. 43. The 2D Cartesian approximation assumes two things. First, the toroidal field is much larger than poloidal magnetic field so that we can neglect $\nabla_\perp$ components in the toroidal direction. This is especially valid in the edge due to the large safety factor. Second, large aspect ratio so that we can neglect the cylindrical metric terms. This latter approximation is straightforward to relax simply by including $1/R$ terns in the finite difference operators discussed below. We define an x and y grid, where $x_i = i\Delta x, i = 0,1,2,...,N_x-1$, and $y_j = j\Delta y, j = 0,1,2,...,N_y-1$. We use the usual second-order finite-difference operator, and a central difference first-order finite difference operator to obtain the following finite-difference equation. $\epsilon_{i,j} = \epsilon(x_j,y_j)$, etc.

$$\begin{aligned}&\epsilon_{i,j}\left(\frac{1}{\Delta x^2}\left(\phi_{i+1,j} - 2\phi_{i,j} + \phi_{i-1,j}\right)\right. \\ &+ \left.\frac{1}{\Delta y^2}\left(\phi_{i,j+1} - 2\phi_{i,j} + \phi_{i,j-1}\right)\right) \\ &+ \frac{1}{4\Delta x^2}\left(\epsilon_{i+1,j} - \epsilon_{i-1,j}\right)\left(\phi_{i+1,j} - \phi_{i-1,j}\right) \\ &+ \frac{1}{4\Delta y^2}\left(\epsilon_{i,j+1} - \epsilon_{i,j-1}\right)\left(\phi_{i,j+1} - \phi_{i,j-1}\right) \\ &= -\rho_{i,j}\end{aligned} \tag{44}$$

The next step is to take this stencil and extend the conventional ∇^2 stencil in the PETSc 2D Poisson solve example. The PETSc matrix is size $N_x Ny \times NxN_y$, zero entries are not stored in memory.