

## **Derivation of gyrokinetic equations for full-f particle simulation with polarization drift**

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### **Introduction**

The research in the field of gyrokinetic theory during the last few decades has resulted in an emergence of a common mathematical framework<sup>1</sup>. This framework includes, among others, the Lie transform perturbation method, which can be used to obtain equations of motion for charged particles in an electromagnetic field, and action principle, which yields the field equations. Together they define a consistent description of the electrodynamic system of charged particles. Despite the common framework the theoretical and numerical implementations vary depending on the preferred assumptions or studied phenomena.

Now the theory basis of electrostatic full-f particle code, ELMFIRE<sup>2</sup>, has been derived in a way which endeavors to use the current standards of formulation. In general terms, the derivation is similar to the other derivations of gyrokinetic equations applying the Lie transform perturbation method, but the difference comes from the definition of the particle velocity where the E×B drift is separated from perpendicular velocity and introduced as a perturbation in the fundamental one-form. This procedure includes then polarization drift in the equations of motion and E×B drift energy in the Hamiltonian. Once the proper Lagrangian is found, variation of the action integral is used to obtain consistent Poisson equation.

### **Particle-in-cell method and ELMFIRE**

The core of a particle-in-cell code consists of equations of motion and the Poisson equation

$$\frac{d\mathbf{R}}{dt} = U\hat{\mathbf{b}}^* + \frac{\mu}{e} \frac{\hat{\mathbf{b}} \times \nabla B}{B_{\parallel}^*} + \frac{\hat{\mathbf{b}} \times \nabla \phi}{B_{\parallel}^*} + \frac{1}{\Omega} \frac{d}{dt} (-\nabla \phi) \quad \frac{dv_{\parallel}}{dt} = \frac{\hat{\mathbf{b}}^*}{m} \cdot (\mu \nabla B + e \nabla \phi) \quad (1)$$

$$\begin{aligned}
-\frac{1}{4\pi e}\nabla^2\phi &= \int d^6Z \left[ F + \frac{\Omega}{B}(\phi - \langle\phi\rangle)\frac{\partial F}{\partial\mu} + \frac{c}{eBB_{\parallel}}\mathbf{F}\cdot[\nabla S_1 + (\mathbf{u}_E - \langle\mathbf{u}_E\rangle)] \right] \cdot \nabla F \\
-\nabla\cdot\frac{m\nabla\phi}{B}F &\Big] \delta_{gc}^3 - n_e(x,t)
\end{aligned} \tag{2}$$

The set of equations above represents the ones ELMFIRE is based on. This approach, based on the theory presented by Sosenko<sup>3</sup>, has been used in order to study an alternative numerical scheme where the computation of the standard polarization density term is not required. Sosenko, however, did not consider if this system is consistent in the Hamiltonian sense. In the standard set<sup>1</sup> the polarization drift is not included in the equations of motion and the 4<sup>th</sup> and 5<sup>th</sup> terms in the Poisson equation are not present. Both sets of equations should in principle form a consistent description of the electrodynamic system comprised of charged particles. Also common to both approaches it that  $\Delta\phi \approx 0$  and the terms involving gradient of the distribution function are considered to be small due to the long equilibrium scale length of density and temperature.

In the standard set the potential is solved from the second term on the RHS of the Poisson equation, i.e. from the polarization density. In the alternative approach, applied in ELMFIRE, the canceling of the second order terms in the long wave length limit is used. Potential is solved by linearizing (particle-wise in each surrounding grid point) the density change caused by the ion polarization drift and the electron parallel acceleration in such a way that the calculated potential (or the shifts in particle positions due to polarization drift/parallel acceleration which are computed after the potential is solved) adjusts the system into quasineutrality. To give a picture of the applied implicit scheme, we first define gyro-averaged ion guiding center density  $\tilde{n}_i(x,t) = \int d^6ZF\delta_{gc}^3$  and vector  $\boldsymbol{\phi}(t) = [\phi(x_{j_1},t), \dots, \phi(x_{j_n},t)]$  containing the potential values which affect all the particles contributing to a certain grid point  $x_j$ . Next we write out the simplified Poisson equation and consider how the densities can be interpreted to change in time

$$\begin{aligned}
0 &= \tilde{n}_i(x_j,t) - n_e(x_j,t) \\
&= \tilde{n}_i(x_j,t - \Delta t) + \delta n_{i,w/o\ pol.\ drift}(x_j,t - \Delta t) + \delta n_{i,pol.\ drift}(x_j,\boldsymbol{\phi}(t) - \boldsymbol{\phi}(t - \Delta t)) \\
&\quad - n_e(x_j,t - \Delta t) - \delta n_{e,w/o\ par.\ acc.}(x_j,t - \Delta t) - \delta n_{e,par.\ acc.}(x_j,\boldsymbol{\phi}(t) - \boldsymbol{\phi}(t - \Delta t))
\end{aligned} \tag{3}$$

By defining short hand notation  $\bar{n}$  which is the density after the particles have gone through all other movement except for the one caused by polarization drift and moving the unknown terms proportional to the potential to the LHS, the equation above can be written in a solvable form as

$$A(x_j)\boldsymbol{\phi}(t) + B(x_j)\boldsymbol{\phi}(t) = \bar{n}_i(x_j,t) - A(x_j)\boldsymbol{\phi}(t - \Delta t) - \bar{n}_e(x_j,t) + B(x_j)\boldsymbol{\phi}(t - \Delta t) \tag{4}$$

## Outline of the derivation - Lie transform perturbation method and action principle

The near identity transform  $T$ , which has following properties

$$\begin{aligned} Tz = \dots T_3 T_2 T_1 z = Z & \quad L_n f = g_n^\mu \frac{\partial f}{\partial z^\mu} & \quad L_n \gamma = i_G d\gamma = g_n^\nu \left( \frac{\partial \gamma_\mu}{\partial z^\nu} - \frac{\partial \gamma_\nu}{\partial z^\mu} \right) \\ T_n = e^{\varepsilon L_n} & \quad \frac{\partial Z^\mu}{\partial \varepsilon^n} = g_n^\mu(\mathbf{Z}) \end{aligned} \quad (5)$$

transforms the particle Lagrangian  $\gamma$  into gyrocenter Lagrangian  $\Gamma = T^{-1}\gamma + dS$ . The fundamental one form defines the Poisson-Lagrange tensor  $\hat{\omega}_j = \partial\Gamma_j/\partial Z^i - \partial\Gamma_i/\partial Z^j$  and thus also the equations of motion  $\hat{\omega}_j dz^j/dt = \partial h/\partial z^i + \partial\Gamma_i/\partial t$ . The Lagrangian for a charged particle is

$$L = \mathbf{p} \cdot \dot{\mathbf{q}} - H = \frac{1}{2} m |\dot{\mathbf{x}}|^2 + \frac{e}{c} \mathbf{A} \cdot \dot{\mathbf{x}} - e\phi \quad \mathbf{q} = \mathbf{x} \quad \mathbf{p} = \frac{\partial L}{\partial \dot{\mathbf{x}}} = \frac{e}{c} \mathbf{A} + m\dot{\mathbf{x}} \quad (6)$$

where  $\mathbf{x} = \mathbf{X} + \mathbf{a}$ ,  $\mathbf{a}$  is the Larmor radius,  $\dot{\mathbf{x}} = \mathbf{v} = U\hat{\mathbf{b}} + \dot{\mathbf{a}} + \mathbf{u}_E$  and  $\mathbf{u}_E = (c\nabla\phi \times \mathbf{B})/\mathbf{B}^2$ . In order to calculate the gyrocenter one form we proceed in a similar fashion as in the standard derivation. Transformation is done separately for each order using the formulae

$$\begin{aligned} \Gamma_0 &= \gamma_0 + dS_0 & \Gamma_2 &= \gamma_2 - L_1 \gamma_1 + \left( \frac{1}{2} L_1^2 - L_2 \right) \gamma_0 + dS_2 \\ \Gamma_1 &= \gamma_1 - L_1 \gamma_0 + dS_1 \end{aligned} \quad (7)$$

The difference comes from the treatment of  $\mathbf{E} \times \mathbf{B}$  drift, which here is due to the fluctuations of the potential. In the standard derivation it is not separated from the perpendicular velocity and in some derivations it is considered to be originating from a strong background electric field. This kind of local velocity transformation was chosen in order to obtain the desired form of the Poisson equation, to avoid the necessity to incorporate a Jacobian into the action integral while transforming from particle space to gyrocenter space and because it gives the guiding center  $\mathbf{E} \times \mathbf{B}$  drift when gyro-averaged. The first and the second order corrections to the Lagrangian are

$$\gamma_1 = m\mathbf{u}_E \cdot d\mathbf{X} - e\phi dt \quad \gamma_2 = -\frac{1}{2} m u_E^2 dt \quad (8)$$

and the generating functions, determined by the requirement that the terms in the gyrocenter one form are gyro-averages of the ones in the particle Lagrangian, are

$$\begin{aligned} g_1^\theta &= -\frac{\Omega}{B} \frac{\partial S_1}{\partial \mu} & g_1^U &= \frac{1}{m} \hat{\mathbf{b}}^* \cdot \nabla S_1 + (\mathbf{u}_E - \langle \mathbf{u}_E \rangle) \cdot \frac{mc}{eB_\parallel} U \nabla \times \hat{\mathbf{b}} \\ g_1^\mu &= \frac{\Omega}{B} \frac{\partial S_1}{\partial \theta} & g_1^{\mathbf{x}} &= \hat{\mathbf{b}}^* \left( \frac{1}{m} \frac{\partial S_1}{\partial U} \right) + \frac{c}{eBB_\parallel} \mathbf{F} \cdot \nabla S_1 + \frac{c}{eBB_\parallel} m \mathbf{F} \cdot (\mathbf{u}_E - \langle \mathbf{u}_E \rangle) \end{aligned} \quad (10)$$

The standard Lie transformation is thus slightly modified, but the new terms originating from  $\mathbf{u}_E$  are smaller than or of the same order as the old ones. The resulting gyrocenter Lagrangian is

$$\begin{aligned} \Gamma = \Gamma_0 + \Gamma_1 + \Gamma_2 = & \left( \frac{e}{c} \mathbf{A} + mU\hat{\mathbf{b}} \right) \cdot d\mathbf{X} + \frac{\mu B}{\Omega} d\theta + (-H_0) dt + \frac{e}{c} m\mathbf{u}_E \cdot d\mathbf{X} - e\langle\phi\rangle dt \\ & + \frac{e}{2} \left[ \langle \nabla \tilde{\phi} \cdot \hat{\mathbf{F}} \cdot \nabla S_1 \rangle + \langle \hat{\mathbf{F}} \cdot (\mathbf{u}_E - \langle \mathbf{u}_E \rangle) \cdot \nabla \tilde{\phi} \rangle + \frac{e}{B} \frac{\partial}{\partial \mu} \langle \tilde{\phi}^2 \rangle \right] dt + \frac{1}{2} m \langle u_E^2 \rangle dt \end{aligned} \quad (11)$$

The action principle is used to find the Poisson equation. First the action integral is transformed from particle space to gyrocenter space  $\int d\mathbf{x} d\mathbf{v} d\mathbf{w} dt F_p H_p \rightarrow \int d^8 Z F_{gy} H_{gy}$ , where  $H_{gy}$  is the time part of the transformed Lagrangian. Varying the action with respect to the potential

$$\frac{1}{4\pi} \int d^4 x \varepsilon \nabla \delta\phi \cdot \nabla \phi - \int d^8 Z \left[ F \int d^3 x \left( \delta\phi(\mathbf{x}) \frac{\delta H}{\delta\phi(\mathbf{x})} + \nabla \delta\phi \cdot \frac{\delta H}{\delta \nabla \phi} \right) \right] = 0 \quad (12)$$

yields the Poisson equation

$$\nabla^2 \phi = -4\pi e \left[ \int d^6 Z F \langle T_{gy}^{-1} \delta_{gc}^3 \rangle - \nabla \cdot \frac{m}{B} \nabla \phi \int d^6 Z F \langle \delta_{gc}^3 \rangle \right] \quad (13)$$

## Conclusions

The benefits of the applied approach include the facts that there is no need to calculate the second order terms in the Poisson equation, approximations about the distribution function are not required and, in general, having an alternative approach which may be benchmarked against other simulation results. The obvious drawback is that long wavelength approximation is required, i.e. the implementation works only for low  $k\rho$ . The approach applied here is not broadly studied and thus further examination is needed. Also the effect of the implicit methods used in solving the potential on the dynamics of the system will be revised. Nevertheless, the derivation shows that the set of equations (1.1)-(1.2) constitutes a proper description of tokamak plasma dynamics.

## References

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