A mixed variable gyrokinetic model for electromagnetic gyrokinetic simulations

Eric Sonnendrücker

Max-Planck Institute for Plasma Physics

and

TU Munich

with: Roman Hatzky, Ralf Kleiber, Axel Könies, Alexey Mishchenko

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Outline

Gyrokinetic Finite Element PIC codes

Gyrokinetic modelling

Gyrokinetic field theories

Avoiding the cancellation problem with the mixed formulation

From the continuous to the discrete action: PIC-FEM
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Motivation

- Solve Alfven eigenmode problems with gyrokinetic PIC codes
- Family of PIC codes started at EPFL
  - ORB5 (EPFL), originally electrostatic Tokamak code
  - NEMORB (IPP Garching), electromagnetic version
  - EUTERPE (IPP Greifswald), electromagnetic stellarator code
  - GYGLES (IPP Garching and Greifswald): simplified 2D version

(Picture: A. Bottino)

- Cancellation problem can be handled with adaptive control variate and meticulous numerics (Hatzky et al. JCP 07)
- Unstable grid modes requiring very low time step
Noise reduction is essential

- PIC is a Monte Carlo approximation. Markers realisations of a stochastic process with probability density $f$.
- The Monte Carlo error for a simulation based on a random variable $X$ is given by $\sqrt{\mathbb{V}(X)/N}$.
- The idea of variance reduction techniques that are essential for efficient Monte Carlo simulations is to find a random variable $\tilde{X}$ so that
  \[ \mathbb{E}(\tilde{X}) = \mathbb{E}(X) \quad \text{and} \quad \mathbb{V}(\tilde{X}) \ll \mathbb{V}(X). \]
- Two such techniques are efficiently used in PIC simulations
  1. Importance sampling: weighted PIC
  2. Control variates: $\delta f$ PIC
- Both have been historically developed for other purposes. First MC interpretation by Aydemir 1994. See also Hatzky.
- Both techniques are still not mainstream in PIC simulations because of weight mixing and weight spreading issues.
Importance sampling to the PIC method

- Instead of initialising the particle positions according to initial particle distribution \( f_0 \), use adequately chosen marker distribution \( g_0 \).
- For each marker \( z_k \) weight is defined by \( w_k = \frac{f_0(z_k)}{g_0(z_k)} \).
- Let marker density evolve like particle density: \( g \) is solution of the same Fokker-Planck (or Vlasov) equation as \( f \), only with different initial condition.
- As \( f \) and \( g \) are conserved along the same characteristics \( w_k \) is constant in time:
  \[
  w_k = \frac{f(t, z_k(t))}{g(t, z_k(t))} = \frac{f_0(z_k(0))}{g_0(z_k(0))}.
  \]
- Good way to initialise marker dependent on physics problem.
Control variates

- Guiding idea: compute as little as possible with noisy particle data.
- In gyrokinetic PIC: use analytical background \( f^0 \) to compute bulk of charge and current densities, e.g.
  \[
  \rho_s = e_s \left( \int f^0_s \, dv + \int (f_s - f^0_s) \, dv \right).
  \]
- Small modification in existing PIC code. Really full \( f \) PIC code carrying in addition time dependent weights for noise reduced computation of source terms for field equations.
- Initialisation: Importance weights for \( \delta f = f - f^0 \) defined by the random variable
  \[
  W^0 = \frac{f_0(Z^0) - f^0(0, Z^0)}{g_0(Z^0)} = W - \frac{f^0(0, Z^0)}{g_0(Z^0)}.
  \]
- Update: (No linearisation involved)
  \[
  W^n = \frac{f(t_n, Z^n) - f^0(t_n, Z^n)}{g(t_n, Z^n)} = \frac{f_0(Z^0) - f^0(t_n, Z^n)}{g_0(Z^0)} = W - \frac{f^0(t_n, Z^n)}{g_0(Z^0)}.
  \]
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Reduction of 6D Vlasov-Maxwell for efficient simulation

- Posed in 6D phase space! Dimension reduction if possible would help.
- Large magnetic field imposes very small time step to resolve the rotation of particles along field lines.

- Physics of interest is low frequency. Remove light waves: Darwin instead of Maxwell.
- Debye length small compared to ion Larmor radius. Quasi-neutrality assumption \( n_e = n_i \) needs to be imposed instead of Poisson equation for electric field.
Towards a reduced model

- **Scale separation**: fast motion around magnetic field lines can be averaged out.
- **Idea**: separate motion of the guiding centre from rotation by a change of coordinates.
- For constant magnetic field can be done by change of coordinates: \( \mathbf{X} = \mathbf{x} - \rho_L \) guiding centre + kind of cylindrical coordinates in \( \mathbf{v} \): \( v_\parallel, \mu = \frac{1}{2} m v_\perp^2 / \omega_c, \theta \).
- Mixes position and velocity variables.
- **Perturbative model for slowly varying magnetic field**.
- **Several small parameters**
  - gyroperiod, Debye length
  - Magnetic field in tokamak varies slowly: \( \epsilon_B = |\nabla B| / |B| \)
  - Time dependent fluctuating fields are small.
Geometric asymptotic reduction

- Long time magnetic confinement of charged particles depends on existence of first adiabatic invariant (Northrop 1963):
  \[ \mu = \frac{1}{2} m v^2_\perp / \omega_c. \]

- Geometric reduction based on making this adiabatic invariant an exact invariant.

- **Two steps procedure:**
  - Start from Vlasov-Maxwell particle Lagrangian and reduce it using Lie transforms such that it is independent of gyromotion up to second order
  - Plug particle Lagrangian into Vlasov-Maxwell field theoretic action and perform further reduction.

- End product is gyrokinetic field theory embodied in Lagrangian. Symmetries of Lagrangian yield **exact conservation laws** thanks to Noether Theorem.
Motion of a particle in an electromagnetic field

Consider given electromagnetic field defined by scalar potential \( \phi \) and vector potential \( \mathbf{A} \) such that

\[
\mathbf{E} = -\frac{\partial \mathbf{A}}{\partial t} - \nabla \phi, \quad \mathbf{B} = \nabla \times \mathbf{A}.
\]

The non relativistic equations of motion of a particle in this electromagnetic field is obtained from Lagrangian (here phase space Lagrangian \( p \cdot \dot{q} - H \) in non canonical variables for later use)

\[
L_s(x, v, \dot{x}, t) = (m_s v + e_s A(t, x)) \cdot \dot{x}^2 - \left( \frac{1}{2} m_s v^2 + e_s \phi(t, x) \right).
\]

where \( p = m_s v + e_s A(t, x) \), \( H = m_s v^2/2 + e_s \phi(t, x) \) are canonical momentum and hamiltonian.
Abstract geometric context

- Lagrangian becomes Poincaré-Cartan 1-form

\[ \gamma = p \cdot dx - H \, dt \]

with \( p = m_s v + e_s A(t, x) \), \( H = m_s v^2 / 2 + e_s \phi(t, x) \).

- \( \omega = d\gamma \) is the Lagrange 2-form, which is non degenerate and so a symplectic form. Its components define the the Lagrange tensor \( \Omega \).

- Then \( J = \Omega^{-1} \) is the Poisson tensor which defines the Poisson bracket

\[ \{ F, G \} = \nabla F^T J \nabla G \]

- The equations of motion can then be expressed from the Poisson matrix and the hamiltonian

\[ \frac{dZ}{dt} = J \nabla H. \]

- Lagrangian contains all necessary information and this structure is preserved by change of coordinates.
Derivation of gyrokinetic particle Lagrangian

- Gyrokinetic particle Lagrangian obtained from Vlasov-Maxwell particle Lagrangian by performing a change of variables, such that lowest order terms independent of gyrophase.
- This is obtained systematically order by order by the Lie transform method (Dragt & Finn 1976, Cary 1981) on the Lagrangian

\[ L_s(x, v, \dot{x}, t) = \left( m_s v + e_s A \right) \cdot \dot{x}^2 - \left( \frac{1}{2} m_s |v|^2 + e_s \phi \right). \]

- Not a unique solution.
  1. \( v_{\parallel} \) formulation. Transform Lagrangian as is keeping fluctuation \( A \) in symplectic form.
  2. \( p_{\parallel} \) formulation, \( p_{\parallel} = v_{\parallel} + (e/m)A_{\parallel} \). Fluctuating \( A_{\parallel} \) in hamiltonian.
  3. \( u_{\parallel} \) formulation. Split fluctuating \( A_{\parallel} \) into two parts. One of them goes into Hamiltonian. Includes others as special case.

- Gyrokinetic codes choose between \( v_{\parallel} \) (symplectic) and \( p_{\parallel} \) (hamiltonian) formulation.
- Both involve severe numerical drawbacks.
The $v_{||}$ formulation

- Physically the most natural
- Involves $\frac{\partial A_{||}}{\partial t}$ term in particles’ equations of motion.
- Straightforward explicit discretisation unstable.
- Similar problems occur in Vlasov-Darwin simulation.
- Momentum equation could in principle be used for stabilisation but not done in practice.
The $p_{\parallel}$ formulation

- Classically used in gyrokinetic simulations
- Gives rise to the so-called cancellation problem in the parallel Ampere Law

\[-\nabla_{\bot}^2 A_{\parallel} + \left( \frac{\omega_{p,i}^2}{c^2} + \frac{\omega_{p,e}^2}{c^2} \right) A_{\parallel} = \mu_0 j_{\parallel}.\]

- Indeed changing variables $p_{\parallel} = v_{\parallel} + (e_s/m_s)A_{\parallel}$

\[j_{\parallel,s} = \int f_s(t, x, v_{\parallel}) v_{\parallel} \, dv_{\parallel} = \int f_s(t, x, p_{\parallel}) p_{\parallel} \, dp_{\parallel} - \frac{e_s}{m_s} A_{\parallel} \int f_s(t, x, p_{\parallel}) \, dp_{\parallel}.\]

- Last term (linearized) leads to large skin term, which must be exactly compensated by the corresponding part of $j_{\parallel}$: Numerically very challenging.
The mixed gyrokinetic particle Lagrangian

- Split $A_{\parallel} = A_{\parallel}^s + A_{\parallel}^h$. Define $u_{\parallel} = v_{\parallel} + (e/m)A_{\parallel}^h$
- $A_{\parallel}^s$ is chosen such that $E_{\parallel} = -\partial_t A_{\parallel} - \nabla_{\parallel}\phi = 0$.
- The gyrokinetic Lagrangian for a single particle always in the form
  \[ L = A^* \cdot \dot{X} + \mu \dot{\theta} - H \]

  with $A^* = A_0 + \left( (m_s/e_s)u_{\parallel} + \langle A_{\parallel}^s \rangle \right) b, \quad b = B/B$,

  \[ H = H_0 + H_1 + H_2, \quad H_0 = \frac{1}{2} m_s u_{\parallel}^2 + \mu B, \quad H_1 = \langle \phi - u_{\parallel} A_{\parallel}^h \rangle \]

  where
  \[ \langle \psi \rangle(x, \mu) \overset{\text{def}}{=} \frac{1}{2\pi} \int \psi(x + \rho) \, d\alpha. \]

- Perpendicular component of fluctuating vector potential $A$ neglected.
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Field theory is action principle from which Vlasov-Maxwell equations are derived. Action proposed by Low (1958) with a Lagrangian formulation for Vlasov, i.e. based on characteristics. Based on particle Lagrangian for species $s$, $L_s$. Such an action, splitting between particle and field Lagrangian, using standard non canonical coordinates, reads:

\[
S = \sum_s \int f_s(z_0, t_0) L_s(X(z_0, t_0; t), \dot{X}(z_0, t_0; t), t) \, dz_0 \, dt + \frac{\epsilon_0}{2} \int |\nabla \phi + \frac{\partial A}{\partial t}|^2 \, dx \, dt - \frac{1}{2 \mu_0} \int |\nabla \times A|^2 \, dx \, dt.
\]

Particle distribution functions $f_s$ taken at initial time.
The electromagnetic gyrokinetic field theory

- Gyrokinetics is a low frequency approximation.
  Darwin approximation: $\partial_t A$ removed from Lagrangian.
- Quasi-neutrality approximation: $|\nabla \phi|^2$ removed:

$$S = \sum_s \int f_s(z_0, t_0)(A^* \cdot \dot{X} - H) \, dz_0 - \frac{1}{2\mu_0} \int |\nabla \times (A_\parallel b)|^2 \, dx.$$  

- Additional approximation made to avoid fully implicit formulation:
  Second order term in Lagrangian linearised (consistent with ordering) by replacing full $f$ by background $f_M$

$$S = \sum_s \int f_s(z_0, t_0)(A^* \cdot \dot{X} - H_0 - H_1) \, dz_0$$

$$- \sum_s \int f_{M,s}(z_0) H_2 \, dz_0 - \frac{1}{2\mu_0} \int |b \times \nabla A_\parallel|^2 \, dx.$$
Derivation of the gyrokinetic equations from the action principle

We denote by $\mathbf{B}^* = \nabla \times \mathbf{A}^*$ and $B^\parallel = \mathbf{B}^* \cdot \mathbf{b}$.

- Setting $\frac{\delta S}{\delta Z_i} = 0, i = 1, 2, 3, 4$ yields:

$$\mathbf{B}^* \times \mathbf{\dot{R}} = -\frac{m}{q} \dot{P}_\parallel \mathbf{b} - \frac{1}{q} \nabla (H_0 + H_1), \quad \mathbf{b} \cdot \mathbf{\dot{R}} = \frac{1}{m} \frac{\partial (H_0 + H_1)}{\partial p_\parallel}.$$ 

- Solving for $\mathbf{\dot{R}}$ and $\dot{P}_\parallel$ we get the equations of motion of the gyrocenters:

$$B^\parallel \mathbf{\dot{R}} = \frac{1}{m} \frac{\partial (H_0 + H_1)}{\partial p_\parallel} \mathbf{B}^* - \frac{1}{q} \nabla (H_0 + H_1) \times \mathbf{b}, \quad B^\parallel \dot{P}_\parallel = -\frac{1}{m} \nabla (H_0 + H_1) \cdot \mathbf{B}^*.$$ 

- These are the characteristics of the gyrokinetic Vlasov equation

$$\frac{\partial f}{\partial t} + \mathbf{\dot{R}} \cdot \nabla f + \dot{P}_\parallel \frac{\partial f}{\partial p_\parallel} = 0.$$
Gyrokinetic Ampere and Poisson equations

- The gyrokinetic Poisson (or rather quasi-neutrality) equation is obtained by variations with respect to $\phi$

$$\int \frac{e_i^2 \rho_i^2 n_{s,0}}{k_B T_i} \nabla_\perp \phi \cdot \nabla \tilde{\phi} \, d\mathbf{x} = \int qn \langle \tilde{\phi} \rangle \, d\mathbf{x}, \quad \forall \tilde{\phi}$$

- The gyrokinetic Ampère equation is obtained by variations with respect to $A_\parallel$:

$$\int \nabla_\perp A_\parallel \cdot \nabla_\perp \tilde{A}_\parallel^h \, d\mathbf{x} + \sum_s \int \frac{\mu_0 q_s^2 n_s}{m_s} \langle A_\parallel^h \rangle \langle \tilde{A}_\parallel^h \rangle \, d\mathbf{x}$$

$$= \mu_0 \int j_\parallel \langle \tilde{A}_\parallel^h \rangle \, d\mathbf{x}, \quad \forall \tilde{A}_\parallel^h$$

- where $A_\parallel = A_\parallel^s + A_\parallel^h$ and $A_\parallel^s$ is related to $\phi$ by the constraint

$$\frac{\partial A_\parallel^s}{\partial t} + \nabla \phi \cdot \mathbf{b} = 0.$$
Conserved quantities

▶ Symmetries of Lagrangian yield invariants using Noether’s theorem
▶ Time translation: Conservation of energy:

\[ \mathcal{E}(t) = \sum_s \int dW_0 dV_0 f_{s,0}(z_0) H_s - \int dV \frac{e_i^2 \rho_i^2 n_{s,0}}{k_B T_i} |\nabla \phi|^2 \]

\[ + \frac{1}{2 \mu_0} \int dV |\nabla \perp A_\parallel|^2. \]

▶ Axisymmetry of background vector potential: Conservation of total canonical angular momentum:

\[ \mathcal{P}_\varphi = \sum_s e_s \int dW_0 dV_0 f_{s,0}(z_0) A_{s,\varphi}^*. \]
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How does the mixed formulation help?

- Evolution of $u_\|$: $\partial_t A^s_\|$ can be replaced by $-\nabla_\| \phi$ to get rid of $\nu_\|$ formulation problem

$$\frac{d u_\|}{dt} = \frac{e_s}{m_s} \left( b \cdot \nabla \left[ \langle \phi \rangle - u_\| \langle A^h_\| \rangle + \frac{e_s}{2m_s} \langle A^h_\| \rangle^2 \right] + \frac{\partial \langle A^s_\| \rangle}{\partial t} ight)$$

$$+ \frac{1}{B^*_\|} \nabla \langle A^s_\| \rangle \cdot b \times \nabla \left[ \langle \phi \rangle - u_\| \langle A^h_\| \rangle + \frac{e_s}{2m_s} \langle A^h_\| \rangle^2 \right]$$

- The mixed Ampere equation: Cancellation problem mitigated if $A^h_\|$ remains small

$$-\nabla_\perp^2 A_\| + \frac{\omega_{p,i}^2 + \omega_{p,e}^2}{c^2} \langle A^h_\| \rangle = \mu_0 j_\|.$$
Adding a pullback at each time step

- Mixed formulation very effective for MHD modes, where $E_\parallel = 0$ and $A_{\parallel,h}$ stays small for all time.
- It does not help so much when $A_{\parallel,h}$ grows with time. What can we do?
- Idea is to perform change of variables (pullback) at each time step to go back to the $v_\parallel$ formulation and evolve in the mixed formulation from there:

$$v_\parallel = u_\parallel - \frac{e_s}{m_s} \langle A_h^h \rangle, \quad f(v_\parallel) = f(u_\parallel), \quad A_\parallel = A_h^h + A_s^s, \quad A_h^h = 0.$$  

- Now $A_h^h$ evolves from 0 at each time step and always stays small, effectively removing the cancellation problem in all cases.
- This can also be seen as an integrating factor method (appropriate change of variable) to solve the $v_\parallel$ gyrokinetic formulation. In this interpretation, mixed gyrokinetic theory not needed.
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Discretisation of the action

- Our action principles rely on a Lagrangian (as opposed to Eulerian) formulation of the Vlasov equation: the functionals on which our action depends are the characteristics of the Vlasov equations $\mathbf{X}$ and $\mathbf{V}$ in addition to the scalar and vector potentials $\phi$ and $\mathbf{A}$.

- A natural discretisation relies on:
  - A Monte-Carlo discretisation of the phase space at the initial time: select randomly some initial positions of the particles.
  - Approximate the continuous function spaces for $\phi$ and $\mathbf{A}$ by discrete subspaces.
  - Yields a discrete action where a finite (large) number of scalars are varied: the particle phase space positions and coefficients in Finite Element basis.

- When performing the variations, we get the classical Particle In Cell Finite Element Method (PIC-FEM).
PIC Finite Element approximation of the Action

- **FE discretisation with B-spline basis functions:**

\[ \phi_h = \sum \phi_i \Lambda_i, \quad A_\parallel = \sum a_i \Lambda_i. \]

- **Particle discretisation of** \( f \approx \sum_k w_k \delta(x - x_k(t))\delta(v - v_k(t)) \)

- **Vlasov-Maxwell action becomes:**

\[ S_{N,h} = \sum_{k=1}^{N} w_k L_s( Z(z_{k,0}, t_0; t), \dot{Z}(z_{k,0}, t_0; t), t ) \]

\[ - \frac{1}{2} \int \left| \sum_{i=1}^{N_g} a_i(t) b \times \nabla \Lambda_i^1(x) \right|^2 \, dx. \]

- **\( Z(z_{k,0}, t_0; t) \) will be traditionally denoted by** \( z_k(t) \) \( is the phase space position at time \( t \) of the particle that was at \( z_{k,0} \) at time \( t_0 \).
Simulation of a TAE in a circular tokamak

Convergence plots with respect to number of electron markers

Convergence plots with respect to time step

Blue: old method
Red: new method
Conclusion and related work

- Variational FE-PIC codes along with control variates for noise reduction at the base of success of PIC simulations of Tokamak turbulence with ORB5 family of codes.
- Pullback idea provides very simple trick to handle cancellation problem.
- Exact conservation properties very useful for code verification
- Ongoing work (with K. Kormann, M. Kraus, P.J. Morrison) highlights finite dimensional Poisson structure for FE-PIC codes