# A mixed variable gyrokinetic model for electromagnetic gyrokinetic simulations

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# Outline

Gyrokinetic Finite Element PIC codes

Gyrokinetic modelling

Gyrokinetic field theories

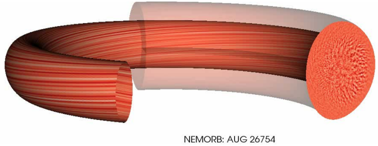
Avoiding the cancellation problem with the mixed formulation

From the continuous to the discrete action: PIC-FEM

# Outline

# 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

$$\mathbb{E}(\tilde{X}) = \mathbb{E}(X) \quad \text{and } \mathbb{V}(\tilde{X}) \ll \mathbb{V}(X).$$

- 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 $w_k = f_0(z_k)/g_0(z_k)$.
- 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:

$$w_k = \frac{f(t, \mathbf{z}_k(t))}{g(t, \mathbf{z}_k(t))} = \frac{f_0(\mathbf{z}_k(0))}{g_0(\mathbf{z}_k(0))}.$$

- 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 an current densities, *e.g.*

$$\rho_s = e_s\left(\int f_s^0 \,\mathrm{d}v + \int (f_s - f_s^0)\,\mathrm{d}v\right).$$

- 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

$$W^0 = \frac{f_0(\mathbf{Z}^0) - f^0(0,\mathbf{Z}^0)}{g_0(\mathbf{Z}^0)} = W - \frac{f^0(0,\mathbf{Z}^0)}{g_0(\mathbf{Z}^0)}.$$

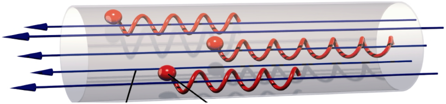
- Update: (No linearisation involved)

$$W^n = \frac{f(t_n,\mathbf{Z}^n) - f^0(t_n,\mathbf{Z}^n)}{g(t_n,\mathbf{Z}^n)} = \frac{f_0(\mathbf{Z}^0) - f^0(t_n,\mathbf{Z}^n)}{g_0(\mathbf{Z}^0)} = W - \frac{f^0(t_n,\mathbf{Z}^n)}{g_0(\mathbf{Z}^0)}.$$

# Outline

# Reduction of 6D Vlasov-Maxwell for efficient simulation

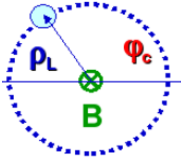
- Posed in 6D phase space! Dimension reduction if possible would help.
- Large magnetic field imposes very small time step to resolve the rotation of particles along field lines.



- 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): $\mu = \frac{1}{2} m v_\perp^2 / \omega_c$.
- 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 $\mathbf{p} \cdot \dot{\mathbf{q}} - H$ in non canonical variables for later use)

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

where $\mathbf{p} = m_s \mathbf{v} + e_s \mathbf{A}(t, \mathbf{x}),\ H = m_s v^2/2 + e_s \phi(t, \mathbf{x})$ are canonical momentum and hamiltonian.

# Abstract geometric context

- Lagrangian becomes Poincaré-Cartan 1-form

$$\gamma = \mathbf{p} \cdot \mathrm{d}\mathbf{x} - H \, \mathrm{d}t$$

  with $\mathbf{p} = m_s \mathbf{v} + e_s \mathbf{A}(t, \mathbf{x})$, $H = m_s v^2/2 + e_s \phi(t, \mathbf{x})$.
- $\omega = \mathrm{d}\gamma$ 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

$$\frac{\mathrm{d}\mathbf{Z}}{\mathrm{d}t} = J \nabla H.$$

- Lagrangian contains all necessary information and this structure is preserved by change of coordintates.

# 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

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

- Not a unique solution.
  1. $v_\parallel$ formulation. Transform Lagrangian as is keeping fluctuation $\mathbf{A}$ 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 $v_\parallel$ formulation

- Physically the most natural
- Involves $\frac{\partial A_\parallel}{\partial t}$ 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

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

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

$$j_{\parallel,s} = \int f_s(t, \mathbf{x}, v_\parallel) v_\parallel \, \mathrm{d}v_\parallel = \int f_s(t, \mathbf{x}, p_\parallel) p_\parallel \, \mathrm{d}p_\parallel - \frac{e_s}{m_s} A_\parallel \int f_s(t, \mathbf{x}, p_\parallel) \, \mathrm{d}p_\parallel .$$

- 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

$$L = \mathbf{A}^* \cdot \dot{\mathbf{X}} + \mu\dot{\theta} - H$$

$$\text{with } \mathbf{A}^* = \mathbf{A}_0 + \left((m_s/e_s)u_\parallel + \langle A_\parallel^s \rangle\right)\mathbf{b}, \quad \mathbf{b} = \mathbf{B}/B,$$

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

where

$$\langle \psi \rangle(\mathbf{x}, \mu) \stackrel{\text{def}}{=} \frac{1}{2\pi}\oint \psi(\mathbf{x} + \rho)\,\mathrm{d}\alpha.$$

- Perpendicular component of fluctuating vector potential $\mathbf{A}$ neglected.

# Outline

# Action principle for the Vlasov-Maxwell equations

- 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:

$$\mathcal{S} = \sum_{\mathrm{s}} \int f_s(\mathbf{z}_0, t_0) L_s(\mathbf{X}(\mathbf{z}_0, t_0; t), \dot{\mathbf{X}}(\mathbf{z}_0, t_0; t), t) \, \mathrm{d}\mathbf{z}_0 \, \mathrm{d}t + \frac{\epsilon_0}{2} \int |\nabla \phi + \frac{\partial \mathbf{A}}{\partial t}|^2 \, \mathrm{d}\mathbf{x} \, \mathrm{d}t - \frac{1}{2\mu_0} \int |\nabla \times \mathbf{A}|^2 \, \mathrm{d}\mathbf{x} \, \mathrm{d}t.$$

Particle distribution functions $f_s$ taken at initial time.

# The electromagnetic gyrokinetic field theory

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

$$\mathcal{S} = \sum_{\mathrm{s}} \int f_s(\mathbf{z}_0, t_0)(\mathbf{A}^* \cdot \dot{\mathbf{X}} - H)\,\mathrm{d}\mathbf{z}_0 - \frac{1}{2\mu_0}\int |\nabla \times (A_{\|}\mathbf{b})|^2\,\mathrm{d}\mathbf{x}.$$

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

$$\mathcal{S} = \sum_{\mathrm{s}} \int f_s(\mathbf{z}_0, t_0)(\mathbf{A}^* \cdot \dot{\mathbf{X}} - H_0 - H_1)\,\mathrm{d}\mathbf{z}_0$$

$$- \sum_{\mathrm{s}} \int f_{M,s}(\mathbf{z}_0) H_2\,\mathrm{d}\mathbf{z}_0 - \frac{1}{2\mu_0}\int |\mathbf{b} \times \nabla A_{\|}|^2\,\mathrm{d}\mathbf{x}.$$

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

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

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

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

- These are the characteristics of the gyrokinetic Vlasov equation

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

# Gyrokinetic Ampere and Poisson equations

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

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

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

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

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

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

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

# Conserved quantities

- Symmetries of Lagrangian yield invariants using Noether's theorem
- Time translation: Conservation of energy:

$$\mathcal{E}(t) = \sum_s \int \mathrm{d}W_0 \mathrm{d}V_0 f_{s,0}(\mathbf{z}_0) H_s - \int \mathrm{d}V \frac{e_i^2 \rho_i^2 n_{s,0}}{k_\mathrm{B} T_i} |\nabla \phi|^2 + \frac{1}{2\mu_0} \int \mathrm{d}V |\nabla_\perp A_\parallel|^2 .$$

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

$$\mathcal{P}_\varphi = \sum_s e_s \int \mathrm{d}W_0 \mathrm{d}V_0 f_{s,0}(\mathbf{z}_0) \mathbf{A}^\star_{s,\varphi}$$

# Outline

# How does the mixed formulation help?

- Evolution of $u_\|$: $\partial_t A_\|^s$ can be replaced by $-\nabla_\| \phi$ to get rid of $v_\|$ formulation problem

$$\frac{\mathrm{d}u_\|}{\mathrm{d}t} = \frac{e_s}{m_s}\left(\mathbf{b}\cdot\nabla\left[\langle\phi\rangle - u_\|\langle A_\|^h\rangle + \frac{e_s}{2m_s}\langle A_\|^h\rangle^2\right] + \frac{\partial\langle A_\|^s\rangle}{\partial t} + \frac{1}{B_\|^*}\nabla\langle A_\|^s\rangle\cdot\mathbf{b}\times\nabla\left[\langle\phi\rangle - u_\|\langle A_\|^h\rangle + \frac{e_s}{2m_s}\langle A_\|^h\rangle^2\right]\right)$$

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

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

- Now $A_\|^h$ 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 $v_\|$ gyrokinetic formulation. In this interpretation, mixed gyrokinetic theory not needed.

# Outline

# 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:

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

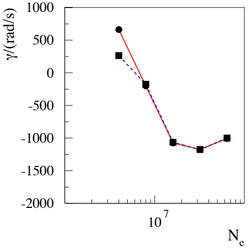
- Particle discretisation of $f \approx \sum_k w_k \delta(x - x_k(t))\delta(v - v_k(t))$
- Vlasov-Maxwell action becomes:

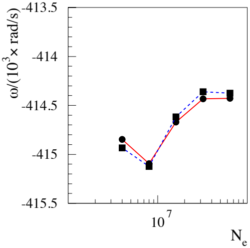
$$\mathcal{S}_{N,h} = \sum_{k=1}^{N} w_k L_s(\mathbf{Z}(\mathbf{z}_{k,0}, t_0; t), \dot{\mathbf{Z}}(\mathbf{z}_{k,0}, t_0; t), t) - \frac{1}{2}\int |\sum_{i=1}^{N_g} a_i(t)\mathbf{b} \times \nabla \Lambda_i^1(\mathbf{x})|^2 \, \mathrm{d}\mathbf{x}.$$

- $\mathbf{Z}(\mathbf{z}_{k,0}, t_0; t)$ will be traditionally denoted by $\mathbf{z}_k(t)$ is the phase space position at time $t$ of the particle that was at $\mathbf{z}_{k,0}$ at time $t_0$.

# Simulation of a TAE in a circular tokamak

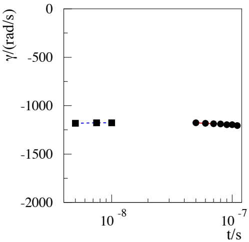
- Convergence plots with respect to number of electron markers

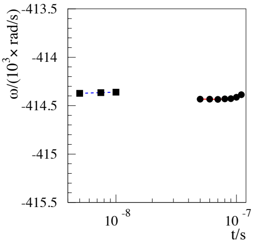



Blue: old method
Red: new method

- Convergence plots with respect to time step



# 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