# Simulation of Drift-Kinetic Dynamics of Charged Particles in Magnetized Plasmas The Guiding Center Approach

September 29, 2009 | Stilianos Louca



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# Simulation of Drift-Kinetic Dynamics of Charged Particles in Magnetized Plasmas Part I: Introduction

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## Introduction to Plasmas

#### Definition of plasmas

Systems on which thermal energies exceed ionization energies of atoms.  $\rightarrow$  Assemblage of unbound electron & ions.

#### Plasma dynamics characterized by:

- High coupling due to internal electromagnetic fields.
- No bound states  $\rightarrow$  complex, vigorous dynamics.



### Particle Kinetics in Plasmas

• Single particle movement governed by Lorentz-Force:

$$\ddot{\mathbf{r}} = \frac{q}{m}\mathbf{E} + \frac{q}{m}\dot{\mathbf{r}} \times \mathbf{B}$$
(1)

with position  $\mathbf{r}$ , charge q, mass m, electric field  $\mathbf{E}$  and magnetic flux density  $\mathbf{B}$ .

- Fusion plasma confinement: requires strong, external magnetic fields <br/>  ${\bf B} \sim 1~{\rm T}.$
- Particle motion characterized by high-frequency gyrations.
- Other interactions: particle collisions, radiation.



# Simulating Fusion Plasmas with PEPC

#### PEPC

Pretty Efficient Parallel Coulomb-solver

Parallel tree-code for rapid computation of long-range Coulomb forces in N-particle systems.

[PEPC]



Figure: Basic PEPC flow-chart

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#### **Gyrations in Magnetic Fields**

- $\mathbf{B}$ -field  $\rightarrow$  charged particles circulate around field axis.
- $\sim$  Particles *approximately* follow **B**-field lines on spiral orbits.



Figure: Electron gyration in homogenic B-field.



# Scales in Fusion Plasma Simulations

Electron gyration radius	$ ho_{ m g}$	$\sim 0.1~{\rm mm}$
Electron gyration period	$T_{\rm g}$	$\sim 10^{-12} { m s}$
Ion gyration period		$\sim 10^{-9} {\rm s}$

- Interesting phenomena at time scales  $\sim 1$  s.
- Problem: Boris Solver requires time-step

$$\delta t \lesssim T_{\rm g} \approx 10^{-13} \, {\rm s}$$
 (2)

for electron gyration.[Parker, Birdsall]

• Idea: Replace exact electron position  $\mathbf{r}$  with gyration center  $\mathbf{R}$ .

# Simulation of Drift-Kinetic Dynamics of Charged Particles in Magnetized Plasmas Part II: Guiding Center Motion

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# Assumptions & scaling parameter

- 1. Only weak field variation within gyration scales.
- 2. Interesting particle interaction scales  $\gg$  gyration scales.
- 3. Radiation neglectable in particle motion.
- 4. Expansion parameter:

$$\varepsilon := \rho_{\rm g} \cdot \frac{\|\nabla \mathbf{B}\|}{B} \stackrel{!}{\ll} 1 \tag{3}$$

with local gyration radius  $\rho_{\rm g}$ .[Northrop]

 $\rightarrow$  Ratio of gyration scales to field-variation scales.



## **Guiding Center: Definition**

- Abstract: Geometrical center of local gyration.
- Exact [Northrop]:

$$\mathbf{R} := \mathbf{r} - \frac{\mathbf{B}}{\omega_{\mathrm{g}}B} \times \left(\dot{\mathbf{r}} - \frac{\mathbf{E} \times \mathbf{B}}{B^2}\right) \tag{4}$$

with local gyration frequency  $\omega_{g}$ , particle position **r** & velocity  $\dot{\mathbf{r}}$ .



Figure: Guiding center of charged particle orbit.



# **Guiding Center: Equation of Motion**

• Equation of motion for guiding center:

$$\ddot{\mathbf{R}} = \frac{q}{m} \left[ \mathbf{E} - \frac{\mu}{q} \nabla B \right] + \frac{q}{m} \dot{\mathbf{R}} \times \mathbf{B} + \mathcal{O}(\varepsilon)$$
(5)

with the magnetic moment

$$\mu := \frac{m}{2} \frac{\dot{\mathbf{r}}_{\perp}^2}{B} \tag{6}$$

and particle velocity  $\dot{\mathbf{r}}_{\perp}$  perpendicular to  $\mathbf{B}$ .[Northrop]

- Same structure as Lorentz-force  $\rightarrow$  same kind of motion in first order.



# **Guiding Center: Perpendicular Drifts**

Projection of the EOM perpendicular to  ${f B}$  leads to:

$$\dot{\mathbf{R}}_{\perp} = \underbrace{\frac{\mathbf{E} \times \mathbf{B}}{B^2}}_{\mathbf{E} \times \mathbf{B} - \text{drift}} + \underbrace{\frac{\mu}{qB} \mathbf{b} \times \nabla B}_{\text{magnetic drift}} - \underbrace{\frac{m}{qB} \ddot{\mathbf{R}} \times \mathbf{b}}_{\text{acceleration drift}} + \mathcal{O}(\varepsilon^2)$$
(7)

with velocity  $\dot{\mathbf{R}}_{\perp}$  perpendicular to  $\mathbf{B}$ .  $\sim$ 

- Guiding center drifting perpendicular to field lines.
- Drifts caused by variations of gyro-radius or gyration speed during gyration period.



# $\mathbf{E} \times \mathbf{B}\text{-}\mathbf{Drift}$

- Caused by variation of gyration speed due to **E**-field.
- Always perpendicular to **E** & **B**-fields.



**Figure:**  $\mathbf{E} \times \mathbf{B}$ -drift of electron guiding center.



### Guiding Center: Start Velocity

• Guiding center start *velocity*:

$$\dot{\mathbf{R}}(0) = \dot{\mathbf{r}}_{\parallel}(0) + \frac{\mathbf{E} \times \mathbf{B}}{B^2} + \mathcal{O}(\varepsilon)$$
(8)

with particle velocity  $\dot{\mathbf{r}}_{\parallel}$  parallel to  $\mathbf{B}$ .

In fusion plasmas:

$$\dot{\mathbf{r}} \sim 10^7 \text{ m} \cdot \text{s}^{-1} \gg \frac{\mathbf{E} \times \mathbf{B}}{\text{B}^2} \sim 1 \text{ m} \cdot \text{s}^{-1}$$
 (9)

 $\rightarrow$  leads to much smaller gyration radius of guiding center.



#### The Magnetic Moment $\mu$

- Interpretation: Magnetic moment of charge orbiting on circle.
- Connected to *mean kinetic energy*:

$$\mathcal{E}_{\rm kin} = \frac{m}{2}\dot{\mathbf{R}}^2 + \mu \cdot B \tag{10}$$

with

$$\frac{d\mathcal{E}_{\rm kin}}{dt} = q \left\langle \dot{\mathbf{R}}, \mathbf{E} \right\rangle + \mu \frac{\partial B}{\partial t} + \mathcal{O}(\varepsilon^2) \tag{11}$$

- **Problem:**  $\mu$  no longer available, since exact particle velocity unknown.
- Solution: Integrate  $\mu \iff \mathcal{E}_{kin}$  along with  $\mathbf{R}, \dot{\mathbf{R}}$  using eq. (11).



# **Guiding Center: Numerical Integration**

- Similarity to original EOM  $\rightarrow$  usage of existing integration scheme.
- **E**-field *modified* by  $\nabla B$ -term.
- Leapfrog integration scheme:

$$\left(\mathbf{R}^{n}, \dot{\mathbf{R}}^{n-\frac{1}{2}}\right) \stackrel{\text{Boris}}{\longrightarrow} \left(\mathbf{R}^{n+1}, \dot{\mathbf{R}}^{n+\frac{1}{2}}\right)$$
(12)

$$\mathcal{E}_{\rm kin}^{n+\frac{1}{2}} := \mathcal{E}_{\rm kin}^{n-\frac{1}{2}} + \delta t \cdot q \cdot \left\langle \mathbf{E}^{n+1}, \dot{\mathbf{R}}^n \right\rangle + \delta t \cdot \frac{\mu^{n-\frac{1}{2}}}{q} \cdot \nabla B^{n+1} \tag{13}$$

#### Fields

- $\mathbf{E}^n \rightarrow \text{calculated using parallel tree-code from positions } \mathbf{R}^n.[\text{PEPC}]$
- $\mathbf{B}^n \to \text{provided as external field at positions } \mathbf{R}^n$ .



## **Example Simulation**

Electron & Guiding Center Orbit in Toroidal B-Field





#### Accuracy of Guiding Center Orbits

Distance Between Calculated Guiding Center & Electron Orbit over Runtime





#### **Spatial Convergence Tests**

Convergence of Guiding Center to Electron Orbit with Varying Time-Steps



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# Simulation of Drift-Kinetic Dynamics of Charged Particles in Magnetized Plasmas Part III: External **B**-Fields

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#### Given Field-Data

- External **B**-field.
- TOKAMAK  $\rightarrow$  cylindrical symmetry.
- External **B**-field given on triangular mesh at  $\varphi = 0$  $\rightarrow$  given as constant on each triangle.
- Need for  $\nabla \mathbf{B} \rightarrow \text{local interpolation}$ .
- Requirement:  $\nabla \cdot \mathbf{B} \stackrel{!}{=} 0!$



# Triangle Mesh & Predefined B-Field

**Projection on**  $\varphi = 0$  plane



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#### Mesh Transformation

- Need for pointwise field definition
   → Transformation of triangular
   mesh.
- Original triangle  $\rightarrow$  3 new triangles.
- New fields defined on triangle vertices.
- 3-point interpolation within each triangle.



New field value: Triangle field

**Figure:** Mesh refinement & definition of new field values



# **Divergence Free Interpolation**

#### Cylindrical symmetry:

Divergence-freeness simplifies to:

$$\frac{\partial}{\partial \rho}(\rho B^{\rho}) + \frac{\partial}{\partial z}(\rho B^{z}) \stackrel{!}{=} 0 \tag{14}$$

- $\varphi$ -component can be interpolated arbitrarily (e.g. linear).
- $\rightarrow$  Problem reduced to 2D-case:  $\mathbf{F} := (\rho B^{\rho}, \rho B^z)$ .

#### 2D-formulation:

Given: 3 base-points  $\mathbf{r}_i \in \mathbb{R}^2$  and base-values  $\mathbf{F}_i \in \mathbb{R}^2$ , i = 1, 2, 3. Sought: Field  $\mathbf{F} : \mathbb{R}^2 \to \mathbb{R}^2$  with  $\mathbf{F}(\mathbf{r}_i) = \mathbf{F}_i \& \nabla \cdot \mathbf{F} = 0$ .



## Ansatz: Component Separation

• General Ansatz for divergence-free field:

$$\begin{pmatrix} F^{x} \\ F^{y} \end{pmatrix} = \begin{pmatrix} F^{x}(y) \\ F^{y}(x) \end{pmatrix}$$
(15)

Idea:

- X component interpolated over Y coordinates of base-points.
- Y component interpolated over X coordinates of base-points.
- $\rightarrow$  simple linear interpolation for each component.
- Prerequisite: Interpolation base-points differ in both coordinates.
- Always possible in some coordinate system!
- Resulting **B**-field: differentiable almost everywhere!



### **Elaboration on Component Separation**



**Figure:** On component separated interpolation: Each component is defined by 1D-interpolation.

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# Example Interpolation



**Figure:** Example component-separated interpolation of  $B^{\rho}$  within 3 points.



# Summary

- Charged particle orbits in **B**-fields characterized by high-frequency gyrations.
- **Problem:** Possible time-steps limited by electron gyration period.
- Solution: Exact particle orbit  $\rightarrow$  replaced with guiding center orbit.
- Implementation: Allows time-step increase of up to  $\times 100$ .
- **B**-field given by divergence-free interpolation.



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# Simulation of Drift-Kinetic Dynamics of Charged Particles in Magnetized Plasmas Part V: Appendix

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# **Magnetic Drift**

- Caused by variation of gyration radius due to **B**-field variation.
- Always perpendicular to **B**-field.



Figure: Magnetic drift of electron guiding center.



#### Acceleration Drift

- Caused by time-varying **B** & **E**-fields and field line curvature.
- In case of stationary fields: Perpendicular to **B**-field lines & curvature center.



**Figure:** Acceleration drift of electron guiding center.



#### Guiding Center: $\mu$ -Convergence Tests



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