Guiding center Fokker-Planck theory and Monte Carlo method

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Outline

1 Fokker-Planck theory and stochastic motion

2 Guiding center formalism

3 High Performance computing

4 Applying the formalism { if time permits

5 Summary

Outline

1 Fokker-Planck theory and stochastic motion
- Motivation
- Derivation of Fokker-Planck equation
- Deboning the FP equation, Part I: the RHS
- Deboning the FP equation, Part II: the LHS
- Equivalence to a stochastic di erential equation

We need an e cient description for a plasma:

- Coulomb interaction has an in nite range
- Motion of each particle is connected to the motion of all other particles
- Number of particles in systems we are interested in is enormous

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Assume small steps due to small-angle Coulomb collisions:

1 Taylor expand f and W around z

$$f(z; t + \quad) = \int d \quad f(z; t) W(z; \quad) \quad \frac{@}{@z}(f(z; t) W(z; \quad)) + \frac{1}{2} \frac{@}{@z} \frac{@}{@z}(f(z; t) W(z; \quad)) : \quad + O(\quad) :$$

2 Rearrange terms

$$\frac{f(z; t + \quad) \quad f(z; t)}{} = \quad \frac{@}{@z} \quad f(z; t) \overline{\quad} + \frac{1}{2} \frac{@}{@z} \frac{@}{@z} : \quad f(z; t) \overline{\quad} \quad + O(\overline{\quad});$$

Here the expectation value with respect to transition probability is

$$h : : : i = \int d \quad W(z; \quad) : : :$$

Include only small-angle collisions:

In fusion plasmas, $\frac{h \quad i}{\quad}$ and $\frac{h \quad\quad i}{\quad\quad}$ dominate higher order terms by a factor ln (# of particles within the Debye-sphere $>> 1$):

$$\frac{@}{@t} f(z; t) = \frac{@}{@z} [(\underline{z} + a(z; t)) f(z; t)] + \frac{@}{@z} \frac{@}{@z} : [D(z; t) f(z; t)]; \qquad (3)$$

where the Hamiltonian part $\underline{z}$ arises from the deterministic motion, $W = (\underline{z} \quad)$, and the collisional friction (or drag) vector and di usion tensor (the Fokker-Planck coe cients) are

$$a(z; t) = \lim_{! 0} \frac{h \quad i}{\quad}; \qquad (4)$$

$$D(z; t) = \lim_{! 0} \frac{h \quad\quad i}{2}: \qquad (5)$$

Careful: ln *determines the* **validity** *of the Fokker-Planck theory. Theory completely breaks down when* ln $!$ 1. **Error** *is proportional to* $1 = \ln$

Guiding center Fokker-Planck l54(F)29(okk)30(er-Planck)-3552ookkland-355(IMonckнck)-3Caokklmetho-350(d)]TJ.2549 0.6784 rg 0 0.2549 0.67127400083392 C

Path of least action in 3D:

z = (r; v), with components z
Minimizing the action in 3D gives

$$\frac{@z}{@t} = fz \; ; Hg \tag{28}$$

where on the RHS we have the *Poisson bracket*,

$$ff; gg \quad \frac{@f}{@z} \quad \frac{@g}{@z}: \tag{29}$$

and is the *Poisson matrix* given as the inverse of the *Lagrange matrix*

$$! \quad = \frac{1}{2} \quad \frac{@}{@z} \quad \frac{@}{@z} \quad ; \tag{30}$$

Note

The Poisson brackets play a crucial role when the GC formalism is derived using Lie transformations. Thus the silly-appearing e ort.

Solving the FP equation I: straightforward approach

Use nite di erence, nite element (FEM) methods !

- In the full 6D phase space, this leads to enormous matrices
- ! mostly applicable when the #

Langevin equation for a test particle

The Fokker-Planck equation

$$\frac{@}{@t} f(z;t) = \frac{@}{@z}\left[(\underline{z} + a(z;t)) f(z;t)\right] + \frac{@}{@z}\frac{@}{@z} : \left[D(z;t) f(z;t)\right];$$

is equivalent to a stochastic di erential equation, the *Langevin equation*

$$dz = [\underline{z} + a(z;t)]\,dt + \quad d \quad ; \tag{36}$$

where the matrix is de ned via a decomposition of the di usion tensor

$$2D = \quad ^{T} : \tag{37}$$

and the stochastic di erential d denotes an in nitesimal change in the random variable which has zero mean and variance t. (The upper index ^{T} denotes a transpose of a matrix.)

Guiding center vs. particle

- Guiding center often misunderstood as the average of the particle position over a single Larmor rotation, i.e., $X \int_0^{2\pi} x\, d\varphi = (2\pi)$.
- However, rigorous definition is a **coordinate transformation**

$$x = X + \rho;$$

where ρ is the vector from the guiding center position to the particle position. Its length, ρ, is called the Larmor radius.

- In principle, for any function we have simple transformation rules

$$f(x) = f(X + \rho) = \sum_n \frac{1}{n!}(\rho \cdot r)^n f(X) = \exp(\rho \cdot r) f(X) \quad F(X);$$

$$F(X) = F(x - \rho) = \sum_n \frac{1}{n!}(-\rho \cdot r)^n F(x) = \exp(-\rho \cdot r) F(x) \quad f(x)$$

Dr. Lie comes to rescue!

The rapid gyro motion can be eliminated formally using the *Lie transform perturbation* method.

Basic idea:
Find a transformation of coordinates such that, in the new coordinates, the transformed Lagrangian is *independent* of the gyro angle.

Things to keep in mind:

- The gyro angle can still be resolved but it is not necessary.
- In the FP equation, the collisional part will still contain the gyro angle *!* has to be averaged

Here, the proceduce will on8qobute of

Basic concepts of the Lie Transformation

Lie transformation is de ned by *pull-back* and *push-forward* operators:

- $T_n = \exp(\ ^n L_{G_n})$
- $T_n\ ^1 = \exp(\quad ^n L_{G_n})$

where

- is a smallness parameter, giving the order of the *near-identity* transformation. Thus the term *'perturbation'*.
- L_{G_n} is the so-called *Lie derivative*, generated by a vector eld G_n.
  - *Lie-derivative of a function reduces to* $L_{G_n} F = G_n @F=@Z$ *so that* $\exp(\ ^n L_{G_n})F = \exp(\ ^n G_n @=@Z\ )F$. *A Lie-transformation is thus*

GC equations of motion

The equations in form ready to be programmed are

$$\dot{X} = f_X; H_{gc} g_{gc} = v_k \frac{B^?}{B_k^?} + \frac{\partial}{qB_k^?} \qquad r_B; \tag{46}$$

$$\dot{v}_k = f_{v_k}; H_{gc} g_{gc} = -\frac{B^?}{m} \frac{}{B_k^?} \quad r_B; \tag{47}$$

$$\dot{} = f_{} ; H$$

Note:

- $X; v_k;$ do not depend on
- is a constant of motion in GC formalism
- we haven't lost any information. The gyro angle can still be followed if so desired.

Transforming the FP equation

So far only LHS = the Hamiltonian part of the FP equation transformed. How to transform the entire FP equation, including the collision operator? Answer: *the Poisson brackets*!

The velocity derivative $@=@v^i$ can be written in terms of Poisson brackets:

$$\frac{@f}{@v^i} = \frac{1}{m} fx^i; Hg \tag{50}$$

! Write the FP equation in terms of Poisson brackets and use the known transformation $ff;gg \; ! \; fF;Gg_{gc}$

$$\frac{@f}{@t} + ff; Hg = fx^i; mK^i f \quad m^2 D^{ij} fx^j; fgg: \tag{51}$$

Here we have used K = a $\frac{@}{@\mathbf{v}}$ D for practical reasons.

Eliminating the last traces of

The GC distribution function $F(Z\ )$ and the friction and di usion coe cients still have dependence $!$ FP has to be averaged over . This tedious job can be found in [EHD2014], yielding

$$\frac{@F}{@t}$$

GC Langevin equation

Now the 'Kolmogorov connection' can be used !

$$dZ = A_{gc}dt + \quad_{gc}\, dW \;; \tag{58}$$

where dW is again a Wiener process with zero mean and variance t, and

$_{gc}$

GC collision operators for numerical implementation: Di usion

$$\langle D^{\mathbf{x}\mathbf{x}} \rangle = {}^{2} \quad (D_k \quad D_?)\frac{B}{2E} + D_? \quad \frac{\text{I} \quad \text{hh}}{(m \quad {}^{?}_{k})^2} + O({}^{3}); \tag{63}$$

$$\langle D^{v_k v_k} \rangle = \frac{D_k}{m^2} + (1 \qquad)\frac{D_? \quad D_k}{m^2}\frac{B}{E} + O({}^{2}); \tag{64}$$

$$\langle D \quad \rangle = (1 \qquad)\frac{2}{mB} \quad (D_k \quad D_?)\frac{B}{E} + D_? \quad + O({}^{2}); \tag{65}$$

$$\langle D^{\mathbf{x}v_k} \rangle = {}^{2}\frac{v_k}{(m \quad {}^{?}_{k})^2}(D_k \quad D_?)\frac{B}{2E}\, r_? \ln B$$

$$+ {}^{2}\frac{v_k}{(m \quad {}^{?}_{k})^2} \quad D_k + \frac{B}{2E}(D_? \quad D_k) \quad r \quad + O({}^{3}); \tag{66}$$

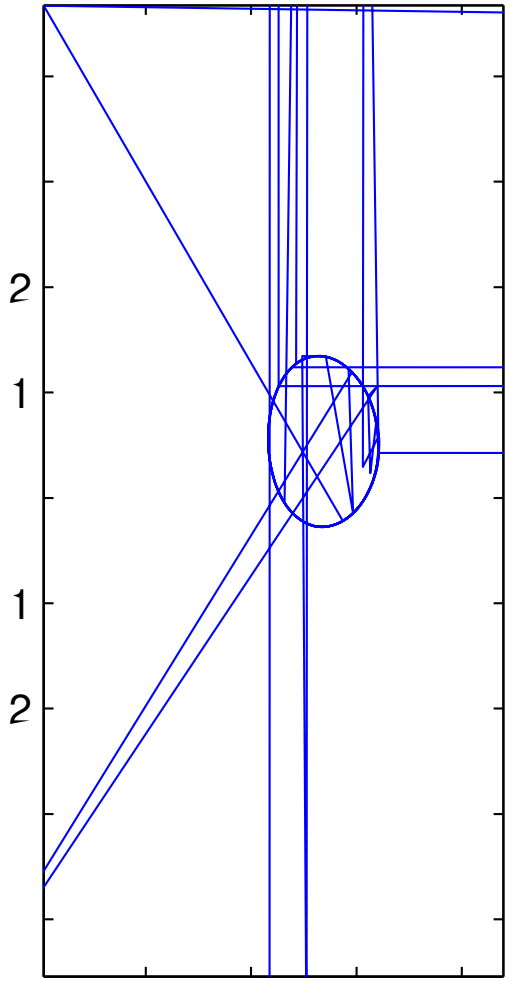
$$\langle D^{\mathbf{x}} \quad \rangle = \quad \frac{}{2mE}(D_k \quad D_?)\frac{}{{}^{?}_{k}} \quad \mathbf{x} + O({}^{3}); \tag{67}$$

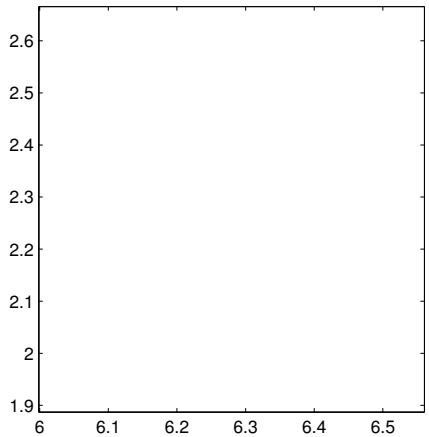
$$\langle D \quad {}^{v_k} \rangle = (1 \qquad)\frac{v_k}{mE}(D_k \quad D_?) + \quad \frac{}{v_k m^2} D_k + O({}^{2}); \tag{68}$$

Drift orbits and neoclassical transport

We now have a powerful tool that allows:

- to follow the *drift orbits*, traced by the guiding centers of a test particle.
- to simulate the *neoclassical transport*, caused by the combined e ect of toroidal geometry and Coulomb collisions, of the test particles.





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Test particles in tokamak magnetic eld

In high performance plasmas, *magnetic eld* dominates the test particle behaviour. How do we get the values of magnetic eld and its derivative, needed for the equations of motion?

- t < 1990's: assume circularly symmetric plasma with simple limiter
  ! analytical expression for B.
  - very fast
  - very accurate
  - has very little to do with the reality of shaped and diverted plasmas
- 1990's { 2000's: introduce diverted geometry with non-circular cross section (ASCOT got experimental backgrounds in 1997.)
  - allows simulations in the SOL and divertor region
  - calculation slows down because 2D interpolation needed
  - choice of interpolation routine not trivial
  - still assumes axisymmetry

How about the still prevailing assumption of axisymmetry???

HPC: super computers needed to simulate fast ions

A 3.5 MeV alpha-particle in ITER slows down in 1 s. Simulating it takes (with realistic 3D B eld and wall and collisions etc)

- 1 min in GC approach as a guiding centre or an
- 1 h in full orbit approach

One needs from thousands to millions of alphas, depending on the quantity of interest ! super computers are a good idea.

HPC: super computers are complicated beasts with many layers and connections of variable speed

Using the (slow) disk e ciently

In any supercomputer the computing nodes outnumber the nodes

Future: GPGPU / Accelerators

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Pros and Cons of Langevin equation with MC

High Performance computing

Your results can only be as good and reliable as your input!
Therefore, before carrying out the simulations check the following

- The quality of your magnetic background: is the eld divergence-free and smooth? (Crazy $r\,B$ -drifts are guaranteed to give crazy results)
- Choose your interpolation routine carefully: you have to navigate between requirements for accuracy and speed.
- Check you orbit-following routine so that it conserves energy and collisionless orbits in axisymmetric case (otherwise you get numerical transport)
- When moving to HPC platforms, check scalability and optimize the code as well as I/O for that particular platform.