UPGRADE OF THE GSP GYROKINETIC CODE

MID-YEAR PROGRESS REPORT

George Wilkie
gwilkie@umd.edu
December 6, 2011

Supervisor: William Dorland, Dept. of Physics
bdorland@umd.edu

Abstract:

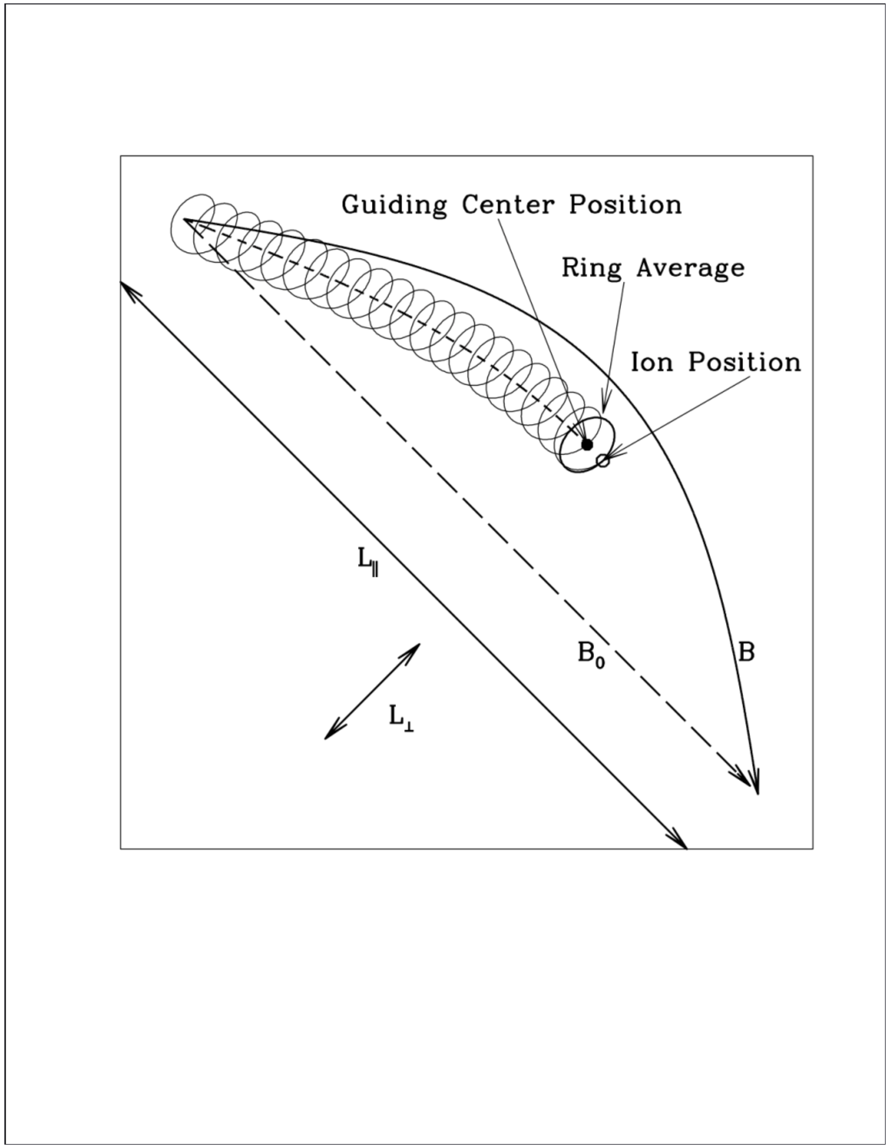
Simulations of turbulent plasma in a strong magnetic field can take advantage of the gyrokinetic approximation, the result of which is a closed set of equations that can be solved numerically. An existing code, GSP, uses a novel and highly efficient solution method to solve the nonlinear 5D gyrokinetic equation. In this project, we will seek to change the velocity-space representation in GSP. This transformation will simplify the inclusion of a new collision operator and make the algorithm more suitable for simulations of turbulence in Tokamak plasmas, while retaining the efficiency and accuracy of the original code.

Outline

- **Overview of Gyrokinetics**
- **Description of GSP**
- **Changes to Algorithm**

Overview

- GSP is a Particle-In-Cell (PIC) code to solve the Gyrokinetic equation to study the evolution of turbulence in highly magnetized plasma
- Gyrokinetic theory treats the many rapidly circulating charges as charged rings
  - These rings drift parallel and perpendicular to the background magnetic field

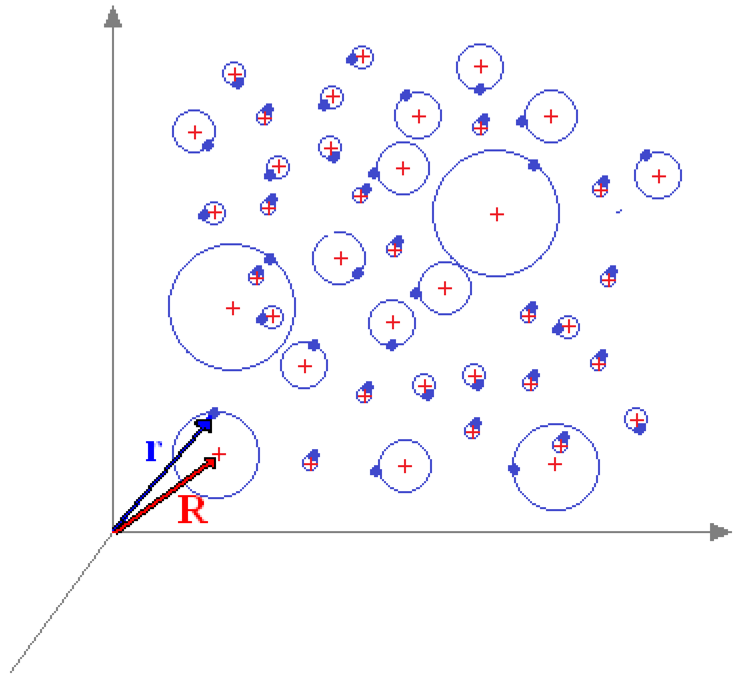


Overview

- The “particles” in the code are *not* intended to simulate the physical particles, nor the “gyro-averaged” rings of charge.
  - The evolution of many physical charges are described by a statistical distribution function in phase space: $f\left(\mathbf{r}, v_{\parallel}, v_{\perp}, \theta\right)$

$$f \approx F_0 + \delta f + \ldots$$

  - Performing an asymptotic expansion and gyroaveraging the Fokker-Planck equation, we can get a dynamical equation for δf : the gyrokinetic equation



The Gyrokinetic Equation

$$\frac{\partial \langle \delta f \rangle}{\partial t} + v_{\parallel} \frac{\partial}{\partial z} \langle \delta f \rangle + \mathbf{v}_D \cdot \nabla \langle \delta f \rangle = \langle C[\delta f] \rangle - \mathbf{v}_D \cdot \nabla F_0 + v_{\parallel} \langle E_z \rangle F_0$$

Where:

- $\langle \delta f \rangle = \langle \delta f \rangle (\mathbf{R}, v_{\perp}, v_{\parallel})$ is the perturbed distribution function to be solved for
- The given background equilibrium distribution is: $F_0 = n\left(\frac{m}{2\pi kT}\right) e^{\frac{-mv^2}{2kT}}$
- The particle "weight" is $w \equiv \frac{\langle \delta f \rangle}{F_0}$
- The (characteristic) drift velocity is: $\mathbf{v}_D = \frac{c}{B_0} \langle \mathbf{E} \rangle \times \hat{\mathbf{z}}$
- $C[\delta f]$ is the collision operator

(angle brackets signify the gyro-averaging operation at constant **R**)

Outline

- Overview of Gyrokinetics
- **Description of GSP**
- Changes to Algorithm

The Gyrokinetic Equation

$$\frac{\partial\langle\delta f\rangle}{\partial t} + v_{\parallel}\frac{\partial}{\partial z}\langle\delta f\rangle + \mathbf{v}_D\cdot\nabla\langle\delta f\rangle = \langle C[\delta f]\rangle - \mathbf{v}_D\cdot\nabla F_0 + v_{\parallel}\langle E_z\rangle F_0$$

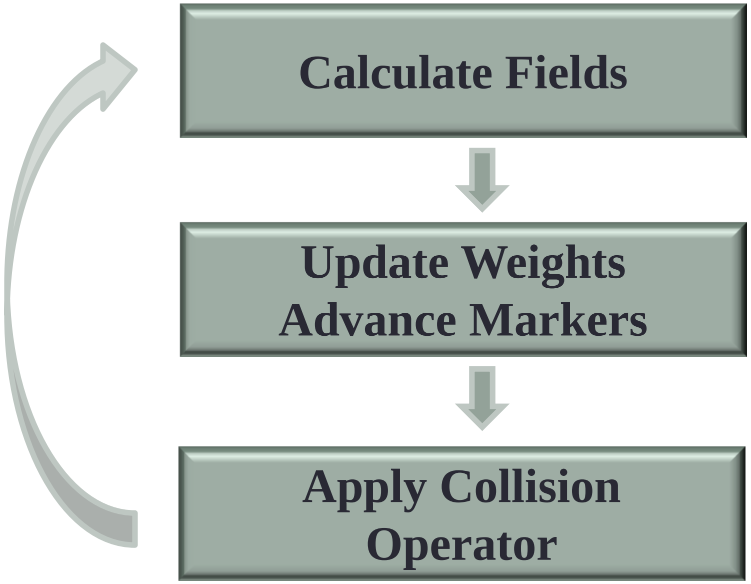
To solve this equation, we identify characteristic trajectories in phase space so that:

- The left hand side becomes $\frac{d}{dt}\langle\delta f\rangle$
- $v_{\parallel}\hat{\mathbf{z}} + \mathbf{v}_D$ is the characteristic velocity
- Characteristic curves are constant in velocity space only under special conditions:
  - Uniform equilibrium magnetic field $\mathbf{B_0}$
  - Special choice of velocity coordinates: $\mu \equiv \frac{m v_{\perp}^2}{2B_0}$ $\mathcal{E} = \frac{1}{2}m\left(v_{\perp}^2 + v_{\parallel}^2\right)$

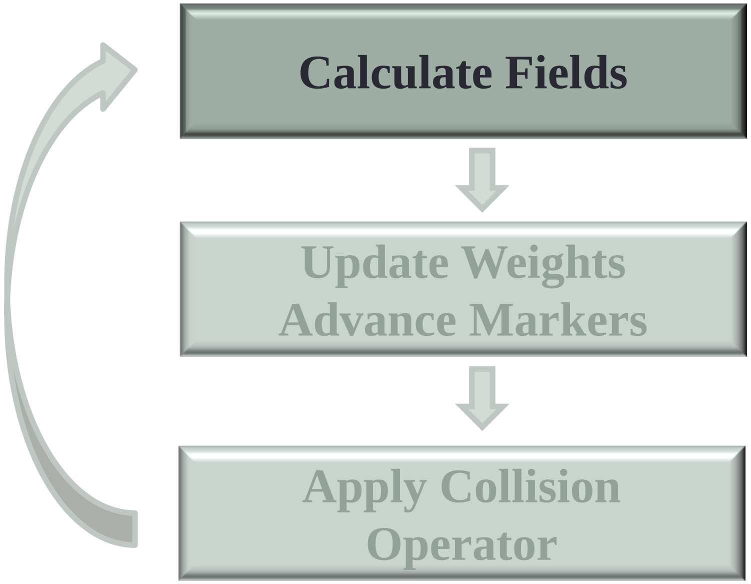
GSP Code

- **Step 1: Initialize particles in phase space**
- **Step 2: Predictor Step:**
  - Calculate fields at step *n*
  - Calculate marker weights along characteristics for step *n+1/2*
  - Advance marker positions for half a timestep
  - Update weights with collision operator for step *n+1/2*
- **Step 3: Corrector Step**:
  - Calculate fields at step *n+1/2*
  - Calculate marker weights along characteristics for step *n+1*
  - Advance marker positions for a full timestep
  - Update weights with collision operator for step *n+1*
- **Step 4: Output results**
- **Repeat Steps 2-4 N_T times**

Flowchart


Calculate Fields
Update Weights
Advance Markers
Apply Collision
Operator

Flowchart


Calculate Fields
Update Weights
Advance Markers
Apply Collision
Operator

Calculate Fields

$$\mathbf{v}_D = \frac{c}{B_0}\langle \mathbf{E} \rangle \times \hat{\mathbf{z}}$$

- Once we know the electrostatic potential, we know the electric field:

$$\mathbf{E} = -\nabla \phi$$

- The gyro-averaging operation is simplified in Fourier space:

$$\langle \tilde{\mathbf{E}} \rangle = J_0\left(\tfrac{k_\perp v_\perp}{\Omega}\right)\tilde{\mathbf{E}} = -i\mathbf{k}\tilde{\phi} J_0\left(\tfrac{k_\perp v_\perp}{\Omega}\right)$$

(J_0 is the 0-th order Bessel function) $\Omega = \frac{eB_0}{mc}$

Calculate Fields

- First, deposit charges onto grid in **R**-space
- Fourier transform grid
- Apply Poisson's equation to calculate the potential:

$$\tilde{\phi} \propto \int dv_{\parallel} \int v_{\perp} dv_{\perp} \langle \delta f \rangle_{\mathbf{R}} J_0\left(\frac{k_{\perp} v_{\perp}}{\Omega}\right)$$

- Issue:
  - J_0 is expensive to calculate explicitly every time
- Solution:
  - Discretize $v_{\perp}$ on a grid in velocity space
  - Store J_0 in a table at the relevant discrete values of $v_{\perp}$ and $k_{\perp}$

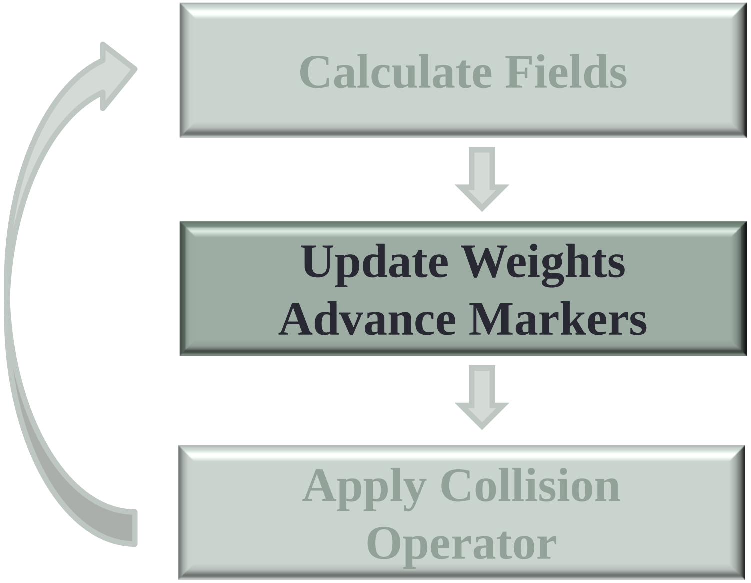
Calculate Fields

- Once potential is calculated, find the gyro-averaged fields in k-space

$$\left\langle \tilde{\mathbf{E}} \right\rangle_{\mathbf{R}} = -i\mathbf{k}\tilde{\phi} J_0\left(\frac{k_\perp v_\perp}{\Omega}\right)$$

- Fourier transform back into grid in **R**-space
- Interpolate to find fields at marker positions

Flowchart


Calculate Fields
Update Weights
Advance Markers
Apply Collision
Operator

Update Weights and Advance Markers

- This Monte Carlo scheme [Aydemir,1994] doesn't model $\left\langle \delta f \right\rangle_{\mathbf{R}}$ explicitly, but rather the function:

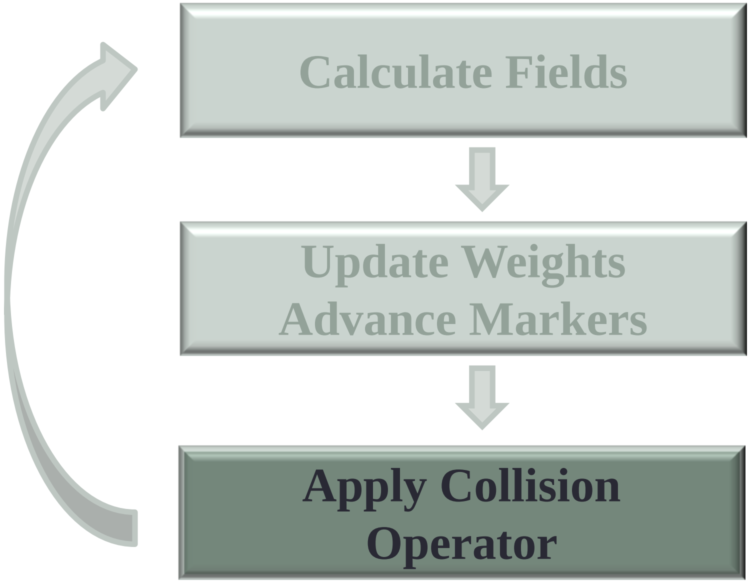
$$w = \frac{\left\langle \delta f \right\rangle_{\mathbf{R}}}{F_0}$$

- The equation for *w* along characteristics is:

$$\dot{w} = \frac{q}{T} v_{\|} \left\langle E_z \right\rangle_{\mathbf{R}} - \frac{\nabla F_0}{F_0} \cdot \mathbf{v}_D$$

- Update marker positions explicitly using $v_{\|}\hat{\mathbf{z}} + \mathbf{v}_D$

Flowchart


Calculate Fields
Update Weights
Advance Markers
Apply Collision
Operator

Collision Operator

- Pitch-angle scattering operator
  - Diffusive in velocity space
  - Energy is conserved with like-particle interactions, or when there's a large disparity in mass (such as ions and electrons)
  - ν is a constant parameter

- Collision operator defined in terms of $h \equiv \langle \delta f \rangle + \langle \phi \rangle F_0$

$$C[h] = \frac{\nu}{2} \frac{\partial}{\partial \xi} \left(1 - \xi^2\right) \frac{\partial h}{\partial \xi} \qquad \xi = \frac{v_\parallel}{v}$$

Collision Operator

- Godunov splitting: We have already applied the non-collisional part of the derivative:

$$\langle \delta f \rangle^{n} \rightarrow \langle \delta f \rangle^{*}$$

- First, convert δf * to h* :

$$h^{*} \equiv \langle \delta f \rangle^{*} + \langle \phi \rangle F_0$$

- Find the derivatives implicitly

$$\frac{h^{n+1} - h^{*}}{\Delta t} = C\left[h^{n+1}\right]$$

- Invert the tri-diagonal matrix to obtain h^{n+1}

- $\langle \delta f \rangle^{n+1} = h^{n+1} - \langle \phi \rangle F$

Collision Operator

- Issues:
  - As implemented, the collision operator does not obey the proper conservations laws

- The update will use the operator from [Abel et al, 2008], which conserves particles, momentum, energy, and obeys the Boltzmann H-theorem

Outline

- Overview of Gyrokinetics
- Description of GSP
- **Changes to Algorithm**

Summary of Changes

Calculate Fields	Most difficult task. Perform calculation with new velocity-space coordinates. Try to keep repeated “calculation” of J_0 efficient.
Update Weights **Advance Markers**	Minor changes if any
Apply Collision Operator	Rework – convert pitch-angle operator to new coordinates. Apply Abel operator.

Coding Status

Calculate Fields	In progress
Update Weights Advance Markers	No changes needed
Apply Collision Operator	

Integral for Electrostatic Potential

$$\tilde{\phi} \propto \int dv_{\parallel} \int v_{\perp} dv_{\perp} \langle \delta f \rangle_{\mathbf{R}} J_0\left(\frac{k_{\perp} v_{\perp}}{\Omega}\right)$$

- We're representing the distribution as:

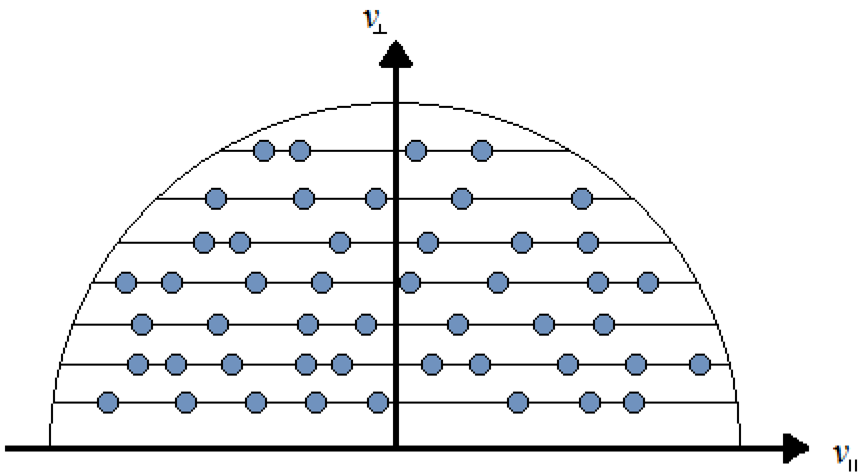
$$\begin{aligned} \langle \delta f \rangle_{\mathbf{R}} &= F_0 w(\mathbf{r}, v_{\parallel}, v_{\perp}) \\ &= F_0 \sum_i w_i \delta(\mathbf{r} - \mathbf{R}_i) \delta(v_{\parallel} - v_{\parallel,i}) \delta(v_{\perp} - v_{\perp i}) \end{aligned}$$

so to calculate the integral, we just sum up the values of $J_0 \cdot w$ for each particle and normalize

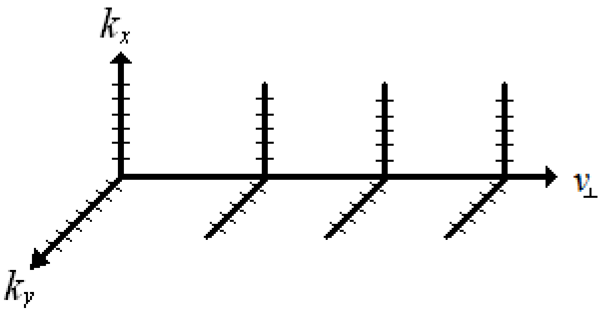
- When $v_{\perp}$ is allowed to change, we need another way to looking up J_0

Current Velocity Grid

- Particles interpolated onto **k** grid
- Particles already have an assigned $v_\perp$

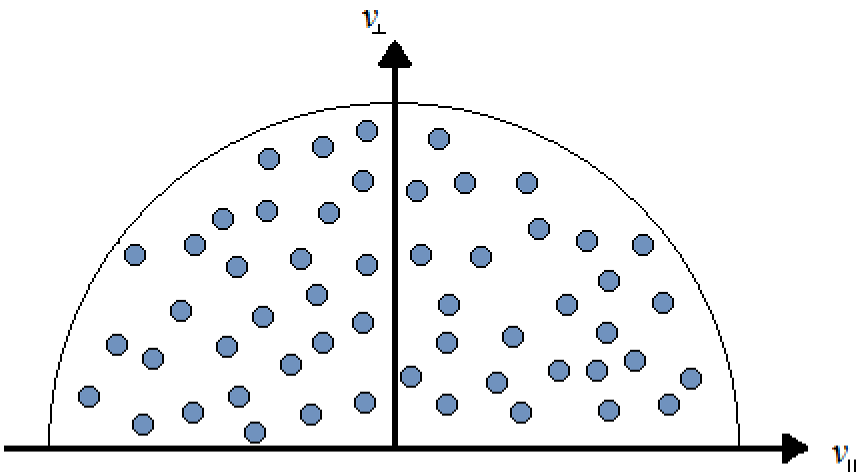


$$J_0 = J_0(k_x, k_y, v_\perp)$$

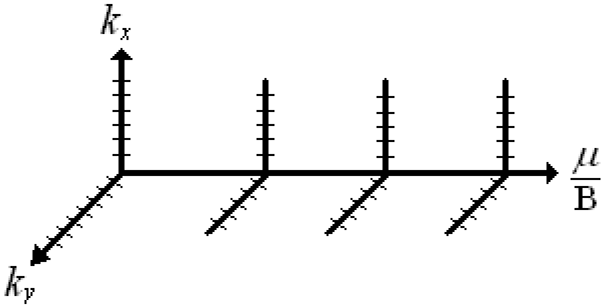


New Velocity "Grid"

- Particles scattered in 2D velocity- space
- Can move around in velocity space depending on the local magnetic field $B(z)$



$$J_0 = J_0(k_x, k_y, v_\perp, B) = J_0\left(k_x, k_y, \frac{\mu}{B}\right)$$



	Timeline	Milestone
Phase I	September – October	Transformed GK equation derived and algorithm understood
Phase II	November – January	Changes coded and debugged
Phase III	February – April	New code validated, tested, and benchmarked
Phase IV	April – May	Results organized, presentation prepared and given

Summary

- Upgrade to GSP progressing slightly behind schedule
  - Phase I (Gyrokinetics analytics and algorithm understanding) took longer than initially expected
  - Currently on Phase II

- Coding still on track to be completed before February

Questions?

Gyrokinetic Derivation Summary

- Start with Fokker-Planck equation
- Gyrokinetic ordering assumptions: $\frac{\omega}{\Omega} \sim \frac{\nu}{\Omega} \sim \frac{k_{\parallel}}{k_{\perp}} \sim \frac{v_D}{v_t} \sim \frac{\delta f}{F_0} \sim \varepsilon$
- Order ε^0:
  - F_0 independent of gyroangle θ
- Order ε^1:
  - F_0 Maxwellian
  - $\delta f = -\frac{q\phi}{T} F_0 + h$ where $\frac{\partial h}{\partial \theta} = 0$
- Order ε^2 :
  - The gyrokinetic equation

Gyroaveraging Fourier Transforms

$$\left\langle e^{i\mathbf{k}\cdot\mathbf{r}} \right\rangle_{\mathbf{R}} = \frac{1}{2\pi}\int e^{i\mathbf{k}\cdot(\mathbf{R}+\rho)} d\theta = \frac{1}{2\pi} e^{i\mathbf{k}\cdot\mathbf{R}} \int e^{-i\mathbf{k}\cdot\frac{\mathbf{v}}{\Omega}} d\theta$$

$$= \frac{1}{2\pi} e^{i\mathbf{k}\cdot\mathbf{R}} \int e^{-i\frac{k_{perp}v_{perp}}{\Omega}\cos\theta} d\theta$$

$$= e^{i\mathbf{k}\cdot\mathbf{R}} J_0\left(\frac{k_{perp}v_{perp}}{\Omega}\right)$$

Maxwell's Equations

- **Poisson's Equation:** $$\nabla^2 \phi = -4\pi\left(q_i n_i + q_e n_e\right)$$

$$n_i = \int \delta f_1(\mathbf{r}, \mathbf{v}, t) d^3\mathbf{v}$$

$$n_e = n_0 \frac{e\phi}{T_e}$$

- **Ampere's Law:** $$\nabla \times \mathbf{B} = \frac{1}{c}\frac{\partial \mathbf{E}}{\partial t} + \frac{4\pi}{c}\mathbf{J}$$

$$\mathbf{J} = e n_i \bar{\mathbf{v}}_i - e n_e \bar{\mathbf{v}}_e$$

$$n_i \bar{\mathbf{v}}_i = \int \delta f_1 \mathbf{v} d^3\mathbf{v}$$

Update Weights and Advance Markers

- Now advance markers along characteristic trajectories:

$$x_i = x_i + \Delta t\left(\hat{\mathbf{x}} \cdot \mathbf{v}_{Di}\right)$$
$$y_i = y_i + \Delta t\left(\hat{\mathbf{y}} \cdot \mathbf{v}_{Di}\right)$$
$$z_i = z_i + \Delta t\left(v_{\parallel i}\right)$$

- The markers' velocity space coordinates do not need updating
- As currently implemented, markers have $v_\parallel$ and $v_\perp$ assigned, which are constants of motion *only in a uniform magnetic field*
    - This update will change coordaintes to *E* and μ which remain constants of motion (up to the order required) even when the magnetic field is non-uniform