AMSC 663 Project Proposal: Upgrade to the GSP Gyrokinetic Code

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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. 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.

1 Background

Plasma physics concerns the collective dynamics of collections of many charged particles interacting self-consistently with their respective electromagnetic fields. In a uniform magnetic field, the motion of a charged particle (we are usually referring to ions unless otherwise specified) in the plane perpendicular to the magnetic field is a circle whose radius (the gyroradius ρ) depends on its velocity in that plane:

$$\rho = \frac{v_\perp}{\Omega}$$

(Ω is the *gyrofrequency*). If this radius is much smaller than the characteristic size of the plasma, we can use that ratio as an expansion parameter. Gyrokinetics specifically is the regime in which turbulent fluctuations *can be* of a size on the order of this gyroradius. This is in contrast to drift-kinetic theory (and by extension, MHD), where the gyroradius needs to be much smaller than the size of the fluctuations. In order to get a closed theory in gyrokinetics, we demand that the drift velocity be small compared to the thermal velocity $v_t \equiv \sqrt{\frac{2k_B T}{m}}$. Such drifts come about when there is curvature or a gradient in the magnetic field or if there exists another force field (such as the electric field).

We can summarize the gyrokinetic assumptions thusly:

$$\frac{\rho}{L} \sim \frac{v_E}{v_t} \sim \frac{\omega}{\Omega} \sim \frac{\nu}{\Omega} \sim \epsilon \ll 1$$

Here, $v_E = \frac{cE}{B_0}$ is the $E \times B$ drift speed, ω is the frequency of turbulent fluctuations, and ν is the characteristic collision frequency. These assumptions are well justified in a wide range of plasmas found in magnetic fusion confinement devices and in astrophysical plasmas.

The gyrokinetic equation results from expanding the distribution function in the small parameter ϵ:

$$f(\mathbf{r}, \mathbf{v}, t) = F_0 + \delta f + \dots$$

Where $\delta f \sim \epsilon F_0$ represents the fluctuations in the distribution function. If we transform coordinates to the center of the gyromotion $\mathbf{R}$, we can write

$$\delta f = F_0 \exp\left(\frac{-q\phi}{k_B T}\right) + h(\mathbf{R}, v_\parallel, v_\perp)$$

The latter function h in the coordinates of the gyrocenter position is what we will be solving for.

2 Approach

The form of the *gyrokinetic equation* (in unconventional notation) is:

$$\frac{\partial h}{\partial t} + \mathbf{A}[h] \cdot \nabla_{\mathbf{R}} h + D_\parallel[h] \frac{\partial h}{\partial v_\parallel} + D_\perp[h] \frac{\partial h}{\partial v_\perp} = S[h]$$

Where the coefficients $\mathbf{A}$, $D_\parallel$, and $D_\perp$ are functions of the local potential χ, which in turn depends on integrals of h in velocity space. This is due to the fact that the fields are calculated from the density and flux of charges, for which the velocity dependence in h must be integrated out. The right hand side $S[f]$ includes, among other terms, the *collision operator*, which is also in general an integral over h. Such nonlinearities make the gyrokinetic equation very difficult to solve even numerically.

The approach we will be taking is a δf particle-in-cell (δf-PIC) algorithm (see [Aydemir, 1994]) that models the gyroaveraged fluctuations from equilibrium as a collection of Lagrangian markers. These are, in a sense, twice removed from the physical particles that make up the plasma, and is more accurately thought of as a Monte-Carlo representation of $\langle \delta f \rangle$. Each marker has a position and a velocity, and a *weight* $w_i \equiv \frac{\langle \delta f \rangle}{F_0}$. The latter is the function δf's value *as represented* by a particle of its position and velocity. The particles follow characteristic trajectories defined by:

$$\begin{aligned}
\frac{\partial \mathbf{R}}{\partial t} &= \mathbf{A} \\
\frac{\partial v_\parallel}{\partial t} &= D_\parallel \\
\frac{\partial v_\perp}{\partial t} &= D_\perp
\end{aligned}$$

In many solutions of the gyrokinetic equation, it is assumed that the equilibrium distribution F_0 and the background field $\mathbf{B_0}$ is uniform and stationary. This simplifies the analysis because the equation that results is:

$$\frac{\partial h}{\partial t} + v_\parallel \frac{\partial h}{\partial z} + \frac{c}{B_0}\hat{\mathbf{z}} \cdot (\nabla_{\mathbf{R}} \langle \chi \rangle \times \nabla_{\mathbf{R}} h) = \langle C[h] \rangle + \frac{q}{T} F_0 \frac{\partial \langle \chi \rangle}{\partial t}$$

Note that there are no terms like $\frac{\partial h}{\partial v_\perp}$. This simplifies the characteristics so that all markers have the same gyroradius. This is the approach of the current GSP code (see [Broemstrup, 2008]).

3 Implementation

Our implementation seeks to generalize the GSP algorithm to handle conditions where there are gradients in the equilibrium distribution function and field. If we follow the same analysis as before, the resulting gyrokinetic equation *does* have terms like $\frac{\partial h}{\partial v_\perp}$. If this were allowed, the integration of h over velocity space (as required to compute the fields) would be significantly slowed down since the particles' velocities are mixed and would require random-access. This is a weakness of the current GSP code since this mixing of particles in velocity space also occurs as a result of collisions. We seek to improve this situation by transforming velocity coordinates. Instead of $v_\perp$ and $v_\parallel$, we will instead represent velocity space with:

$$\mu = \frac{m v_\perp^2}{2B_0}$$

and

$$\mathcal{E} = \frac{1}{2} m \left(v_\perp^2 + v_\parallel^2 \right)$$

the magnetic moment and kinetic energy, respectively. This is a particularly wise choice because both $\mathcal{E}$ and μ are *constants of motion*, so that $\frac{d\mu}{dt} = \frac{d\mathcal{E}}{dt} = 0$. Now the "velocity" derivatives do not appear in the gyrokinetic equation whether there are gradients or not.

Let us now discuss the collision operator. It consists of two terms: $C[h] = C_\xi[h] + C_\mathcal{E}[h]$, each of which discribes the diffusion through the velocity polar angle ξ and through energy $\mathcal{E}$ respectively. The latter process is relatively very slow and will not be part of our overall analysis. This is justified by considering the dynamics of two-body interactions: when there is a large disparity in masses (such as between an electron and an ion), the transfer of energy $\Delta\mathcal{E} = \frac{2m_e}{M_i}$ is very small. Furthermore, when the colliding partners' masses are identical, they exchange momenta and the collision can be represented by a different scattering angle of particles with the *same* energy. Therefore, in plasmas with only one ion species $\frac{d\mathcal{E}}{dt} = 0$ is a good approximation.

The collision operator is expected to be diffusive in velocity space, serving to smooth out fine structure in h. However, in evaluating the collision operator, an interpolation in velocity space onto a polar grid is required. This results in an

artificial diffusion that does not follow the proper physics that the true collision operator does. The fact that the interpolation is two-dimensional exacerbates this effect. Therefore, by choosing our velocity grid to be polar to begin with, this interpolation is only one dimensional.

We conclude that successfully making this change of velocity coordinates in GSP will result in a code that is more accurate (by minimizing artificial diffusion) and more efficient (by minimizing random access) when generalized to systems with background gradients.

The algorithm implemented in GSP is illustrated here:

1. Initialization
   - Place particles as sampled from the equilibrium distribution function
   - Integrate to obtain initial potential χ
2. Simulation
   - For each particle i:
     - $\mathbf{R}_i^{n+\frac{1}{2}} = \mathbf{R}_i^n + \frac{\Delta t}{2}\mathbf{v}_i^n$
     - $\langle\chi\rangle^{n+\frac{1}{2}}$ calculated on a grid in Fourier space, using $\mathbf{R}_j^{n+\frac{1}{2}}$
     - $S_i^{n+\frac{1}{2}}[h]$ (RHS of GK equation) calculated from $\langle\chi\rangle^{n+\frac{1}{2}}$ and $w_j^n(\forall j)$
     - $w_i^{n+1} = w_i^n + \Delta t S_i^{n+\frac{1}{2}}[h]$
     - $\mathbf{v}_i^{n+\frac{1}{2}}$ calculated from $\langle\chi\rangle^{n+\frac{1}{2}}$
     - $\mathbf{R}_i^{n+1} = \mathbf{R}_i^n + \Delta t \mathbf{v}_i^{n+\frac{1}{2}}$
     - $\langle\chi\rangle^{n+1}$ calculated on a grid in Fourier space, using $\mathbf{R}_j^{n+1}$
     - $\mathbf{v}_i^{n+1}$ calculated from $\langle\chi\rangle^{n+1}$
3. Repeat Step 2 as needed
4. Obtain moments of $\langle\delta f\rangle$ such as density, temperature, and flux

A crucial step of the algorithm is where the fields are computed. In the current implemention of GSP, this is done in Fourier space with:

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

The Bessel function J_0 comes from the calculation of the gyroaverage in Fourier space. Translating this integral into a suitable, equally efficient method to calculate the potential when using the transformed velocity coordinates $\mathcal{E}$ and μ represents the most significant challenge of this project. Failure to do so is a risk and would will result in a code that does not retain the efficiency of the original GSP. Considering the complexity of the code, it is also possible that the student fails to sufficiently grasp the algorithm to make and debug the needed changes.

4 Databases

- GSP Source code:
  http://gyrokinetics.svn.sourceforge.net/viewvc/gyrokinetics/gsp/
- Article with analytic result:
  - Ricci, et al, "Gyrokinetic linear theory of the entropy mode in a Z pinch." *Physics of Plasmas*, **13**: 062102
- Article with computational benchmark:
  - Dimits, et al, "Comparisons and physics basis of tokamak transport models and turbulence simulations." *Physics of Plasmas*, **7**: 969

5 Validation

To ensure we have built a code that gives physical results, we will compare results obtained from both the old version of GSP and the update. Both should agree remarkably well in regimes in which the original GSP is accurate since a coordinate change shall not change the physics being simulated.

A standard computational benchmark for gyrokinetics is given in [Dimits et al, 2000]. We will use this reference to compare results obtained from GSP.

Furthermore, an analytical condition necessary for stability in a gyrokinetic plasma has been obtained in Appendix B of [Ricci et al, 2006]. Comparing this to the conditions at which the code predicts an unstable plasma would provide a good test of the physical fidelity of the code. Application of this test would require a translation in position coordinates as well, which is beyond the immediate scope of this project, although it is hoped to be accomplished.

6 Testing

Even if we have built a code with robust physics, it is possible that such an effort may be in vain. This would occur if the "updated" version of GSP is not an update at all and instead is considerably less efficient than the original code. Therefore, we shall benchmark the performance of the update against the original code and ensure that it scales well from a parallelization standpoint.

7 Schedule and Milestones

Phase I: Analytics
September - October 2011

- Understand rigorous derivation of the gyrokinetic equation
- Become familiar with analytical aspects of the gyrokinetic equation
- Make velocity coordinate change

- Understand algorithm used by GSP to solve GK equation
- Understand Abel collision operator and how it is to be implemented in GSP
- **Milestone:** Derive GK equation in velocity coordinates E and μ.

Phase II: Numerics
October 2011 - January 2012

- Become familiar with GSP code
- Make proposed changes to the code
- Ensure code still runs
- **Milestone:** GSP Code updated with new velocity coordinates.

Phase III: Testing and Validation
February - April 2012

- Debug updated GSP code
- Validate and test against previous version and known results
- Run test cases, organize results
- **Milestone:** GSP code in new velocity coordinates validated and tested

Phase IV: Communication
April - May 2012

- Prepare final presentation
- **Milestone:** Final presentation given

8 Deliverables

- Updated GSP source code
- Sample input files of test cases
- Test case comparison data
- Mid-year progress report
- Final presentation

9 Bibliography

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