Gyrokinetic Turbulence Simulations

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Overview

1. General geometry, coordinates
2. Flux tube vs. global
3. GK equations
4. Higher order effects
5. Numerical issues
6. Outstanding near-term problems
   (a) Second microstability
   (b) Finite β effects on secondary instabilities, transport
   (c) Basics of electron energy transport in the absence of ITG modes
   (d) Testing simulation predictions of multi-channel transport
   (e) Testing simulation predictions in unconventional settings (ST, dipole, stellarator)
   (f) Dissipation/coupling of waves to particles (natural plasmas)

General Geometry

- Metric coefficients for general geometry calculations are well known. Given a Clebsch representation of the magnetic field:

$$\mathbf{B} = \nabla\alpha \times \nabla\psi$$

and an axisymmetric magnetic field defined by

$$\mathbf{B} = I(\Psi)\nabla\phi + \nabla\Psi \times \nabla\phi,$$

we use `June4` (available on-line) to calculate all needed quantities.

- In the field-line-following (ballooning) limit, perturbed quantities are represented by

$$A = \hat{A}(\theta)\exp(iS)$$

where $\hat{\mathbf{b}} \cdot \nabla S = 0$. This takes into account the fact that the perturbations tend to be slowly varying along the field line, and allows for rapid variation across the field line.

- To make contact with the ballooning approximation and with field-line following coordinates, choose

$$S = n_0\left(\alpha + q\theta_0\right),$$

where n_0 is an integer, θ_0 is the ballooning parameter, $q(\Psi) = d\Psi_T/d\Psi$, $\Psi_T = (2\pi)^{-2}\int_V d\tau \mathbf{B}\cdot\nabla\phi$ is the toroidal flux, and $d\tau$ is the volume element.

General Geometry Coordinates

- The coordinate α is defined by

$$\alpha = \int_0^\theta d\theta \frac{\mathbf{B} \cdot \nabla\phi}{\nabla\theta \times \nabla\Psi \cdot \nabla\phi}$$

  where θ is the poloidal angle and ϕ is the toroidal angle.

- Use arbitrary flux surface label $\rho = \rho(\Psi)$.

- In some cases, it is convenient to replace the θ coordinate with a new coordinate θ', which measures the arc length. The operator $\hat{\mathbf{b}} \cdot \nabla$ is then

$$\hat{\mathbf{b}} \cdot \nabla \rightarrow \frac{2\pi}{L_{\text{arc}}} \frac{\partial}{\partial\theta'}.$$

- The Jacobian is $J = (d\Psi/d\rho)\,(L_{\text{arc}}/2\pi B)$. The flux surface average of a quantity Γ is

$$\langle\Gamma\rangle = \lim_{\Delta\rho\rightarrow 0} \frac{\int \Gamma J\, d\theta'\, d\alpha\, d\rho}{\int J\, d\theta'\, d\alpha\, d\rho}.$$

- The flux surface average of a radially directed quantity (such as the radial heat flux) is given by

$$Q_{\text{sim}} = \frac{\langle \mathbf{Q} \cdot \nabla\rho \rangle}{\langle \nabla\rho \rangle}$$

  which will appear in the transport equation as

$$\frac{3}{2}\frac{d}{dt}\langle nT\rangle + \frac{1}{V'}\frac{d}{d\rho} A Q_{\text{sim}} + \ldots = 0,$$

  where the surface area $A = 2\pi\langle\,|\nabla\rho|\,\rangle \int J d\theta'$.

General Geometry Operators

- The linear part of the ∇B drift is given by

$$\frac{v_\perp^2}{2}\frac{1}{\Omega B^2}\mathbf{B}\times\nabla B\cdot\nabla S=\left(\frac{k_\theta\rho_i}{2}\right)\frac{v_\perp^2}{2}\left[\omega_{\nabla B}+\omega_{\nabla B}^{(0)}\theta_0\right],$$

  where

$$\omega_{\nabla B}=\frac{2}{B^2}\frac{d\Psi}{d\rho}\hat{\mathbf{b}}\times\nabla B\cdot\nabla\alpha,\qquad\omega_{\nabla B}^{(0)}=\frac{2}{B^2}\frac{d\Psi}{d\rho}\hat{\mathbf{b}}\times\nabla B\cdot\nabla q.$$

- Similarly, the curvature drift is given by

$$\omega_\kappa=\omega_{\nabla B}+\frac{8\pi}{B^2}\frac{dp}{d\rho}.$$

- The only remaining geometric dependence occurs in $|\nabla S|^2$:

$$|\nabla S|^2=\frac{n_0^2}{a^2}\left|\nabla\left(\alpha+q\theta_0\right)\right|^2$$

  which is calculated in straightforward fashion:

$$|\nabla S|^2=k_\theta^2\left(\frac{d\Psi}{d\rho}\right)^2\left|\nabla\alpha\cdot\nabla\alpha+2\theta_0\nabla\alpha\cdot\nabla q+\theta_0^2\nabla q\cdot\nabla q\right|.$$

Flux-Tube *vs.* Global

- Flux-tube
  - Simulation domain has a "small" perpendicular cross-section:
    The simulation domain should be at least a few turbulent correlation lengths long in each direction.
  - The variation of the gradient scale lengths across the simulation domain is assumed to be small.
  - The energy, momentum and/or particle sources and sinks inside the flux-tube are assumed to be small.
  - Radial periodicity prevents artificial flattening of driving gradients.
  - For small ρ/a, flux tube assumptions reduce the total simulation volume significantly.
- Global
  - Change in scale lengths across the simulation domain not assumed small. *Equilibrium shear may be treated non-perturbatively.*
  - Radial periodicity not assumed, but sources are needed.
  - Large devices cannot be simulated with existing computers, particularly when small scales are important (such as ρ_e or c/ω_{pe}).

Gyrokinetic Equation

- Gyrokinetic equation appropriate if

$$\frac{\omega}{\Omega} \sim \frac{k_\parallel}{k_\perp} \sim \frac{\delta f}{f} \sim \frac{e\delta\Phi}{T} \sim \frac{\delta B}{B} \sim \frac{\rho}{L} \ll 1$$

- Gyrokinetic equation describes evolution of perturbed distribution function $h = h_s(\rho, \alpha, \theta, \epsilon, \mu; t)$. For $F_0 = F_0(\epsilon, \Psi)$:

$$\left(\frac{d}{dt} + v_\parallel \hat{\mathbf{b}} \cdot \nabla + i\omega_d + C\right) h = i\omega_*^T \chi - q\frac{\partial F_0}{\partial \epsilon}\frac{\partial \chi}{\partial t}.$$

- The total derivative is

$$\frac{dh}{dt} = \frac{\partial h}{\partial t} + \frac{c}{B}\{\chi, h\}.$$

- The drift frequency $i\omega_*^T = n_0 c\, \partial F_0/\partial\Psi$, where n_0 is the toroidal mode number of the perturbation and Ψ is the equilibrium poloidal magnetic flux enclosed by the magnetic surface of interest.

- The perpendicular drifts (curvature, grad-B) are

$$\omega_d = \mathbf{k}_\perp \cdot \mathbf{B}_0 \times \left(m v_\parallel^2 \hat{\mathbf{b}} \cdot \nabla \hat{\mathbf{b}} + \mu \nabla B_0\right) / (m B_0 \Omega),$$

- The fields are represented by

$$\chi = J_0(\gamma)\left(\Phi - \frac{v_\parallel}{c} A_\parallel\right) + \frac{J_1(\gamma)}{\gamma}\frac{m v_\perp^2}{q}\frac{\delta B_\parallel}{B}.$$

Here, $\gamma = k_\perp v_\perp / \Omega$.

Gyrokinetic Maxwell Equations

- Fields determined by Maxwell equations, neglecting displacement current.
- Poisson's equation:

$$\nabla_\perp^2 \Phi = 4\pi \sum_s \int d^3v\, q \left[q\Phi \frac{\partial F_0}{\partial \epsilon} + h \exp\left(iL\right) \right],$$

  where $L = (\mathbf{v} \times \hat{\mathbf{b}} \cdot k_\perp)/\Omega$ accounts for the gyrophase dependence.
- Preferred velocity space coordinates are (ϵ, μ, ξ), so that

$$\int d^3v = \frac{B}{m^2} \int \frac{d\epsilon\, d\mu\, d\xi}{|v_\parallel|} \equiv \frac{1}{2\pi} \int d^2v\, d\xi$$

- Integrate over the gyrophase to find

$$\nabla_\perp^2 \Phi = 4\pi \sum_s \int d^2v\, q \left[q\Phi \frac{\partial F_0}{\partial \epsilon} + J_0(\gamma) h \right]$$

- Similarly, Ampere's equation provides the two components of the perturbed magnetic field:

$$\nabla_\perp^2 A_\parallel = -\frac{4\pi}{c} \sum_s \int d^2v\, q v_\parallel J_0(\gamma) h$$

$$\frac{\delta B_\parallel}{B} = -\frac{4\pi}{B^2} \sum_s \int d^2v\, m v_\perp^2 \frac{J_1(\gamma)}{\gamma} h$$

Summary of Gyrokinetic Ordering

- As stated before:

$$\frac{\omega}{\Omega} \sim \frac{k_\parallel}{k_\perp} \sim \frac{\delta f}{f} \sim \frac{e\delta\Phi}{T} \sim \frac{\delta B}{B} \sim \frac{\rho}{L} \ll 1$$

- Also, $\mathbf{E}\times\mathbf{B}$ velocity must remain small

$$\frac{v_E}{v_t} \sim \frac{\rho}{L} \ll 1$$

- And equilibrium quantities may evolve only very slowly:

$$\frac{\frac{\partial}{\partial t}\big|_{eq}}{\omega} \sim \left(\frac{\rho}{L}\right)^2$$

- No specific assumptions about size of any of:

$$\beta, \quad k_\perp\rho, \quad \frac{\omega}{k_\parallel v_t}, \quad \frac{\omega}{\omega_d}, \quad \frac{\omega}{\omega_b}, \quad \frac{\omega}{\nu}, \quad \frac{\omega}{\omega_{NL}}$$

Higher-Order Effects

- "Parallel nonlinearity":

$$\hat{\mathbf{b}} \cdot \nabla \delta\Phi \times \left(\frac{\partial\, \delta f}{\partial v_{\parallel}} \right)$$

  - Formally small because gradients in velocity space are ordered $1/v_t$.

- Nonlinearities without gradients, *e.g.*, terms like the last one in:

$$\delta(n\Phi) \sim n_0\, \delta\Phi + \delta n\, \Phi_0 + \delta n\, \delta\Phi$$

  which are sometimes kept in PIC implementations.

- Evolution of equilibrium – *i.e.*, evolution of longest perpendicular wavelengths of global simulation

Numerical Issues

- Coordinate choices: flux coordinates universal, but
  - Details differ. *E.g.,* how to define k_θ in general geometry, whether to let simulation domain become severely distorted, *etc.*
  - Parallel extent of simulation domain
- Integration schemes
  - Eulerian *vs.* Lagrangian
  - Implicit *vs.* explicit
  - Pseudo-spectral *vs.* finite difference
- Sources of error/inaccuracy
  - Particle noise
  - Velocity-space filamentation
- Consistency
  - Flux tube large enough?
  - Resolution adequate?
  - Orderings satisfied?

Integration Scheme: GS2

- Convenient to advance

$$f = h + q\frac{\partial F_0}{\partial \epsilon}\left[J_0(\gamma)\Phi + \frac{J_1(\gamma)}{\gamma}\frac{mv_\perp^2}{q}\frac{\delta B_\parallel}{B}\right]$$

- GKE becomes

$$\left(\frac{\partial}{\partial t} + \mathcal{L}\right) f = C(f) + S\left(\Phi, A_\parallel, \frac{\delta B_\parallel}{B}\right) - [\chi, h]$$

- Method of fractional steps used:
  - $\mathcal{L}$ and source term S treated implicitly with finite differencing along the field line.
  - Momentum-conserving Lorentz collision operator $C(f)$ treated implicitly in pitch-angle space.
  - Nonlinear term evaluated explicitly with dealiased pseudo-spectral algorithm. Time-stepping scheme is second-order Adams-Bashforth.
- Time step adjusted dynamically to satisfy Courant condition for nonlinear term. Limiting velocity is $\mathbf{v}_\chi \propto \hat{\mathbf{b}} \times \nabla\chi$.
- Maxwell's equations solved with "implicit supercell" technique since boundary condition couples different k_ρ's along the field line.

Implicit Algorithm Automatically Recovers Low Mass Approximation

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- Consider relevant terms:

$$\frac{\partial f}{\partial t} + v_{\parallel} \frac{\partial f}{\partial \theta} = \mathcal{S}$$

- Centered, implicit time and space differences:

$$\frac{f^{n+1}_{j+1/2} - f^{n}_{j+1/2}}{\Delta t} + v_{\parallel\, j+1/2} \left(\frac{f^{n+1/2}_{j+1} - f^{n+1/2}_{j}}{\Delta \theta} \right) = \mathcal{S}^{n+1/2}_{j+1/2}$$

where $f^{n+1}_{j+1/2} \equiv \frac{1}{2}\left(f^{n+1}_{j+1} + f^{n+1}_{j}\right)$ and $f^{n+1/2}_{j+1} \equiv \frac{1}{2}\left(f^{n+1}_{j+1} + f^{n}_{j+1}\right)$.

- Leads to an upper diagonal system, easily inverted.
- Trapped particles and parallelism made easy by homogeneous, inhomogenous sweeps in spatial coordinate j.
- For large Δt and simple source

$$\mathcal{S} = v_{\parallel\, j+1/2} \left(\frac{\Phi^{n+1/2}_{j+1} - \Phi^{n+1/2}_{j}}{\Delta \theta} \right) F_m$$

  the solution is easy:

$$f^{n+1}_{j} = \Phi^{n+1}_{j} F_m$$

Implicit Algorithm Automatically Recovers Low Mass Approximation

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- Electromagnetic source give $\frac{\partial A_\parallel}{\partial t}$ contribution.
- In general, one finds

$$f^{n+1}(z) = \int^z \frac{dz'}{v_\parallel} \left(\frac{\mathcal{S}^{n+1} + \mathcal{S}^n}{2} \right)$$

  so that this scheme has recovered the bounce (or orbit) average when $\Delta t > t_{\text{bounce}}$.

- As the amplitudes get large enough to limit the time step, the correct non-bounce-averaged response is recovered. *No subsidiary ordering of the nonlinear terms is required.*

Implicit Integration of Collision Operator

- Lorentz collision operator:

$$C(f) = \frac{\nu(E)}{2}\frac{\partial}{\partial \xi}(1-\xi^2)\frac{\partial f}{\partial \xi}$$

  with optional momentum-conserving terms allowed.

- For example, for electron-ion collisions:

$$\nu(E) = \frac{\nu_{ei}}{(v/v_{te})^3}\left[Z_{\text{eff}} + \frac{v_{te}}{v\sqrt{\pi}}e^{-(\frac{v}{v_{te}})^2} + \left(1 - \frac{v_{te}}{2v^2}\right)\text{erf}(\frac{v}{v_{te}})\right]$$

  where

$$\nu_{ei} = \frac{4\pi n e^4 \ln\Lambda}{(2T_e)^{3/2} m_e^{1/2}}$$

  and

$$\xi = \frac{v_\parallel}{v} = \sqrt{1-\lambda B}$$

- Implicit, tridiagonal solve

- Second derivative in velocity space implies realistic collision level is enough to keep f smooth. Removes filamentation problem for typically resolved distribution function.

Pseudo-Spectral Evaluation of Nonlinear Terms

- Simple bracket form of nonlinear term valid in general geometry

$$[\chi, h] = \frac{\partial \chi}{\partial \rho}\frac{\partial h}{\partial \alpha} - \frac{\partial \chi}{\partial \alpha}\frac{\partial h}{\partial \rho}$$

  can be evaluated with standard pseudo-spectral algorithm.

- Derivatives evaluated in transform space, multiplication carried our in real space.

- Time-integration is second-order Adams-Bashforth, which requires only one evaluation of nonlinear term per timestep.

- Issues: de-aliasing, spectral blocking

- Advantages: Fast, highly accurate (no numerical dissipation such as occurs with finite-differencing schemes)

Why Pseudo-Spectral?

1. "Exponentially convergent" derivatives.

   - Compare with finite difference:

$$\frac{\partial f}{\partial x} \sim \frac{f(x+h) - f(x-h)}{2h} + \mathcal{O}(h^2)$$

   or

$$\frac{\partial f}{\partial x} \sim \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h} + \mathcal{O}(h^4)$$

   - Pseudo-spectral is much better: error in $\frac{\partial f}{\partial x} \sim \mathcal{O}(h^N)$ at fixed h but

$$\text{error} \sim \mathcal{O}\left(\left(\frac{1}{N}\right)^N\right)$$

     since h decreases as N increases.

2. At fixed accuracy, pseudo-spectral is memory minimizing.

   - To resolve a function with 1% accuracy, spectral requires $N/2$ (compared to non-spectral scheme with N points)
   - `GS2` is spectral in ρ, α, E, λ, implying $\sim$ factor of 16 savings.
   - Advantages greater at higher resolution – but probably not important for turbulence.

Why Pseudo-Spectral?

3. Integrals more accurate

   - Simple rules like

     $$\int_a^b f(x)\,dx = \sum_{i=1}^{N} f(x_i) w_i$$

     integrate polynomial of degree $N+1$ accurately over finite domain with equally spaced grid points.
   - But, use freedom to choose x_i to minimize error; increases degree of polynomials that are exactly integrated to $2N+1$.
   - No free lunch: x_i, w_i must be precomputed.

Summary of Numerical Issues

- `GS2` uses spectral decomposition in the two directions perpendicular to the field line and for energy and pitch angle for good accuracy with minimal memory & CPU usage.
- Implicit integration of fast motion along field lines reduces time step restrictions and automatically recovers appropriate orbit averages, without any subsidiary ordering of nonlinear terms.
- Velocity-space filamentation not a problem for realistic colliion frequencies with Lorentz collision operator.
- Electrostatic and electromagnetic perturbations treated on equal footing.
- Pseudo-spectral evaluation of nonlinear terms is fast, without introducing numerical dissipation.
- Flux-tube simulation domain is maximally consistent with GK ordering.