A Fokker-Planck collision model for gyrokinetic simulations in stellarators

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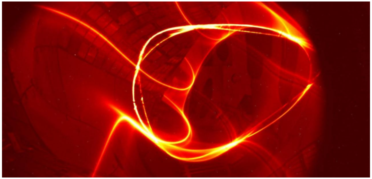
Outline

Turbulence in stellarators

- Optimised stellarators: designed to control neoclassical losses
- → Turbulent losses are important
- Microinstabilities known from tokamaks also found in stellarators [cf. Klinger et al, 2019]
- Can the geometry of stellarators be used to control turbulence?
- → Numerical simulations of turbulence in stellarators



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Gyrokinetic simulations with stella

- stella (Barnes, Parra, Landreman; 2018) is δf-gyrokinetic code
- General magnetic geometry: 3D equilibrium from VMEC
- With $f = F + \delta f$, $g = \langle \delta f \rangle$

$$\frac{\partial g}{\partial t} + \overbrace{v_{\|}\hat{\mathrm{b}}\cdot\nabla\left(g + \frac{Ze}{T}\langle\phi\rangle F\right) - \frac{\mu}{m}\hat{\mathrm{b}}\cdot\nabla B\frac{\partial g}{\partial v_{\|}}}^{\text{par. dynamics}}$$

$$+ \underbrace{\mathrm{v}_M\cdot\left(\nabla_\perp g + \frac{Ze}{T}\nabla_\perp\langle\phi\rangle F\right)}_{\text{mag. drifts}} + \underbrace{\langle\mathrm{v}_E\rangle\cdot\left(\nabla_\perp g + \nabla|_E F\right)}_{E\times B\text{ drifts}} = \underbrace{C[g]}_{\text{collisions}}$$

- Split parallel (fast) and perpendicular (slow) dynamics
- Treat parallel dynamics implicitly to avoid CFL constraint

The collision operator

- Collisions are required for dissipation of energy into heat at small scales
- Described by the Landau-Fokker-Planck operator:

$$\boxed{C_{ab}[f_a, f_b] = \frac{\partial}{\partial v_k}\left[A_k^{ab} f_a + \frac{\partial}{\partial v_l}\left(D_{kl}^{ab} f_a\right)\right]}$$

$$A_k := L^{ab}[1+\frac{m_a}{m_b}]\frac{\partial}{\partial v_k}\underbrace{\int \frac{f_b(\mathrm{v}')}{u}\; d^3 v'}_{\phi_b(\mathrm{v})}, \;\; D_{kl} := -L^{ab}\frac{\partial^2}{\partial v_k \partial v_l}\underbrace{\int u f_b(\mathrm{v}')\; d^3 v'}_{\psi_b(\mathrm{v})},$$

with $u := |\mathrm{v} - \mathrm{v}'|$ and L^{ab} a constant.

- C_{ab} conserves particles, momentum and energy
- C_{ab} is self-adjoint $\rightarrow$ satisfies Boltzmann's H-theorem

The linearised operator

- Assume $f_s = f_{s0} + \delta f_s$; f_{s0} Maxwellian; $\delta f_s / f_{s0} \sim \epsilon \ll 1$.
- For species approximately in thermodynamic equilibrium

$$C_{ab}[f_a, f_b] = \underbrace{C_{ab}[f_{a1}, f_{b0}]}_{test\ \ particle\ \ coll.} + \underbrace{C_{ab}[f_{a0}, f_{b1}]}_{field\ \ particle\ \ coll.} + O(\epsilon^2)$$

- Rosenbluth potentials of Maxwellian, $\phi_{b0}(v)$, $\psi_{b0}(v)$, can be calculated explicitly
- Examine the test-particle operator first, return later to field particle component

Test particle operator

- With $v, \xi = \cos\theta$, ϕ velocity coordinates:

$$C_{ab}[f_{a1}, f_{b0}] = \overbrace{\frac{1}{2}\nu_D \frac{\partial}{\partial \xi}(1-\xi^2)\frac{\partial f_a}{\partial \xi}}^{=:pitch\ angle\ scattering} + \frac{1}{2}\nu_D \frac{1}{1-\xi^2}\frac{\partial^2 f_a}{\partial \phi^2} + \underbrace{\frac{1}{v^2}\frac{\partial}{\partial v}\left[\frac{1}{2}\nu_\parallel v^4 F_0 \frac{\partial}{\partial v}\frac{f_a}{F_0}\right]}_{energy\ diffusion}$$

- With collision frequency, ν^{ab}, and $x_b = \frac{v}{v_{th,b}}$

$$\nu_D^{ab}(v) := \nu^{ab}\frac{\mathrm{erf}(x_b) - G(x_b)}{x_a^3},\ \nu_\parallel^{ab}(v) := \nu^{ab}\frac{2G(x_b)}{x_a^3}$$
$$\text{with Chandrasekhar function, } G. \tag{1}$$

Test particle operator (II)

- In stella, use $v_\parallel$, $\mu = \frac{mv_\perp^2}{2B}$ coordinates. Then (with normalisations)

$$C_{ab}[f_{a1}, f_{b0}] = \frac{\partial}{\partial v_\parallel}\left[\gamma_{v_\parallel} F_0 \frac{\partial}{\partial v_\parallel}\frac{\delta f_a}{F_0} + v_\parallel \mu \nu_x^{ab} F_0 \frac{\partial}{\partial \mu}\frac{\delta f_a}{F_0}\right]$$
$$+ \frac{\partial}{\partial \mu}\left[\gamma_\mu F_0 \frac{\partial}{\partial \mu}\frac{\delta f_a}{F_0} + v_\parallel \mu \nu_x^{ab} F_0 \frac{\partial}{\partial v_\parallel}\frac{\delta f_a}{F_0}\right]$$
$$+ \frac{\nu_D^{ab}}{2}\left[1 + \frac{v_\parallel^2}{2B_0\mu}\right]\frac{\partial \delta f_a^2}{\partial \phi^2},$$

where $\nu_x^{ab} = \nu_\parallel^{ab} - \nu_D^{ab}$, and

$$\gamma_{v_\parallel}^{ab} := \frac{1}{2}\left[\nu_\parallel^{ab} v_\parallel^2 + 2\nu_D^{ab} B_0 \mu\right], \quad \gamma_\mu^{ab} := 2\left[\nu_\parallel^{ab}\mu^2 + \nu_D^{ab}\frac{v_\parallel^2}{2B_0}\mu\right]$$

Gyroaveraged test particle operator

- Denote $h := \delta f_a + \frac{q}{T}\phi F_0$; Fourier analyze: $h = \sum_{\mathbf{k}_\perp} e^{i\mathbf{k}_\perp \cdot \mathbf{R}} h_{\mathbf{k}_\perp}$
- Perform gyroaverage, $\langle \cdot \rangle = 1/2\pi \int_0^{2\pi} \cdot \, d\phi$

$$C_{GK}[h_{\mathrm{k}_\perp}] = \langle e^{i\mathrm{k}_\perp \cdot \boldsymbol{\rho}} C[e^{-i\mathrm{k}_\perp \cdot \boldsymbol{\rho}} h_{\mathrm{k}_\perp}] \rangle_{\mathrm{R}}$$

- Gyrokinetic test-particle operator:

$$C^{ab}_{\mathrm{GK}}[h_{\mathbf{k}}] = C^{ab}_{v_\parallel,\mu}[h_{\mathbf{k}}] - \underbrace{\frac{1}{2}\left[\nu^{ab}_\parallel B_0\mu + \nu^{ab}_D[v_\parallel^2 + B_0\mu]\right] k_\perp^2 \rho_s^2 h_{\mathbf{k}}}_{gyrodiff.\ term} .$$

Implementation in stella

- stella advances GKE in terms of $g = \langle \delta f \rangle = h - \frac{q}{T} \langle \phi \rangle F_0$
- Treat collisions implicitly, to avoid CFL constraint $[\Delta t_{\mathrm{CFL}} \sim (\Delta v)^2]$
- Split non-collisional and collisional physics. For implicit treatment:

$$\frac{g^{n+1} - g^*}{\Delta t} = C_{GK}^{\mathrm{test}}[h^{n+1}]$$

where g^* is g after advancing non-collisional part of GKE

Implicit algorithm

- Implicit solve:

$$\boxed{(1 - \Delta t C_{\mathrm{GK}}) h^{n+1} = g^* + \frac{q}{T} \langle \phi^{n+1} \rangle F_0} \quad (2)$$

- Write $h^{n+1} = h^{n+1}_{hom} + h^{n+1}_{inh}$, then

$$(1 - \Delta t C_{\mathrm{GK}}) h^{n+1}_{inh} = g^* \quad (3)$$

$$(1 - \Delta t C_{\mathrm{GK}}) h^{n+1}_{hom} - \frac{q}{T} \langle \phi^{n+1} \rangle F_0 = 0 \quad (4)$$

- Solve Eq. [3] with band matrix solver
- Use Green's function method to solve Eq. [4]

Green's function method

- Use Green's function method to solve

$$(1 - \Delta t C_{\mathrm{GK}}) h_{hom}^{n+1} = \frac{q}{T} \phi^{n+1} J_0 F_0 \tag{5}$$

- Supply unit impulse to potential and solve $(1 - \Delta t C_{\mathrm{GK}}) \delta h / \delta \phi = q J_0 F_0 / T$ for response $\delta h / \delta \phi$. Then

$$h_{hom}^{n+1} = \frac{\delta h}{\delta \phi} \phi^{n+1} \tag{6}$$

- Potential ϕ^{n+1} is obtained via quasineutrality $\phi^{n+1} = Q[h^{n+1}]$. Q is a velocity space integral operator. Then

$$\phi_{hom}^{n+1} = \phi^{n+1} Q \left[\frac{\delta h}{\delta \phi} \right] \tag{7}$$

Green's function method (II)

- Then

$$\phi_{inh}^{n+1} = \phi^{n+1}\left(1 - Q\left[\frac{\delta h}{\delta \phi}\right]\right)$$

- Solve for ϕ^{n+1} (know $\phi_{inh}^{n+1} = Q[h_{inh}^{n+1}]$ from inhomogeneous equation)
- Advance from g^* to h^{n+1} by solving

$$(1 - \Delta t C_{\mathrm{GK}})h^{n+1} = g^* + \frac{q}{T}\phi^{n+1}J_0F_0 \qquad (8)$$

Field particle operator

- The field particle operator is required for momentum and energy conservation
- After linearising the collision operator, the field particle component is

$$C^{ab}_{\mathrm{field}}[f_{a0}, f_{b1}] = \frac{\partial}{\partial v_k}\left[L^{ab}\left(1+\frac{m_a}{m_b}\right)\frac{\partial \phi_{b1}}{\partial v_k} f_{a0} + \frac{\partial}{\partial v_l}\left(-L^{ab}\frac{\partial^2 \psi_{b1}}{\partial v_k \partial v_l} f_{a0}\right)\right] \tag{9}$$

where the Rosenbluth potentials are integrals in v' over the perturbed distribution function $f_b(v - v')$

- Inversion of the integro-differential operator [9] is slow
- **How do we include this operator efficiently in `stella`'s implicit collision model?**

Spherical harmonic expansion

- Collisions are spherically symmetric → spherical harmonics (SH) are eigenfunctions of the collision operator
- Expand in spherical harmonics:

$$C^{ab}_{\mathrm{field}}[f_{a0}, f_{b1}] = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} Y_{lm}(\theta, \phi) C^{ab}_{v} \left[f_b^{(lm)}(v) \right] \tag{10}$$

- $f_b^{(lm)}$ are the SH expansion coefficients; $C^{ab}_v[f_b^{(lm)}]$ is an isotropic operator, but still complicated
- How can $C^{ab}_v[f_b^{(lm)}]$ be expanded while retaining the conservation properties, self-adjointness and null-space of the exact operator?

Hirshman-Sigmar expansion

- Hirshman & Sigmar (1976): expansion that can be truncated and retains the pertinent properties of the collision operator

$$C_v^{(N)}\left[f_b^{lm}\right] = \sum_{j=0}^{N} \psi_j^{*(l)}[f_b^{lm}]\Delta_j\left[x_b^l L_j^{(l+\frac{1}{2})}(x_b^2) f_{b0}(x_b^2)\right],$$

- Basis functions via Gram-Schmidt orthogonalisation

$$\Delta_0[f] = C_v[f]$$
$$\Delta_{j+1}[f] = \Delta_j[f] - \psi_j^{(l)}\Delta_j\left[x_b^l L_j^{(l+\frac{1}{2})}(x_b^2) f_{b0}(x_b^2)\right].$$

- with coefficients to ensure moment conservation and self-adjointness

$$\psi_j^*(f_b^{(l)}) = \frac{\int_0^\infty v^l L_j^{(l+\frac{1}{2})}(x_b^2)\Delta_j(f_b^{(l)})\ v^2 dv}{\int_0^\infty v^l L_j^{(l+\frac{1}{2})}(x_b^2)\Delta_j\left[x_b^l L_j^{(l+\frac{1}{2})}(x_b^2) f_{b0}(x_b^2)\right]\ v^2 dv}$$

Field particle operator

- Truncating the Hirshman-Sigmar expansion after N terms exactly retains the first $N+1$ velocity moments of the full collision operator
- Combine the spherical harmonic and Hirshman-Sigmar expansion and gyroaverage
- $\rightarrow$ the k-th Fourier component of the field particle operator is

$$C_{\mathrm{GK}}^{\mathrm{field},ab}[h_{\boldsymbol{k}_\perp}] = \sum_{l=0}^{\infty} \sum_{m=-l}^{m=+l} \sum_{j=0}^{\infty} c_{lm} P_{lm}(v_\parallel / v) J_m \left(\frac{k_\perp v_\perp}{\Omega} \right) \psi_j^{(l,ab)}[h_{\boldsymbol{k}_\perp}] \Delta_j^{(l,ab)}$$

- where P_{lm} are Legendre polynomials and coefficients are given by

$$\psi_j^{(l,ab)}[h_{\boldsymbol{k}_\perp}^{lm}(v)] = 2\pi(-1)^m c_{l,-m} \int\int J_m P_{l,-m} h_{\boldsymbol{k}_\perp}(z, v_\parallel, \mu) \Delta_j^{(l,ba)} \, dv_\parallel d\mu$$

Implementation of the field particle operator

- In the implicit time advance scheme we now have

$$(1 - \Delta t C_{\mathrm{test}}) h_{hom}^{n+1} = \frac{q\phi^{n+1}}{T} f_0 + \Delta t C_{\mathrm{field}}[h^{n+1}] \tag{11}$$

- Applying the Green's function method to the fields $\psi_j^{ab,l}$ in C_{field}:

$$h_{hom}^{n+1} = \phi^{n+1} \frac{\delta h_{hom,\phi}}{\delta \phi} + \sum_{jlm} \psi_j^{lm,n+1} \frac{\delta h_{hom,\psi_j^{lm}}}{\delta \psi_j^{lm}} \tag{12}$$

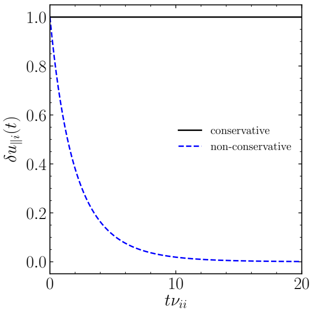
- $\rightarrow$ Linear system of equations for ϕ^{n+1} and fields $\psi_j^{lm,n+1}$:

$$[\boldsymbol{I} - \boldsymbol{R}]\, \boldsymbol{f}^{n+1} = \boldsymbol{f}_{inh}^{n+1} \tag{13}$$

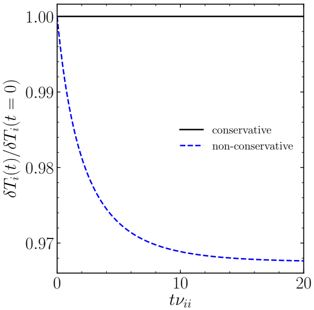
where $\boldsymbol{R}$ contains the responses, and $\boldsymbol{f}^{n+1}$ and $\boldsymbol{f}_{inh}^{n+1}$ are vectors of the fields $[\phi^{n+1}, \{\psi_j^{lm,n+1}\}]$ and $[\phi_{inh}^{n+1}, \{\psi_{j,inh}^{lm,n+1}\}]$, respectively

Conservation tests

- In the limit $k_\perp = 0$ the gyrokinetic collision operator should conserve density, momentum and energy
- Evolution of these moments over 20 collision times, with field particle terms (black) and without (blue, dashed):



Momentum



Energy

The Spitzer problem

- To test the accuracy of the collision model we solve:

$$C_{ee}[f_e] + C_{ei}[f_e, f_{0i}] = -\Bigg[v_\| \underbrace{\left(\frac{q_e E_\|}{T_e} - \nabla_\| \ln p_{0e} \right)}_{=:I_1} + v_\| \left(x_e^2 - \frac{5}{2} \right) \underbrace{\left[-\nabla_\| \ln T_{0e} \right]}_{=:I_2} \Bigg] F_{0e}. \quad (14)$$

- Calculate Spitzer transport coefficients L_{11}, $L_{12} = L_{21}$ and L_{22}:

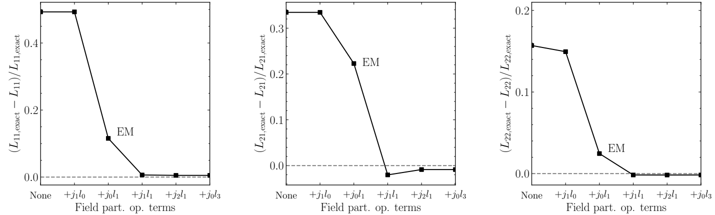
$$c_{ei} \int d^3v \; v_\| f_e = L_{11} I_1 + L_{12} I_2 \quad (15)$$

and

$$c_{ei} \int d^3v \; v_\| \left(x_e^2 - 5/2 \right) f_e = L_{12} I_1 + L_{22} I_2. \quad (16)$$

Spitzer coefficients

- Comparison with exact Fokker-Planck operator [Belli & Candy 2011, PPCF]



L_{11} $L_{12} = L_{21}$ L_{22}

- Including field particle terms up to $j_2 l_1$ yields Spitzer coefficients that are accurate to within 1%

Summary

- Implemented a linearised Fokker-Planck collision model in `stella`
  - Implicit scheme $\rightarrow$ no CFL constraint
  - Satisfies conservation laws
  - Flexible, scalable accuracy
- Next steps:
  - test self-adjointness: currently only guaranteed on uniform μ-grid in `stella`
  - GK simulations in stellarators