Comparison of collision operators and particle trajectories in stellarators using the SFINCS code

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Motivation

- Neoclassical physics is very important in stellarators:
  - At low $v_*$, neoclassical radial transport exceeds turbulent transport.
  - W7-X is sensitive to $j_{bs}$: divertor requires $q = 1$ at LCFS.

However,

- Design & modelling of W7-X has used an ad-hoc kinetic equation, & simplistic collision operator.
- Generally, coupling in the energy coordinate has been neglected to reduce kinetic equation from 4D $\rightarrow$ 3D.

*With modern computing power, we can now solve the 4D equation.*
SFINCS (Stellarator Fokker-Planck Iterative Neoclassical Conservative Solver)

- Solves time-independent linear drift-kinetic equations for $f_s(\theta, \zeta, v_\perp, v_\parallel)$.

- Several options for terms in the kinetic equation involving $E_r$ – “effective particle trajectories.”

- Several options for collision operator, including full linearized Fokker-Planck (so no “momentum correction” is required.)

- Continuum discretization, with mix of finite-difference, spectral, and pseudospectral methods.

- General nested flux surface geometry allowed, with interface to equilibrium data.

- Arbitrary number of species.

- Uses preconditioned GMRES solver (via PETSc library).

- Closely related to the tokamak code PERFECT for finite-orbit-width neoclassical calculations in tokamak pedestals: $f_s(\theta, \psi, v_\perp, v_\parallel)$.  
  \textit{PPCF 56, 045005 (2014).}
1. “DKES trajectories” (Incompressible ExB drift, van Rij & Hirshman (1989)):

\[
\left( v_b + \frac{c}{B^2} \frac{d\Phi}{d\psi} B \times \nabla \psi \right) \cdot \nabla f_1 - \frac{(1 - \xi^2)}{2B} \nu (\nabla B) \frac{\partial f_1}{\partial \xi} - C \{ f_1 \} = -v_m \cdot \nabla \psi \frac{\partial f_m}{\partial \psi} 
\]

\[
\xi = \frac{v_\parallel}{v}
\]
Several choices are available for the $E_r$ terms

1. “DKES trajectories” (Incompressible ExB drift, van Rij & Hirshman (1989)):

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\left( v_\parallel b + \frac{c}{\langle B^2 \rangle} \frac{d\Phi}{d\psi} B \times \nabla \psi \right) \cdot \nabla f_1 - \frac{1 - \xi^2}{2B} \nu \left( \nabla_\parallel B \right) \frac{\partial f_1}{\partial \xi} - C \{ f_1 \} = -v_m \cdot \nabla \psi \frac{\partial f_m}{\partial \psi}
$$

$$\xi = \nu_\parallel / \nu$$

2. “Partial trajectories” (Correct ExB drift):

$$
\left( v_\parallel b + \frac{c}{B^2} \frac{d\Phi}{d\psi} B \times \nabla \psi \right) \cdot \nabla f_1 - \frac{1 - \xi^2}{2B} \nu \left( \nabla_\parallel B \right) \frac{\partial f_1}{\partial \xi} - C \{ f_1 \} = -v_m \cdot \nabla \psi \frac{\partial f_m}{\partial \psi}
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1. "DKES trajectories" (Incompressible ExB drift, van Rij & Hirshman (1989)):

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\left( v_{||} \mathbf{b} + \frac{c}{\langle B^2 \rangle} \frac{d\Phi}{d\psi} \mathbf{B} \times \nabla \psi \right) \cdot \nabla f_1 - \left( 1 - \xi^2 \right) \nu \left( \nabla_{||} B \right) \frac{\partial f_1}{\partial \xi} - C \left\{ f_1 \right\} = - \mathbf{v}_m \cdot \nabla \psi \frac{\partial f_M}{\partial \psi}
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$$\xi = \frac{v_{||}}{v}$$

2. "Partial trajectories" (Correct ExB drift):

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$$

3. "Full trajectories" (Including other terms required to conserve $\mu$ & correct viscous force):

$$
\left( v_{||} \mathbf{b} + \frac{c}{\langle B^2 \rangle} \frac{d\Phi}{d\psi} \mathbf{B} \times \nabla \psi \right) \cdot \nabla f_1 + \left[ - \left( 1 - \xi^2 \right) \nu \left( \nabla_{||} B \right) + \frac{c \xi \left( 1 - \xi^2 \right)}{2 B^3} \frac{d\Phi}{d\psi} \mathbf{B} \times \nabla \psi \cdot \nabla B \right] \frac{\partial f_1}{\partial \xi}

+ \frac{c v}{2 B^3} \left( 1 + \xi^2 \right) \frac{d\Phi}{d\psi} \left( \mathbf{B} \times \nabla \psi \cdot \nabla B \right) \frac{\partial f_1}{\partial \psi} - C \left\{ f_1 \right\} = - \mathbf{v}_m \cdot \nabla \psi \frac{\partial f_M}{\partial \psi}
$$
Several choices are available for the $E_r$ terms

1. “DKES trajectories” (Incompressible ExB drift, van Rij & Hirshman (1989)):

$$
\left( \nu b + \frac{c}{B^2} \frac{d \Phi}{d \psi} B \times \nabla \psi \right) \cdot \nabla f_1 - \frac{(1 - \xi^2)}{2B} \nu \left( \nabla_{B1} \right) \frac{\partial f_1}{\partial \xi} - C \{ f_1 \} = -v_m \cdot \nabla \psi \frac{\partial f_M}{\partial \psi}
$$

$$
\xi = \nu_{L} / \nu
$$

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\left( \nu b + \frac{c}{B^2} \frac{d \Phi}{d \psi} B \times \nabla \psi \right) \cdot \nabla f_1 + \left[ -\frac{(1 - \xi^2)}{2B} \nu \left( \nabla_{B1} \right) + \frac{c \xi (1 - \xi^2)}{2B^3} \frac{d \Phi}{d \psi} B \times \nabla \psi \cdot \nabla B \frac{\partial f_1}{\partial \xi} \right]
$$

$$
+ \frac{c \nu}{2B^3} (1 + \xi^2) \frac{d \Phi}{d \psi} (B \times \nabla \psi \cdot \nabla B) \frac{\partial f_1}{\partial \nu} - C \{ f_1 \} = -v_m \cdot \nabla \psi \frac{\partial f_M}{\partial \psi}
$$

These models are ordered from least to most accurate, in a sense, but care is required…
In the partial and full trajectory models, unphysical constraints will be imposed on \( f \) unless you are careful.

Example: partial trajectories:

\[
\left( v_{||} b + \frac{c}{B^2} \frac{d\Phi}{d\psi} \mathbf{B} \times \nabla \psi \right) \cdot \nabla f - \frac{1 - \xi^2}{2B} \nu \left( \nabla_B \right) \frac{\partial f_i}{\partial \xi} - C \{ f_i \} = -v_m \cdot \nabla \psi \frac{\partial f_M}{\partial \psi}
\]

Consider the \( \left\langle \int d^3\nu \ldots \right\rangle \) moment:

\[
\frac{d\Phi}{d\psi} \left\langle \int d^3\nu f_i \mathbf{B} \times \nabla \psi \cdot \nabla \frac{1}{B^2} \right\rangle = 0
\]
In the partial and full trajectory models, unphysical constraints will be imposed on \( f \) unless you are careful.

Example: partial trajectories:

\[
\left( v_{\parallel} \mathbf{b} + \frac{c}{B^2} \frac{d\Phi}{d\psi} \mathbf{B} \times \nabla \psi \right) \cdot \nabla f_1 - \frac{1 - \xi^2}{2B} \nu \left( \nabla B \right) \frac{\partial f_1}{\partial \xi} - C\{f_1\} = -\mathbf{v}_m \cdot \nabla \psi \frac{\partial f_M}{\partial \psi}
\]

Consider the \( \left\langle \int d^3\nu (\ldots) \right\rangle \) moment:

\[
\frac{d\Phi}{d\psi} \left\langle \int d^3\nu f_1 \mathbf{B} \times \nabla \psi \cdot \nabla \frac{1}{B^2} \right\rangle = 0
\]

If \( \frac{d\Phi}{d\psi} = 0 \),

\[ 0 = 0. \text{ No problem.} \]
In the partial and full trajectory models, unphysical constraints will be imposed on $f$ unless you are careful.

Example: partial trajectories:

$$\left(v \parallel b + \frac{c}{B^2} \frac{d\Phi}{d\psi} B \times \nabla \psi\right) \cdot \nabla f_1 - \left(1 - \frac{\xi^2}{2B}\right) v \left(\nabla \parallel B\right) \frac{\partial f_1}{\partial \xi} - C\{f_1\} = -v_m \cdot \nabla \psi \frac{\partial f_M}{\partial \psi}$$

Consider the $\left\langle \int d^3\nu (\ldots) \right\rangle$ moment:

$$\frac{d\Phi}{d\psi} \left\langle \int d^3\nu f_1 \ B \times \nabla \psi \cdot \nabla \frac{1}{B^2} \right\rangle = 0$$

If $\frac{d\Phi}{d\psi} = 0$, $0 = 0$. No problem.

If $\frac{d\Phi}{d\psi} \neq 0$, $\left\langle \int d^3\nu f_1 \ B \times \nabla \psi \cdot \nabla \frac{1}{B^2} \right\rangle = 0$

Unphysical constraint on $f_1$.

Solution for $\frac{d\Phi}{d\psi} = 0$ is very different from solution for $\frac{d\Phi}{d\psi} = \epsilon$. 
In the partial and full trajectory models, unphysical constraints will be imposed on $f$ unless you are careful.

Example: partial trajectories:

\[
\left( v \mathbf{b} + \frac{c}{B^2} \frac{d\Phi}{d\psi} \mathbf{B} \times \nabla \psi \right) \cdot \nabla f_1 - \left( \frac{1 - \xi^2}{2B} \right) v \left( \nabla \cdot \mathbf{B} \right) \frac{\partial f_1}{\partial \xi} - C\{f_1\} = -\mathbf{v}_m \cdot \nabla \psi \frac{\partial f_M}{\partial \psi}
\]

Consider the $\left\langle \int d^3\nu \left( \ldots \right) \right\rangle$ moment:

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\frac{d\Phi}{d\psi} \left\langle \int d^3\nu f_1 \mathbf{B} \times \nabla \psi \cdot \nabla \frac{1}{B^2} \right\rangle = 0
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If $\frac{d\Phi}{d\psi} = 0$, $0 = 0$. No problem.

If $\frac{d\Phi}{d\psi} \neq 0$, $\left\langle \int d^3\nu f_1 \mathbf{B} \times \nabla \psi \cdot \nabla \frac{1}{B^2} \right\rangle = 0$

Unphysical constraint on $f_1$.

Solution for $\frac{d\Phi}{d\psi} = 0$ is very different from solution for $\frac{d\Phi}{d\psi} = \varepsilon$. Similar problem for the $\left\langle \int d^3\nu \nu^2 \left( \ldots \right) \right\rangle$ moment, & for full trajectories.
The partial and full trajectory models become well-behaved if you include sources.

\[
\left( v_{\parallel b} + v_E \right) \cdot \nabla f_1 + \dot{\xi} \frac{\partial f_1}{\partial \xi} - C_\ell \{ f_1 \} - S_p f_M \left( \frac{mv^2}{2T} - \frac{5}{2} \right) - S_h f_M \left( \frac{mv^2}{2T} - \frac{3}{2} \right) = -v_d \cdot \nabla f_M
\]
The partial and full trajectory models become well-behaved if you include sources.

\[
\left( \nu_{\parallel} b + \nu_E \right) \cdot \nabla f_1 + \dot{\xi} \frac{\partial f_1}{\partial \xi} - C_\ell \{ f_1 \} - S_p f_M \left( \frac{mv^2}{2T} - \frac{5}{2} \right) - S_h f_M \left( \frac{mv^2}{2T} - \frac{3}{2} \right) = -\mathbf{v}_d \cdot \nabla f_M
\]

2 extra unknowns \((S_p \text{ and } S_h)\) require 2 extra equations.

Kinetic equation \{ \}

\[
\left\langle \int d^3\nu f_1 \right\rangle_\nu = 0 \quad \begin{bmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} f_1 \\ S_p \\ S_h \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}
\]

Vector of unknowns

\[
\left\langle \int d^3\nu f_1 \nu^2 \right\rangle_\nu = 0 \quad \begin{bmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} f_1 \\ S_p \\ S_h \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}
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The partial and full trajectory models become well-behaved if you include sources.

\[
\left( \mathbf{v}_b + \mathbf{v}_E \right) \cdot \nabla f_1 + \dot{\xi} \frac{\partial f_1}{\partial \xi} - C_\ell \{ f_1 \} - S_p f_M \left( \frac{mv^2}{2T} - \frac{5}{2} \right) - S_h f_M \left( \frac{mv^2}{2T} - \frac{3}{2} \right) = -\mathbf{v}_d \cdot \nabla f_M
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<table>
<thead>
<tr>
<th>Kinetic equation</th>
<th>( \left\langle \int d^3 \nu f_1 \right\rangle )</th>
<th>( \begin{bmatrix} 0 &amp; 0 \ 0 &amp; 0 \end{bmatrix} )</th>
<th>( \begin{bmatrix} f_1 \ S_p \ S_h \end{bmatrix} )</th>
<th>( -\mathbf{v}_d \cdot \nabla f_M )</th>
</tr>
</thead>
<tbody>
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DKES trajectories: \( S_p = 0, \quad S_h = 0. \)

Partial trajectories: \( S_p \neq 0, \quad S_h \neq 0. \)

Full trajectories: \( S_p = 0, \quad S_h 
eq 0 \) except at the ambipolar \( E_r. \)
The partial and full trajectory models become well-behaved if you include sources.

\[(\nu_{\parallel} \mathbf{b} + \mathbf{v}_E) \cdot \nabla f_1 + \dot{\xi} \frac{\partial f_1}{\partial \xi} - C_\ell \{ f_1 \} - S_p f_M \left( \frac{mv^2}{2T} - \frac{5}{2} \right) - S_h f_M \left( \frac{mv^2}{2T} - \frac{3}{2} \right) = -\mathbf{v}_d \cdot \nabla f_M \]

2 extra unknowns \((S_p\) and \(S_h\)) require 2 extra equations.

• Only the full trajectory model preserves intrinsic ambipolarity in quasisymmetric \(B\) fields.

• Only the full trajectory model gives the correct parallel viscous force associated with \(E_r\)-driven gyroviscosity:

\[\bar{\Pi}_E = (b \mathbf{v}_E + v_E \mathbf{b}) mnV_{\parallel}, \quad \mathbf{b} \cdot (\nabla \cdot \bar{\Pi}_E) = cmB \frac{d\Phi}{d\psi} \mathbf{B} \times \nabla \psi \cdot \nabla \left( \frac{nV_{\parallel}}{B^3} \right)\]

DKES trajectories: \(S_p = 0, \quad S_h = 0\).

Partial trajectories: \(S_p \neq 0, \quad S_h \neq 0\).

Full trajectories: \(S_p = 0, \quad S_h \neq 0\) except at the ambipolar \(E_r\).
SFINCS can use the full linearized Fokker-Planck collision operator.

\[ C_i \{ f_1 \} = \left\{ \begin{array}{l} \text{pitch-angle \& energy scattering} \\ \text{(test particle part)} \end{array} \right\} + \nu_{ii} 3e^{-\nu^2/\nu_{th,i}^2} \left[ f_1 - \frac{H}{2\pi \nu_{th,i}^2} + \frac{\nu^2}{2\pi \nu_{th,i}^4} \frac{\partial^2 G}{\partial \nu^2} \right] \left\{ \begin{array}{l} \text{field particle part} \end{array} \right\} \]

\[ \nabla_\nu^2 H + 4\pi f_1 = 0 \]

\[ \nabla_\nu^2 G - 2H = 0 \]
SFINCS can use the full linearized Fokker-Planck collision operator.

\[ C_i \{ f_1 \} = \begin{cases} \text{pitch-angle & energy scattering} \\ \text{test particle part} \end{cases} + \nu_{ii} 3e^{-\nu^2/\nu_{th,i}^2} \begin{bmatrix} f_1 - \frac{H}{2\pi \nu_{th,i}^2} + \frac{\nu^2}{2\pi \nu_{th,i}^4} \frac{\partial^2 G}{\partial \nu^2} \end{bmatrix} \]

Kinetic equation:

\[ \nabla_v^2 H + 4\pi f_1 = 0 \]

\[ \nabla_v^2 G - 2H = 0 \]

Vector of unknowns

Similar to independent work in Lyons et al, *PoP* 19, 082515 (2012)
SFINCS allows comparison between collision operators

\[ v' = v_{ii} R / v_{th,i}, \quad \text{W7-X geometry,} \quad E_r = 0. \]
When $E_*=E_r/E_r^{res}$ is < 0.3, the 3 models are nearly identical; otherwise differences can be significant.

\[ \nu_{ii} R / \nu_{th,i} = 0.01, \quad E_r^{res} = B \nu_{th,i} tr / R \]
Example: W7-X edge.

Example: W7-X edge. Trajectory model has little impact on ambipolar $E_r$, modest effect on $j_{bs}$.
Example: W7-X edge. Trajectory model has little impact on ambipolar $E_r$, modest effect on $j_{bs}$.

$E_r^{res} = B\nu_{th,i}tr / R = 100\text{kV/m}$
For expected W7X profiles, trajectory model and collision operator have little effect on $E_r$ or radial fluxes.
For expected W7X profiles, trajectory model and collision operator have modest effect on flows and $j_{\text{bs}}$.

**Ion contribution to bootstrap current**

**Total bootstrap current**

- DKES calculations by Turkin, with momentum correction
- DKES calculations by Turkin, without momentum correction
- SFINCS: Fokker–Planck, full trajectories
- SFINCS: Fokker–Planck, monoenergetic trajectories
- SFINCS: Pitch–angle scattering, full trajectories
- SFINCS: Pitch–angle scattering, monoenergetic trajectories
Summary

• Our new code SFINCS allows a comparison of several variants of the drift-kinetic equation, differing in the $E_r$ terms.
  
  – The trick of including particle & heat sources allows for steady-state solution of a wide variety of kinetic equations, even if conservation is imperfect.
  
  – Below $\sim 1/3$ of the $E_r$ resonance, the variants give nearly identical results. This is probably the case for W7-X.
  
  – For larger $E_r/E_r^{\text{res}}$, there can be substantial differences.
  
  – The “full trajectory” model is probably the best of the 3 models considered here, but radial coupling could also be important.
Future work & opportunities for collaboration

- Use existing version of SFINCS to study impurity transport. Fokker-Planck collision operator may make a difference.

- Clarify orderings. Is there a superior version of the kinetic equation?

- Include poloidal & toroidal magnetic drifts.

- Applications for $f_1$, $n_1(\theta, \zeta)$, adiabatic $\Phi_1(\theta, \zeta)$?

- Nonlinear $\Phi_1(\theta, \zeta)$ terms (García-Regaña et al, PPCF (2013))

- Code, documentation, & examples online: www.github.com/landreman/sfincs