Impurities in a non-axisymmetric plasma: transport and effect on bootstrap current

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Background

- Helically trapped particles can drift out of plasma ⇒ collisionless trajectories not always confined.
- Radial electric field $E_r = -\frac{d\Phi}{dr}$, restore ambipolarity.
- $E_r$ often points radially inwards ⇒ impurity accumulation.

W7-AS measurements:

[Burhenn et al, Nucl Fusion (2009)]
[Giannone et al, PPCF (2000)]
Stellarator neoclassical calculations have predominantly been performed using simplified models for collisions, e.g. pitch-angle scattering + momentum correction.

"Monoenergetic" approximation, dropping derivatives of distribution function with respect to speed.
Solves the radially local 4D drift-kinetic equation, two spatial ($\theta, \zeta$) two velocity ($x, \xi$) variables.

- Arbitrary number of species.
- $C_a$ – Full linearized Fokker-Planck collisions.
- $N_{\text{species}} \times N_\theta \times N_\zeta \times N_x \times N_\xi \sim 10^6 – 10^7$ degrees of freedom.
Transport matrix

Impurity particle transport

N.B. $L_{jk}^{ab}$ depends on $E_r$, we use $E_r = 0$.

Fluxes

\[
\begin{pmatrix}
\langle \int d^3v f_z v_m \cdot \nabla \psi \rangle \\
\langle \int d^3v f_z \frac{m_n^2}{2T} v_m \cdot \nabla \psi \rangle \\
\langle BV \rangle_z \\
\langle \int d^3v f_i v_m \cdot \nabla \psi \rangle \\
\langle \int d^3v f_i \frac{m_n^2}{2T} v_m \cdot \nabla \psi \rangle \\
\langle BV \rangle_i \\
\end{pmatrix}
= 
\begin{pmatrix}
L_{11}^{zz} & L_{12}^{zz} & L_{11}^{zi} & L_{12}^{zi} & L_{13}^{zi} \\
L_{21}^{zz} & L_{22}^{zz} & L_{21}^{zi} & L_{22}^{zi} & L_{23}^{zi} \\
L_{31}^{zz} & L_{32}^{zz} & L_{31}^{zi} & L_{32}^{zi} & L_{33}^{zi} \\
L_{11}^{iz} & L_{12}^{iz} & L_{11}^{ii} & L_{12}^{ii} & L_{13}^{ii} \\
L_{21}^{iz} & L_{22}^{iz} & L_{21}^{ii} & L_{22}^{ii} & L_{23}^{ii} \\
L_{31}^{iz} & L_{32}^{iz} & L_{31}^{ii} & L_{32}^{ii} & L_{33}^{ii} \\
\end{pmatrix}
\]

Assume $T_i = T_z$

\[
\langle \Gamma_z \cdot \nabla \psi \rangle = \mathcal{K} \{ L_{11}^{zz} A_{z_1} + L_{11}^{zi} A_{i_1} + (L_{12}^{zz} + L_{12}^{zi}) A_2 \} 
\]

Thermodynamic forces

\[
\begin{pmatrix}
\mathcal{K} \left[ \frac{1}{n_z} \frac{dn_z}{d\psi} + \frac{Z e}{T_z} \frac{d\Phi}{d\psi} - \frac{3}{2T} \frac{dT_z}{d\psi} \right] \\
\mathcal{K} \left[ \frac{1}{T_z} \frac{dT_z}{d\psi} \right] \\
\mathcal{J} \left[ \frac{E_{||B}}{B^2} \right] \\
\mathcal{K} \left[ \frac{1}{n_i} \frac{dn_i}{d\psi} + \frac{e}{T_i} \frac{d\Phi}{d\psi} - \frac{3}{2T_i} \frac{dT_i}{d\psi} \right] \\
\mathcal{K} \left[ \frac{1}{T_i} \frac{dT_i}{d\psi} \right] \\
\mathcal{J} \left[ \frac{E_{||B}}{B^2} \right] \\
\end{pmatrix}
\]
SFINCS calculations

• We have used SFINCS to calculate $L_{11} zz$, $L_{11} zi$ and $L_{12} = L_{12} zz + L_{12} zi$. 
Linearized Fokker-Planck collisions vs pitch-angle scattering.

$C^{6+}$ impurity and $H^+$ main ions, $Z_{\text{eff}} = 1.05$ and $Z_{\text{eff}} = 2.0$. 
W7-X vacuum configuration.

• Compare to analytical modeling in the high collisionality regime. [Braun, Helander, PoP (2010)]

• Compare to calculations with the DKES (Drift Kinetic Equation Solver) code. [Hirshman et al, Phys. Fluids (1986)], [van Rij, Hirshman, Phys. Fluids B (1989)]
Carbon flux $\propto \nabla n_z$

- Negative $\Rightarrow$ drives outward flux.
- Pitch-angle scattering a relatively good approximation for $L_{11zz}$.
  However, some difference for $Z_{\text{eff}}=2.0$ at high collisionality.
Carbon flux $\propto \nabla n_i$

- Pure pitch-angle scattering $\Rightarrow$ inter-species coefficients vanish.
- DKES + momentum corr. fail to find the sign change at low collisionality.
  Difference caused by even part in $v_{\parallel}$ of the field term in the collision operator.

N.B. Logarithmic scale separated by linear region around axis.
Carbon flux $\propto \nabla T$

- All collision models find temperature screening at low collisionality.
- Pure pitch-angle scattering always finds inward drive at high collisionality. For SFINCS Fokker-Planck calculations it depends on the impurity content.
Benchmark at high collisionality

[Braun, Helander, PoP (2010)] Short mean-free-path expansion of $f_{z1}$. Transport coefficients depend on $u \propto J_\parallel$ (depend on geometry).

![Graphs showing $L_{11}$ and $L_{12}$ vs $\nu'$ with linear y-axis regions.](image)
Bootstrap current calculations

- $r/a = 0.2$, zero-flux carbon gradient, Fokker-Planck
- $r/a = 0.2$, $Z_{\text{eff}}$ independent of $r$, Fokker-Planck
- $r/a = 0.8$, zero-flux carbon gradient, Fokker-Planck
- $r/a = 0.8$, $Z_{\text{eff}}$ independent of $r$, Fokker-Planck

- W7-X magnetic configuration with $\langle \beta \rangle \sim 2.9\%$, $H^+, e^-$ and $C^{6+}$.
- Bootstrap current density decreases with $Z_{\text{eff}}$. 
Bootstrap current calculations

- Changes of $\Delta Z_{\text{eff}} \sim 1 \Rightarrow \Delta j_{\text{bs}} \gtrsim 20 \text{ kA/m}^2$.
- If such a change happens across the entire plasma $\Rightarrow \Delta I_{\text{bs}} \gtrsim 10 \text{ kA} \Rightarrow$ Changes in island divertor strike point locations.
Conclusions

We have used SFINCS to demonstrate

- At low collisionality, pitch-angle scattering sufficient to describe $\Gamma_z \propto \nabla n_z, \nabla T$. However to correctly describe $\Gamma_z \propto \nabla n_i$, full linearized Fokker-Planck collisions necessary.

- At intermediate/high collisionality, lack of momentum conservation can lead to transport predictions in the wrong direction.

- At low collisionality we find impurity screening for all coefficients. However in reality $E_r$ plays a major role.

- Bootstrap current calculations should be performed with a realistic ion composition, important for divertor strike point locations.

Note: SFINCS Fokker-Planck calculations typically demanding compared to e.g. DKES calculations, particularly at low collisionality.

SFINCS available at [www.github.com/landreman/sfincs](http://www.github.com/landreman/sfincs)
Backup slides
Transport matrix

Impurities and main ions

Fluxes

\[
\begin{pmatrix}
\langle \int d^3 v f_z v_m \cdot \nabla \psi \rangle \\
\langle \int d^3 v f_z \frac{mv^2}{2T} v_m \cdot \nabla \psi \rangle \\
\langle BV_{||z} \rangle \\
\langle \int d^3 v f_i v_m \cdot \nabla \psi \rangle \\
\langle \int d^3 v f_i \frac{mv^2}{2T} v_m \cdot \nabla \psi \rangle \\
\langle BV_{||i} \rangle \\
\end{pmatrix}
= 
\begin{pmatrix}
L_{11}^{zz} & L_{12}^{zz} & L_{13}^{zz} & L_{11}^{zi} & L_{12}^{zi} & L_{13}^{zi} \\
L_{21}^{zz} & L_{22}^{zz} & L_{23}^{zz} & L_{21}^{zi} & L_{22}^{zi} & L_{23}^{zi} \\
L_{31}^{zz} & L_{32}^{zz} & L_{33}^{zz} & L_{31}^{zi} & L_{32}^{zi} & L_{33}^{zi} \\
L_{11}^{iz} & L_{12}^{iz} & L_{13}^{iz} & L_{11}^{ui} & L_{12}^{ui} & L_{13}^{ui} \\
L_{21}^{iz} & L_{22}^{iz} & L_{23}^{iz} & L_{21}^{ui} & L_{22}^{ui} & L_{23}^{ui} \\
L_{31}^{iz} & L_{32}^{iz} & L_{33}^{iz} & L_{31}^{ui} & L_{32}^{ui} & L_{33}^{ui}
\end{pmatrix}
\begin{pmatrix}
\mathcal{K} \left[ \frac{1}{n_z} \frac{dn_z}{d\psi} + \frac{Ze}{T_z} \frac{d\Phi}{d\psi} - \frac{3}{2T} \frac{dT_z}{d\psi} \right] \\
\mathcal{K} \frac{1}{T_z} \frac{dT_z}{d\psi} \langle E_{||B} \rangle \\
\mathcal{J} \langle B^2 \rangle \\
\mathcal{K} \left[ \frac{1}{n_i} \frac{dn_i}{d\psi} + \frac{e}{T_i} \frac{d\Phi}{d\psi} - \frac{3}{2T_i} \frac{dT_i}{d\psi} \right] \\
\mathcal{K} \frac{1}{T_i} \frac{dT_i}{d\psi} \langle E_{||B} \rangle \\
\mathcal{J} \langle B^2 \rangle 
\end{pmatrix}
\]

Normalization factors \( \mathcal{K}, \mathcal{J} \) contain geometrical quantities.

Boozer coordinates

\[
\mathbf{B} = K (\psi, \theta, \zeta) \nabla \psi + I (\psi) \nabla \theta + G (\psi) \nabla \zeta
\]
Transport matrix

Impurities and main ions

Fluxes

\[
\begin{bmatrix}
\frac{Ze(G+iI)}{n_z c T_z G} \left< \int d^3 v f_z v_m \cdot \nabla \psi \right>
+ \frac{1}{v_z B_0} \left< BV \right>_z \\
\frac{e(G+iI)}{n_i c T_i G} \left< \int d^3 v f_i v_m \cdot \nabla \psi \right>
+ \frac{1}{v_i B_0} \left< BV \right>_i
\end{bmatrix}
= \begin{bmatrix}
L^{zz} & L^{zz} & L^{zi} & L^{zi} & L^{zi} & L^{zi} \\
L^{zz} & L^{zz} & L^{zi} & L^{zi} & L^{zi} & L^{zi} \\
L^{zz} & L^{zz} & L^{zi} & L^{zi} & L^{zi} & L^{zi} \\
L^{iz} & L^{iz} & L^{i2} & L^{i2} & L^{i2} & L^{i2} \\
L^{iz} & L^{iz} & L^{i2} & L^{i2} & L^{i2} & L^{i2} \\
L^{iz} & L^{iz} & L^{i2} & L^{i2} & L^{i2} & L^{i2}
\end{bmatrix}
\begin{bmatrix}
\frac{GT_z c}{Ze B_0 v_z} \frac{1}{n_z} \frac{dn_z}{d \psi} + \frac{Ze}{T_z} \frac{d \Phi}{d \psi} - \frac{3}{2T_z} \frac{dT_z}{d \psi} \\
\frac{GT_z c}{Ze B_0 v_z} \frac{1}{n_i} \frac{dn_i}{d \psi} + \frac{e}{T_i} \frac{d \Phi}{d \psi} - \frac{3}{2T_i} \frac{dT_i}{d \psi} \\
\frac{Ze}{T_z} (G+iI) \frac{\langle E_i B \rangle}{\langle B^2 \rangle} \\
\frac{GT_z c}{Ze B_0 v_z} \frac{1}{n_i} \frac{dn_i}{d \psi} + \frac{e}{T_i} \frac{d \Phi}{d \psi} - \frac{3}{2T_i} \frac{dT_i}{d \psi} \\
\frac{Ze}{T_z} (G+iI) \frac{\langle E_i B \rangle}{\langle B^2 \rangle}
\end{bmatrix}
\]

Thermodynamic forces

Geometry in Boozer coordinates

\[ B = K(\psi, \theta, \zeta) \nabla \psi + I(\psi) \nabla \theta + G(\psi) \nabla \zeta \]
Carbon flux \( \propto \nabla n_i \)

Collisionality

\[
v_{\parallel} \nabla_{\parallel} f_{z1} = C_{zz} [f_{z1}, f_{Mz}] + C_{zz} [f_{Mz}, f_{z1}] + C_{zi} [f_{z1}, f_{Mi}] + C_{zi} [f_{Mz}, f_{i1}]
\]

\( \downarrow \) Bounce average

\[
0 = C_{zz} [f_{z1}, f_{Mz}] + C_{zz} [f_{Mz}, f_{z1}] + C_{zi} [f_{z1}, f_{Mi}] + C_{zi} [f_{Mz}, f_{i1}]
\]
Benchmark at high collisionality

[Braun, Helander, PoP (2010)] Short mean-free-path expansion of $f_{z1}$. Transport coefficients depend on $u \propto J_\parallel$ (depend on geometry).

\[
L_{11}^{zz} = \frac{3\sqrt{\pi}}{2Z^4} \left( \frac{\beta_{i1}}{\alpha_{i1} \beta_0 - \alpha_0 \beta_{i1}} \right) \frac{n_i^2}{n_z^2} \frac{m_i^{1/2}}{m_z^{1/2}} \frac{1}{G^2} B_0^2 H(\psi) \nu_z',
\]

\[
L_{11}^{zi} = -Z L_{11}^{zz},
\]

\[
L_{12}^{zz} + L_{12}^{zi} = -\frac{3\sqrt{\pi}}{2Z^4} \left( \frac{5}{2} (Z - 1) \beta_{i1} + \beta_0 \right) \frac{n_i^2}{n_z^2} \frac{m_i^{1/2}}{m_z^{1/2}} \frac{1}{G^2} B_0^2 H(\psi) \nu_z'
\]

\[
H(\psi) = \frac{\langle uB^2 \rangle^2}{\langle B^2 \rangle} - \langle u^2 B^2 \rangle \leq 0
\]

$\alpha_0$, $\alpha_{i1}$, $\beta_0$ and $\beta_{i1}$ are coefficients of $f_{i1}^{(0)}$ expanded in Sonine polynomials.
Bootstrap current calculations

- W7-X magnetic configuration with $\langle \beta \rangle \sim 2.9\%$, $H^+, e^-$ and $C^{6+}$.
- Assumed $n_e$, predicted $T_e$, $T_i$. [Turkin et al, PoP (2011)]
Finding ambipolar $E_r$
Future

• SFINCS is evolving, e.g. account for flux-surface variation of $\Phi$ which is particularly important in impurity transport studies.

• Benchmarking to other codes; including several species and non-zero $E_r$.

• Looking at ideas for minimizing neoclassical impurity accumulation.