Drift-Kinetic Simulations of Neoclassical Transport

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Motivation for the NEO code

• Develop a practical tool for high-accuracy neoclassical calculations, which includes:
  – Self-consistent coupled ion-electron physics
  – Multiple ion species
  – Poloidal correction to the potential
  – General geometry
  – Rotation effects
  – Finite-orbit-width effects

• Provide a stepping-stone toward a full-F Gyrokinetic + Neoclassical solver
  – Serve as a framework to explore new formulations which will allow calculation of the neoclassical $E_r^0$
  – Provide a tool for use in steady-state gyrokinetic transport simulations: TGYRO $\rightarrow$ coupled GYRO + NEO simulations
NEO solves a hierarchy of equations based on an expansion of the DKP eqns in powers of $\rho_{*i}$.

**$O(1)$:**

$$v_{\parallel b} \cdot \nabla f_{0a} - \frac{Z_a e}{m_a} v_{\parallel b} \cdot \nabla \Phi_0 \frac{\partial f_{0a}}{\partial \epsilon} - C_{aa}(f_{0a}, f_{0a}) = 0$$

$$\sum_a Z_a e n_{0a} = 0$$

**$O(\rho_{*i})$:**

$$v_{\parallel b} \cdot \nabla f_{1a} - \frac{Z_a e}{m_a} v_{\parallel b} \cdot \nabla \Phi_1 \frac{\partial f_{0a}}{\partial \epsilon} - \sum_b C_{ab}(f_{1a}, f_{1b}) = -\vec{v}_D \cdot \nabla f_{0a} + \frac{Z_a e}{m_a} \vec{v}_b \cdot \nabla \Phi_0 \frac{\partial f_{0a}}{\partial \epsilon}$$

$$0 = \sum_a Z_a e \int d^3 v f_{1a}$$

**$O(\rho_{*i}^2)$:**

$$v_{\parallel b} \cdot \nabla f_{2a} - \frac{Z_a e}{m_a} v_{\parallel b} \cdot \nabla \Phi_2 \frac{\partial f_{0a}}{\partial \epsilon} - \sum_b C_{ab}(f_{2a}, f_{2b}) = -\vec{v}_D \cdot \nabla f_{1a} + \frac{Z_a e}{m_a} \vec{v}_b \cdot \nabla \Phi_1 \frac{\partial f_{0a}}{\partial \epsilon} + \vec{v}_E^{(0)} \cdot \nabla f_{1a} + \vec{v}_E^{(1)} \cdot \nabla f_{0a}$$

$$+ \frac{Z_a e}{m_a} \left( v_{\parallel b} \cdot \nabla \Phi_1 + \vec{v}_D \cdot \nabla \Phi_0 \right) \frac{\partial f_{1a}}{\partial \epsilon} + \mu \frac{\partial f_{1a}}{\partial \mu} + S_{2a}$$

$$- \sum_a n_{0a} Z_a^2 e^2 \frac{\rho_a^2 |\nabla n|^2}{T_{0a}^2} \frac{\partial^2 \Phi_0}{\partial r^2} = \sum_a Z_a e \int d^3 v f_{2a}$$

**Standard neoclassical**

$$\Gamma_{2a} = \left\langle \int d^3 v \left( f_{0a} \vec{v}_E^{(1)} \cdot \nabla r + f_{1a} \vec{v}_D \cdot \nabla r \right) \right\rangle$$

$$Q_{2a} = \left\langle \int d^3 v m_a e \left( f_{0a} \vec{v}_E^{(1)} \cdot \nabla r + f_{1a} \vec{v}_D \cdot \nabla r \right) \right\rangle$$

**Finite-orbit-width correction**

$$\Gamma_{3a} = \left\langle \int d^3 v \left( f_{0a} \vec{v}_E^{(2)} \cdot \nabla r + f_{2a} \vec{v}_D \cdot \nabla r + f_{1a} \vec{v}_E^{(1)} \cdot \nabla r \right) \right\rangle$$

$$Q_{3a} = \left\langle \int d^3 v m_a e \left( f_{0a} \vec{v}_E^{(2)} \cdot \nabla r + f_{2a} \vec{v}_D \cdot \nabla r + f_{1a} \vec{v}_E^{(1)} \cdot \nabla r \right) \right\rangle$$

* required for solvability

$f_{0a} = F_{Ma}$
The ambipolarity relation, which requires complete cross-species collisional coupling, is preserved.

Operate on the kinetic equation with $\langle \int d^3v (v||/B) \rangle$:

$$\Gamma_{2a} = -\left( \frac{I}{\psi'\Omega_a} \int d^3v v|| \sum_b C_{ab} g_{1b} \right)$$

\Downarrow

$$\sum_a Z_a \Gamma_{2a} = -c \left( \frac{I}{\psi'eB} \int d^3v \sum_{a,b} m_a v|| C_{ab} g_{1b} \right)$$

$$f_{ia} = g_{ia} - \frac{f_{0a} Z_a e}{T_{0a}} \Phi_1$$

$$I(\psi) = RB_i$$

$\psi$: poloidal flux / (2$\pi$)

$$\frac{I}{\psi'} \rightarrow \frac{qR_0}{r} (s - \alpha \text{ geometry})$$

The plasma maintains ambipolarity only if the momentum conservation properties of $C_{ab}$ are properly maintained.
Three model forms of the linearized collision operator are implemented and compared.

- **Connor Model**

\[
C_{ab}^L = v_{ab} L f_{1a} + P_1(v_{||}/v) \left( v_{ab} v \frac{r_{ba}}{v_{ta}^2} \right) f_{0a}
\]

- **Zeroth Order Hirshman-Sigmar Operator**

\[
C_{ab}^L = v_{ab}^D L f_{1a} + P_1(v_{||}/v) \left[ v_{ab}^s v \frac{r_{ba}}{v_{ta}^2} + \left( v_{ab}^D - v_{ab}^s \right) \frac{u_{a1}(v)}{v} \right] f_{0a}
\]

- **Full Hirshman-Sigmar Operator**

\[
C_{ab}^L = v_{ab}^D L f_{1a} + P_1(v_{||}/v) \left[ v_{ab}^s v \frac{r_{ba}}{v_{ta}^2} + \left( v_{ab}^D - v_{ab}^s \right) \frac{u_{a1}(v)}{v} + \left( v_{ab}^h h_{ba} + v_{ab}^k k_{ab} \right) \frac{v^3}{v_{ta}^4} \right] f_{0a}
\]

\[
+ \frac{1}{v^2} \frac{\partial}{\partial v} \left[ \frac{1}{2} v_{ab}^2 v^4 \left( \frac{\partial n_{la}}{\partial v} - \frac{v}{v_{ta}^2} q_{ba} \right) f_{0a} \right] + P_2(v_{||}/v) \left[ v_{ab}^p v^2 \frac{5\pi_{ba}}{4v_{ta}^4} - v_{ab}^E \frac{\pi_{la}(v)}{v^2} \right] f_{0a}
\]

The NEO algorithm is highly accurate and time efficient.

\[
g_{ka}(r, \theta, \xi, \varepsilon) = f_{0a}(r, \varepsilon) \sum_{m=0}^{N_{r}-1} \sum_{n=0}^{N_{\xi}-1} P_m(\xi) T_n(z) c_{m,n}^a(r, \theta) \]

\[
f_{ka} = g_{ka} - f_{0a} \frac{Z_a e}{T_{0a}} \Phi_k
\]

- Mesh in \{r_i, \theta_j\}
- Legendre polynomials in \(\xi = v_{||}/v\)
  - collocation integrals done exactly
- Chebyshev polynomials in \(\varepsilon = v^2/2\)
  \(z = 2(\varepsilon/\varepsilon_{\text{max}})^{1/2} - 1, \text{ typically } \varepsilon_{\text{max}} = 16v_{\text{ta}}^2\)
  - collocation integrals done with composite higher-order Gauss-Legendre quadrature
- collision integrals, which are multi-scale, can be done to high accuracy (8-10 significant digits)

\[\Rightarrow \text{Sparse matrix system:}\]

\[
c_{m',n'}^{a',j'} A_{mm',nn'}^{aa',jj'} = b_{m,n}^{a,j}
\]

Typical sim time is < 1min.
Verification: With the full HS collision op, NEO recovers Taguchi’s theory, which is the most accurate analytic result in the banana regime.

The Connor & HS0 collision ops underestimate $Q_i$.

Chang-Hinton theory overestimates $Q_i$.

GA standard parameters: 
(s-α geometry) 
$r/a=0.5$  $R_0/a=3$  $q=2$  
$\alpha/L_n=1$  $\alpha/L_T=3$  $T_{0i}=T_{0e}$

Chang & Hinton, PF 25, 1493 (1982).
Taguchi, PPCF 30, 1897 (1988).
With self-consistent electron dynamics, the 2nd order fluxes have been successfully benchmarked with analytic theory.

Ambipolarity is confirmed.

The Connor & HS0 collision ops consistently underestimate Q.

Full electron-deuterium mass ratio used.
With NEO, we find that the Sauter model overestimates the bootstrap current.

Standard neoclassical relation:

\[
\langle u_i B \rangle_i = \frac{c T_{0i}}{Z_i e \psi'} \left( \frac{Z_i e}{T_{0i}} \frac{\partial \Phi_0}{\partial r} + \frac{1}{L_{ni}} + (1 - k_i) \frac{1}{L_{Ti}} \right)
\]

Sauter et al, PoP 6, 2834 (1999); PoP 9, 5140 (2002).

Dependence of \( k_i \) on \( \varepsilon \) & \( \nu_{*i} \) is coupled and difficult to predict analytically.
Studies of the effects of impurities find that the HS multi-species analytic theory is poor.

Comparison of 2nd order particle fluxes with analytic theory

For the NEO results, the Connor model is largely inaccurate.

GA standard parameters + Carbon: $Z_I n_{0I}/n_{0e}=0.1$, $T_I = T_i$

The multi-species analytic theory is qualitatively better for \( Q_i \) but still poor for \( Q_i \).

Comparison of 2nd order energy fluxes with analytic theory
The effects of rapid toroidal rotation, which introduces 0th-order density asymmetries, are also included in NEO.

Generalize the DKEs to allow for flow speeds $\sim O(v_{th})$:

$$\Phi = \Phi_{-1} + \Phi_0 + \Phi_1 + \Phi_2 + \ldots$$

$$\vec{V}_{0a} = \omega R^2 \nabla \varphi, \quad \omega(\psi) = -c \frac{d\Phi_{-1}}{d\psi}$$

$O(1)$:

$$f_{0a} = \frac{n_{0a}}{(2\pi T_{0a}/m_a)^{3/2}} e^{-v^2/2v_{ta}^2} \quad \nabla \rightarrow \text{rotating frame speed}$$

$$n_{0a}(\psi, \theta) = N_{0a}(\psi) \exp \left( -\frac{Z_e e}{T_{0a}} \Phi_0(\theta) + \frac{\omega^2 R(\theta)^2}{2v_{ta}^2} \right)$$

$$\Phi_0 = \Phi_0 - \langle \Phi_0 \rangle$$

determined by quasi-neutrality

(solve w/ Newton’s method)

formation of potential wells, which can enhance the effective fraction of trapped particles.

However, the effects of toroidal rotation are weak in experiments.

\[ \frac{k_i}{k_I} = 1.30 \quad (30\%) \]

\[ \frac{k_i}{k_I} = 0.73 \quad (27\%) \]

\[ \tilde{U}_a = \hat{\omega}_a R^2 \nabla \varphi + \frac{K_a}{n_0a} B \]

\[ K_a = -k_a \left( \frac{cT_{0a} I}{Z_a e L_{Ta} \psi' \left( B^2 / n_0a \right)} \right), \quad \hat{\omega}_a = - \left( \frac{cT_{0a}}{Z_a e \psi'} \left[ \frac{d \ln p_{0a}}{dr} + \frac{z_a e d \langle \Phi_o \rangle}{T_{0a} dr} \right] \right) \]

* Experimental data is being re-analyzed for accuracy.
Good overall agreement is found between NEO and NCLASS, although NCLASS slightly underestimates $|v_{pol}|$. 

- ~30% difference
- ~17% difference
Higher-order solution of the DKEs identifies a break-down of the $\delta f$ formalism due to FOW effects in the region $r < r_{\text{potato}}$.

Consistency check:
Verification of s.s. transport relation

$$\frac{1}{V'} \frac{\partial}{\partial r} (V' Q_{2a}) + Z_a e^2 \frac{\partial \Phi}{\partial r} \Gamma_{2a} = \left\langle \int d^3 v m_a \epsilon S_{2a} \right\rangle$$

Deviations from $Q_{2i}$ identify the break-down of the $\delta f$ formalism

R$_0$=4 m, a=1m, q=3, B$_0$=4 T, $(n_{oi}, T_{oi}) \sim c_1 + c_2 \exp(-c_3 (r/a)^3)$, s-\alpha geometry, adiabatic ele
However, for typical DIII-D plasmas, only a weak FOW effect is found due to steep gradients in the H-mode edge.

DIII-D H-mode profiles
shot#132010, t=2.5-3.5s

Higher-order NEO results

Pedestal region

DIII-D data provided by A. Leonard, T. Osborne, & R. Groebner. Simulations done with s-a geometry.
Summary: NEO provides a first-principles DKP-based calculation of the neoclassical transport coefficients.

- **Verification/analytic comparisons**
  - Agreement with Taguchi’s theory for the full HS collision op.
  - CH theory overestimates $Q_i$ for intermediate $\varepsilon$.
  - The Sauter model overestimates the bootstrap current.

- **Comparisons w/ NCLASS**
  - Corrections $\sim 17\%$ for the bootstrap current and $\sim 30\%$ for $v_{\theta}$.

- **Impurity transport**
  - The HS multi-species theory gives a poor prediction of the ion and impurity fluxes.

- **Rotation effects**
  - Generally weak in experiments.

- **FOW effects**
  - Break-down of the $\delta f$ formalism in the small region $r < r_{potato} \Rightarrow$ full $F$ required.
  - Only a weak FOW effect in the DIII-D H-mode edge.