Reduced kinetic neutral model for neutral-plasma interaction

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Background and motivation

• Neutral interactions:
  – provide sources or sinks of plasma density, momentum and energy
• Important process include
  – ionization, charge exchange and radiation
• Motivation for studying:
  – energetic neutrals impacting wall ⇒ erosion, sputtering, possible damage
  – recycled and puffed neutrals impact the shape of the plasma profiles
  – profiles drive turbulence and transport to wall ⇒ closed loop

• Challenges:
  – Neutral mean free path (MFP) is not necessarily short ⇒ fluid theory questionable
  – Difficult to run kinetic turbulence simulations on the transport (equilibrium profile) timescale
Reduced modeling approach

- Retain essential ingredients
- Avoid burdensome computational requirements

Plasma
- SOLT (Scrape-off Layer Turbulence) code
  - 2D fluid code describing outboard midplane region of tokamak
  - evolves $n_e$, $\Phi$, $T_e$, $T_i$ in plane $\perp B$
  - analytic closures describe parallel physics: sheath-connected filaments are flute-like; disconnected structures are collision limited
  - blob turbulence with $\delta n/n \sim 1$ permitted

Neutrals
- Reduced model developed in the following:
  - 2D fluid model molecules: typical cold, near wall, with short MFP
  - 1D kinetic model for atoms: $> 3eV$ and can be hot, longer MFP
2D fluid model for neutral molecules
(not yet implemented in SOLT)

• Neutral molecules are created near the wall by recycling and/or gas puff
• May be treated as a 2D fluid (like the SOLT plasma)
• Fluid treatment for molecules justified by typical short MFP
  – molecules emerge from the wall cold
  – exist mainly near the wall (then dissociate into atoms)
• 2D treatment motivated by short MFP:
  – molecules can interact with blob structures in the plasma
• In reality many molecular species can be present
  – model developed for a single dominant (effective) species
1D-1V kinetic model for atoms
(recently implemented in SOLT – see Russell, poster B-24)

• Atoms created by dissociation:
  – Franck-Condon process created at ~ 3eV
  – longer MFP than molecules

• Multiple charge exchange interactions with edge plasma ⇒ hot atoms
  – can have very long MFP
  – direct ballistic loss to wall
  – radial profile of edge $n_i$ and $T_i$ important for good CX model

• Long MFP ⇒ turbulence and blob structures are transparent to atoms
  – motivates 1D model that only retains spatial variations in $x$ (radial)
  – most important velocity variable for neutral transport is $x$ (radial)
Reduced model geometry and physics

Simulation plane \( \perp B \)

neutral atoms (1D-1V)

wall

blobs

LCFS

neutral molecules (2D)

x (radial)

y (binormal)
Kinetic equation for neutral atoms and ions

neutral atoms: \[
\frac{\partial g}{\partial t} + \mathbf{v} \cdot \nabla g = X(f_i, g) - h_{iz} n_e g + s_0
\]

plasma ions: \[
\frac{\partial f_i}{\partial t} + \mathbf{v} \cdot \nabla f_i + a \cdot \nabla f_i = -X(f_i, g) + h_{iz} n_e g
\]

CX: \[
X(f, g) = \int d^3\mathbf{v}' \sigma_{cx} |\mathbf{v}' - \mathbf{v}| [f_i(\mathbf{v})g'(\mathbf{v}') - f_i(\mathbf{v}')g(\mathbf{v})]
\]

- Make the (non-essential) assumption that CX rate coefficient is independent of \( \mathbf{v}' \): \( \sigma_{cx} |\mathbf{v}' - \mathbf{v}| \rightarrow h_{cx}(E_0, T_i) \)

\[
X(f, g) = h_{cx} n_0 f_i(\mathbf{v}) - h_{cx} n_i g(\mathbf{v})
\]

charge exchange rate coefficient

\( n_0 = \text{neutral atom density} \)
\( n_i = n_e = \text{plasma density} \)
1D-1V kinetic equation for neutral atoms
(implemented model)

\[
\frac{\partial G}{\partial t} + v_x \frac{\partial G}{\partial x} = h_{cx} n_0 \langle F \rangle_y - h_{cx} \langle n_i \rangle_y G - h_{iz} \langle n_e \rangle_y G + S_0
\]

- \( G(x,v_x) \) is the 1D-1V distribution function
- In addition to \( G \) and \( n_0 \) the \( y \)-velocity moment of the neutrals is needed and separately evolved

\[
n_0 = \int dv_x G(v_x)
\]

\[
\partial_t v_{0y} = -v_{0x} \partial_x (v_{0y}) + h_{cx} \langle n_i \rangle_y \left( \langle v_y \rangle_y - v_{0y} \right) - \frac{1}{n_0} S_n n_0 v_{0y}
\]

\[
v_0 = e_x \int dv_x v_x G(v_x)/n_0 + e_y v_{0y}
\]

neutrals are born with \( v_y = 0 \)
Plasma equations – 2D SOLT limit

- Warm ion, no Boussinesq approximation

\[
\partial_t n_e + v_E \cdot \nabla n_e = -\nabla ||\Gamma|| + h_{iz} n_e n_0 - \nabla \cdot \Gamma_{||n} + S_n
\]

\[
\nabla \cdot \left( \frac{n_i m_i c^2}{B^2} \nabla \Phi \right) + T_i \text{ terms} = \nabla ||J|| - \frac{2c}{B} b \times \nabla \cdot \kappa + \frac{m_i c}{B} b \cdot \nabla \times F_{i0}
\]

\[
\partial_t T_e + v_E \cdot \nabla T_e = -\frac{2}{3n_e} \nabla ||q_e|| + \frac{T_e}{n_e} \nabla ||\Gamma|| - h_{iz} n_0 \left( \frac{2}{3} E_{iz} + T_e \right) - \frac{2}{3n_e} \nabla \cdot q_{\perp e} + \frac{T_e}{n_e} \nabla \cdot \Gamma_{||n} + S_{Te}
\]

\[
\partial_t T_i + v_E \cdot \nabla T_i = -\frac{2}{3n_e} \nabla ||q_i|| + \frac{T_i}{n_e} \nabla ||\Gamma|| + (h_{iz} + h_{cx}) n_0 \left( \frac{2}{3} E_0 - T_i \right) - \frac{2}{3n_e} \nabla \cdot q_{\perp i} + \frac{T_i}{n_e} \nabla \cdot \Gamma_{||n} + S_{Ti}
\]

- Definitions:

\[
v_i = v_E + v_{di}
\]

\[
F_{i0} = h_{cx} n_i n_0 (v_0 - v_i) + h_{iz} n_e n_0 v_0
\]

\[
q_{\perp j} = -n_e D_{Tj} \nabla T_j
\]

\[
S_{Tj} = \frac{1}{n_e} \left( \frac{2}{3} H_j - T_j S_n \right)
\]

\[
n_0 E_0 = \frac{1}{2} m_i \alpha^2 \int \nabla_x v_x^2 G(v_x), \ 1 \leq \alpha^2 \leq 3
\]

\[
\Gamma_{||n} = -D_n \nabla n_e
\]

isotropization factor

\[
E_{iz} = \text{ionization energy cost}
\]
**Fluid model for neutral molecules**  
*(extended model)*

- Model the molecules explicitly in the **diffusive short MFP approximation**
  - balances neutral pressure gradient against neutral collisions

\[
\partial_t n_{m0} = \nabla \cdot (D_{m0} \nabla n_{m0}) - h_{md} n_e n_{m0} + S_{m0}
\]

\[
D_{m0} = \frac{v_{tm0}^2}{2v_{m0}}
\]

- Source term for the neutral atom equation:
  - atoms created by dissociation have the **Franck-Condon energy** \( \sim 3eV = m_i v_{FC}^2 \)

\[
S_0 = 2h_{md} n_e n_{m0} \frac{e^{-v_x^2/2v_{FC}^2}}{(2\pi)^{1/2}v_{FC}}
\]
Wall recycling boundary condition

molecular flux from wall \[ \Gamma_{m0}^+ = -\frac{1}{2} R_i \Gamma_i^+ - \frac{1}{2} R_0 \Gamma_0^- - R_m \Gamma_{m0}^- \]
ion flux to wall
neutral atom and molecular flux to wall

\[ R_j = \text{recycling coefficient} \]

\[ \Gamma_i^- = n_i v_{ix}, \quad v_{ix} > 0 \]
\[ \Gamma_0^- = \int_0^\infty dv_x v_x G(x_w, v_x) \]
\[ \Gamma_{m0}^- = n_{m0} v_{m0x} = -D_{m0} \partial_x n_{m0}, \quad v_{m0x} > 0 \]

- Limit of rapid molecular dissociation, \( h_{md} \to \infty \): neglect \( n_{m0} \) and \( \Gamma_{m0}^- \)

\[ \Gamma_0^+ \equiv 2 \Gamma_{m0}^+ = -(R_i \Gamma_i^- + R_0 \Gamma_0^-) \]

- equivalent to specifying a boundary condition on \( G \) at the wall:

\[ G(x_w, v_x) = (R_i \Gamma_i^- + R_0 \Gamma_0^-) \frac{e^{-v_x^2/2v_{FC}^2}}{v_{FC}^2}, \quad v_x < 0 \]
Charge exchange and energy conservation

• Recall the definition of the neutral energy $E_0$ in terms of the 1D distribution function and the isotropization factor $\alpha$

$$n_0 E_0 = \frac{1}{2} m_i \alpha^2 \int dv_x v_x^2 G(v_x)$$

• Total ion + neutral energy obeys

$$\partial_t (n_0 E_0 + \frac{3}{2} n_i T_i) + \partial_x (\frac{m_i \alpha^2}{2} \int dv_x v_x^3 G) + \mathbf{v}_E \cdot \nabla (\frac{3}{2} n_i T_i) = \frac{(\alpha^2 - 3)}{2} h_{cx} n_0 n_i T_i$$

• In the presence of isotropic ions, charge exchange provides a sink for the total energy density unless the neutrals are also isotropic ($\alpha^2 = 3$)
  - short MFP limit $\Rightarrow$ frequent collisions $\Rightarrow$ isotropic
  - long MFP limit $\Rightarrow$ anisotropic in SOL, but in this limit lost energy flux to the wall exceeds the non-conservative term

$$\partial_x (\frac{m_i \alpha^2}{2} \int dv_x v_x^3 G) \gg \frac{(\alpha^2 - 3)}{2} h_{cx} n_0 n_i T_i$$

$$\frac{1}{L_x} E_0 \gg h_{cx} n_i T_i \quad \Leftrightarrow \quad E_0 \gg \frac{L_x}{\lambda_{0,MFP}} T_i$$
**Total power balance**

- Total (plasma + neutral) energy $W$ is lost through ionization (radiation), $\perp$ and $\parallel$ transport to the walls, and gained by plasma heating $H_e$ and $H_i$

$$\partial_t W + \partial_x Q_x = -h_{iz} n_e n_0 E_{iz} + \partial_x n_e D_T e \partial_x T_e + \partial_x n_e D_{Ti} \partial_x T_i - \frac{q_\parallel}{L_{\parallel}} + H_e + H_i$$

**energy density**

$$W = \frac{3}{2} n_e (T_e + T_i) + n_0 E_0$$

**energy flux**

$$Q_x = Q_{px} + Q_0 = \frac{3}{2} n_e (T_e + T_i) v_{Ex} + \frac{m_i \alpha^2}{2} \int dv_x v_x^3 G$$
Conclusions

• A reduced model describing neutrals and plasma with computation cost similar to that of the original (plasma) SOLT model has been developed.
• The reduced model employs a fluid plasma and 1D kinetic neutral-atom description, with an extension for 2D fluid neutral molecules.
• The model contains the essential physics of
  – charge exchange
  – ionization
  – recycling
• The model respects conservative density, momentum and energy terms
  – with a noted caveat on energy
• The new model will be used to study neutral interactions with the plasma and the wall, and to enable
  – an assessment of neutral vs. ion sputtering, erosion
  – self-consistent sources and plasma profiles for edge/SOL turbulence simulations