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 $\Rightarrow$ erosion, sputtering, possible damage
  - recycled and puffed neutrals impact the shape of the plasma profiles
  - profiles drive turbulence and transport to wall $\Rightarrow$ closed loop

- Challenges:
  - Neutral mean free path (MFP) is not necessarily short $\Rightarrow$ 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, Φ, 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)

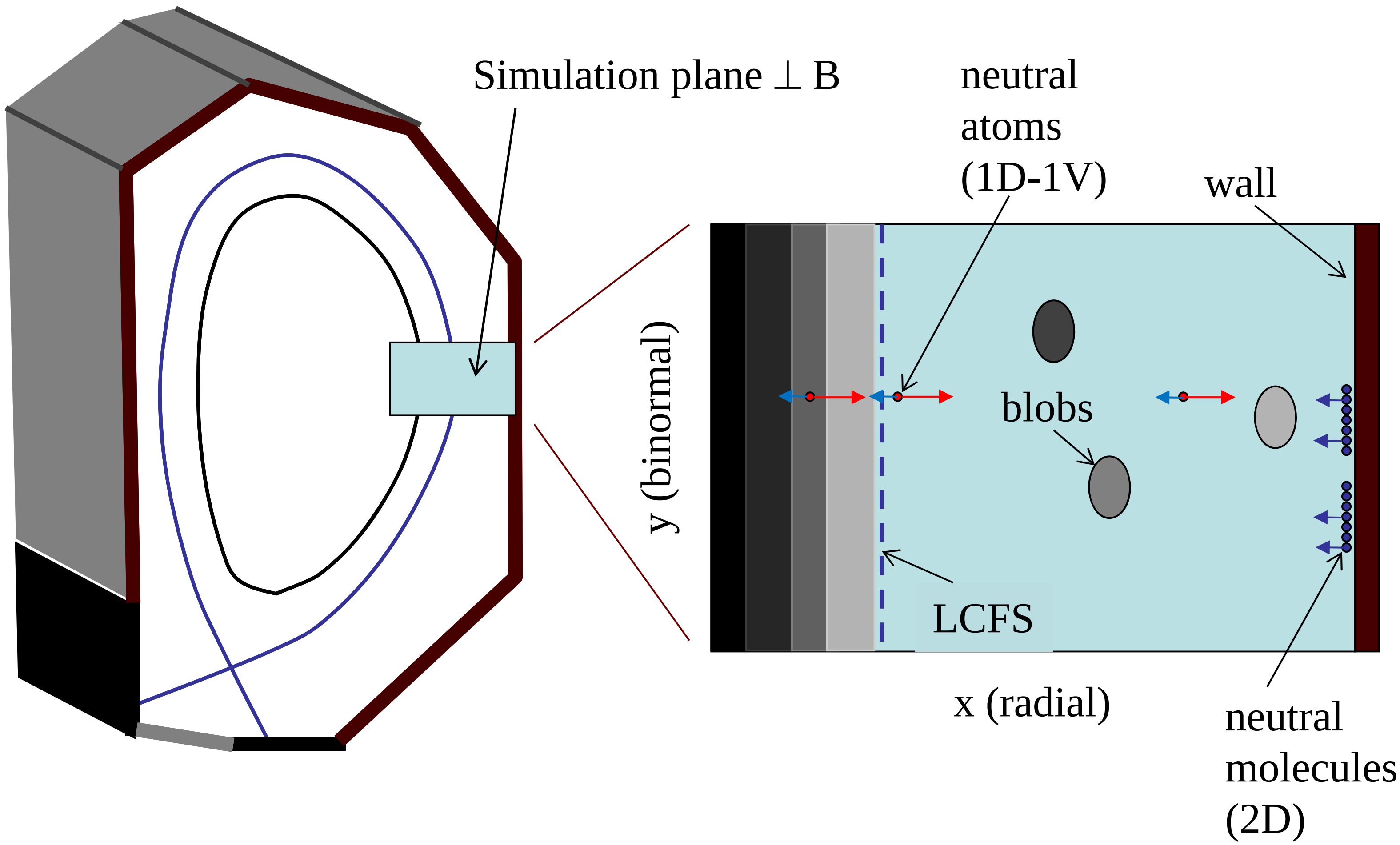
- Neutral molecules are created near the wall by recycling and/or gas puff
- May be treated as a 2D fluid (like the SOLT plasma)
- Fluid treatment for molecules justified by typical short MFP
  - molecules emerge from the wall cold
  - exist mainly near the wall (then dissociate into atoms)
- 2D treatment 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



Kinetic equation for neutral atoms and ions

kinetic source

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

ionization

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

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

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

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

charge exchange rate coefficient

n_0 = neutral atom density
$n_i = n_e$ = 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

$$n_0 = \int dv_x G(v_x)$$

$$\partial_t v_{0y} = -v_{0x} \partial_x (v_{0y}) + h_{cx} \langle n_i \rangle_y \left(\langle v_y \rangle_y - v_{0y} \right) - \frac{1}{n_0} S_{n0} v_{0y}$$

$$\mathbf{v}_0 = \mathbf{e}_x \int dv_x v_x G(v_x) / n_0 + \mathbf{e}_y v_{0y}$$

neutrals are born with $v_y = 0$

Plasma equations – 2D SOLT limit

- Warm ion, no Boussinesq approximation

$$\partial_t n_e + \mathbf{v}_E \cdot \nabla n_e = -\nabla_\| \Gamma_\| + h_{iz} n_e n_0 - \nabla \cdot \Gamma_{\perp n} + S_n$$

$$\nabla \cdot \frac{d}{dt}\left(\frac{n_i m_i c^2}{B^2}\nabla_\perp \Phi\right) + T_i \text{ terms} = \nabla_\| J_\| - \frac{2c}{B}\mathbf{b}\times\nabla p \cdot \kappa + \frac{m_i c}{B}\mathbf{b}\cdot\nabla\times\mathbf{F}_{i0}$$

$$\partial_t T_e + \mathbf{v}_E \cdot \nabla T_e = -\frac{2}{3n_e}\nabla_\| q_{e\|} + \frac{T_e}{n_e}\nabla_\| \Gamma_\| - h_{iz} n_0 (\frac{2}{3}E_{iz} + T_e) - \frac{2}{3n_e}\nabla \cdot \mathbf{q}_{\perp e} + \frac{T_e}{n_e}\nabla \cdot \Gamma_{\perp n} + S_{Te}$$

$$\partial_t T_i + \mathbf{v}_E \cdot \nabla T_i = -\frac{2}{3n_e}\nabla_\| q_{i\|} + \frac{T_i}{n_e}\nabla_\| \Gamma_\| + (h_{iz} + h_{cx}) n_0 (\frac{2}{3}E_0 - T_i) - \frac{2}{3n_e}\nabla \cdot \mathbf{q}_{\perp i} + \frac{T_i}{n_e}\nabla \cdot \Gamma_{\perp n} + S_{Ti}$$

- Definitions:

$$\mathbf{v}_i = \mathbf{v}_E + \mathbf{v}_{di}$$

$$\mathbf{F}_{i0} = h_{cx} n_i n_0 (\mathbf{v}_0 - \mathbf{v}_i) + h_{iz} n_e n_0 \mathbf{v}_0$$

$$\mathbf{q}_{\perp j} = -n_e D_{Tj} \nabla T_j$$

$$S_{Tj} = \frac{1}{n_e}(\frac{2}{3}H_j - T_j S_n)$$

$$n_0 E_0 \equiv \frac{1}{2} m_i \alpha^2 \int dv_x\, v_x^2\, G(v_x),\ 1 \le \alpha^2 \le 3$$

isotropization factor

$$\Gamma_{\perp n} = -D_n \nabla n_e$$

$$E_{iz} = \text{ionization energy cost}$$

Fluid model for neutral molecules
(extended model)

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

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

puff or recycling

$$D_{m0} = \frac{v_{tm0}^2}{2\nu_{m0}}$$

molecular dissociation

- Source term for the neutral atom equation:
  - atoms created by dissociation have the Franck-Condon energy ~ 3eV = $m_i v_{FC}^2$

$$S_0 = 2 h_{md} n_e n_{m0} \frac{e^{-v_x^2/2v_{FC}^2}}{(2\pi)^{1/2} v_{FC}}$$

Wall recycling boundary condition

molecular flux from wall ion flux to wall neutral atom and molecular flux to wall

$$\Gamma_{m0}^{+} = -\frac{1}{2}R_i\Gamma_i^{-} - \frac{1}{2}R_0\Gamma_0^{-} - R_{m0}\Gamma_{m0}^{-}$$

R_j = recycling coefficient

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

- Limit of rapid molecular dissociation, $h_{md} \to \infty$: neglect n_{m0} and Γ_{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:

$$G(x_w, v_x) = (R_i\Gamma_i^{-} + R_0\Gamma_0^{-})\frac{e^{-v_x^2/2v_{FC}^2}}{v_{FC}^2},\ v_x < 0$$

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 α

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

- 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

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

$$\frac{1}{L_x} E_0 >> h_{cx} n_i T_i \quad \Leftrightarrow \quad E_0 >> \frac{L_x}{\lambda_{0,MFP}} T_i$$

Total power balance

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

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

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

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

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