Effects of neutral transport on plasma scrape-off layer turbulence in gyrokinetic simulations

by

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in collaboration with

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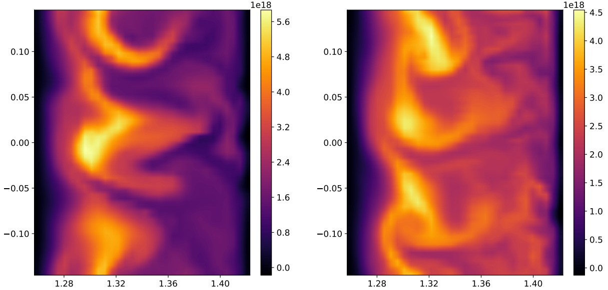
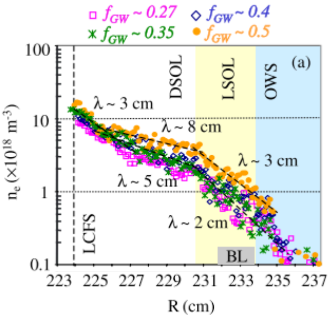


Neutrals play key role in tokamak boundary physics

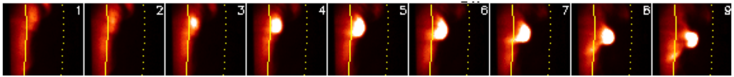
- Scrape-off layer (SOL) sets boundary conditions for the core and determines how heat and particles are exhausted

- Neutrals present via neutral beam injection, gas puffing, and recycling

- Necessary to explore how neutrals dynamically impact SOL plasma properties such as
  - Plasma profiles and density shoulder formation
  - Turbulence and blob dynamics
  - Heat flux width



DIII-D SOL density profiles
(Rudakov et al. NF 2005)



GPI images of blobs from NSTX

Coupled first-principles models of plasma and neutral dynamics necessary for predictive SOL modeling

How do neutral interactions affect plasma turbulence in the SOL?

Plasma model (columns) / **Neutral model** (rows)

	fluid	gyrokinetic
fluid	nHESEL (2D) GRILLIX trans-neut, Hermes	
kinetic	GBS nSOLT (2D)	XGC1 **Gkeyll**

- Gkeyll couples continuum gyrokinetic solver with continuum kinetic solver
  - ***Why GK plasma?*** SOL mean free paths not small enough to justify the Braginskii fluid closure and kinetic flux limiting of parallel heat transport is important.
  - ***Why kinetic neutrals?*** Valid for large range of SOL parameters, including long mean free path neutrals.
  - ***What's new?*** Continuum coupling avoids noise issues, achieves improved accuracy for given resolution at reasonable computational cost

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Continuum kinetic neutral transport model coupled to continuum gyrokinetic code in SOL simulations to probe effects of neutrals on plasma dynamics

- Description of Gkeyll and kinetic neutral model
- NSTX SOL simulations in simplified geometry
- Extension to shaped SOL geometries with seeded blob simulations
- Conclusions and outlook

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Gkeyll facilitates a kinetic model for neutrals

- A computational framework for modeling fusion, astrophysical, and space plasmas and neutral fluids with continuum kinetic and fluid solvers
- Uses a discontinuous Galerkin (DG) algorithm, which preserves conservation properties
- Modular “App” system facilitates development
- Contains full-*f* continuum GK solver with options for
  - EM fluctuations (Mandell JPP 2020, PhD Thesis 2021)
  - Shaped geometries of open and closed field lines without an X-point (Francisquez arXiv:2110.02249)
  - Atomic neutral interactions (Bernard PoP 2022)

https://github.com/ammarhakim/gkyl

https://gkeyll.readthedocs.io

Continuum kinetic models coupled via collisional terms

- Plasma species modeled with full-f electrostatic GK equation in the long-wavelength limit, $f_s(\boldsymbol{R}, v_\parallel, \mu, t)$:

$$\frac{\partial \mathcal{J}_s f_s}{\partial t} + \nabla \cdot (\mathcal{J}_s \{\boldsymbol{R}, H_s\} f_s) + \frac{\partial}{\partial v_\parallel}(\mathcal{J}_s \{v_\parallel, H_s\} f_s) = \mathcal{J}_s C[f_s] + \mathcal{J}_s S_s \tag{1}$$

$$H_s = \frac{1}{2} m v_\parallel^2 + \mu B + q_s \phi, \tag{2}$$

$$-\nabla \cdot \left(\frac{n_{i0}^g e^2 \rho_{s0}^2}{T_{e0}} \nabla_\perp \phi \right) = \sigma_g = e[n_i^g(\boldsymbol{R}, t) - n_e(\boldsymbol{R}, t)]. \tag{3}$$

- Neutral dynamics modeled using the Vlasov solver including **electron-impact ionization** and **charge exchange** via collisional terms:

$$\frac{\partial f_n}{\partial t} + \nabla \cdot (\boldsymbol{v} f_n) = C[f_n] \tag{4}$$

- **Wall recycling** included as boundary condition in parallel direction

Maxwellian distribution functions used for interaction terms on different phase-space grids

- Plasma species are evolved on GK grid and neutrals on Vlasov grid
- Shared configuration space but different velocity space
- Use fluid moments to project ion and neutral distribution function as Maxwellian on other grid

$$\frac{d}{dt}\mathcal{J}f_e(\boldsymbol{R}, v_\parallel, \mu, t) = n_n\langle\sigma_{iz}v_e\rangle[2\mathcal{J}F_{M,gk}(n_e, u_{z,n}, v_{th,iz}^2) - \mathcal{J}f_e] \quad (5)$$

$$\frac{d}{dt}\mathcal{J}f_i(\boldsymbol{R}, v_\parallel, \mu, t) = n_e\langle\sigma_{iz}v_e\rangle\mathcal{J}F_{M,gk}(n_n, u_{z,n}, v_{th,n}^2) + \sigma_{cx}V_{cx}[n_i\mathcal{J}F_{M,gk}(n_n, u_{z,n}, v_{th,n}^2) - n_n\mathcal{J}f_i], \quad (6)$$

$$\frac{d}{dt}f_n(\boldsymbol{x}, \boldsymbol{v}, t) = -n_e f_n\langle\sigma_{iz}v_e\rangle - \sigma_{cx}V_{cx}[n_i f_n - n_n F_M(n_i, u_{\parallel i}, v_{th,i}^2)], \quad (7)$$

Total time derivative $\frac{d}{dt}$ used as shorthand for LHS of GK and Vlasov equations.

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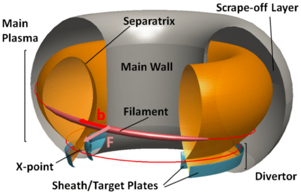
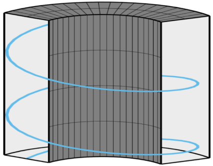
NSTX SOL simulated with Gkeyll in simplified geometry

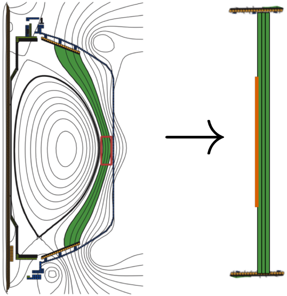
- Simple helical SOL: constant curvature and $L_{||}$, no shear or X-point, open-field lines only



(Carralero PRL 2015)

$\approx$

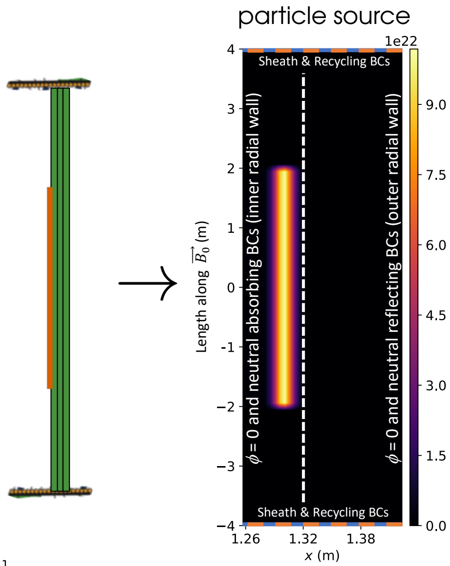




- Field lines are straight in non-orthogonal field-line following coordinate system:
  - z is along $\boldsymbol{B}$, with conducting sheath BCs
  - x is radial coordinate, with Dirichlet ($\phi = 0$) BCs
  - y is binormal coordinate, with periodic BCs

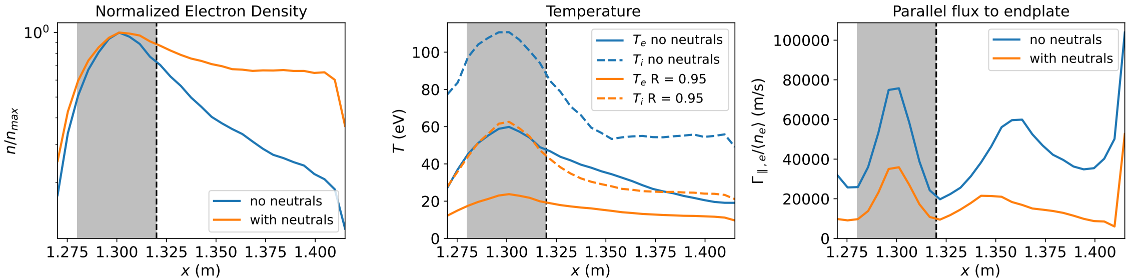
(Images adapted from Mandell APS-DPP 2020)

NSTX SOL simulation with neutrals compared to baseline case without neutrals



- Simulations based on (Shi PoP 2019; Mandell JPP 2020) and include:
  - $L_{||} = 8$ m, $L_x = 50\rho_s \approx 14.6$ cm
  - Deuterium plasma, electrostatic GK electron and ion species (3D2V)
  - Particle and heat source at the midplane mimics flux across "quasi-separatrix" into SOL ($P_{SOL} = 1.35$ MW)
- Simulation with 3D3V Vlasov neutrals include:
  - endplate recycling rate $\alpha_r = 0.95$, $T_{n,rec} = 10$ eV
  - ionization and charge exchange (CX)
  - volumetric particle source floor for neutrals approximates recombination rate

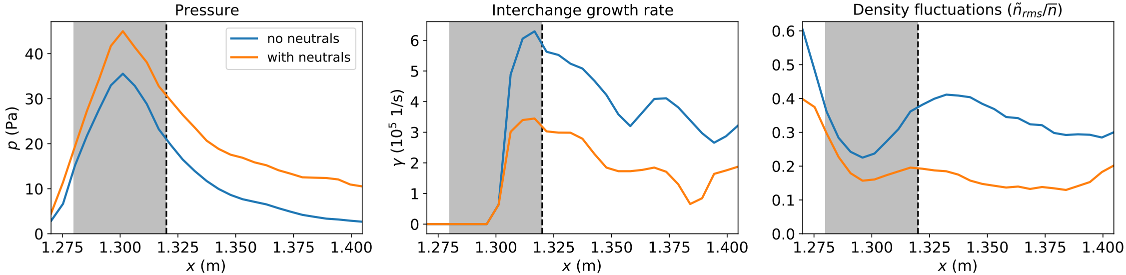
Neutral interactions introduce density profile flattening



Steady-state profiles at midplane, with source region in gray and quasi-separatrix denoted by black dashed line.

- Neutrals increase n_e by factor of 3 via ionization (not shown)
- Density profile flattening similar to experimental observations (Rudakov NF 2005, Vianello NF 2017) and GBS simulations (Mancini NF 2021)
- Neutrals decrease T_i and T_e through CX and ionization, respectively
- Parallel flux is reduced

Neutrals decrease normalized density fluctuations



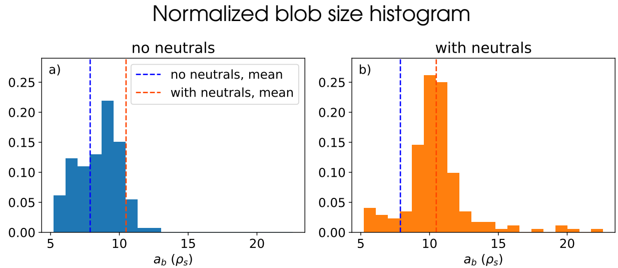
- Decreased temperature for neutrals case results in similar pressure profiles
- Slightly decreased interchange growth rate, $\gamma_I = c_s\sqrt{2/(RL_p)}$
- Corresponding decrease in normalized density fluctuations

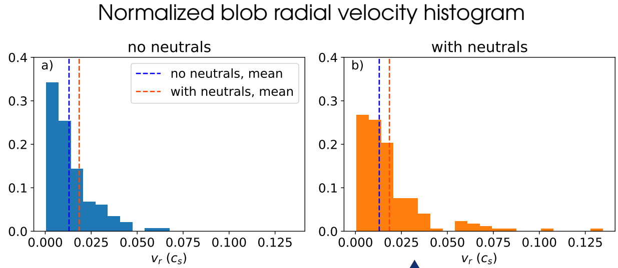
(Bernard PoP 2022)

GENERAL ATOMICS

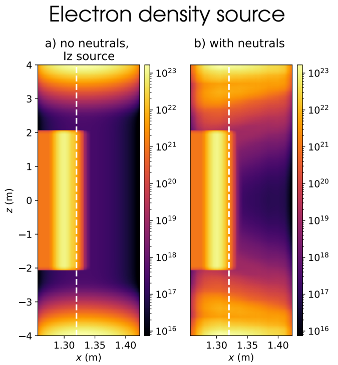
Normalized blob size and uniformity increases with neutrals

- Blob tracking algorithm identifies blobs by density contours that are 2σ above $\langle n_e \rangle$
- Neutrals case has 20% more blobs (200 μs interval at midplane)
- Larger and more uniform blobs for case with neutrals
- Radial velocities similar for both

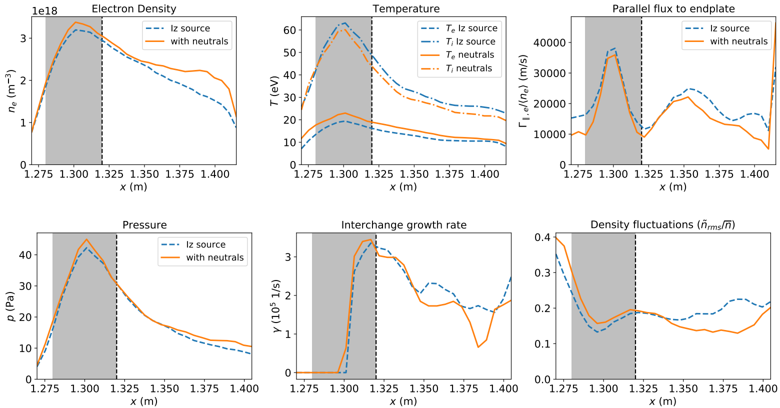




Effective ionization source added to isolate sourcing effects from CX collisions



Source term added to simulation without neutrals (a) to mimic ionization particle source in (b).



- Ionization source accounts for most differences
- Does not capture density flattening and reduced fluctuations at large radii

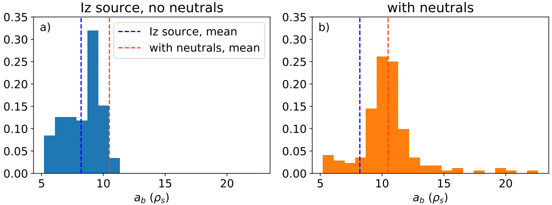
GENERAL ATOMICS

CX collisions result in larger, slower blobs

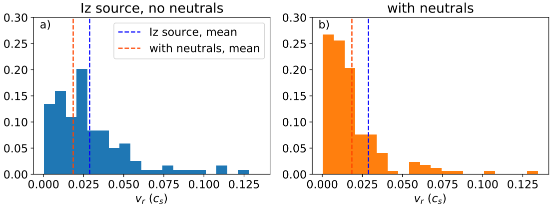
- Simulation with neutrals had 25% more blobs compared to case with ionization source and no neutrals
- Blobs are larger and slower in case with neutrals

(Bernard PoP, in preparation)

Normalized blob size histogram



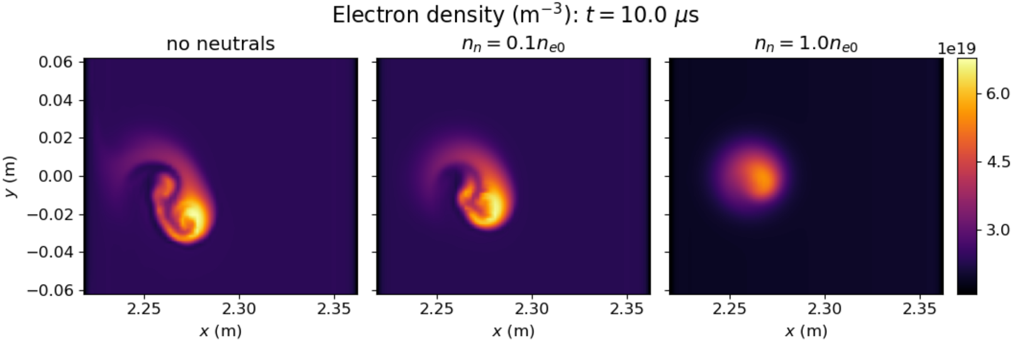
Normalized blob radial velocity histogram



GENERAL ATOMICS

Charge exchange increases blob coherency and reduces radial velocity in seeded blob simulations

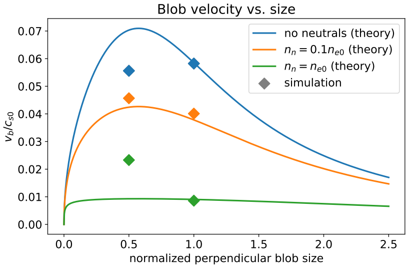
- Seeded blob simulations conducted with DIII-D SOL parameters
- Static background neutrals, only CX
- 3 cases: $n_n = [0.0, 0.1, 1] \cdot n_{e0}$
- Blobs more compact as neutral density is increased (left to right below)

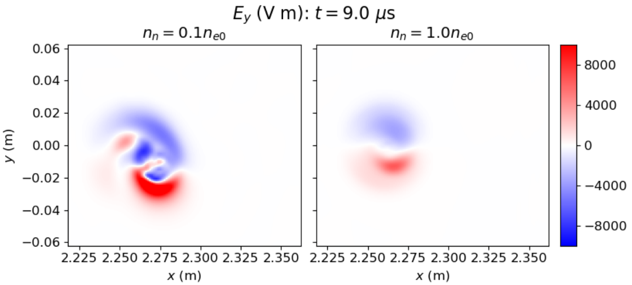


GENERAL ATOMICS

Neutrals reduce blob polarization

- Simulations follow theoretical scaling predictions (Krasheninnikov JPP 2008) that CX neutral collisions will decrease radial velocity
- As neutral density is increased, binormal electric field magnitude E_y decreases





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Neutral model adapted for shaped geometries

- Neutral distribution function evolved in mixed coordinates: $f_n(x, y, z, v_X, v_Y, v_Z)$
- Physical space is field-line following and velocity space is Cartesian
- Geometric terms enter through Jacobian and streaming term in Vlasov equation

$$\frac{\partial \mathcal{J} f_n}{\partial t} + \nabla \cdot (\mathcal{J} \mathbf{v} f_n) = C[\mathcal{J} f_n] \tag{8}$$

$$\nabla \cdot (\mathcal{J} \mathbf{v} f_n) = \frac{\partial}{\partial x}(\mathcal{J} \mathbf{v} \cdot \nabla x) + \frac{\partial}{\partial y}(\mathcal{J} \mathbf{v} \cdot \nabla y) + \frac{\partial}{\partial z}(\mathcal{J} \mathbf{v} \cdot \nabla z) \tag{9}$$

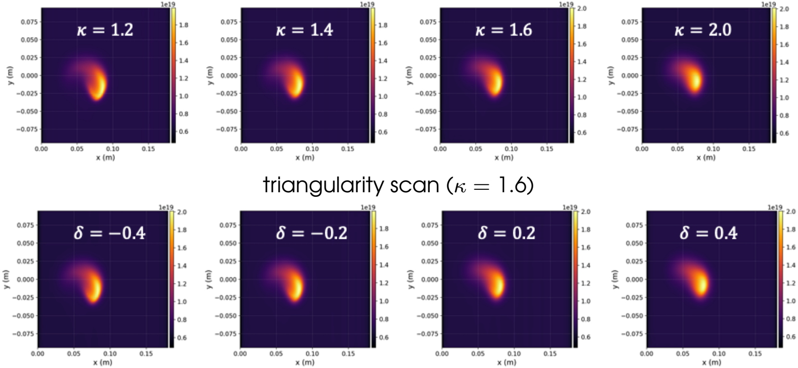
- Geometric terms calculated in code from mapping given in input file (currently using analytic Miller approximation for equilibrium)

Seeded blob simulations scan elongation and triangularity with static neutrals

- Inner-wall limited geometry with DIII-D parameters
- Constant background n, T, no source
- $n_0 = 7 \times 10^{18}\ \mathrm{m}^{-3}$, $T_{e0} = T_{i0} = 40$ eV
- Static atomic D neutrals with ionization and CX
- Density profiles assume endplate and main chamber recycling
- $T_n = 10$ eV

Electron density at 10 μs

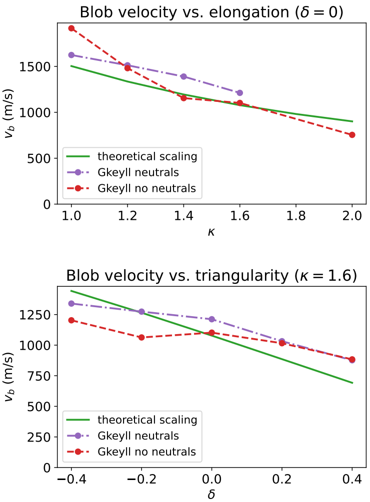
elongation scan ($\delta = 0$)



GENERAL ATOMICS

Shaping affects blob dynamics more than neutral interactions

- Curvature drive decreases as elongation and triangularity increase → radial blob velocities decrease
- Neutral interactions affect sheath-balanced term in velocity scaling
- Increase in sheath density and decrease in parallel outflow nearly offset each other, leaving sheath term relatively unchanged
- Radial blob velocities similar to simulations without neutral interactions



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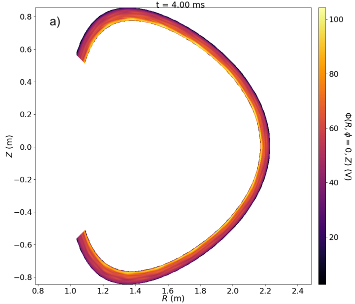
Conclusions

- Presented results of a continuum kinetic neutral transport model coupled to the continuum gyrokinetic code in Gkeyll
- Including neutrals in helical geometry NSTX SOL simulations resulted lower n, T, flatter density profile and reduced fluctuations and flows (Bernard PoP 2022)
- CX effects contribute to density flattening, reduced turbulence levels, and larger, slower blobs (Bernard PoP, in preparation)
- Neutral model extended to general geometries
- Static neutrals have small effect in shaped SOL seeded blob simulations
- Radial blob velocities decrease as κ, δ are increased, consistent with theoretical scalings

Ongoing and future work



ϕ from DIII-D $+\delta$ SOL simulation

- Fully turbulent shaped SOL simulations of DIII-D ($\pm\delta$) without neutrals have been carried out
- DIII-D $+\delta$ simulations with open+closed field line geometry now running, inner-wall limited
- Parallelization over species available and GPU-ification of GK solver+neutral interactions nearly complete
- Validation with DIII-D experimental data
- **Future developments**: models for recombination and impurity radiation, X-point geometry, interpolation scheme to retain all kinetic effects from neutrals ...

Thanks for your attention!

For more information:
https://github.com/ammarhakim/gkyl
https://gkeyll.readthedocs.io

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Extra Slides

Electron-impact ionization model uses average reaction rate

$$e^- + n \rightarrow i^+ + 2e^- - E_{iz},$$

- Integral over velocity space is approximated by statistical average (Wersal & Ricci NF 2015):

$$\frac{d}{dt}\mathcal{J} f_e(\boldsymbol{R}, v_\parallel, \mu, t) = n_n \langle \sigma_{iz} v_e \rangle [2\mathcal{J} f_{M,e}(n_e, \boldsymbol{u}_n, v_{th,iz}^2) - \mathcal{J} f_e], \quad (10)$$

where f_M accounts for low-energy electrons and $v_{th,iz}^2 = \frac{v_{th,e}^2}{2} - \frac{E_{iz}}{3m_e}$.

- Ion and neutral equations given by simply

$$\frac{d}{dt}\mathcal{J} f_i(\boldsymbol{R}, v_\parallel, \mu, t) = n_e \mathcal{J} f_n \langle \sigma_{iz} v_e \rangle, \quad (11)$$

$$\frac{d}{dt} f_n(\boldsymbol{R}, \boldsymbol{v}, t) = -f_n n_e \langle \sigma_{iz} v_e \rangle, \quad (12)$$

- Fitting function (Voronov AD&NDT 1997) is used to approximate $\langle \sigma_{iz} v_e \rangle$.

Charge exchange model uses effective ‘relative velocity’

$$i^+ + n \rightarrow n + i^+$$

- Integrals over velocity space are approximated as in (Meier & Shumlak PoP 2012):

$$\frac{d}{dt}\mathcal{J} f_i(\boldsymbol{R}, v_\parallel, \mu, t) = \sigma_{cx} V_{cx} (n_i \mathcal{J} f_n - n_n \mathcal{J} f_i), \quad (13)$$

$$\frac{d}{dt} f_n(\boldsymbol{R}, \boldsymbol{v}, t) = -\sigma_{cx} V_{cx} (n_i f_n - n_n f_i), \quad (14)$$

where the “relative velocity” is defined as

$$V_{cx}^2 \equiv \frac{4}{\pi}(v_{t,i}^2 + v_{t,n}^2) + (\boldsymbol{u}_i - \boldsymbol{u}_n)^2 \quad (15)$$

- CX cross section σ_{cx} is approximated by a fitting function.

Model for wall recycling implemented

- In 1D3V (1 spatial dimension and 3 velocity space dimensions), neutral distribution function at the boundary defined by:

$$f_n(v_x, v_y, v_z, z = z_{ghost}) = \alpha_b f_n(v_x, v_y, -v_z, z_{\min}) + C f_{M,rec}(T = T_{n,rec}), \quad (16)$$

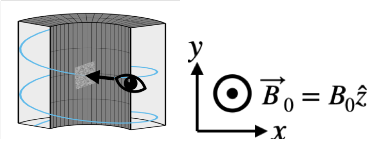
  where z and v_z directed along B and α_b is reflection coefficient.

- Maxwellian is scaled such that incoming flux of neutrals equals outgoing flux of ions multiplied by recycling fraction α_r:

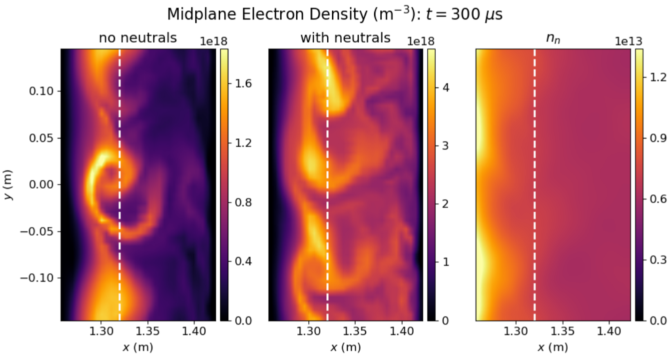
$$C \int_{v_{x,\min}}^{v_{x,\max}} \int_{v_{y,\min}}^{v_{y,\max}} \int_{0}^{v_{z,\max}} dv_x dv_y dv_z \; v_z \, f_{M,rec} \doteq \alpha_r \frac{2\pi}{m} \int_0^{\mu_{\max}} \int_{v_{\| i,\min}}^{0} dv_\| \, d\mu \; v_{\| i} \mathcal{J} f_i(z = z_{\min}). \quad (17)$$

Qualitative differences in density evolution observed

- **"no neutrals"**: only GK species, similar to closed divertor scenario
- **"with neutrals"**: couples to Vlasov neutrals with $\alpha_r = 0.95$, similar to open divertor scenario
- Simulations run to 0.4 ms ($\sim 4\tau_i$):
  - **no neutrals** 1.5 days on 512 CPUs
  - **with neutrals** 7.5 days on 512 CPUs ($\sim$5x longer)

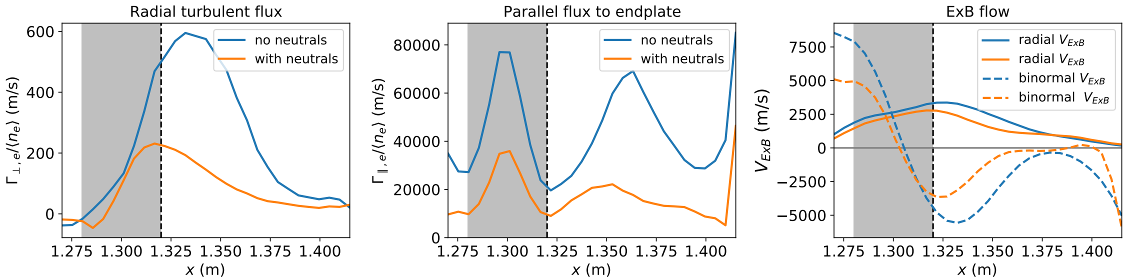


Midplane view visual aides



From left to right, electron density (n_e) in simulation without neutrals, electron density (n_e) in simulation with neutrals, and neutral density (n_n).

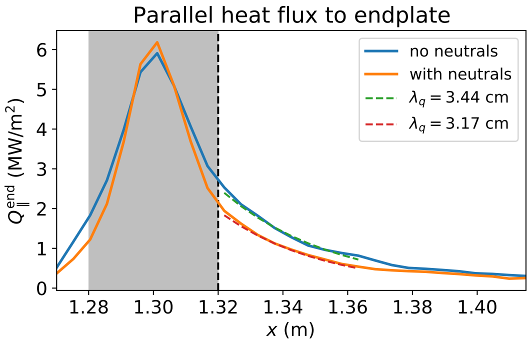
Neutrals decrease plasma flows

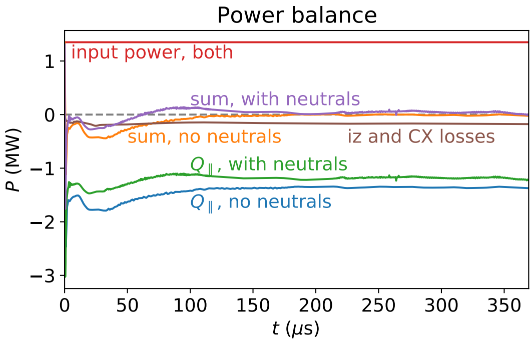


- Radial flux ($\Gamma_r = \langle \tilde{n}_e \tilde{v}_r \rangle$) normalized to n_e decreases with neutrals
- Parallel electron particle flux normalized to n_e decreases with neutrals
- ExB flow magnitudes decrease slightly with neutrals

GENERAL ATOMICS

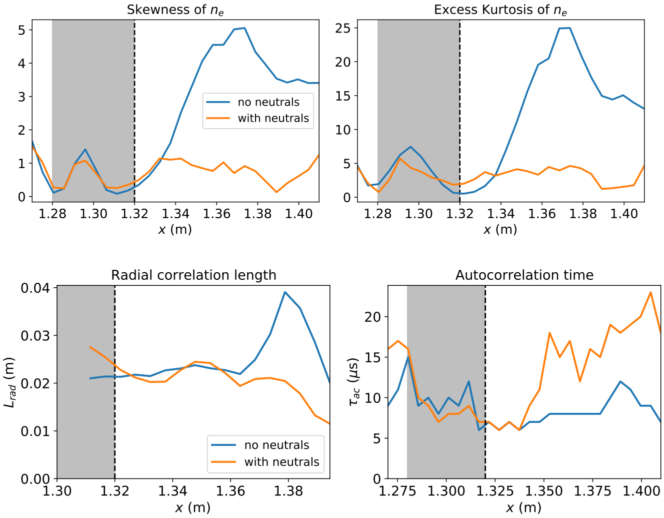
Parallel heat flux width slightly reduced with neutrals





- Heat flux is calculated at upper endplate ($z = L_z/2$), sum of ion and electron contributions
- Profiles fit to exponential to estimate width at quasi-separatrix: $Q_\parallel^{end}(x = 1.32)e^{-x/\lambda_q}$
- Neutrals decrease width and magnitude slightly

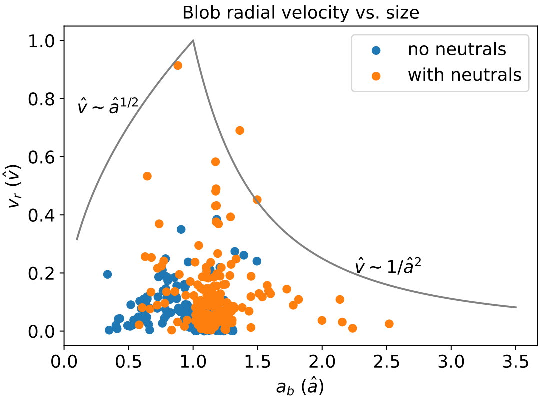
Neutrals increase temporal coherency of turbulent structures



$$\text{Skewness} = E[\tilde{n}^3]/\sigma^3$$
$$\text{Excess kurtosis} = E[\tilde{n}^4]/\sigma^4 - 3$$

- Neutral interactions decreased intermittency with lower skewness and kurtosis on LFS
- Radial correlation lengths are comparable but autocorrelation times longer with neutrals
- Suggests longer temporal coherency of blobs when neutrals included

Blob velocity scalings indicate sheath-interchange regime dominates

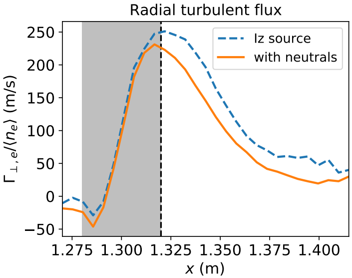


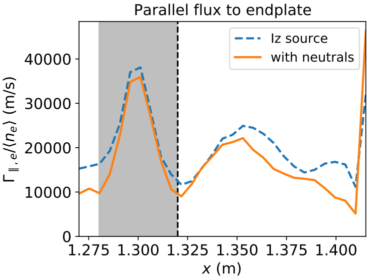
- Data bounded by theoretical scaling laws (Myra et al. PoP 2006).
- Reference velocity and size given by:

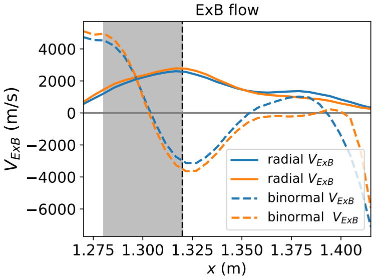
$$\hat{a} = \left(\frac{4L_C^2}{\rho_s R}\right)^{1/5} \rho_s, \qquad \hat{v} = \left(\frac{2L_C\rho_s^2}{R^3}\right)^{1/5} c_s.$$

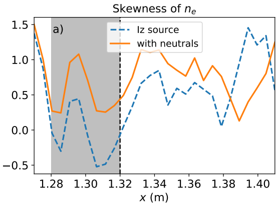
- Blobs likely in sheath-interchange regime
- Scans in collisionality and including general geometry required to access other regimes.

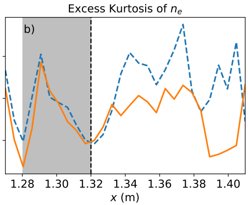
Ionization source plots

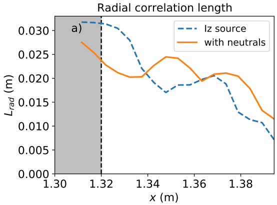


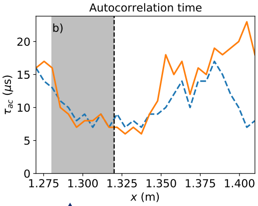








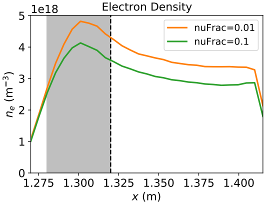


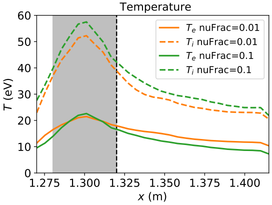


GENERAL ATOMICS

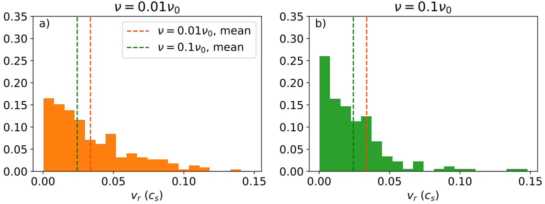
Increased plasma collisionality has small effect on neutral simulations

- Plasma collisions modeled with Lenard-Bernstein operator with a constant Spitzer collision frequency ν_0 calculated from input parameters
- Previous neutral simulation used reduced collisionality $\nu = 0.01\nu_0$ for faster computation
- Simulations with neutrals run with collisionalities, $\nu = [0.01, 0.1] \cdot \nu_0$ and recycling rate $\alpha_r = 0.75$
- Results similar except for minor differences in density, temperature and blob speed.



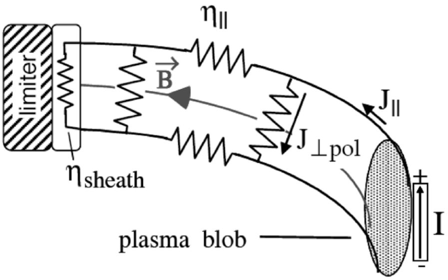


Normalized blob radial velocity



CX neutrals reduce radial blob velocity

- Estimate radial blob velocity by modeling blob as a circuit and using quasineutrality condition $\nabla \cdot \boldsymbol{j} = 0$.



From (Krasheninnikov JPP 2008)

$$v_b = \frac{2\sqrt{\frac{a_b}{R}}c_s}{1 + \frac{2\sqrt{R}}{\rho_s^2 L_{\|}}\sigma a_b^{5/2} + \frac{\sqrt{R a_b \nu_{cx}}}{2c_s}} \frac{\delta p}{p} \qquad (18)$$

curvature drive
sheath current damping term
neutral CX damping term