A kinetic model of ions and neutrals with wall boundary conditions in edge plasmas

M. Barnes
M. R. Hardman, J. Omotani, F. I. Parra, and S. L. Newton

ExCALIBUR

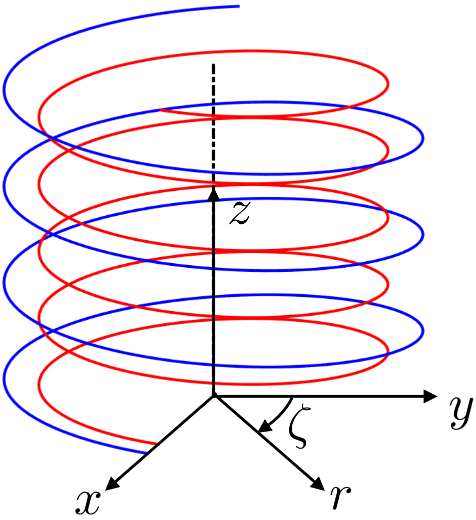
Turbulent Dynamics of Tokamak Plasmas (TDoTP)

Research challenges for models of the Edge

- Variation in the profiles on the scale of the eddies
  ⇒ **Global models**
- Transition from closed to open field lines
  ⇒ **Avoid coordinate singularity at the separatrix**
- Large fluctuation sizes
  ⇒ **Full-f models**
- Wall boundary conditions
  ⇒ **Sheath physics must be captured**
- Transition from hot 'collisionless' core to cold 'fluid' edge
  ⇒ **Need appropriate representation of velocity space**
- Complex interactions between charged and neutral particles
  ⇒ **Kinetic treatment of neutrals and ions**

Minimal model for investigating kinetic edge physics

- Full-f Drift Kinetic equations
- 2D-2V Drift kinetics for ions
- 2D-3V Kinetics for neutrals
- (plus moments-based evolution in 1D-1V)
- Electrostatic, with Boltzmann Electrons
- Helical Geometry
- Wall boundaries for the sheath
- Model Charge-exchange (CX) and Ionization (IZ) collisions



z
y
ζ
x
r

Model drift-kinetic equations: part I

- Gyroaveraged equation for $F_i = F_i(r, z, v_\parallel, v_\perp)$:

$$\frac{\partial F_i}{\partial t} + \left(b_z v_\parallel - \frac{E_r}{B} \right) \frac{\partial F_i}{\partial z} + \frac{E_z}{B} \frac{\partial F_i}{\partial r} + \frac{e b_z E_z}{m_i} \frac{\partial F_i}{\partial v_\parallel} = - R_{\mathrm{in}} \left(n_n F_i - n_i \langle F_n \rangle \right) + R_{\mathrm{ion}} n_e \langle F_n \rangle + S_i.$$

- Equation for $F_n = F_n(r, z, v_r, v_z, v_\zeta)$:

$$\frac{\partial F_n}{\partial t} + v_z \frac{\partial F_n}{\partial z} + v_r \frac{\partial F_n}{\partial r} = -R_{\mathrm{in}} \left(n_i F_n - n_n F_i \right) - R_{\mathrm{ion}} n_e F_n + S_n.$$

- R_{in}, the CX rate; R_{ion}, the IZ rate; S_i, the ion source function; S_n, the neutral source function.

Model drift-kinetic equations: part II

- Definitions of the ion and neutral densities:

$$n_i(z,r,t) = 2\pi \int_{-\infty}^{\infty} dv_\parallel \int_0^{\infty} dv_\perp v_\perp F_i(z,r,v_\perp,v_\parallel,t),$$

$$n_n(z,r,t) = \int_{-\infty}^{\infty} dv_\zeta \int_{-\infty}^{\infty} dv_r \int_{-\infty}^{\infty} dv_z F_n(z,r,v_\zeta,v_r,v_z,t).$$

- Assumption of Boltzmann (adiabatic) electrons:

$$n_i = n_e = N_e \exp\left(\frac{e\phi}{T_e}\right).$$

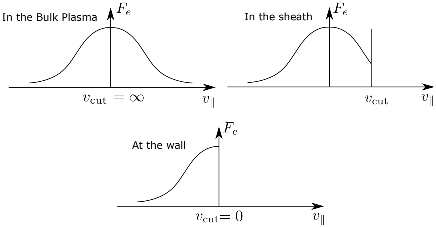
- Definition of the electric field:

$$E_z = -\frac{\partial \phi}{\partial z}, \text{ and } \quad E_r = -\frac{\partial \phi}{\partial r}.$$

Wall boundary conditions: part I – electrons and ions

- Logical sheath for electrons that is compatible with a Boltzmann response in the bulk plasma Stangeby (2000)

Electron distribution F_e at $z = -L_z/2$



$$J_{\|} = 0 \text{ at the wall plates} \Rightarrow N_e = -\sqrt{\frac{4\pi m_e}{m_i}} \exp\left(-\frac{e\phi_W}{T_e}\right) \frac{J_{\|,i}}{e c_s}.$$

- Sheath is electron repelling
  (low-energy electrons are reflected into the bulk plasma)
- Ions do not return from the wall

$$F_i(z = -L_z/2, v_{\|} > E_r/B_z, v_{\perp}, t) = 0$$
$$F_i(z = L_z/2, v_{\|} < E_r/B_z, v_{\perp}, t) = 0.$$

Wall boundary conditions: part II – neutrals

- Neutrals are thermally emitted from the wall with a Knudsen cosine distribution F_{Kw}

- The neutrals are sourced by the inward flux of ions $\Gamma_{i,\pm L_z/2}$ and neutrals $\Gamma_{n,\pm L_z/2}$ at $z = \pm L_z/2$

$$F_n(z=-L_z/2, v_z>0, v_r, v_\zeta, t) = \left(\Gamma_{i,-L_z/2} + \Gamma_{n,-L_z/2}\right) F_{Kw}\left(v_z, \sqrt{v_r^2 + v_\zeta^2}\right),$$

$$F_n(z=L_z/2, v_z<0, v_r, v_\zeta, t) = \left(\Gamma_{i,L_z/2} + \Gamma_{n,L_z/2}\right) F_{Kw}\left(v_z, \sqrt{v_r^2 + v_\zeta^2}\right),$$

- F_{Kw} is defined by

$$F_{Kw}(v_z, v_t) \doteq \frac{3}{\pi}\left(\frac{m_i}{2T_w}\right)^2 \frac{|v_z|}{\sqrt{v_z^2 + v_t^2}} \exp\left(-\frac{m_i\left(v_z^2 + v_t^2\right)}{2T_w}\right)$$

Moment-based evolution

- We can reformulate drift-kinetics in terms of a distribution function normalised by its moments, which are then evolved separately
- E.g., in the 1D-1V case

$$\hat{g}_s(z, \hat{w}_\parallel, t) \doteq f_s(z, \hat{w}_\parallel, t) \frac{v_{\mathrm{th},s}(z,t)}{n_s(z,t)},$$

where $\hat{g}_s$ is a function of the normalised peculiar velocity

$$\hat{w}_\parallel \doteq \frac{v_\parallel - u_s}{v_{\mathrm{th},s}}.$$

The lowest three moments of $\hat{g}_s$ satisfy

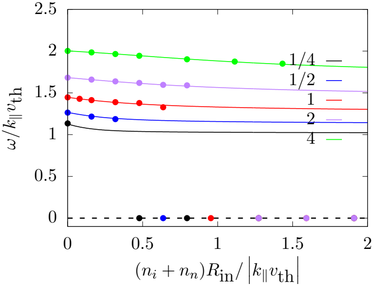
$$\int d\hat{w}_\parallel \left(1, \hat{w}_\parallel, \hat{w}_\parallel^2\right) \hat{g}_s = \left(1, 0, \frac{1}{2}\right).$$

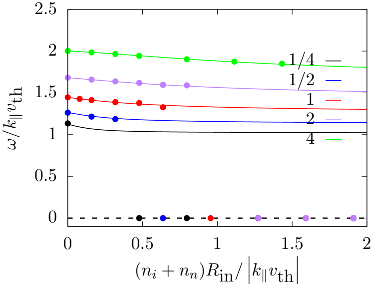
- These constraints must be enforced as we evolve $\hat{g}_s$, n_s, $v_{\mathrm{th},s}$, and u_s.
- This method may be advantageous in the Edge where 'fluid' models are appropriate in the colder parts of the plasma.

Numerical Implementation

- For time stepping, we utilise a Strong Stability Preserving (SSP) Runge-Kutta (RK) scheme Shu and Osher (1988); Gottlieb and Shu (1998); Gottlieb et al. (2001).
- For the spatial and velocity discretisation both finite difference and Chebyshev spectral methods are implemented.
- Finite differences: uniform grid; third order upwind derivatives Durran (1999); integration by the composite Simpson's rule.
- Chebyshev spectral elements: Gauss-Chebyshev-Lobatto grid on each element Abramowitz and Stegun (1972); Fast Fourier Transforms for derivatives Frigo and Johnson (2005. Special issue on Program Generation, Optimization, and Platform Adaptation); integration via Clenshaw-Curtis quadrature rules Clenshaw and Curtis (1960).
- OpenMPI support Byrne et al. (2021). Symbolic algebra via the `Symbolics.jl` package Gowda et al. (2021); Sym. Interpolation via `Interpolations.jl` Int.
- All revisions of the 'moment kinetics' code are written in the Julia programming language.
- The master 1D-1V code currently available on GitHub at `https://github.com/mabarnes/moment_kinetics`.
- The latest 2D-3V code is held in the branch `https://github.com/mabarnes/moment_kinetics/tree/radial-vperp-standard-DKE-with-neutrals`.

- Solving the 1D-1V system for perturbations about an equilibrium Maxwellian, we obtain frequencies and damping rates that vary with neutral density in agreement with analytical theory.

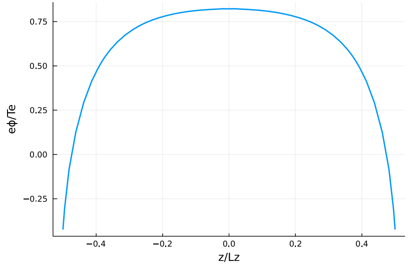


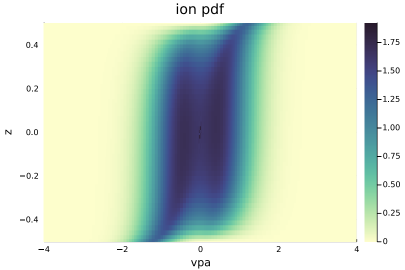


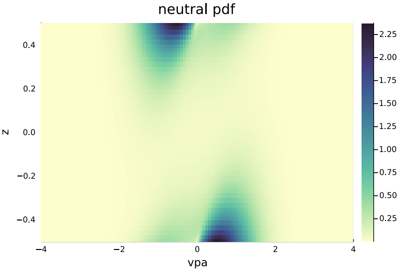
Plasma on open field lines: physics study – neutral accumulation

- Allowing the 1D-1V system to run to steady state, with $R_{\text{in}} = R_{\text{ion}} = 2$, we find a solution that satisfies the kinetic Bohm criterion (Harrison and Thompson, 1959)

$$\int dv_{\parallel} \frac{c_s^2}{v_{\parallel}^2} f_i(v_{\parallel}) \leq 2n_i,$$





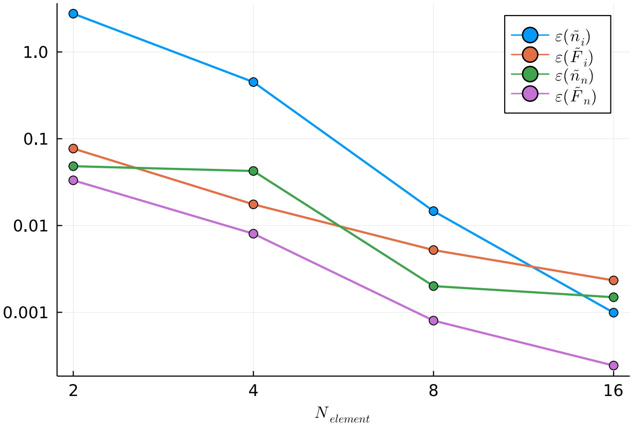


Method of manufactured solutions (MMS) tests

- Analytical solutions are difficult to obtain in general.
- Instead use a ‘manufactured’ target solution (MS) to test the code.
- Specify a desired output F_s, and find S_s such that F_s is the solution.
- We (partially) automate the computation of S_s with the Julia `Symbolics.jl` package.
- Caveat: F_s must satisfy the right boundary conditions.
- The form of the MS determines which operators are tested.

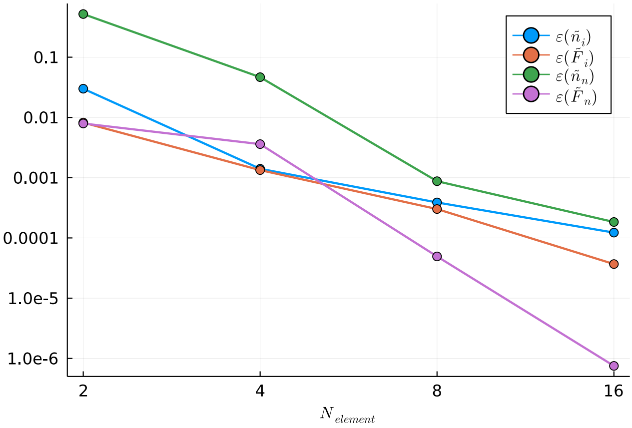
MMS test – Periodic boundary conditions

- Here we show a case with CX and IZ collisions, in 2D, with periodic boundary conditions in (r, z).
- We scan in the number of velocity elements $N_{element}$ in the spectral-element $\mathbf{v}$ grids $\Rightarrow$ Convergence!



MMS test – Wall boundary conditions

- Here we show a case without collisions, in 1D, with wall boundary conditions in z, and all velocity coordinates.
- We scan in the number of velocity elements $N_{element}$ in the spectral-element $\mathbf{v}$ grids $\Rightarrow$ Convergence!



- These tests currently do not converge well with $E_r \neq 0$.

Conclusions

- We have a full-f model that contains features relevant to edge physics.
- The model is comprehensively covered by MMS tests.
- Standard drift kinetic and moment kinetic models agree for periodic BCs, but moment kinetic model challenging for wall BCs.
- Some cases with wall boundary conditions and $E_r \neq 0$ do not (yet) converge well.
- More physics still to include (see talk by J. Omotani this afternoon)
- Test-driven development allows for rapid progress in well defined programming challenges.

References I

S. Wiesen et al. *J. Nucl. Mater.*, 463:480, 2015.

F.D. Halpern et al. *J. Comput. Phys.*, 315:388, 2016.

S. Ku et al. *J. Comput. Phys.*, 315:467, 2016.

A.H. Hakim et al. *Phys. Plasmas*, 27:042304, 2020.

M.A. Dorf et al. *Phys. Plasmas*, 23:056102, 2016.

A. Geraldini, F.I. Parra, and F. Militello. *Plasma Phys. Control. Fusion*, 60: 125002, 2018.

C. Wersal and P. Ricci. *Nucl. Fusion*, 55:123014, 2015.

H. Bufferand et al. *Nucl. Fusion*, 61:116052, 2021.

P. C. Stangeby. *The Plasma Boundary of Magnetic Fusion Devices*. Institute of Physics Publishing, Bristol and Philadelphia, 2000.

C.-W. Shu and S. Osher. Efficient implementation of essentially non-oscillator shock-capturing schemes. *J. Comp. Phys.*, pages 77:439–471, 1988.

S. Gottlieb and C.-W. Shu. Total variation diminishing runge-kutta methods. *Mathematics of Computation*, pages 67:73–85, 1998.

S. Gottlieb, C.-W. Shu, and E. Tadmor. Strong stability-preserving high-order time discretization methods. *SIAM Rev.*, page 43:89, 2001.

D. R. Durran. *Numerical methods for wave equations in geophysical fluid dynamics*. Springer, 1999.

References II

M. Abramowitz and I. Stegun. *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*. Dover, New York, 1972.

Matteo Frigo and Steven G. Johnson. The design and implementation of fftw3. *Proceedings of the IEEE*, pages 93(2):216–231, 2005. Special issue on Program Generation, Optimization, and Platform Adaptation.

C. W. Clenshaw and A. R Curtis. A method for numerical integration on an automatic computer. *Numerische Mathematik*, page 2:197, 1960.

Simon Byrne, Lucas C. Wilcox, and Valentin Churavy. Mpi.jl: Julia bindings for the message passing interface. *JuliaCon Proceedings*, pages 1(1), 68, 2021. doi: 10.21105/jcon.00068.

Shashi Gowda, Yingbo Ma, Alessandro Cheli, Maja Gwozdz, Viral B Shah, Alan Edelman, and Christopher Rackauckas. High-performance symbolic-numerics via multiple dispatch. *arXiv preprint arXiv:2105.03949*, 2021.

`Symbolics.jl`. URL `https://symbolics.juliasymbolics.org/dev/`.

`Interpolations.jl`. URL `https://github.com/JuliaMath/Interpolations.jl`.

E. R. Harrison and W. B. Thompson. The low pressure plane symmetric discharge. *Proc. Phys. Soc.*, page 74:145, 1959.

Background

- Fluid models dominate the field of edge transport modelling, see, e.g. Wiesen et al. (2015); Halpern et al. (2016).
- There is increasing interest in developing edge kinetic models, see, e.g. Ku et al. (2016); Hakim et al. (2020); Dorf et al. (2016).
- Kinetic effects are needed to accomodate kinetic wall boundary conditions, see, e.g. Geraldini et al. (2018).
- Kinetic effects are needed to capture the impact of collisions between neutrals and ions, see, e.g., Wersal and Ricci (2015); Bufferand et al. (2021).

Wall boundary conditions: part III – neutrals definitions

The fluxes are defined by

$$\Gamma_{i,-L_z/2} \doteq 2\pi \int_{-\infty}^{E_r/B} dv_\parallel \int_0^\infty dv_\perp v_\perp \left| b_z v_\parallel - \frac{E_r}{B} \right| F_i(z = -L_z/2, r, v_\parallel, v_\perp, t)$$

$$\Gamma_{n,-L_z/2} \doteq \int_{-\infty}^{0} dv_z \int_{-\infty}^{\infty} dv_r \int_{-\infty}^{\infty} dv_\zeta \, |v_z| \, F_n(z = -L_z/2, r, v_z, v_r, v_\zeta, t)$$

and

$$\Gamma_{i,L_z/2} \doteq 2\pi \int_{E_r/B}^{\infty} dv_\parallel \int_0^\infty dv_\perp v_\perp \left| b_z v_\parallel - \frac{E_r}{B} \right| F_i(z = L_z/2, v_\parallel, v_\perp, t)$$

$$\Gamma_{n,L_z/2} \doteq \int_{0}^{\infty} dv_z \int_{-\infty}^{\infty} dv_r \int_{-\infty}^{\infty} dv_\zeta \, |v_z| \, F_n(z = L_z/2, v_z, v_r, v_\zeta, t)$$

Measuring errors in the MMS tests

- We define an error on the densities

$$\epsilon(\widetilde{n}_s) = \sqrt{\frac{\sum_{i,j} |\widetilde{n}_s(z_i, r_j) - \widetilde{n}_s^{MS}(z_i, r_j)|^2}{N_r N_z}}.$$

- We define an error on the ion distribution function

$$\epsilon(\widetilde{F}_i) = \sqrt{\frac{\sum_{i,j,k,l} |\widetilde{F}_i(v_{\| i}, v_{\perp j}, z_k, r_l) - \widetilde{F}_i^{MS}(v_{\| i}, v_{\perp j}, z_k, r_l)|^2}{N_{v_\|} N_{v_\perp} N_r N_z}}.$$

- We define an error on the neutral distribution function

$$\epsilon(\widetilde{F}_n) = \sqrt{\frac{\sum_{i,j,k,l,m} |\widetilde{F}_n(v_{zi}, v_{rj}, v_{\zeta k}, z_l, r_m) - \widetilde{F}_n^{MS}(v_{zi}, v_{rj}, v_{\zeta k}, z_l, r_m)|^2}{N_{v_z} N_{v_r} N_{v_\zeta} N_r N_z}}.$$

- We specify the following target solutions (2D+3V):

$$\widetilde{n}_i = \frac{3}{2} + \frac{\sin(2\pi\tilde{t})}{10}\left(\sin\left(\frac{2\pi r}{L_r}\right) + \sin\left(\frac{2\pi z}{L_z}\right)\right)$$

$$\widetilde{n}_n = \frac{3}{2} + \frac{\sin(2\pi\tilde{t})}{10}\left(\cos\left(\frac{2\pi r}{L_r}\right) + \cos\left(\frac{2\pi z}{L_z}\right)\right)$$

$$\widetilde{F}_i = \widetilde{n}_i \exp\left(-\tilde{v}_\parallel^2 - \tilde{v}_\perp^2\right)$$

$$\widetilde{F}_n = \widetilde{n}_n \exp\left(-\tilde{v}_z^2 - \tilde{v}_r^2 - \tilde{v}_\zeta^2\right)$$

- We can use this MMS test to investigate any case with periodic boundary conditions

MMS test – Wall boundary conditions: part I

- We specify the following target solution for ions:

$$\widetilde{F}_i = \Bigg[H\left(\overline{v}_\parallel\right)\overline{v}_\parallel^2\left(\frac{1}{2}+\frac{z}{L_z}\right)n_+(r) + H\left(-\overline{v}_\parallel\right)\overline{v}_\parallel^2\left(\frac{1}{2}-\frac{z}{L_z}\right)n_-(r)$$
$$+\left(\frac{1}{2}-\frac{z}{L_z}\right)\left(\frac{1}{2}+\frac{z}{L_z}\right)n_0(r)\Bigg]\exp\left(-\overline{v}_\parallel^2-\tilde{v}_\perp^2\right).$$

$\overline{v}_\parallel = \tilde{v}_\parallel - \rho_*\widetilde{E}_r/2b_z$, $n_+ = n_- = n_0 = 1 + (1/20)\sin(2\pi r/L_r)$.

- We specify the following target solution for neutrals:

$$\widetilde{F}_n = H\left(\tilde{v}_z\right)\left[\widetilde{\Gamma}_{i,-L_z/2}\left(\frac{1}{2}-\frac{z}{L_z}\right)^2+\widetilde{\Gamma}_n\right]\widetilde{F}_{Kw}\left(\tilde{v}_z,\sqrt{\tilde{v}_r^2+\tilde{v}_\zeta^2}\right)$$
$$+H\left(-\tilde{v}_z\right)\left[\widetilde{\Gamma}_{i,L_z/2}\left(\frac{1}{2}+\frac{z}{L_z}\right)^2+\widetilde{\Gamma}_n\right]\widetilde{F}_{Kw}\left(\tilde{v}_z,\sqrt{\tilde{v}_r^2+\tilde{v}_\zeta^2}\right).$$

- We can make the test a 1D-3V test by taking $r = 0$, $b_z = 1$ and $\rho_* = 0$.