Algorithms and results from first continuum full-F simulations of turbulence in tokamak scrape-off-layer

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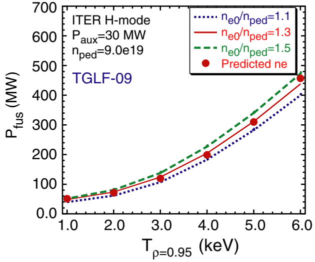
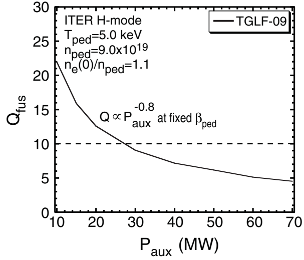
Boundary-plasma strongly affect fusion performance

- Boundary plasma (edge and SOL) believed to set boundary conditions on the core
- Improved confinement associated with transient suppression of edge turbulence[1]
- ITER projections show fusion performance highly sensitive to the H-mode-pedestal temperature, relatively insensitive to auxiliary power heating ('core profile stiffness')
- Need reliable, fully predictive simulations of the pedestal to quantitatively model the core
- How to increase the pedestal pressure?

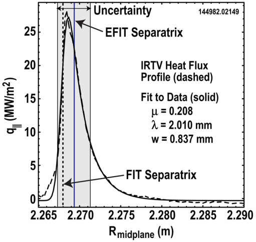




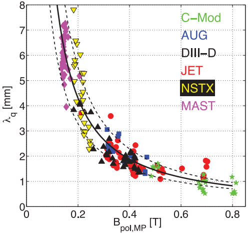
From Kinsey et al., (2011)

SOL power-exhaust problem is potential show-stopper

- Most of power (100 MW on ITER) released in the SOL flows in an extremely narrow channel $\sim$1 mm
- On ITER, need to dissipate most ($\sim$95% (Goldston, 2015)) of this power somehow before it reaches the divertor plates
  - Material limitations $\sim$10 MW m^{-2}, ITER operation can 'easily' reach $\sim$30 MW m^{-2}
- If SOL heat-flux width is too narrow, even steady-state power loads can result in material erosion
  - ITER designs have assumed $\lambda_q = 5$ mm, empirical extrapolation[2] of 1 mm ($B_{\text{pol}} \approx 1.2$ T)



DIII-D from Makowski et al. (2012)



Eich et al. (2013)

Approaches for boundary-plasma simulation

- Sophisticated codes for fluid-based modeling of the boundary plasma have been developed.
  - Fluid **transport** codes: Model cross-field transport as diffusion and employ free parameters to match experimental profiles (interpretive use). SOLPS/UEDGE remain the principal tool for ITER boundary-plasma modeling.
  - Fluid **turbulence** codes (fluid and gyrofluid): Qualitatively useful, but cannot fully capture potentially important kinetic effects.
- We need kinetic codes solving 5D $(\boldsymbol{R}, v_{\|}, \mu)$ gyrokinetic equations in the edge and SOL for quantitative prediction
  - First-principles-based approach valid across a wide range of collisionality regimes
  - Parallel variations in T, n, ϕ on order of mean free paths
  - Help improve models and boundary conditions used in much cheaper fluid codes
  - Check empirical extrapolations to ITER

Attempts at gyrokinetic *continuum* code for boundary

We are not the first ones to attempt this!

- TEMPEST (LLNL, ∼2005–2010) — Finite-difference scheme, performed some axisymmetric studies. Conservation issues?
- G5D (JAEA, ∼2007–present) — Conservative finite-difference scheme, stated goal of open-field-line turbulence appears to have been dropped.
- FEFI (IPP Garching, ∼2009–?) — 4th-order Arakawa scheme. Went directly to electromagnetics. Issues with Alfvén dynamics and sheath-model stability.
- COGENT (LLNL, ∼2008–present) — 4th-order finite volume. Axisymmetric 4D transport simulations in realistic divertor geometry and initial tests in a 5D performed

This is a very hard problem and has required us to overcome many numerical and physics challenges.

Status of gyrokinetics in Gkeyll

- Initial work by Eric Shi[3] led to 5D electrostatic full-F GK simulations of LAPD and NSTX-like helical SOL with sheath BCs
- Discontinuous Galerkin (DG) discretization scheme
  - high order method, local and parallelizable
  - conserves energy for Hamiltonian systems (like GK)
- Over past year, we have been developing a new version of Gkeyll
  - Moving from nodal to modal DG representation $\rightarrow$ orthonormal basis functions, quadrature-free, computer algebra-generated solver kernels (much easier to generalize to higher dimensionality/polynomial order), $\mathcal{O}(10)$ faster
  - Much simpler user interface, details abstracted away
- Have reproduced many of Shi's results with new version of Gkeyll
- **New nonlinear SOL simulations with electromagnetics**

[3] See 2017 thesis; JPP 2017 paper on LAPD; and PoP 2019 paper on Helical SOL

Gyrokinetic Model in Gkeyll (electrostatic)

- Gkeyll solves the gyrokinetic system in the **long-wavelength (drift-kinetic) limit** for the gyrocenter distribution function $f(\boldsymbol{R}, v_\parallel, \mu, t)$:

$$\frac{\partial \mathcal{J} f}{\partial t} + \nabla \cdot (\mathcal{J} \{\boldsymbol{R}, H\} f) + \frac{\partial}{\partial v_\parallel} (\mathcal{J} \{v_\parallel, H\} f) = \mathcal{J} C[f] + \mathcal{J} S,$$

$$-\nabla_\perp \cdot \left(\frac{n_0^g m_i}{B^2} \nabla_\perp \phi \right) = \sigma_g = e \left[n_i^g(\boldsymbol{R}) - n_e(\boldsymbol{R}) \right],$$

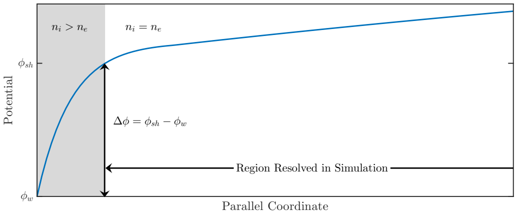
$$H = \frac{1}{2} m v_\parallel^2 + \mu B + e\phi,$$

where $\mathcal{J} = B_\parallel^*$, $C[f]$ represents a model of collisions, and

$$\{F, G\} = \frac{\mathbf{B}^*}{m B_\parallel^*} \cdot \left(\nabla F \frac{\partial G}{\partial v_\parallel} - \frac{\partial F}{\partial v_\parallel} \nabla G \right) - \frac{\hat{\mathrm{b}}}{q B_\parallel^*} \times \nabla F \cdot \nabla G$$

- Linearized ion polarization density for now (constant n_0^g)

Conducting-Sheath Boundary Conditions



- Need to model effects of non-neutral sheath using BCs
- Get ϕ_{sh}(x,y) from solving GK Poisson equation, then use $\Delta\phi = \phi_{sh} - \phi_w$ to reflect low-$v_{||}$ electrons entering sheath
  - Kinetic version of sheath BCs used in some fluid models (also similar to some gyrofluid sheath BCs)
- Potential self-consistently relaxes to ambipolar-parallel-outflow state
- Allows local currents into and out of the wall
- No BC applied at sheath to ions (free outflow)

Sheath-Model Boundary Conditions for Electrons

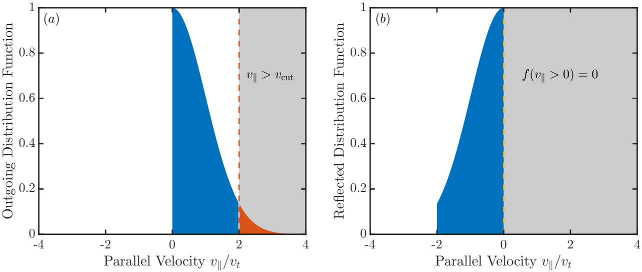


Figure: Illustration of sheath-model boundary condition. (a) Outgoing electrons with $v_\parallel > v_{\rm cut} = \sqrt{2e\Delta\phi/m}$ are lost into the wall, where $\Delta\phi = \phi_{sh} - \phi_w$, ϕ_{sh} is determined from the GK Poisson equation, and $\phi_w = 0$ for a grounded wall. (b) The rest of the outgoing particles $(0 < v_\parallel < v_{\rm cut})$ are reflected back into the plasma.

Heat-flux profiles narrow with increased B_p

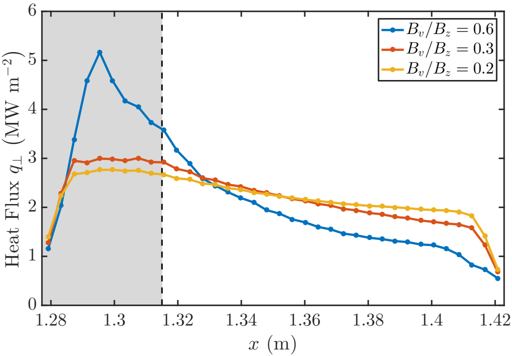


Figure: Time-averaged radial profiles of the total perpendicular heat flux $q_\perp = q_\| \sin\theta = q_\| B_v/B_z$ measured at the sheath entrance for three simulations with different magnetic-field-line pitches. A larger B_v/B_z results in a steeper heat-flux profile, similar to how the SOL heat-flux width scales with B_p in present-day tokamaks.

Particle-flux as function of poloidal field

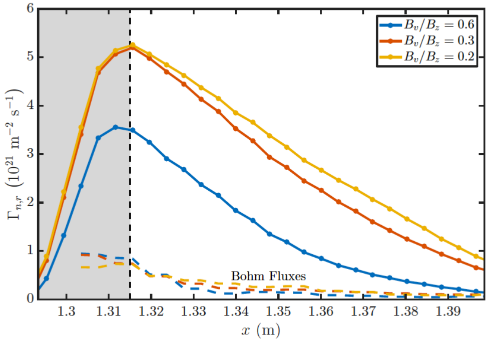


Figure: Comparison of radial $E \times B$ particle flux evaluated at the midplane for three different poloidal fields. Increasing the poloidal field decreases the radial flux, consistent with the heat-flux profiles on the divertor plate. For comparison, Bohm fluxes estimates are shown as dashed lines.

Larger amplitude, more intermittent blobs in SOL

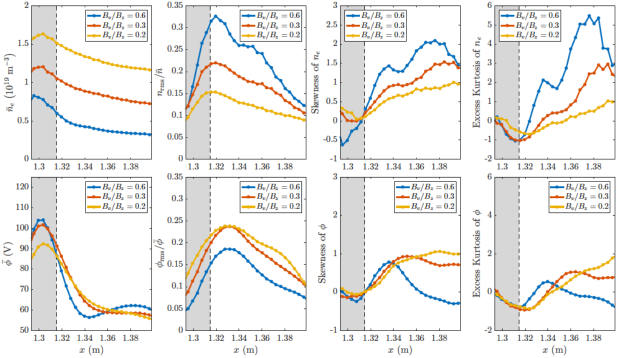


Figure: Comparison of electron-density fluctuations (top row) and electrostatic fluctuations (bottom row) at mid-plane. The density fluctuations (blobs) are larger amplitude and more intermittent than the potential fluctuations which show much smaller skewness and kurtosis.

Ion and electron temperatures are not in equilibrium

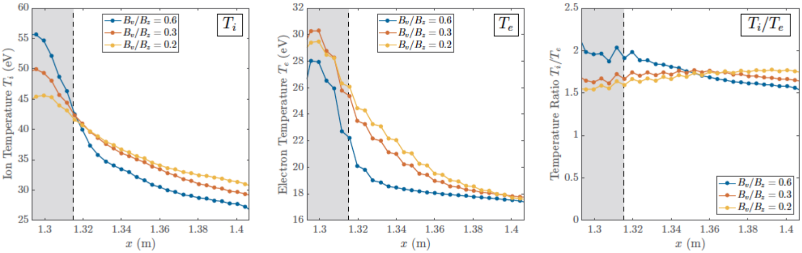


Figure: Radial profiles of steady-state ion (left) and electron (middle) profiles near midplane. Right plot shows ion-to-electron temperature ratio. Although both electrons and ions are sourced at the same temperature, the sheath allows rapid loss of high energy electrons to wall, resulting in lower electron temperatures in the SOL.

What about electromagnetics?

- Electromagnetic effects are especially important in the edge and SOL, where steep gradients can push the plasma close to the ideal-MHD stability threshold and produce stronger turbulence
- Including electromagnetic fluctuations has proved challenging in some PIC codes, in part due to the well-known Ampère cancellation problem
- Continuum gyrokinetic codes for core turbulence have avoided the Ampère cancellation issue
- As `Gkeyll` uses a continuum formulation, we expect that we can handle electromagnetic effects in the edge and SOL in a stable and efficient manner

Hamiltonian ($p_\parallel$) vs. Symplectic ($v_\parallel$) formulation of EMGK

In the Hamiltonian gyrokinetic formalism (see e.g. Brizard & Hahm, 2007), there are two formulations for including electromagnetic fluctuations:

- Hamiltonian formulation: $p_\parallel = mv_\parallel + qA_\parallel$

$$\frac{\partial f}{\partial t} = \{H, f\}$$

$$H = \frac{1}{2m} p_\parallel^2 + \mu B + q\phi = \frac{1}{2m}(mv_\parallel + qA_\parallel)^2 + \mu B + q\phi \qquad \mathbf{B}^* = \mathbf{B_0} + \frac{1}{q} p_\parallel \nabla \times \hat{\mathrm{b}}$$

- Symplectic formulation: $p_\parallel = mv_\parallel$

$$\frac{\partial f}{\partial t} = \{H, f\} + \frac{q}{m}\frac{\partial f}{\partial v_\parallel}\frac{\partial A_\parallel}{\partial t}$$

$$H = \frac{1}{2} mv_\parallel^2 + \mu B + q\phi \qquad \mathbf{B}^* = \mathbf{B_0} + \frac{m}{q} v_\parallel \nabla \times \hat{\mathrm{b}} + \delta \mathbf{B}_\perp$$

Poisson bracket:

$$\{F, G\} = \frac{\mathbf{B}^*}{B_\parallel^*} \cdot \left(\nabla F \frac{\partial G}{\partial p_\parallel} - \frac{\partial F}{\partial p_\parallel} \nabla G \right) - \frac{\hat{\mathrm{b}}}{qB_\parallel^*} \times \nabla F \cdot \nabla G$$

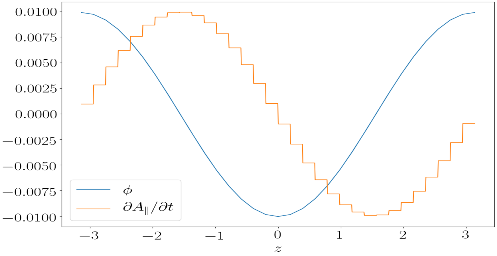
Hamiltonian ($p_\parallel$) vs. Symplectic ($v_\parallel$) formulation of EMGK

In `Gkeyll`'s DG scheme, the distribution function and other fields can be discontinuous across cell boundaries, but **energy is conserved only if the Hamiltonian is continuous**

- Hamiltonian ($p_\parallel$) $\Rightarrow$ both ϕ & $A_\parallel$ must be continuous
- Symplectic ($v_\parallel$) $\Rightarrow$ ϕ must be continuous, but $A_\parallel$ (and $\frac{\partial A_\parallel}{\partial t}$) can be discontinuous in parallel direction

Ex) MHD limit, $E_\parallel = 0 \Rightarrow \frac{\partial \phi}{\partial z} = -\frac{\partial A_\parallel}{\partial t}$

Piecewise linear ϕ $\Rightarrow$ piecewise constant $\frac{\partial \phi}{\partial z}$ $\Rightarrow$ piecewise constant $\frac{\partial A_\parallel}{\partial t}$



Ampère cancellation problem: Hamiltonian formulation

In Hamiltonian formulation, Ampère's law becomes

$$\left(-\nabla_\perp^2 + C_n \sum_s \frac{\mu_0 q}{m} \int d^3p\ f\right) A_\parallel = C_j\ \mu_0 \sum_s \frac{q}{m^2} \int d^3p\ p_\parallel f$$

The "cancellation problem" arises when there are small errors in the calculation of the integrals. These errors are represented by C_n and C_j (which should both be exactly 1 in the exact system).

The simplest Alfvén wave dispersion relation (slab geometry, uniform Maxwellian background with stationary ions) becomes (with $\hat{\beta} \equiv \frac{\beta_e}{2}\frac{m_i}{m_e}$)

$$\omega^2 = \frac{k_\parallel^2 v_A^2}{C_n + k_\perp^2 \rho_s^2/\hat{\beta}} \left[1 + (C_n - C_j)\frac{\hat{\beta}}{k_\perp^2 \rho_s^2}\right]$$

This reduces to the correct result if integrals calculated consistently, so that $C_n = C_j$, but if not there will be large errors for modes with $\hat{\beta}/k_\perp^2 \rho_s^2 \gg 1$.

Ampère cancellation problem: symplectic formulation

In symplectic formulation, Ampère's law is

$$-\nabla_\perp^2 A_\parallel = \mu_0 \sum_s q \int d^3v \ v_\parallel f$$

However, we need a way to handle the $\frac{\partial A_\parallel}{\partial t}$ term that appears in the GK equation. One way is to take $\frac{\partial}{\partial t}$ of Ampère's law, which gives an Ohm's law:

$$-\nabla_\perp^2 \frac{\partial A_\parallel}{\partial t} = \mu_0 \sum_s q \int d^3v \ v_\parallel \frac{\partial f}{\partial t} = \mu_0 \sum_s q \int d^3v \ v_\parallel \left[\{H, f\} + \frac{q}{m} \frac{\partial f}{\partial v_\parallel} \frac{\partial A_\parallel}{\partial t} \right]$$

$$\Rightarrow \left(-\nabla_\perp^2 + C_n \sum_s \frac{\mu_0 q^2}{m} \int d^3v \ f \right) \frac{\partial A_\parallel}{\partial t} = C_j \ \mu_0 \sum_s q \int d^3v \ v_\parallel \{H, f\}$$

Same dispersion relation, but integrals over $v_\parallel$, not $p_\parallel$. These can easily be calculated consistently so that $C_n = C_j$ and there is no cancellation problem.

We choose symplectic formulation of EMGK

Electromagnetic GK equation:

$$\frac{\partial f}{\partial t} = \{H, f\} + \frac{q}{m}\frac{\partial f}{\partial v_\parallel}\frac{\partial A_\parallel}{\partial t} + C[f] + S \tag{1}$$
$$= \frac{\partial f^\star}{\partial t} + \frac{q}{m}\frac{\partial f}{\partial v_\parallel}\frac{\partial A_\parallel}{\partial t},$$

with $H = \frac{1}{2}mv_\parallel^2 + \mu B + q\phi$, and $\frac{\partial f^\star}{\partial t} \equiv \{H, f\} + C[f] + S$

Quasineutrality equation (long-wavelength):

$$-\nabla \cdot \sum_s \frac{mn_0}{B^2}\nabla_\perp \phi = \sum_s q \int d^3v\ f \tag{2}$$

Ohm's law: *solve directly for $\partial A_\parallel / \partial t$*

$$\left(-\nabla_\perp^2 + \sum_s \frac{\mu_0 q^2}{m}\int d^3v\ f\right)\frac{\partial A_\parallel}{\partial t} = \mu_0 \sum_s q \int d^3v\ v_\parallel \frac{\partial f^\star}{\partial t} \tag{3}$$

Parallel Ampère equation: *only used for initial condition on $A_\parallel$*

$$-\nabla_\perp^2 A_\parallel = \mu_0 \sum_s q \int d^3v\ v_\parallel f \tag{4}$$

Explicit time-advance scheme

Given f^n and $A_\parallel^n$ at the beginning of timestep n,

1. Calculate ϕ^n:

$$-\nabla\cdot\sum_s \frac{mn_0}{B^2}\nabla_\perp\phi^n = \sum_s q\int d^3v\ f^n$$

2. Calculate partial GK RHS:

$$\left(\frac{\partial f^\star}{\partial t}\right)^n = \{H^n, f^n\}^n + C[f^n] + S^n$$

3. Calculate $\left(\frac{\partial A_\parallel}{\partial t}\right)^n$:

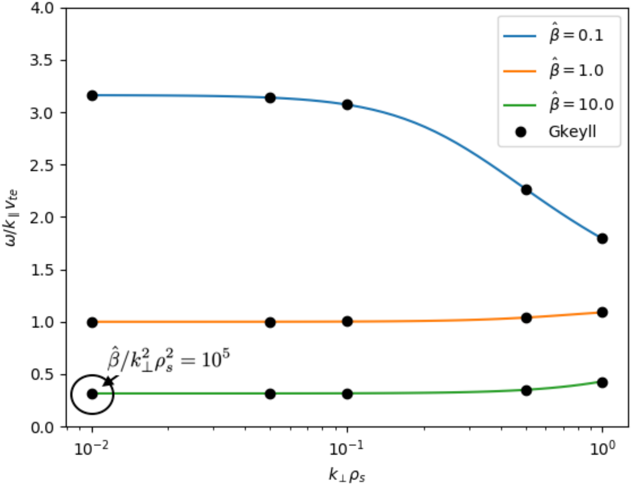
$$\left(-\nabla_\perp^2 + \sum_s \frac{\mu_0 q^2}{m}\int d^3v\ f^n\right)\left(\frac{\partial A_\parallel}{\partial t}\right)^n = \mu_0\sum_s q\int d^3v\ v_\parallel\left(\frac{\partial f^\star}{\partial t}\right)^n$$

4. Advance f^{n+1} and $A_\parallel^{n+1}$:

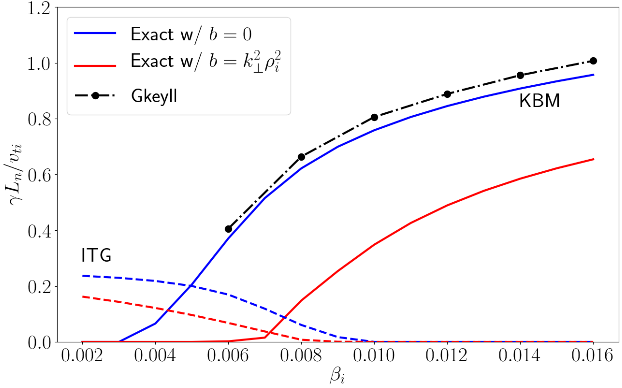
$$f^{n+1} = f^n + \Delta t\left[\left(\frac{\partial f^\star}{\partial t}\right)^n + \frac{q}{m}\frac{\partial f^n}{\partial v_\parallel}\left(\frac{\partial A_\parallel}{\partial t}\right)^n\right]$$

$$A_\parallel^{n+1} = A_\parallel^n + \Delta t\left(\frac{\partial A_\parallel}{\partial t}\right)^n$$

Linear Benchmark: Kinetic Alfvén Waves



Linear Benchmark: Kinetic Ballooning Mode Instability



$$k_\perp \rho_i = 0.5,\ k_\| L_n = 0.1,\ R/L_n = 5,\ R/L_{Ti} = 12.5,\ R/L_{Te} = 10,\ \tau = 1$$

Summary & Future Work

- We have a new version of the `Gkeyll` code that is faster and includes EM
- We have demonstrated that our formulation and scheme for EMGK is effective and avoids the Ampère cancellation problem
- We have successfully completed some basic linear EMGK benchmarks
- **We have performed preliminary nonlinear full-F continuum EMGK SOL simulations**
- In-progress/Future Work:
  - Detailed comparison of ES and EM GK simulations in helical SOL geometry
  - Generalize the geometry to better model NSTX SOL, and also to include closed field line regions
  - Include FLR effects (beyond the first order polarization drift)