Continuum Electromagnetic Gyrokinetic Simulations of Turbulence in the Tokamak Scrape-Off Layer and Laboratory Devices

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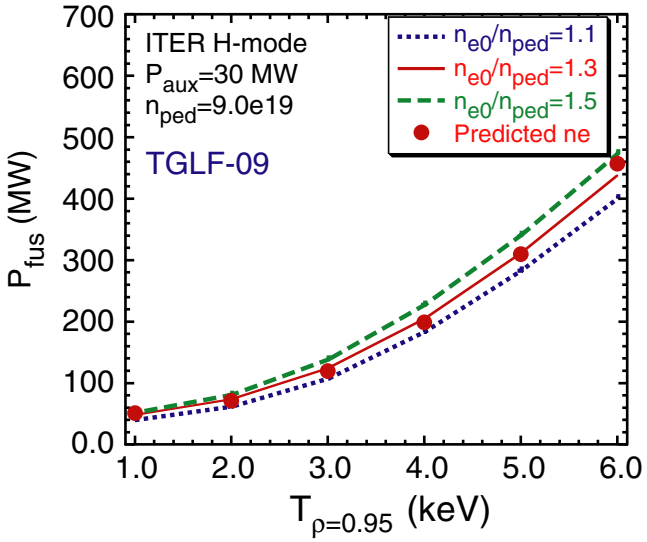
Boundary-plasma strongly affect fusion performance

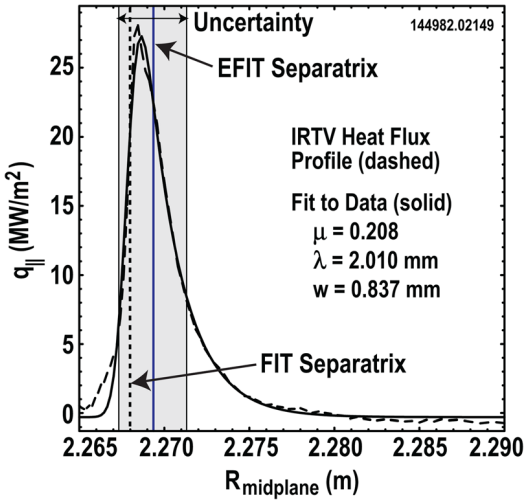
- Boundary plasma (edge and SOL) believed to set boundary conditions on the core
- Improved confinement associated with suppression of edge turbulence[1]
- ITER projections show fusion performance highly sensitive to the H-mode-pedestal temperature
- Need reliable, fully predictive simulations of the pedestal to quantitatively model the core



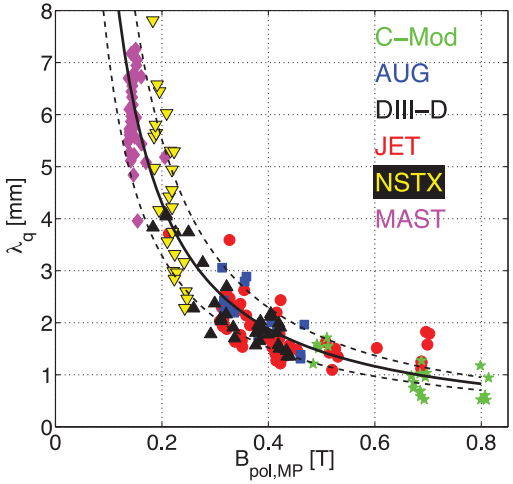
From Kinsey et al., (2011)

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 ∼1 mm
- On ITER, need to dissipate most (∼95% (Goldston, 2015)) of this power somehow before it reaches the divertor plates
  - Material limitations ∼10 MW m^{-2}, ITER operation can 'easily' reach ∼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 ($B_{pol} \approx 1.2$ 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. GBS/GDB, BOUT++, ...
- 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
  - Allow parallel variations in T, n, ϕ on order of mean free paths

Boundary-plasma simulation: prior/current work

Edge is difficult: large fluctuations, open-field lines, interacting with material walls (sheaths, recycling), significant neutral interactions etc.

- XGC is leading edge PIC code, able to handle X-point geometries and do core and edge in the same simulation box.
- COGENT (LLNL, ∼2008–present) is a continuum code — uses 4th-order finite volume. Axisymmetric 4D transport simulations in realistic divertor geometry and initial work in 5D.

We are the first continuum code to do fully non-linear full-F simulations of electromagnetic gyrokinetics with sheath-boundary conditions.

Electromagnetic Gyrokinetic Model

- 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 historically proven challenging in some PIC codes, in part due to the well-known Ampère cancellation problem. Significant progress in recent years.
- 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:

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

We choose symplectic formulation of EM gyrokinetics

Electromagnetic GK equation:

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

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):

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

Parallel Ampère equation for $A_\parallel$

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

Take time-derivative: parallel momentum equation to *solve directly for* $\partial A_\parallel/\partial t$

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

Important to preserve quadratic invariants

For any Hamiltonian system we can show that

$$\int_K H\{f, H\}\, d\mathbf{z} = \int_K f\{f, H\}\, d\mathbf{z} = 0$$

The first of this leads to conservation of total energy (on use of field equations), while the second leads to conservation of $\int_K f^2 d\mathbf{z}$ (called *enstrophy* for incompressible fluids, and related to entropy).

- Energy conservation in Hamiltonian systems is *indirect*: we evolve the distribution function and field equation. In fluid models, in contrast, the energy conservation is *direct*, as we evolve the total energy equation (in addition to density and momentum density equations). Hence, ensuring energy conservation for Hamiltonian system is non-trivial, and difficult in finite-volume schemes.
- Energy conservation can be ensured using the famous finite-difference *Arakawa* scheme (widely used in climate modeling and one of the top-twenty algorithms ever published in JCP). However, Arakawa scheme is *dispersive* and can lead to huge oscillations for grid-scale modes.

Can one construct conservative schemes?

Answer: Yes, using a version of discontinuous Galerkin schemes.
Summary:

- Distribution function is discretized using *discontinuous* basis functions. Key: Hamiltonian is assumed to be in a continuous subspace
- With these assumptions, our algorithm conserves energy *exactly* in the time-continuous limit, while can optionally conserve the second quadratic invariant *or* decay it monotonically.
- The conservation of total energy is independent of upwinding! This is a surprising result, as upwinding adds diffusion to the system. This diffusion is actually *desirable*, as it gets rid of grid-scale oscillations.
- Momentum conservation is independent of velocity space resolution, and converges rapidly with resolution in configuration space.

DG represents state-of-art for hyperbolic PDEs

DG algorithms hot topic in CFD and applied mathematics.

- First introduced by Reed and Hill in 1973 as a conference paper to solve steady-state neutron transport equations. More than 2100 citations.
- Some earlier work on solving *elliptic* equations by Nitsche in 1971 (original paper in German). Introduced the idea of "interior penalty". Usually, though, DG is not used for elliptic problems. Paradoxically, perhaps DG may be even better for certain elliptic/parabolic problems.
- Key paper for nonlinear systems in multiple dimensions is by Cockburn and Shu (JCP, **141**, 199-224, 1998). More than 1700 citations.
- Almost continuous stream of papers in DG, both for fundamental formulations and applications to physics and engineering problems. This continues to be an active area of research.

What are discontinuous Galerkin schemes?

Discontinuous Galerkin schemes are a class of *Galerkin* schemes in which the solution is represented using *piecewise discontinuous* functions.

- *Galerkin* minimization
- Piecewise *discontinuous* representation[3]

[3] *Representation* being discontinuous is not cause for alarm: the underlying solution can still have the needed continuity.

The Ampère cancellation problem

In symplectic formulation, recall we use parallel momentum equation to update $A_\parallel$

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

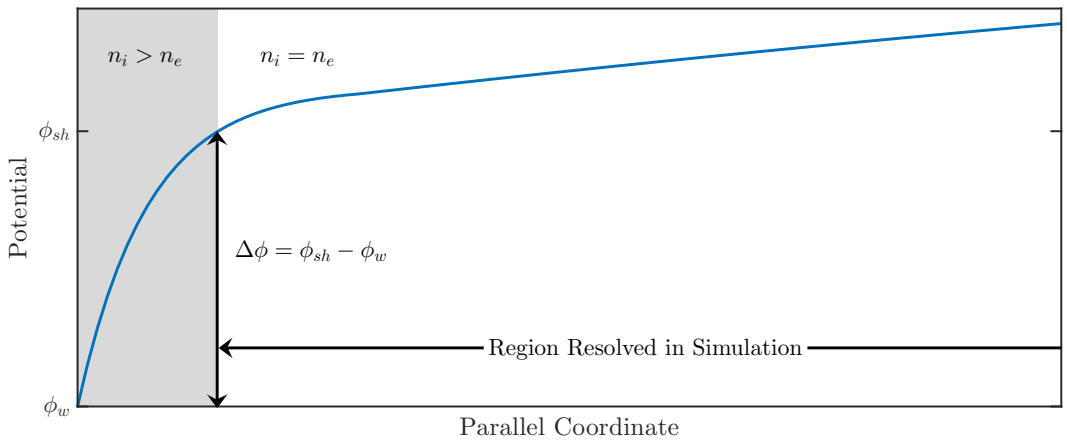
The simplest Alfvén wave dispersion relation (slab geometry, uniform Maxwellian background with stationary ions) becomes (with $\hat{\beta} \equiv \frac{\beta_e}{2}\frac{m_i}{m_e}$)

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

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 $\hat{\beta}/k_\perp^2\rho_s^2 \gg 1$.

In our DG scheme we compute moments of f consistently, ensuring $C_n = C_j$ and hence there is no cancellation problem!

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

Sheath-Model Boundary Conditions for Electrons

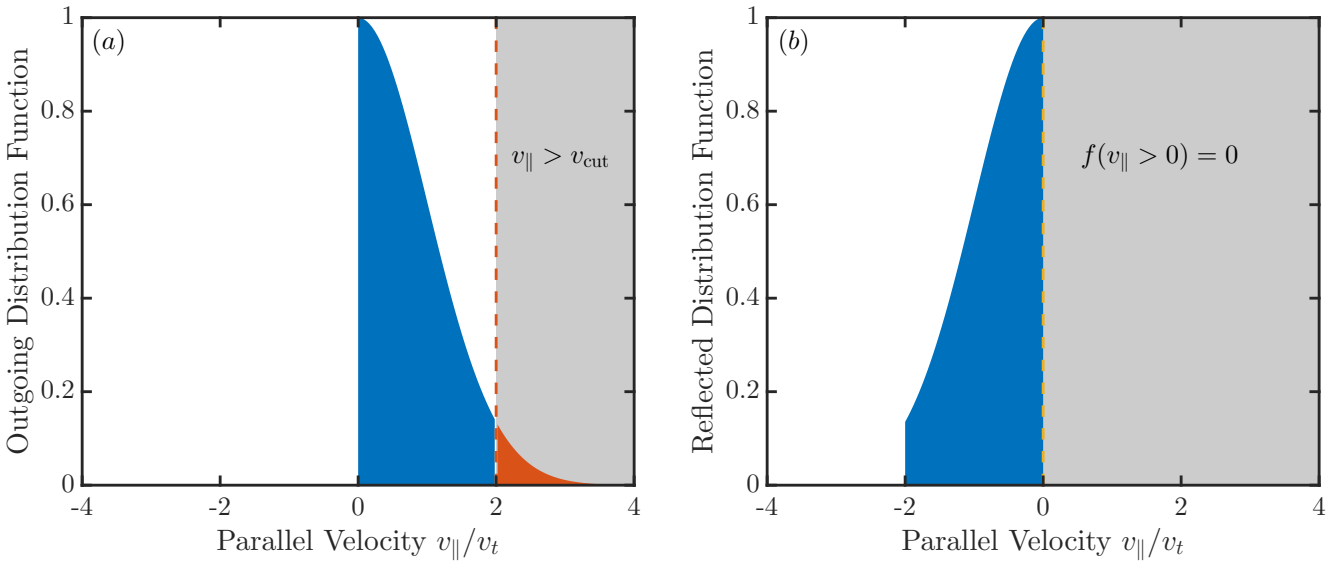
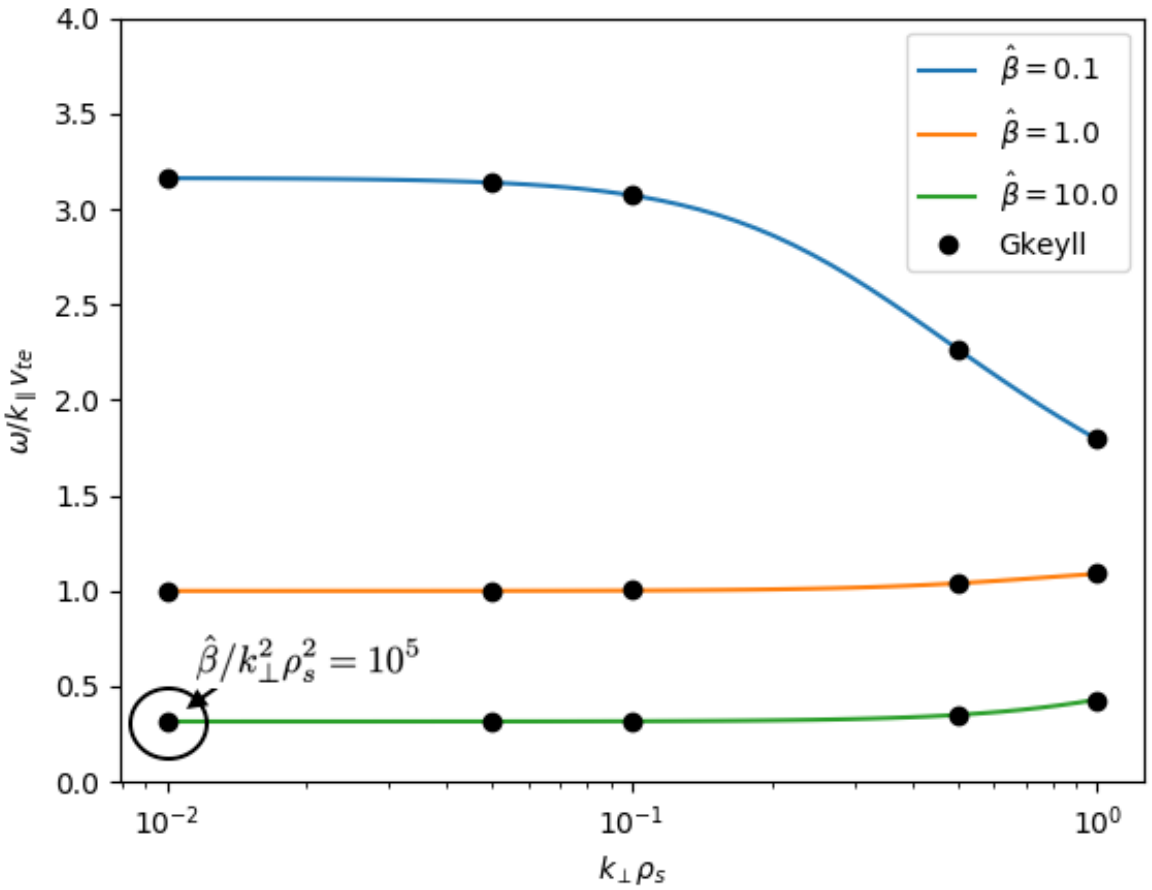


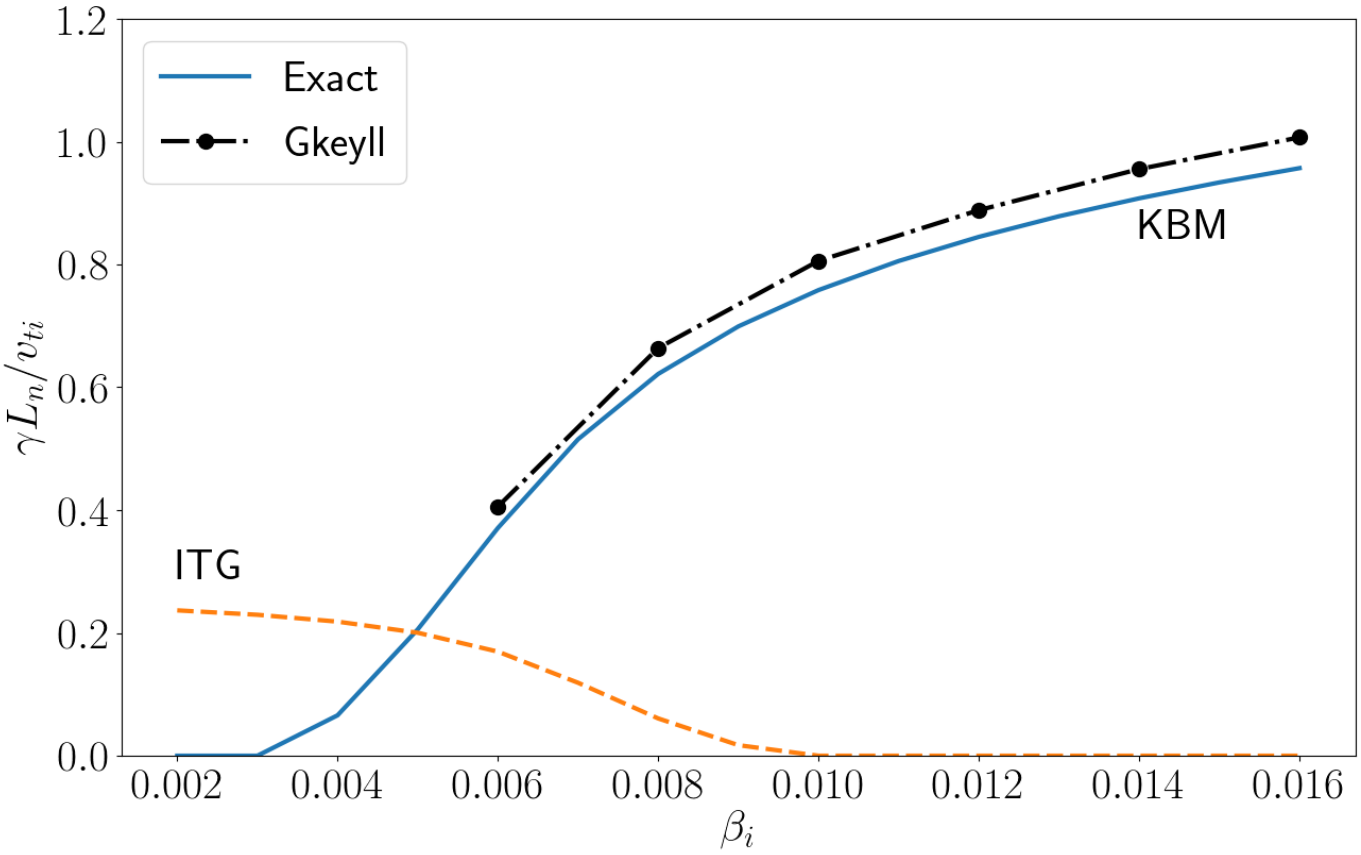
Figure: Illustration of sheath-model boundary condition. (a) Outgoing electrons with $v_\parallel > v_{\rm cut} = \sqrt{2e\Delta\phi/m}$ are lost into the wall, where $\Delta\phi = \phi_{sh} - \phi_w$, ϕ_{sh} is determined from the GK Poisson equation, and $\phi_w = 0$ for a grounded wall. (b) The rest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

Linear Benchmark: Kinetic Alfvén Waves



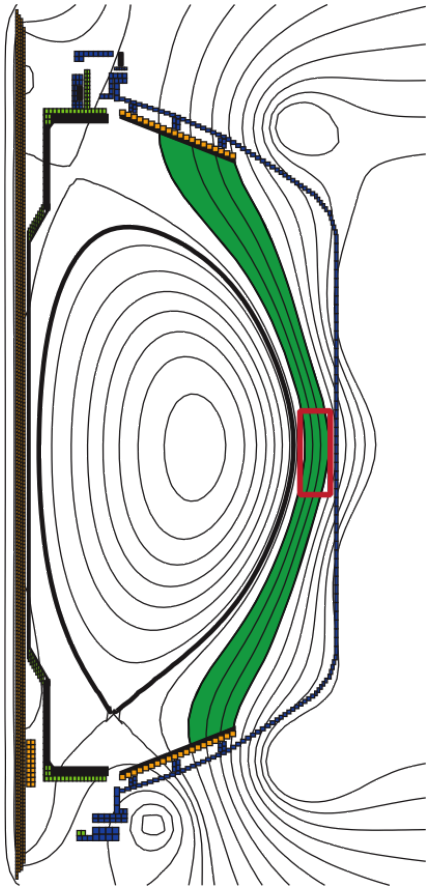
Numerical results match very well, even for case of $\hat{\beta}/k_\perp^2 \rho_s^2 = 10^5$.

Linear Benchmark: Kinetic Ballooning Model



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

Modelling NSTX-like SOL



- Simple helical model of tokamak SOL
  - Like the green region, but straightened out to vertical flux surfaces
  - Field-aligned simulation domain that follows field lines from bottom divertor plate, around the torus, to the top divertor plate
  - All bad curvature; brings in interchange instability drive
- Parameters taken from NSTX SOL measurements; Real deuterium mass ratio, Lenard-Bernstein collisions. $10\times$ n_0 **to stress-test EM effects**
- Conducting sheath boundary conditions at the divertor plates
- Radially-localized source to model flux of particles and heat across separatrix from core

Blob formation due bad-curvature drive

Bad curvature drive causes interchange instability, "peeling off" highly intermittent blobs radially outwards.

More intermittent structures in EM simulations

More intermittent structures in EM simulations

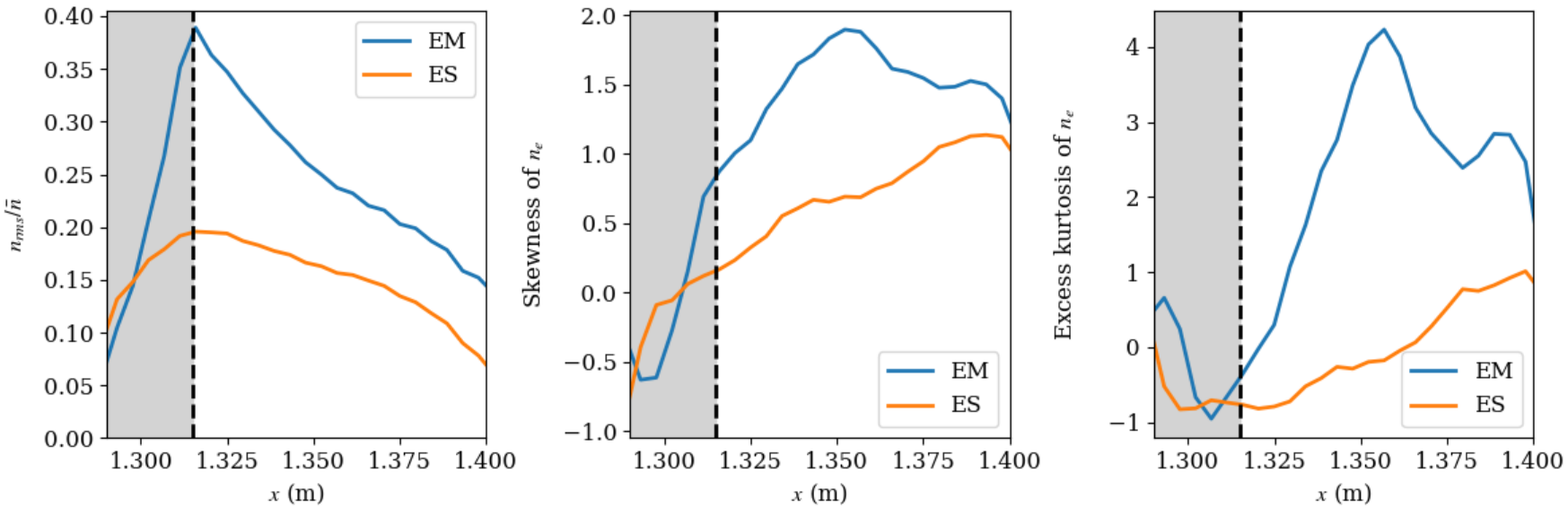


Figure: Statistics of density fluctuations from EM and ES gyrokinetic simulations

Radial particle transport and heat-flux

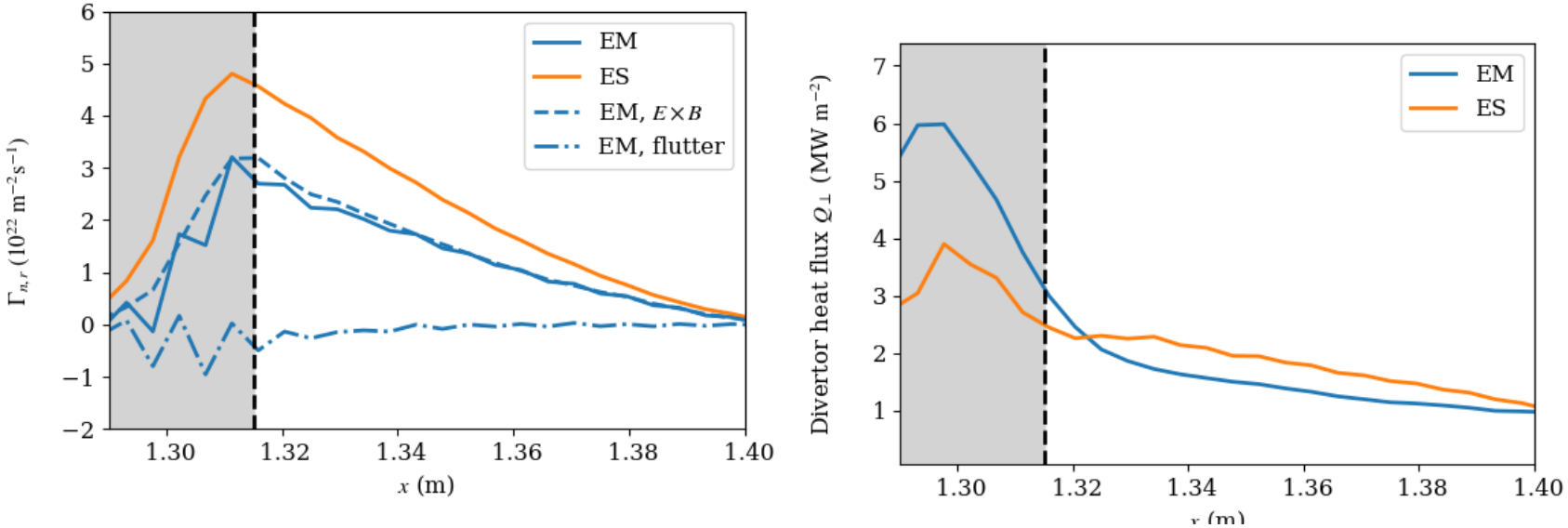
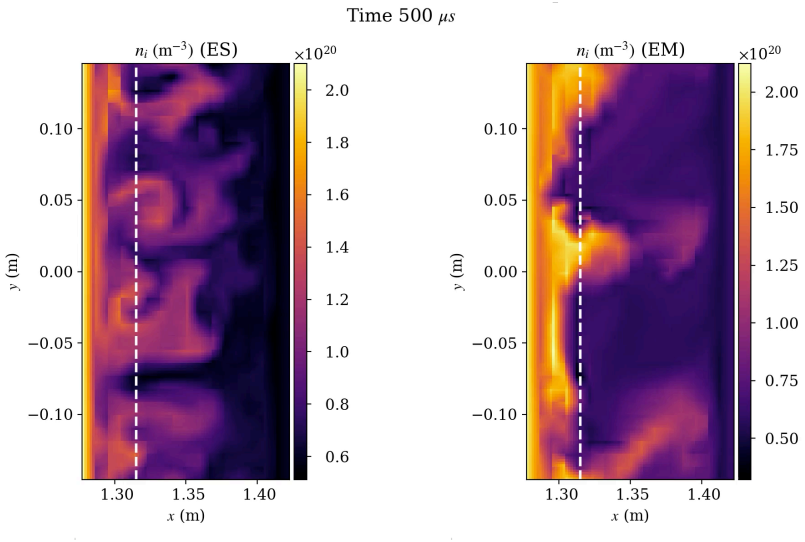


Figure: Left: Radial particle transport **reduced** in EM. Right: Heat-flux to divertor is **more peaked**

Dance of the field-lines

Play/Pause

Simulation cost is modest: even with EM terms!



(Nx, Ny, Nz, Nv, Nm) ~(32, 64, 20, 20, 10)	Electrostatic	Electromagnetic
Total compute time (128 cores)	8,320 core-hrs	10,496 core-hrs
Time/timestep (wall clock)	0.41 s	0.68 s

Beyond gyrokinetics: `Gkeyll` Vlasov-Maxwell solvers

For use in detailed kinetic study, we have implemented a Vlasov-Maxwell solver that directly discretizes the Vlasov equations in 6D.

$$\frac{\partial f_s}{\partial t} + \nabla_{\mathbf{x}} \cdot (\mathbf{v} f_s) + \nabla_{\mathbf{v}} \cdot (\mathbf{F}_s f_s) = \left(\frac{\partial f_s}{\partial t}\right)_c$$

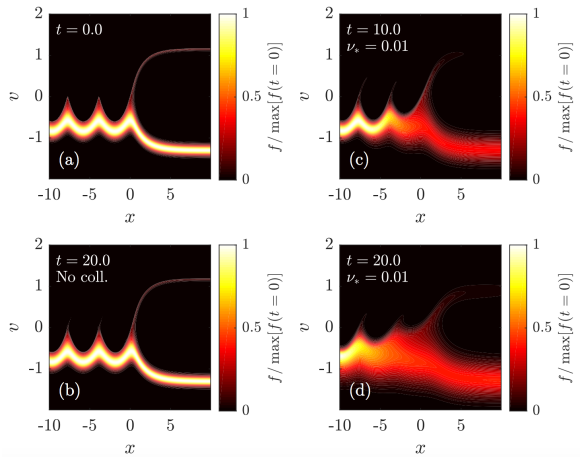
where $\mathbf{F}_s = q_s/m_s(\mathbf{E} + \mathbf{v} \times \mathbf{B})$. The EM fields are determined from Maxwell equations

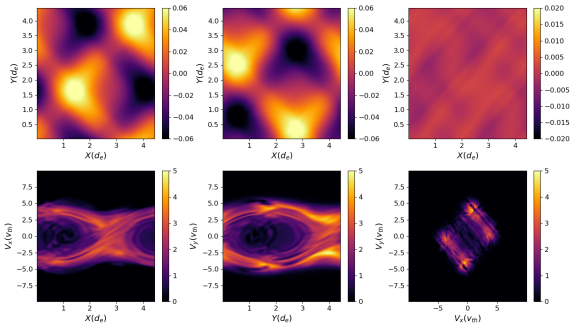
$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = 0$$
$$\epsilon_0 \mu_0 \frac{\partial \mathbf{E}}{\partial t} - \nabla \times \mathbf{B} = -\mu_0 \mathbf{J}$$

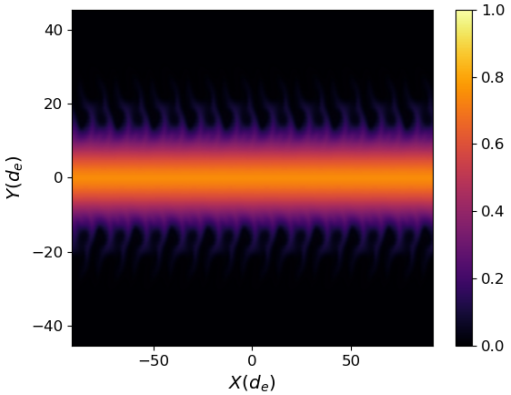
Beyond gyrokinetics: `Gkeyll` Vlasov-Maxwell solvers

For use in detailed kinetic study, we have implemented a Vlasov-Maxwell solver that directly discretizes the Vlasov equations in 6D. Many applications, including

- First-principles sheath-physics study and (Cagas PhD Thesis 2017, Cagas et. al. PoP 2018).
- Electrostatic shocks (with and without collisions). See Pustvai *et al.* 2018 PPCF, Sundström *et al.* 2019 JPP
- Weibel instability (in 1D and 2D) Cagas *et al.* 2017 PoP, Skoutnev *et al.* ApJ letters 2019
- Lower hybrid drift instability Ng *et al.* JGR 2019

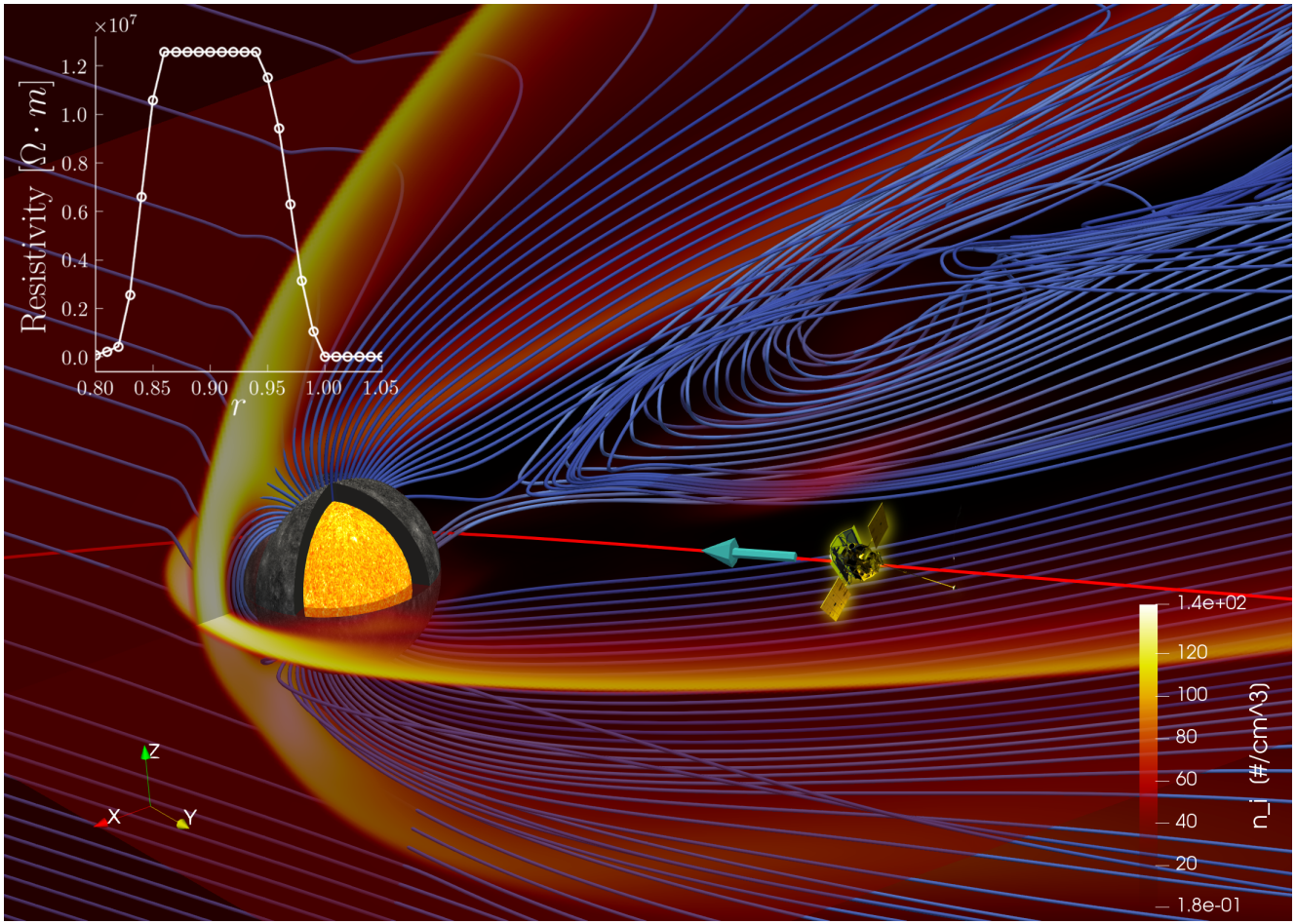




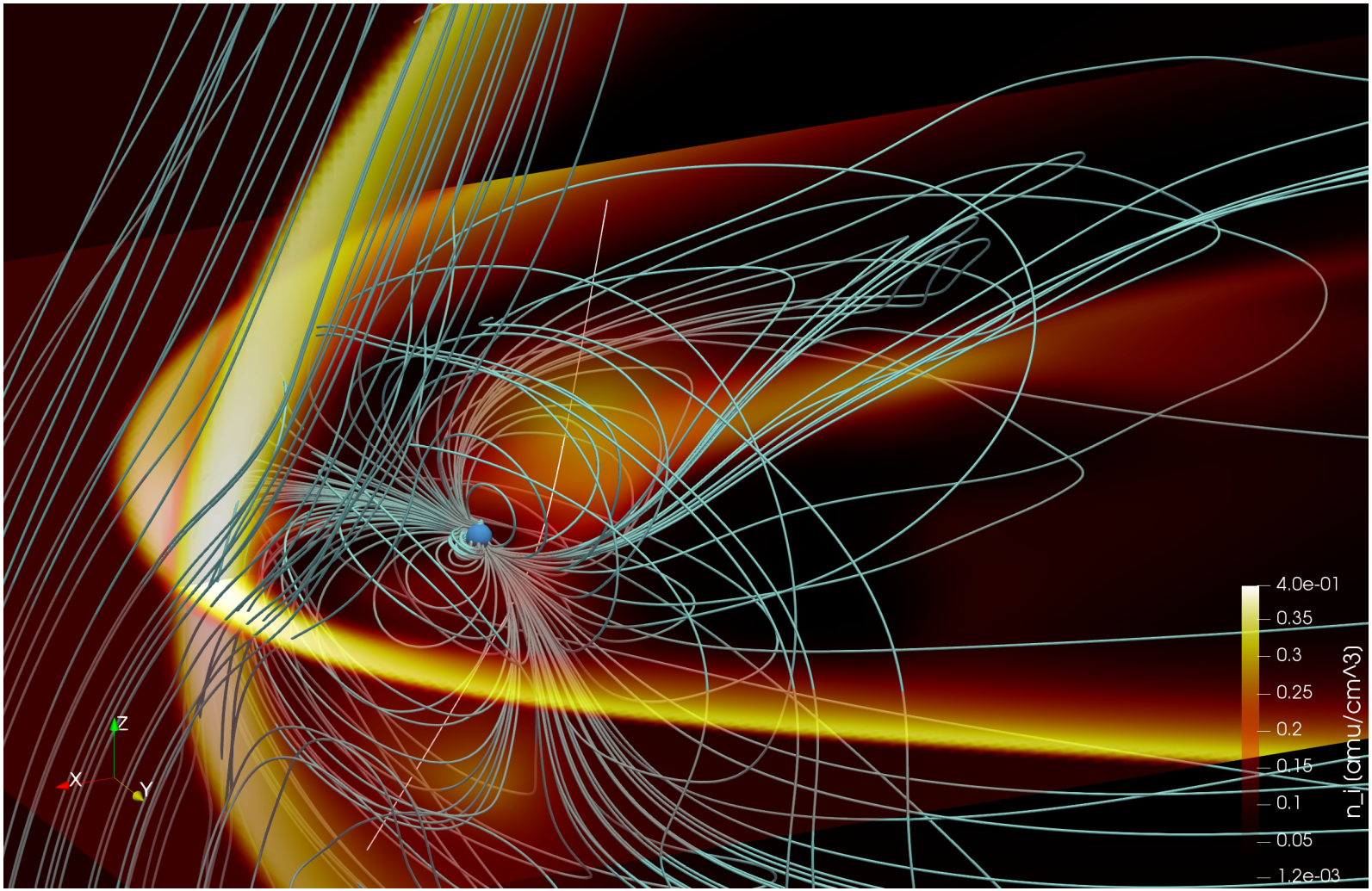


Beyond gyrokinetics: `Gkeyll` Multi-fluid solvers

For global simulation of fusion and space-plasma problems we have implemented advanced multi-fluid moment models that retain some kinetic effects via collisionless closures.



Beyond gyrokinetics: `Gkeyll` Multi-fluid solvers



Summary & Current/Future Work

- We have a new version of the `Gkeyll` gyrokinetic code that is faster and includes electromagnetic effects
- 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 first nonlinear full-F continuum EMGK SOL simulations**
- In-progress/Future Work:
  - Generalize the geometry to better model tokamaks SOL, and also to include closed field line regions
  - Include FLR effects (beyond the first order polarization drift)

The Gkeyll Project spans nearly all scales: gyrokinetics, full Vlasov-Maxwell to multi-moment fluid models. Many more exciting results to come!

Extra slides

Dance of the field-lines: Real NSTX parameters