Initial SOL turbulence results from the Gkeyll code, including first electromagnetic effects.

Greg Hammett, for:
Noah Mandell (grad student, EM gyrokinetics),
Ammar Hakim (Gkeyll Group Leader),
M. Francisquez, T. Bernard, E. Shi

AUG Seminar, 27/1/2020

PRINCETON UNIVERSITY

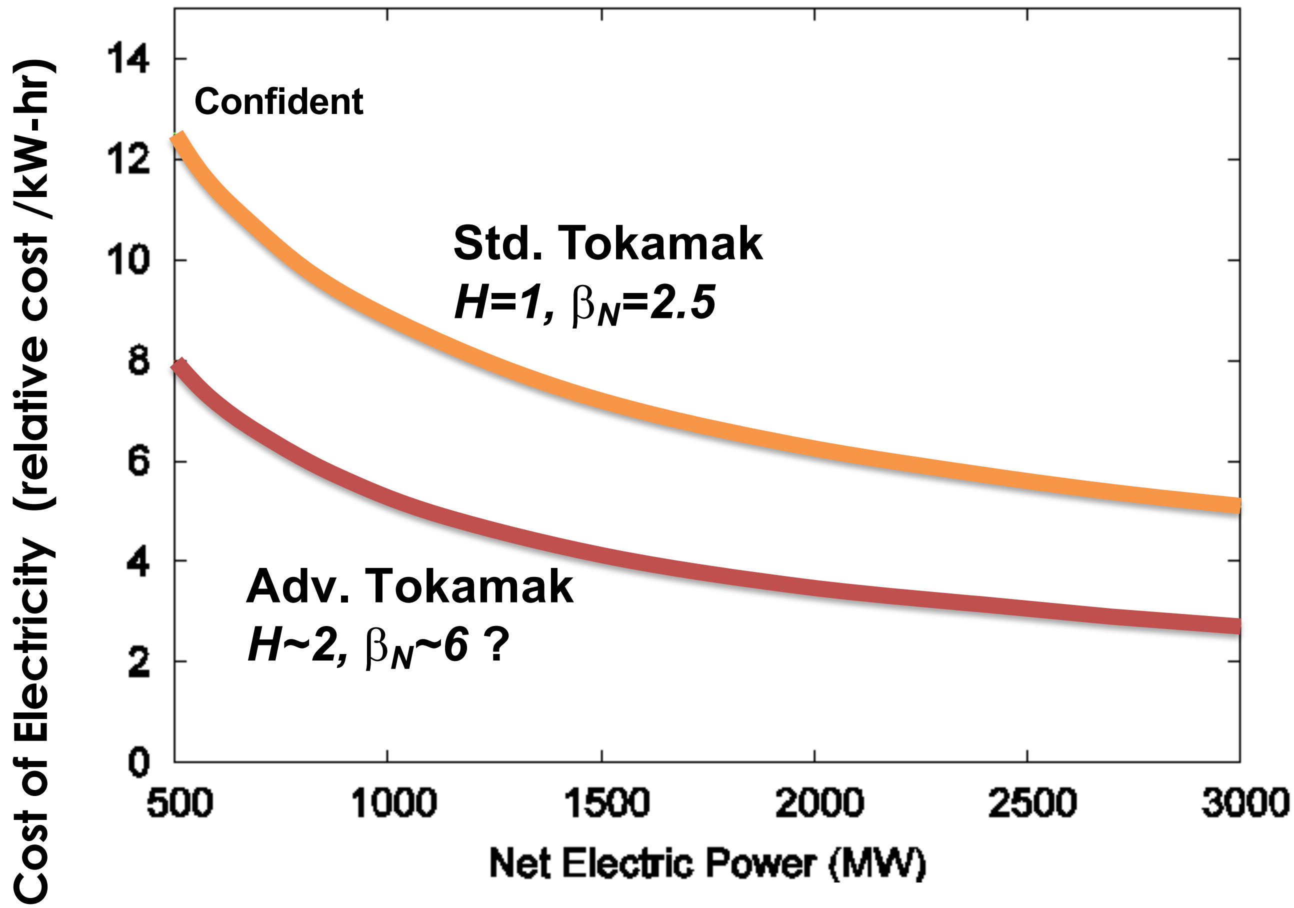
PPPL
PRINCETON PLASMA PHYSICS LABORATORY

Motivation: ↓ turbulence & ↑ pressure limits could significantly reduce cost of fusion

Regimes of Improved confinement and pressure limits have been achieved in experiments, but we are less confident in how they scale to reactors.

Comprehensive simulations can help improve design of future reactors.

Comprehensive simulations also needed to maximize results from ITER.

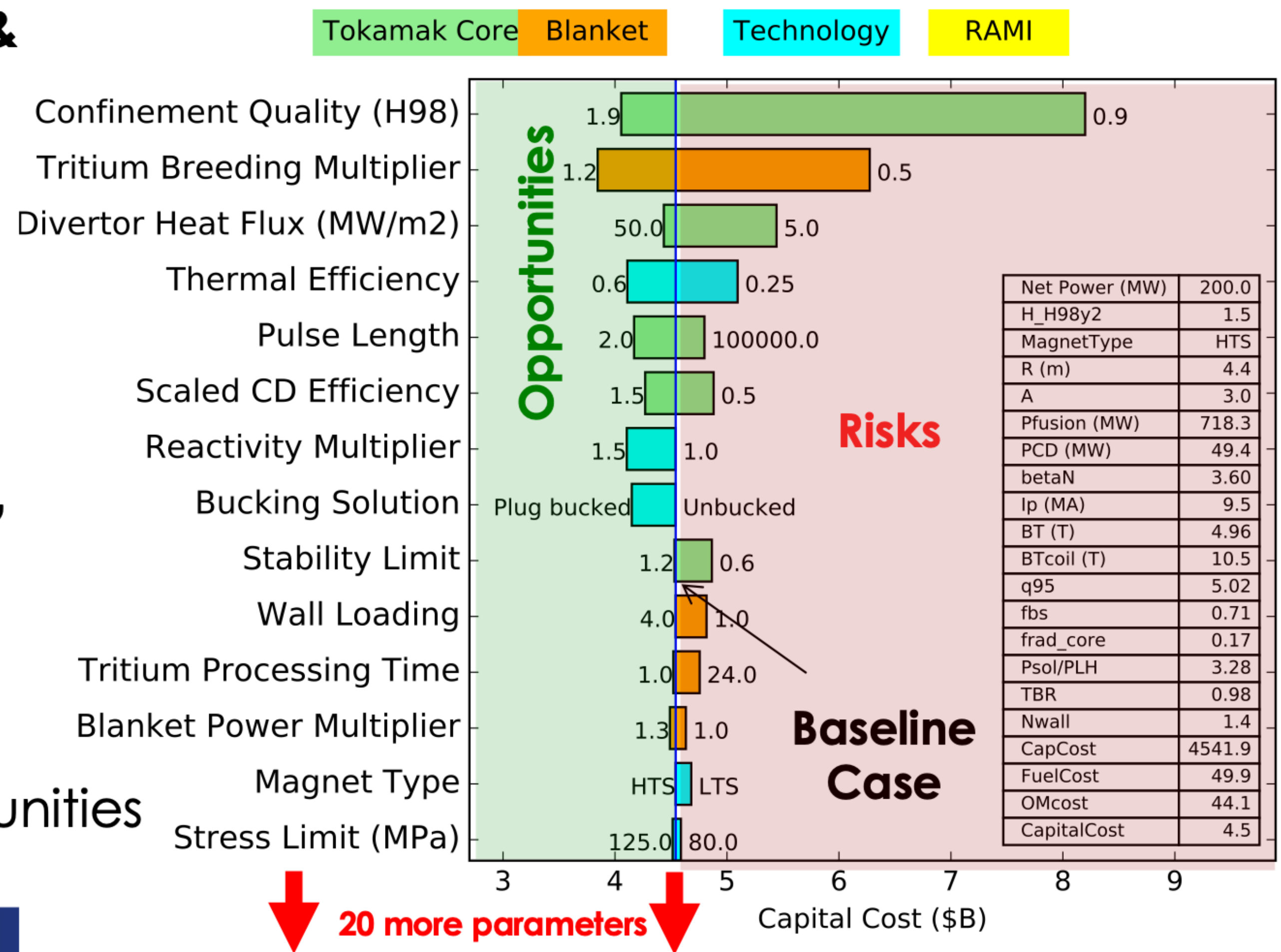


Galambos, Perkins, Haney, & Mandrekas 1995 Nucl.Fus.

Even larger reduction possible in construction cost for lower-power pilot plants, focus of U.S. National Academy report (2018).

Example of Capital Cost Sensitivity Analysis for 200 MWe Pilot Plant with $H_{98y2} < 1.5$, A = 3.0, REBCO Magnets

- **Key baseline assumptions & constraints**
  - Free standing TF
  - TBR = 1.0; $\eta_{th} = 0.4$
  - $f_{GW} < 1$; $\beta_N/\beta_{N,limit} < 0.75$
  - $q_{div,max} < 10\ MW/m^2$
- **Vary each parameter independently→ "Tornado" Chart**
  - Identifies most sensitive variables
  - As well as risks & opportunities

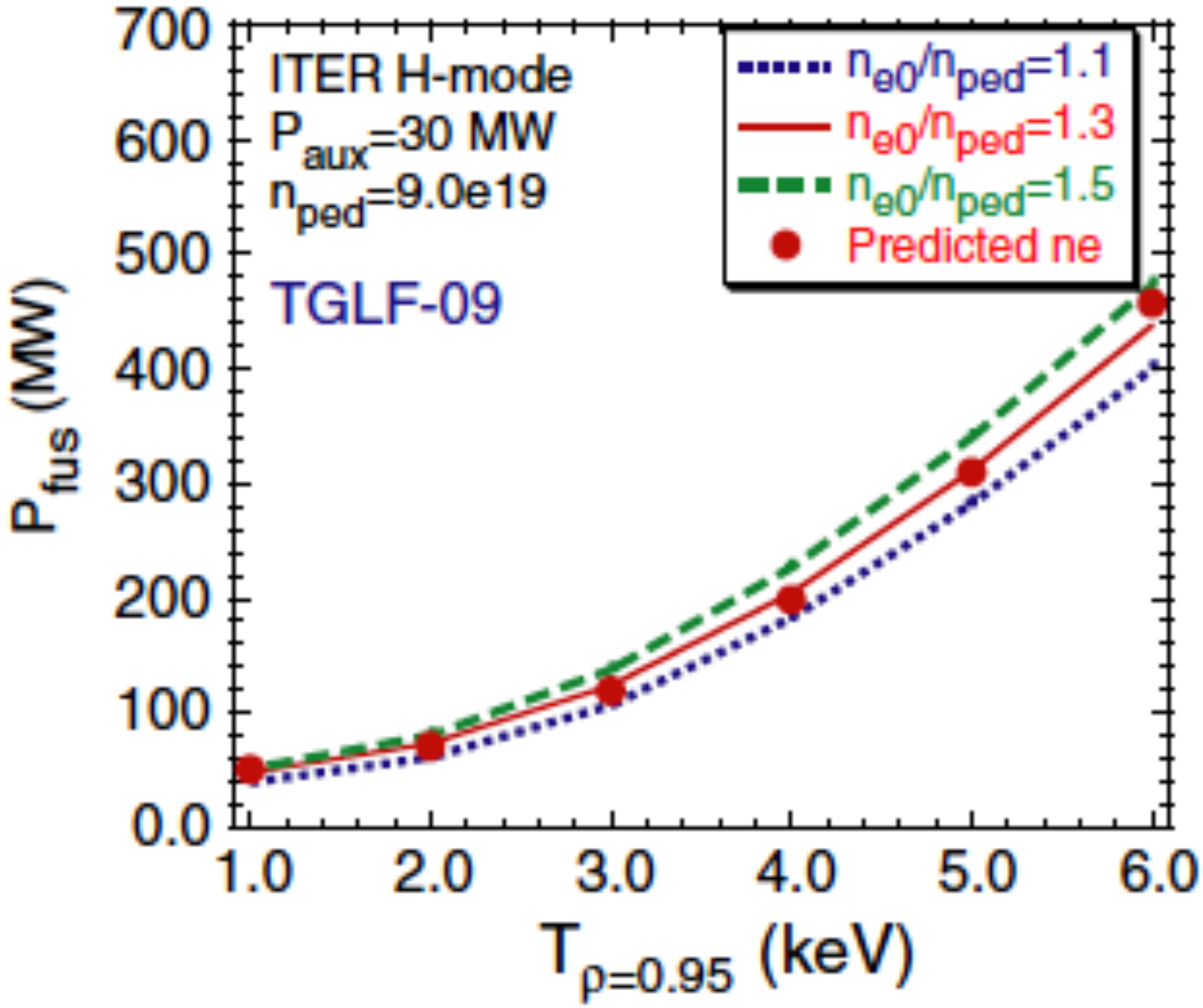


(from M. Wade, SOFE 2019)

Motivation: Pedestal Temperature Has a Big Effect on Fusion Performance

TGLF/TGYRO core transport simulations of ITER, strongly depends on assumed pedestal temperature.

The edge pedestal is the tail that wags the dog.

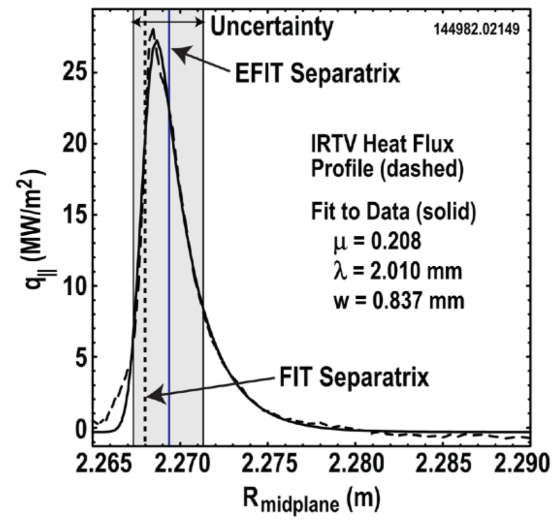


Need full nonlinear gyrokinetic simulations to confidently predict boundary turbulence and optimize pedestal temperature. (Also need nonlinear GK simulations to handle core turbulence that can be subcritical.)

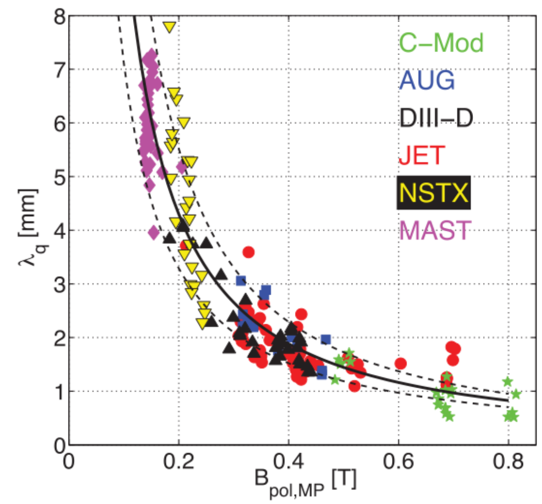
Kinsey et al. Nucl. Fus. 2011 http://stacks.iop.org/NF/51/083001 General effect known since 90's IFS-PPPL model,, see Dimits et al., 2000

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)

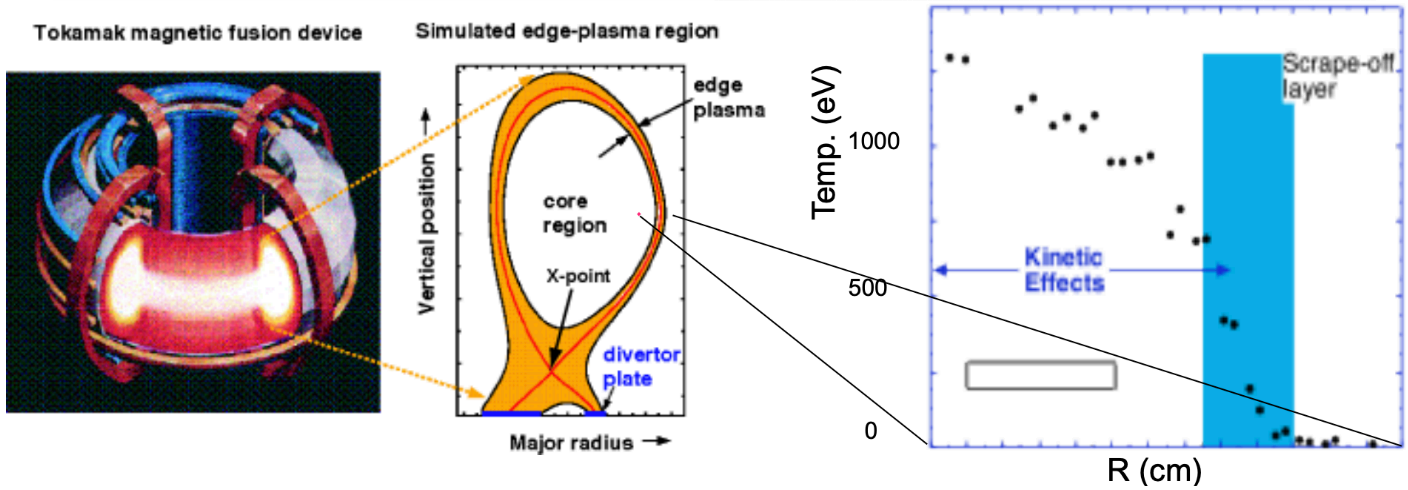


DIII-D from Makowski et al. (2012)



Eich et al. (2013)

Modeling edge region is very difficult



- Plasma properties in the edge/SOL constrain performance and component lifetime
  - Heat exhausted in SOL could damage divertor plates
  - Sets boundary condition on core profiles (e.g. H mode)
- Open/closed field lines, plasma-wall interactions, large-amplitude fluctuations, atomic physics
- Electromagnetic effects can be important in the edge/SOL, $\beta\, m_e/m_i > \sim 1$, steep pressure gradients can push plasma close to ideal-MHD threshold and produce stronger turbulence
- Most present turbulence codes optimized for core, need specialized codes for edge
- Codes like XGC1 making great progress, but essential to have several independent codes to cross-check on difficult turbulence problems

The Gkeyll Plasma Framework

- Flexible suite of solvers for plasma physics, Ammar Hakim, architect & group leader.
  - Continuum solvers for full-F gyrokinetics and Vlasov-Maxwell w/ DG methods; also multi-fluids with FV methods
- Novel discontinuous Galerkin (DG) scheme conserve energy for Hamiltonian systems (like GK)
  - A. Hakim et al., arXiv:1908.01814
  - A. Hakim et al., arXiv: 1903.08062
- First successful <u>continuum</u> GK code on open field lines (E. L. Shi, Princeton Ph.D. thesis 2017)
  - E. L. Shi et al, JPP 2017 (LAPD)
  - E. L. Shi et al, PoP 2019 (NSTX SOL)
  - T. Bernard et al, PoP 2019 (Helimak)
  - GENE also did LAPD: Q. Pan et al. PoP 2018
- **First electromagnetic GK on open field lines: N. R. Mandell et al, arXiv:1908.05653**

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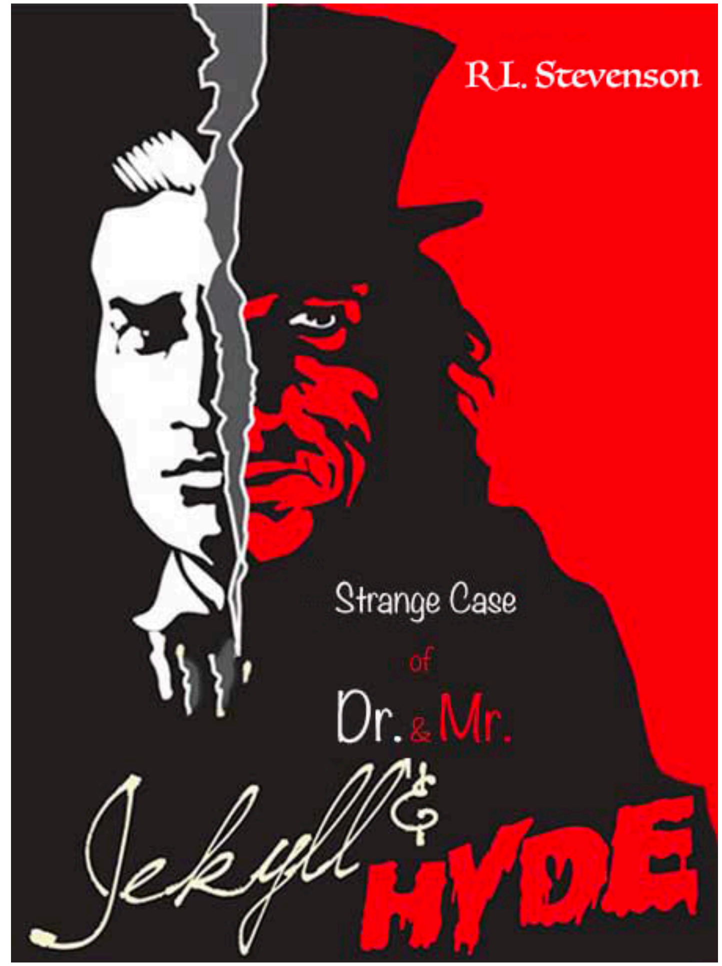


https://github.com/ammarhakim/gkyl/

https://gkeyll.readthedocs.io/en/latest/index.html

- Present slides borrowed from:
  - Ammar Hakim, APS invited talk, 2019
  - Noah Mandell, MPPC talk, Göttingen, 2019.
  - Tess Bernard, Sherwood & TTF invited talks, 2019.
  - Papers on previous page

Full-F electromagnetic gyrokinetics

EMGK equation, $f_s = f_s(\boldsymbol{R}, v_\parallel, \mu; t)$

$$\frac{\partial f_s}{\partial t} + \dot{\boldsymbol{R}} \cdot \nabla f_s + \dot{v}_\parallel \frac{\partial f_s}{\partial v_\parallel} = C[f_s] + S_s$$

with nonlinear phase-space trajectories

$$\dot{\boldsymbol{R}} = \{\boldsymbol{R}, H_s\} = \frac{\boldsymbol{B_0^*} + \delta \boldsymbol{B}_\perp}{B_\parallel^*} v_\parallel + \frac{\hat{\mathbf{b}}}{q_s B_\parallel^*} \times (\mu \nabla B + q_s \nabla \phi)$$

$$\dot{v}_\parallel = \{v_\parallel, H_s\} - \frac{q_s}{m_s}\frac{\partial A_\parallel}{\partial t} = -\frac{\boldsymbol{B_0^*} + \delta \boldsymbol{B}_\perp}{m_s B_\parallel^*} \cdot (\mu \nabla B + q_s \nabla \phi) - \frac{q_s}{m_s}\frac{\partial A_\parallel}{\partial t}$$

where $\boldsymbol{B_0^*} = \boldsymbol{B_0} + (m_s v_\parallel / q_s) \nabla \times \hat{\mathbf{b}}$ and $\delta \boldsymbol{B}_\perp = \nabla A_\parallel \times \hat{\mathbf{b}}$.

Using symplectic ($v_\parallel$) formulation of EMGK, so $\frac{\partial A_\parallel}{\partial t}$ appears explicitly

Full-F electromagnetic gyrokinetics

Quasineutrality equation (long-wavelength):

$$-\nabla\cdot\sum_s \frac{m_s n_{0s}}{B^2}\nabla_\perp\phi = \sum_s q_s \int d^3v\ f_s$$

Parallel Ampère equation:

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

Can take $\frac{\partial}{\partial t}$ to get an exact Ohm's law:

$$-\nabla_\perp^2 \frac{\partial A_\parallel}{\partial t} = \mu_0 \sum_s q_s \int d^3v\ v_\parallel \frac{\partial f_s}{\partial t}$$

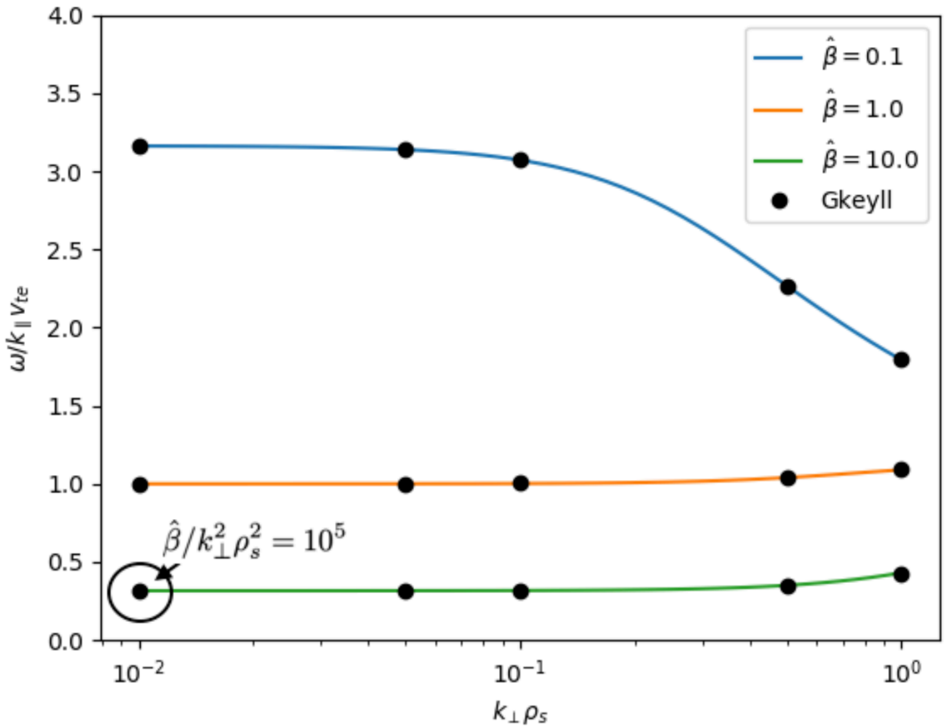
Writing GK eq. as

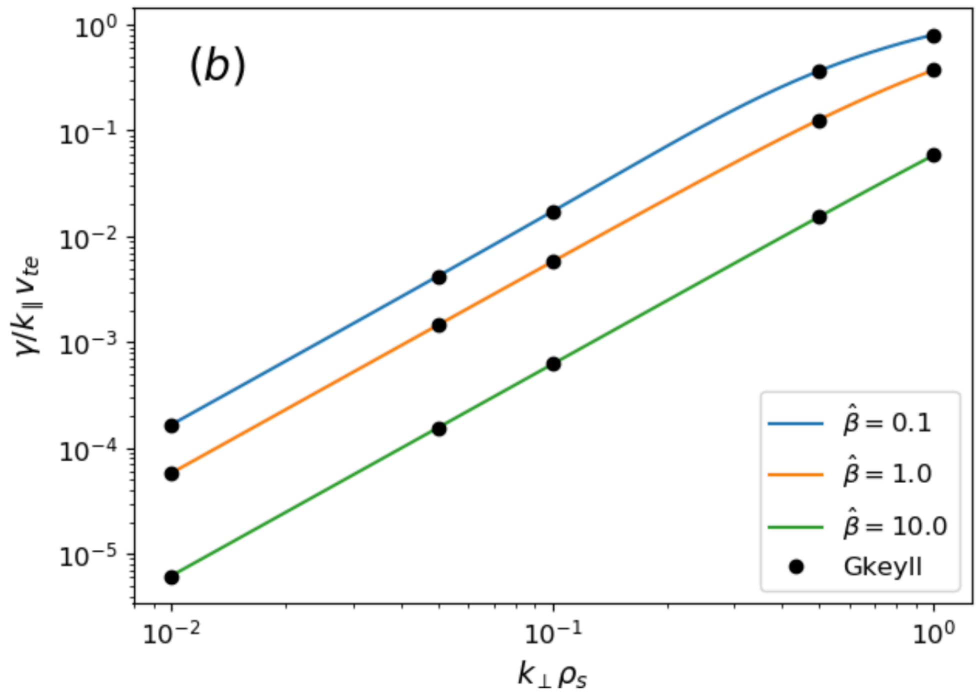
$$\frac{\partial f_s}{\partial t} = \frac{\partial f_s}{\partial t}^\star + \frac{q_s}{m_s}\frac{\partial A_\parallel}{\partial t}\frac{\partial f_s}{\partial v_\parallel},$$

where $\frac{\partial f_s}{\partial t}^\star$ denotes all the terms in the gyrokinetic equation except the $\frac{\partial A_\parallel}{\partial t}$ term, can write Ohm's law as (DG preserves integration by parts exactly.)

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

Linear benchmark: kinetic Alfvén wave





$$\hat{\beta} = \frac{\beta_e}{2}\frac{m_i}{m_e}$$

Gkeyll results match theory very well, even for case with $\frac{\hat{\beta}}{k_\perp^2\rho_s^2} = 10^5$

No cancellation problem!

Texas Helimak is useful for code validation

- Allows investigation of SOL-like turbulence in simple cylindrical geometry
- 500+ Langmuir probes
- Baffled probes directly measure ϕ
- Ion species: He^+, Ne^+, $\mathbf{Ar}^+$
- Turbulent drives are interchange and drift-wave
- Bias voltage applied to end plates to study effect of velocity shear on turbulence

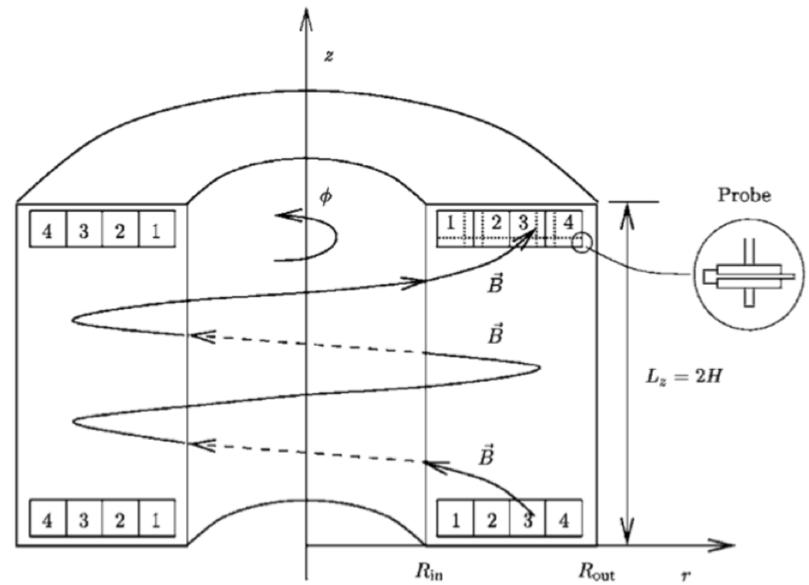
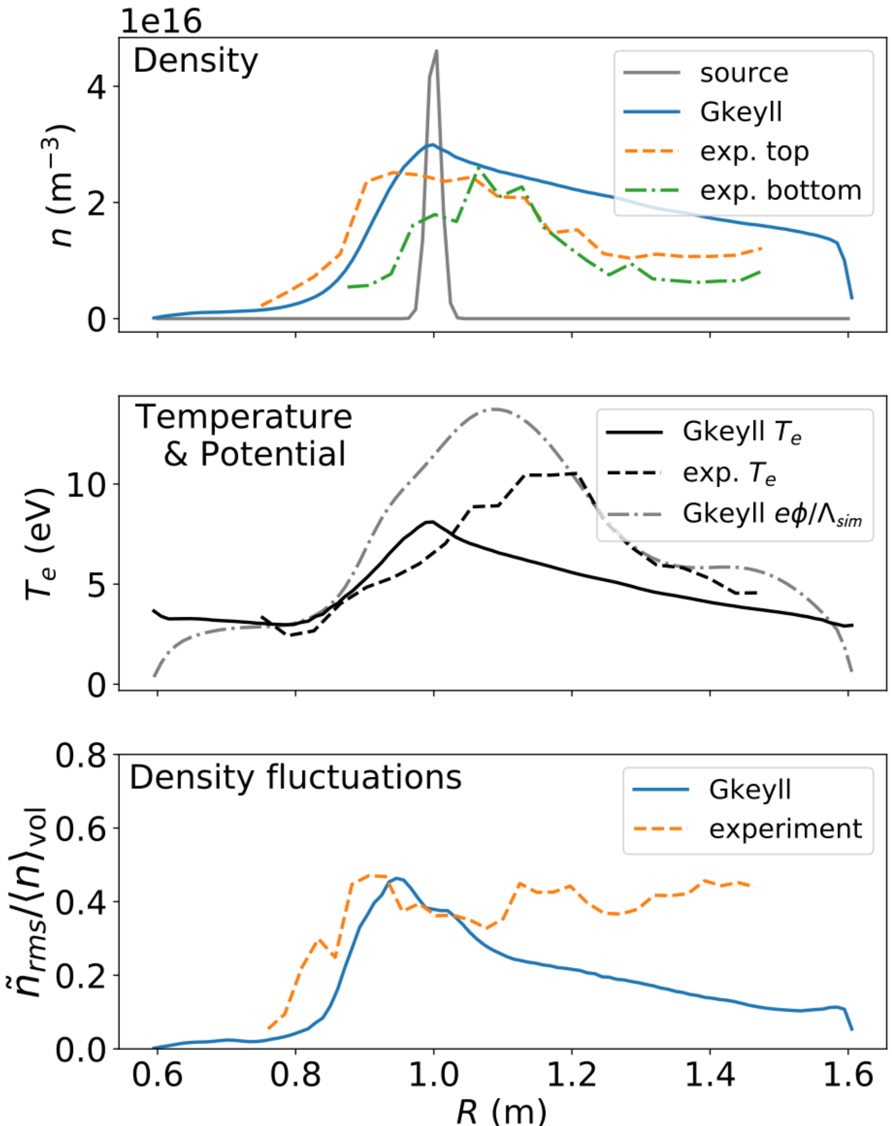


Figure: Texas Helimak (left) and cross section (above)

T. Bernard et al, PoP 2019

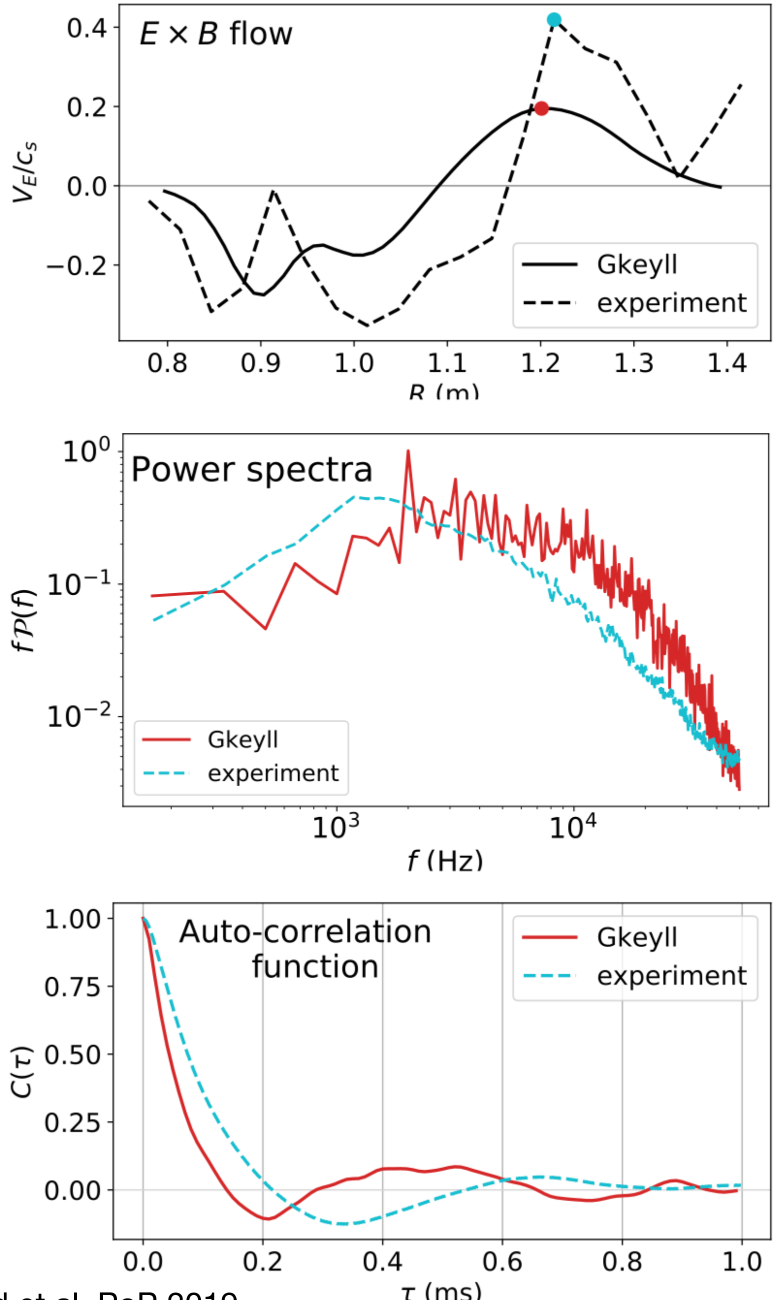
Simulation captures features of experimental equilibrium profiles



T. Bernard et al, PoP 2019

- Narrow source (in gray) broadened by turbulence.
- Simulation reproduces density magnitude and gradients relatively well.
- Top-bottom asymmetry in experiment not captured: simulations currently do not have vertical $E \times B$ flow.
- Slightly underpredicts T_e magnitude and gradient at high R.
- Fluctuation levels approach experimental values but not at high R.
- Could improve with full non-linear Poisson equation.

Turbulence statistics compared at max(V_E)



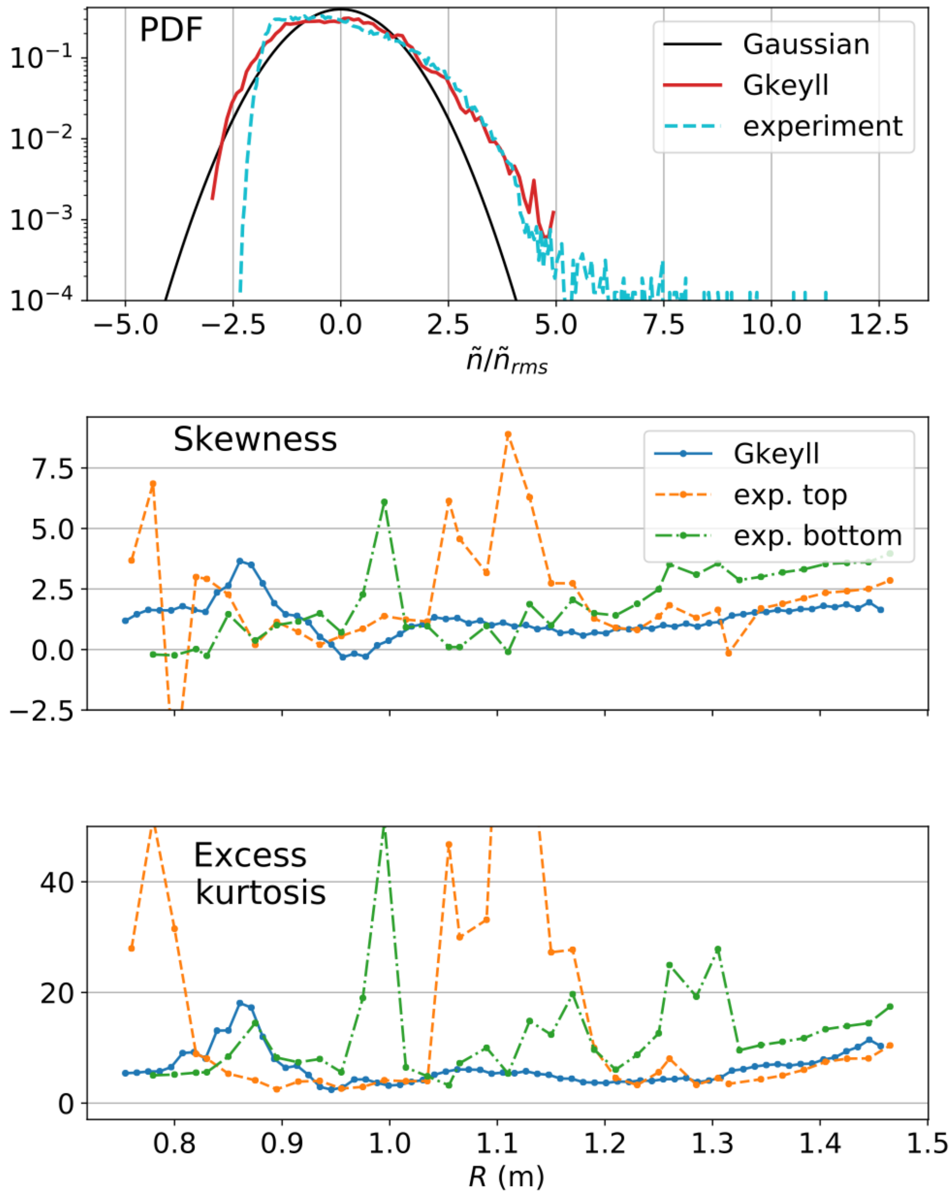
- $V_E = -(d\phi_0/dx)/B_0$.
- Experimental V_E calculated from T_e profiles, assuming adiabatic electrons.

- Power spectra normalized to total energy $f\mathcal{P}(f)$ at radial locations where V_E is maximal.
- Simulation is noisier, peaks at a higher frequency, and decays more quickly.

- $C(\tau) = \langle \tilde{n}(t)\tilde{n}(t+\tau)\rangle / \langle \tilde{n}(t)^2\rangle$
- Correlation time for the simulation data is shorter.

T. Bernard et al, PoP 2019

Simulation captures turbulence intermittency



- Positive tails of the simulation PDF's approach the experimental values until $5\tilde{n}/n_{\mathrm{rms}}$.
- Longer simulations could attain longer experimental tails.
- Positive skewness and excess kurtosis signal intermittent turbulence, a sign of blob transport.
- Skewness $= E[\tilde{n}^3]/\sigma^3$
- Excess kurtosis $= E[\tilde{n}^4]/\sigma^4 - 3$

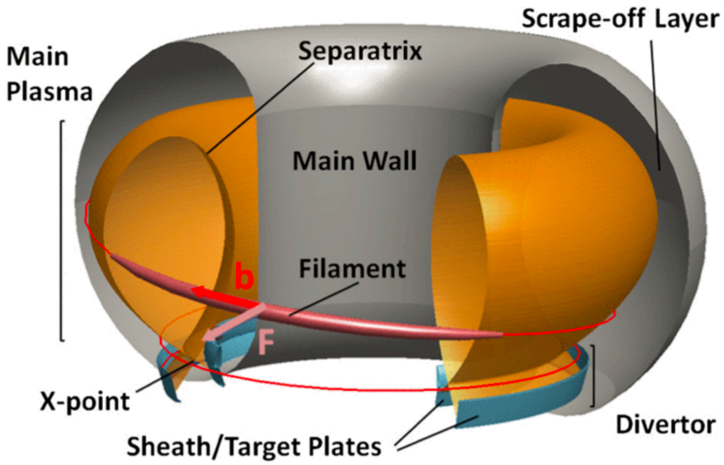
T. Bernard et al, PoP 2019

Additional features could improve comparison

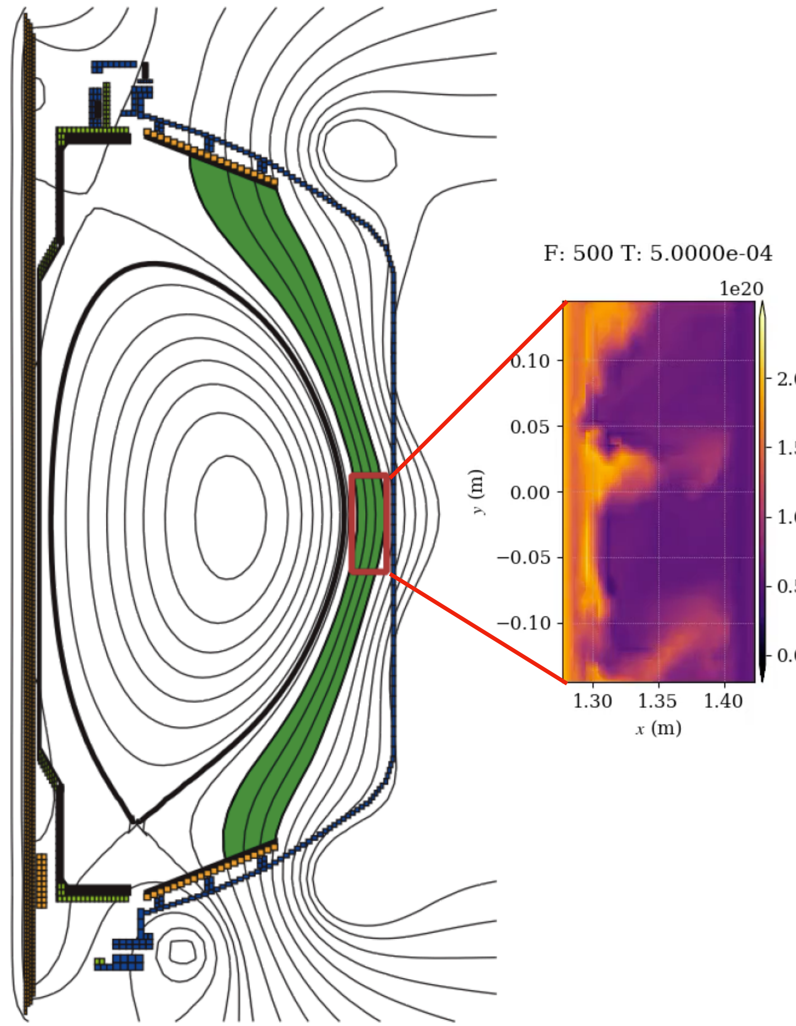
- Vertical $E \times B$ flow: transport and equilibrium profiles
- Magnetic shear: turbulence statistics
- Real electron mass: turbulence levels (by increasing response of electrostatic potential to temperature fluctuations at sheath)
- Full non-linear Poisson equation
- Other considerations: radiation, neutral model, improved sheath BCs

T. Bernard et al, PoP 2019

Modeling the NSTX SOL with Gkeyll

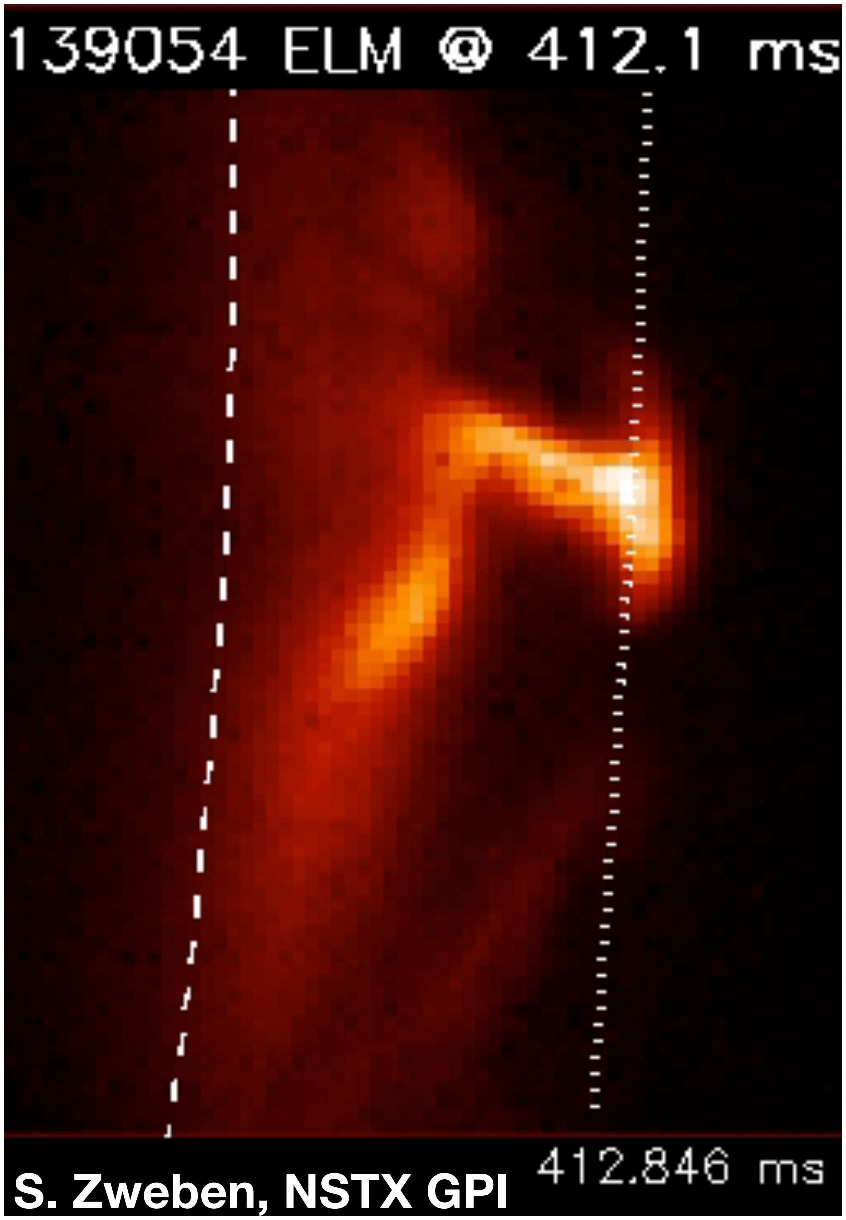


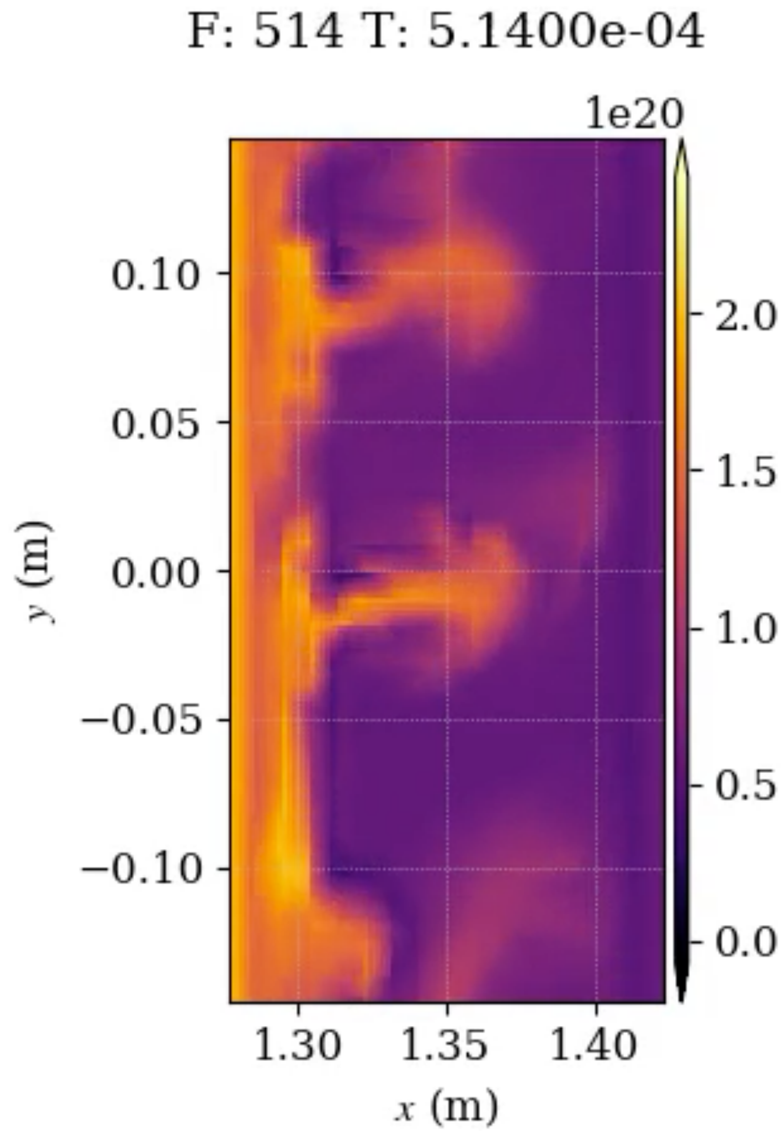
Carralero et al, 2015



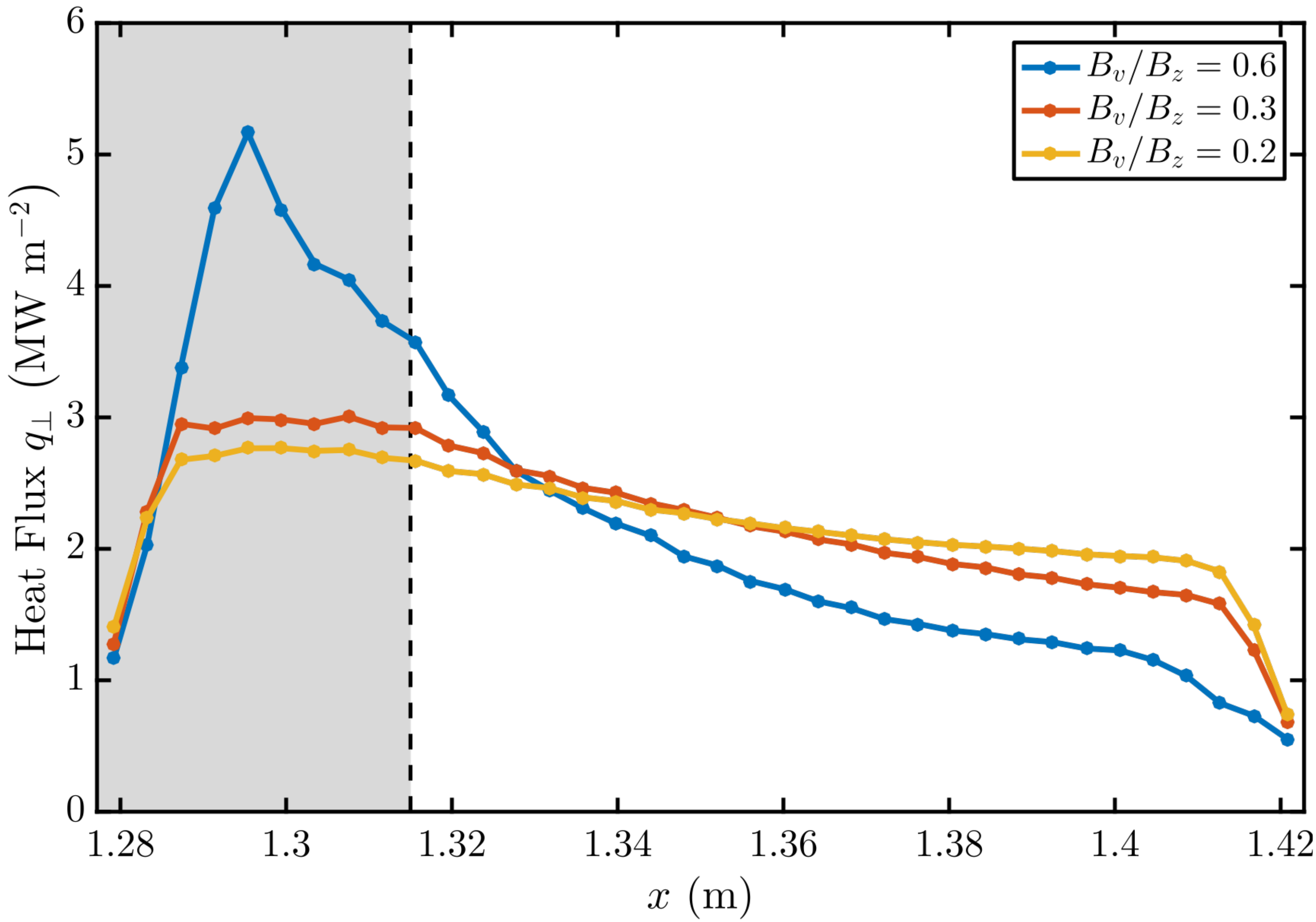
- Simple helical model of tokamak SOL
  - Field-aligned simulation domain that follows field lines from bottom divertor plate, around the torus, to the top divertor plate
  - Like the green region, but straightened out to vertical flux surfaces
  - All bad curvature brings interchange instability drive
- Parameters from NSTX SOL, but with 10x β_0 to stress-test EM effects (could happen in ELM?)
- Real deuterium mass ratio, Lenard-Bernstein collisions
- Radially-localized source models flux of heat and particles across separatrix from core
- Boundary conditions: Dirichlet in *x*, periodic in *y* (toroidal), conducting sheath in *z* (allows current fluctuations)

Modeling the NSTX SOL with Gkeyll





Divertor heat flux narrows ~ $1/\theta \sim 1/B_{pol}$ at high B_{pol}



E. Shi (Ph.D. 2017, PoP 2019)

(Present simulation neglects magnetic shear and related stabilization near x-point, shortened parallel length to divertor plates to approximately compensate.)

radial heat flux weakens at high B_{pol}

(not just that faster parallel losses reduces net radial transport)

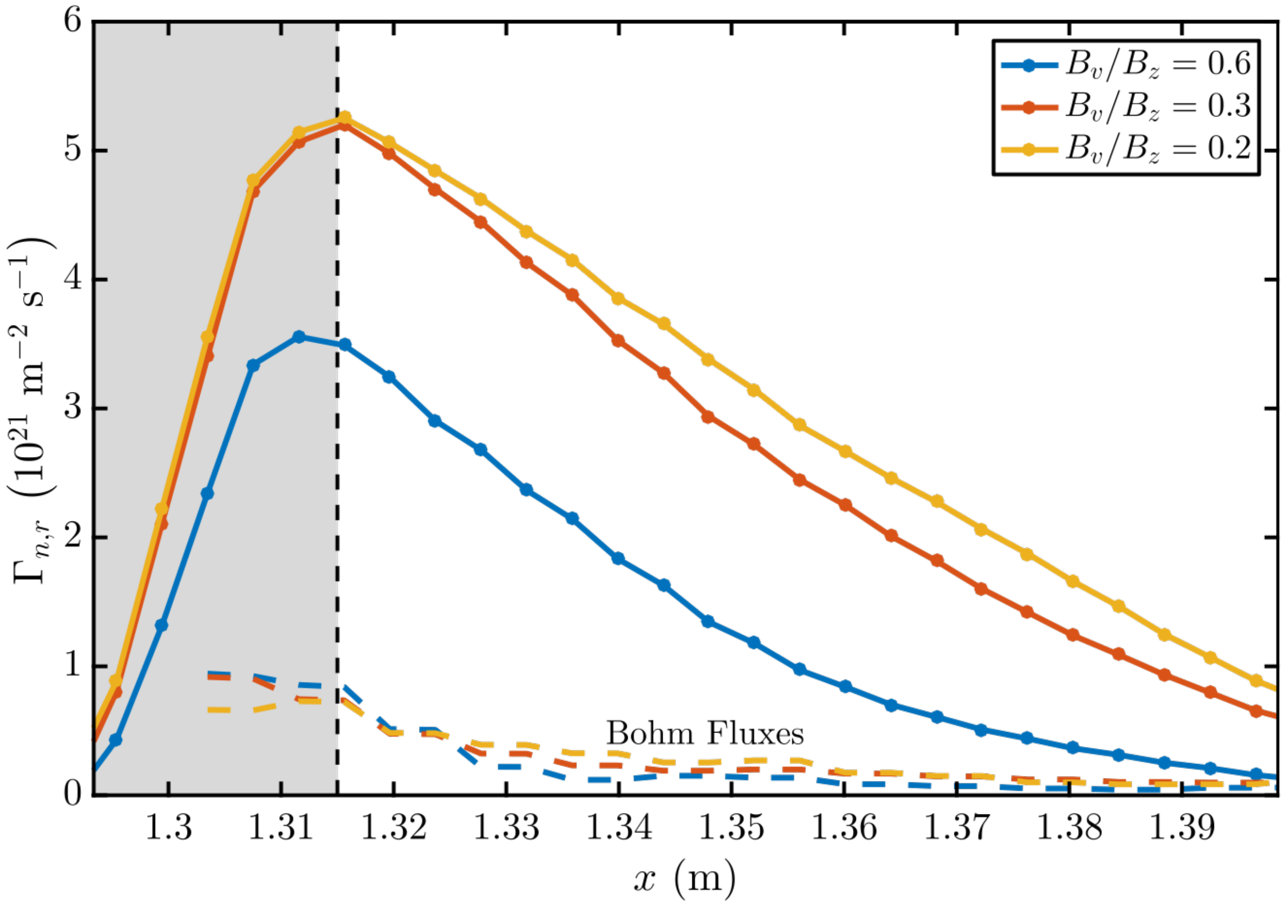
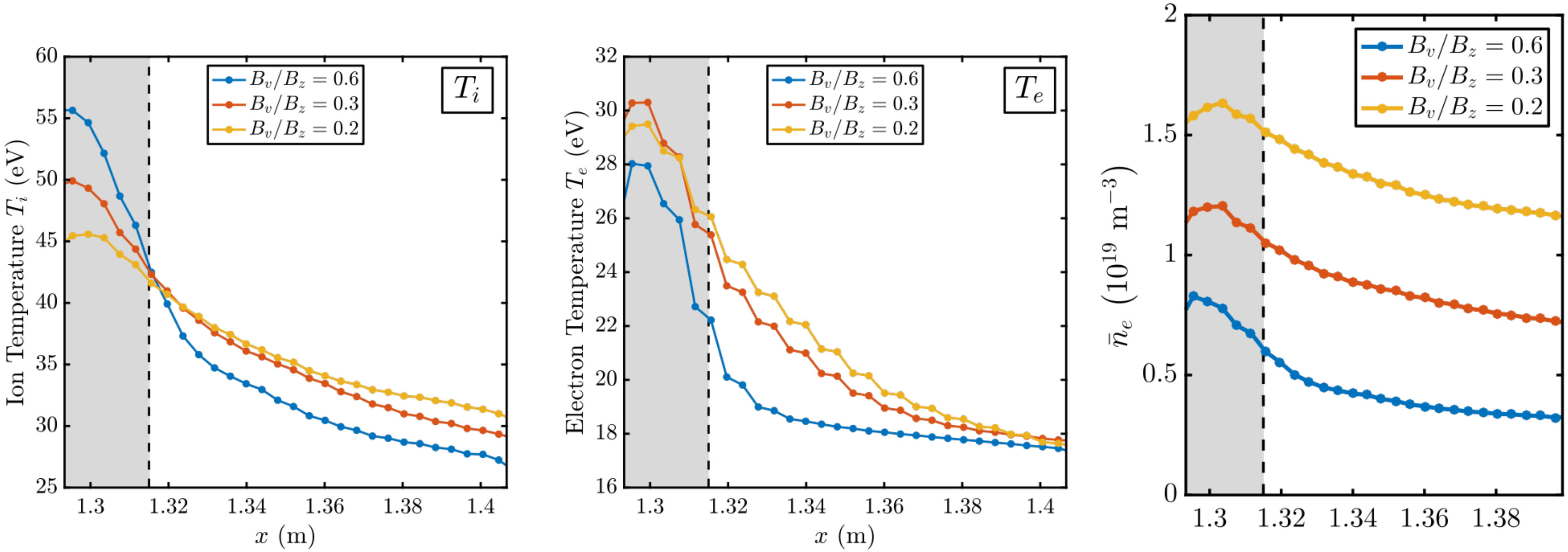


FIG. 6. Comparison of the radial $E \times B$ particle flux evaluated near the midplane for three cases with different magnetic-field-line pitches. The shaded area indicates the region in which the source is concentrated. The dashed lines are Bohm-flux estimates for comparison.

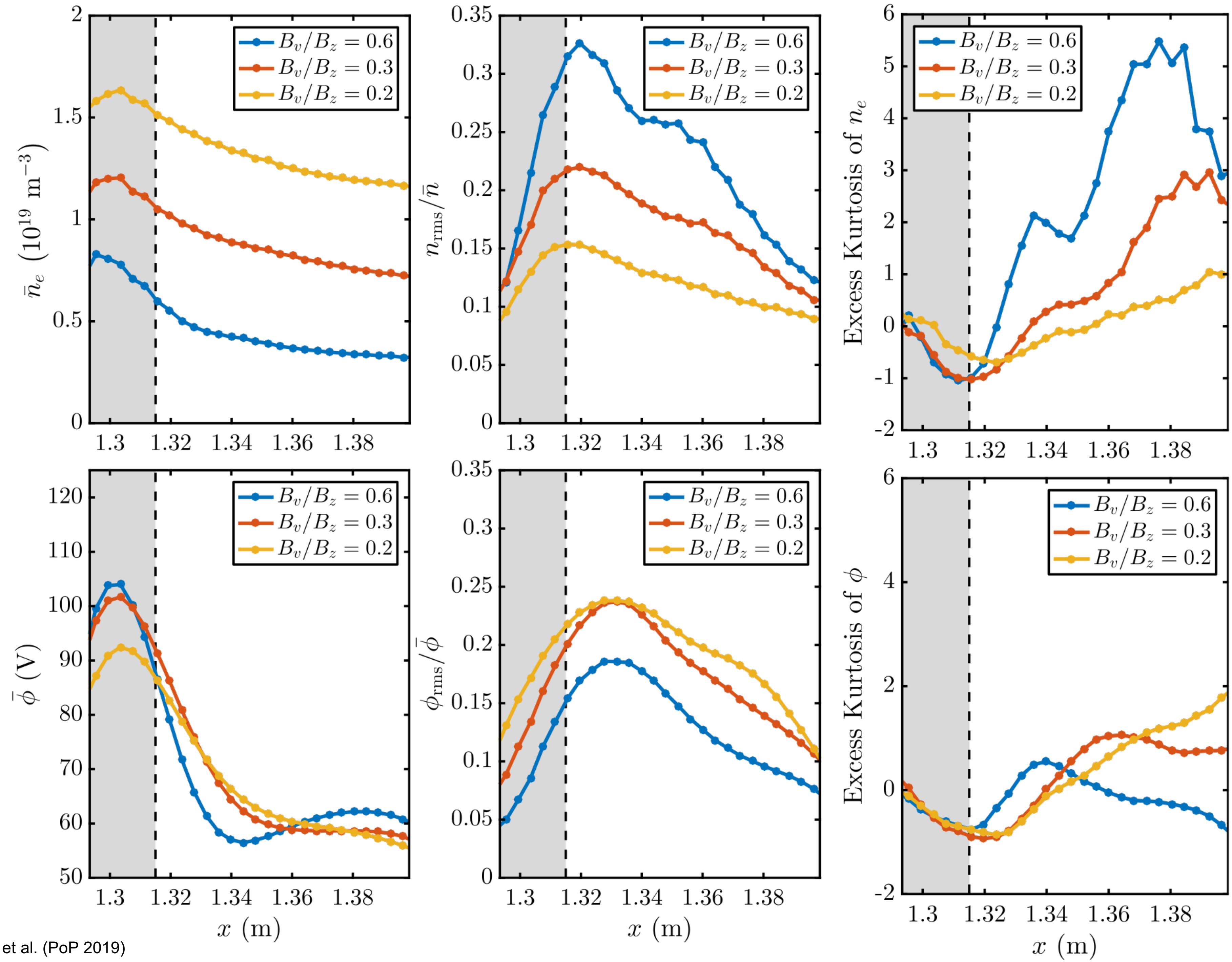
E. Shi et al. (PoP 2019)

SOL profiles narrow ~ $1/\theta \sim 1/B_{pol}$ at high B_{pol}



E. Shi et al. (PoP 2019)

SOL profiles narrow ~ $1/\theta$ ~ $1/B_{pol}$ at high B_{pol}



E. Shi et al. (PoP 2019)

Gkeyll predicts non-zero currents into divertor plates: compare with experiments?

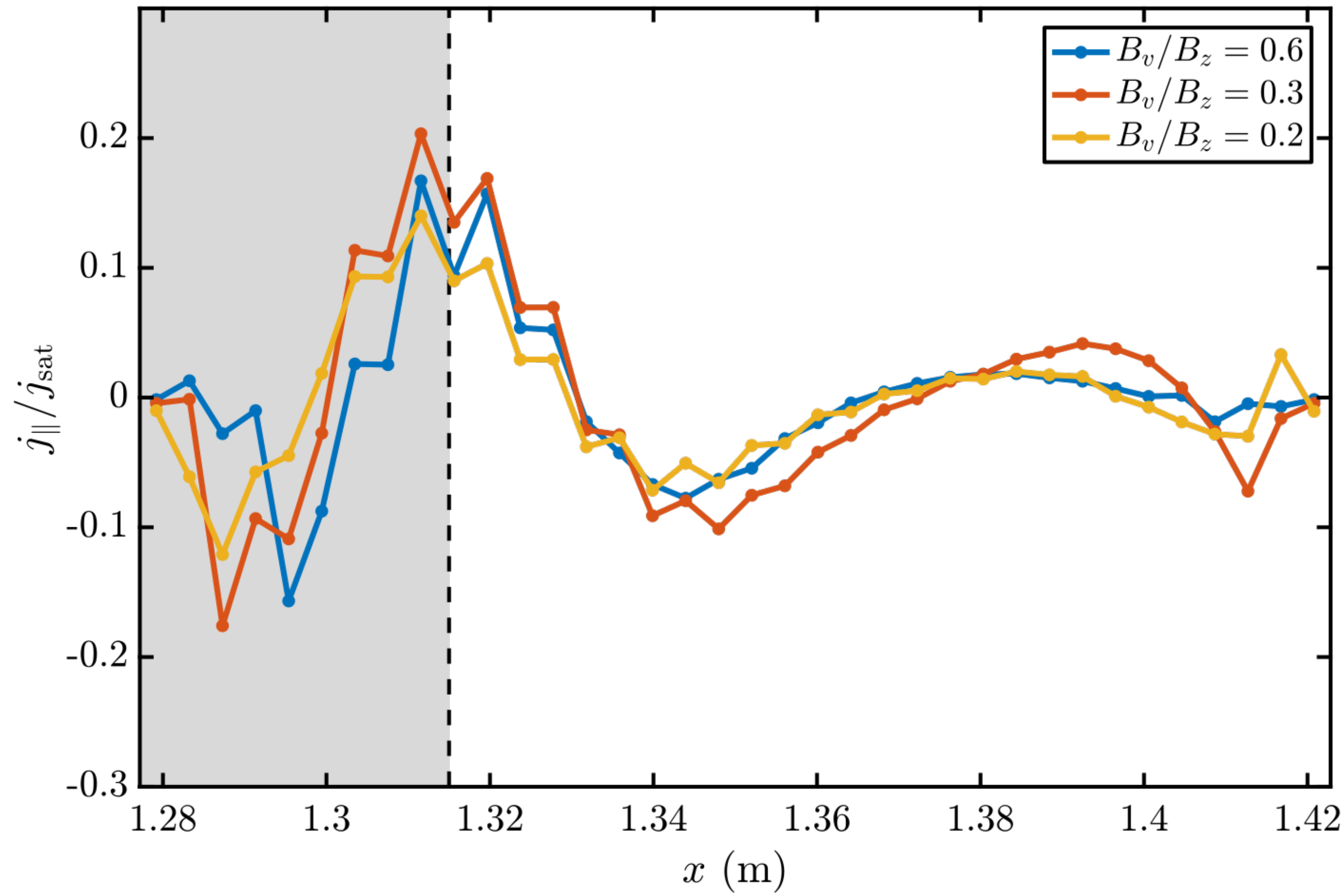
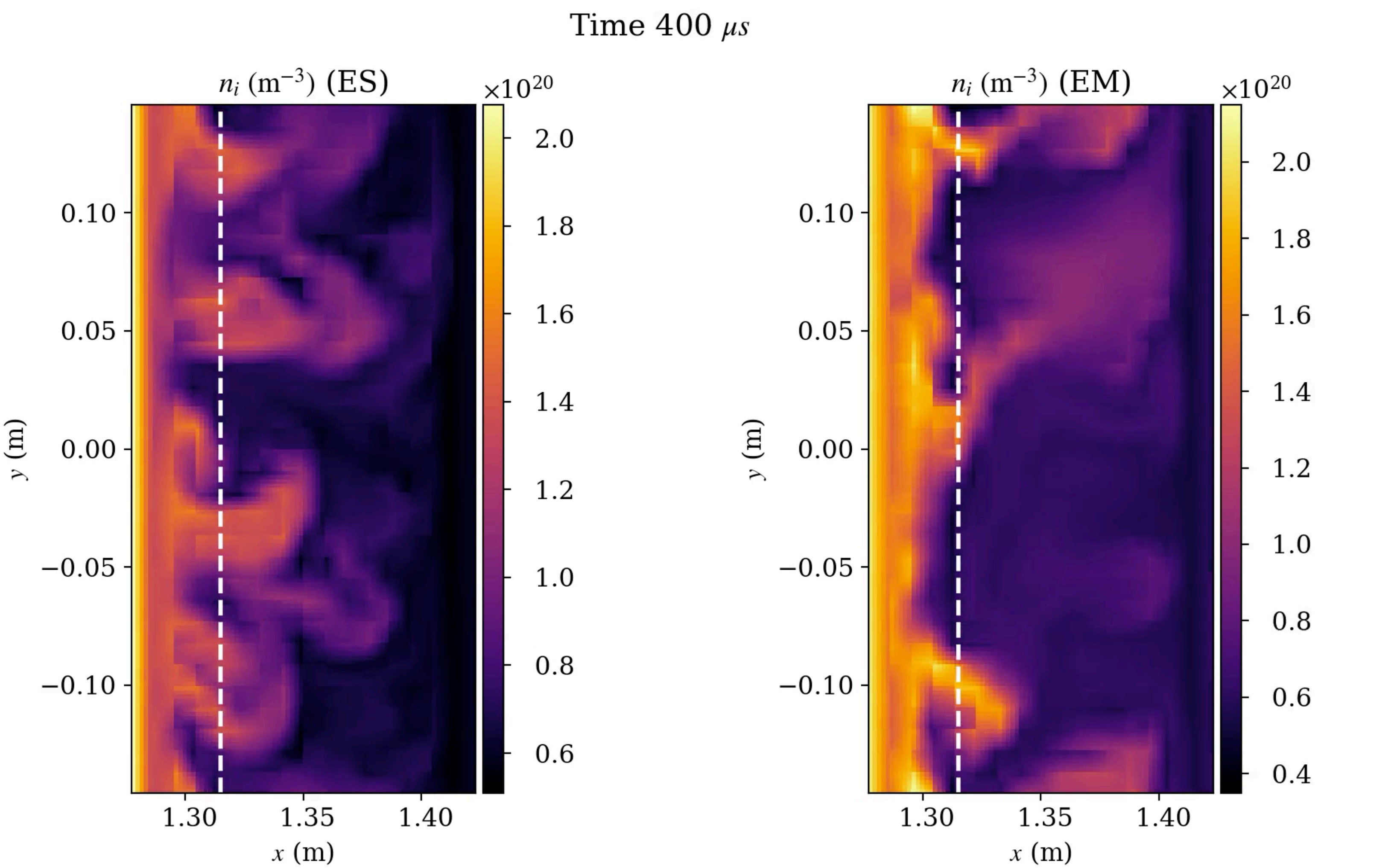


FIG. 12. Radial profiles of the steady-state parallel currents into the sheaths for cases with different magnetic-field-line pitches. The current is normalized to the peak value of the steady-state ion saturation current $j_{\mathrm{sat}} = q_i n_i c_s$ for each simulation. All three cases are quite quantitatively similar, featuring a large excess electron outflow in the source region which is balanced by a large excess ion outflow just outside of the source region.

E. Shi et al. (PoP 2019)

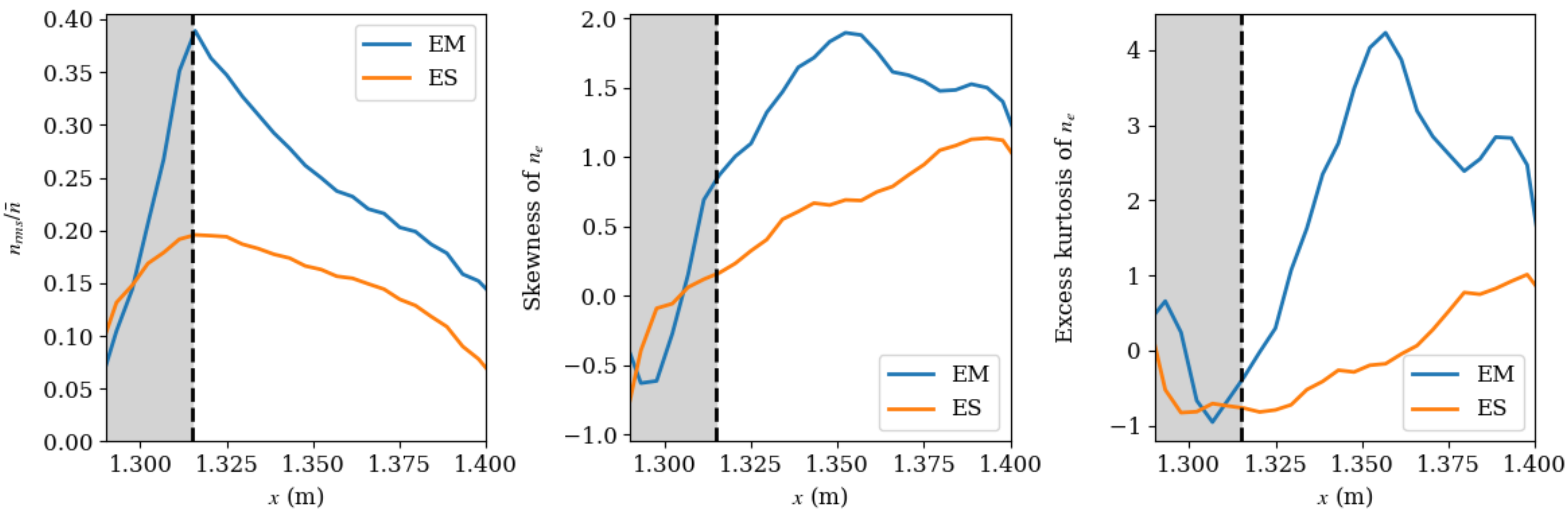
Electrostatic/electromagnetic comparison



Electrostatic/electromagnetic comparison

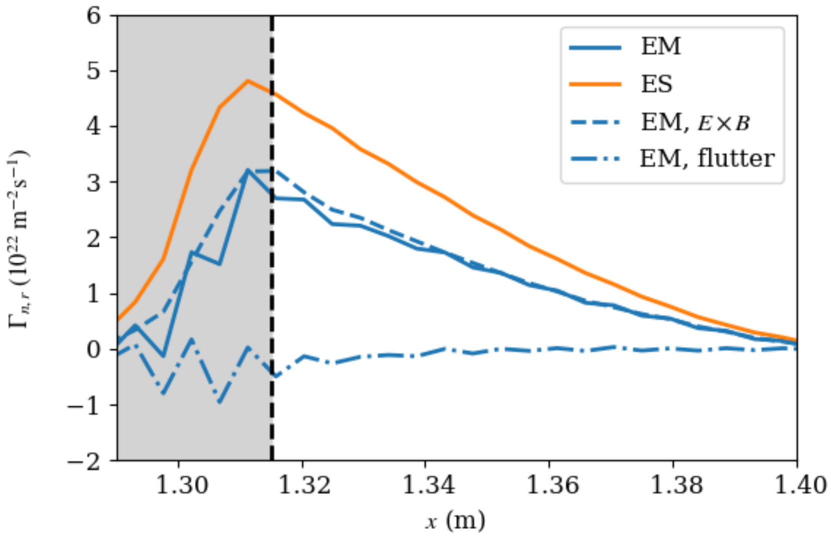
$$\frac{n_{\mathrm{rms}}}{\bar{n}}$$

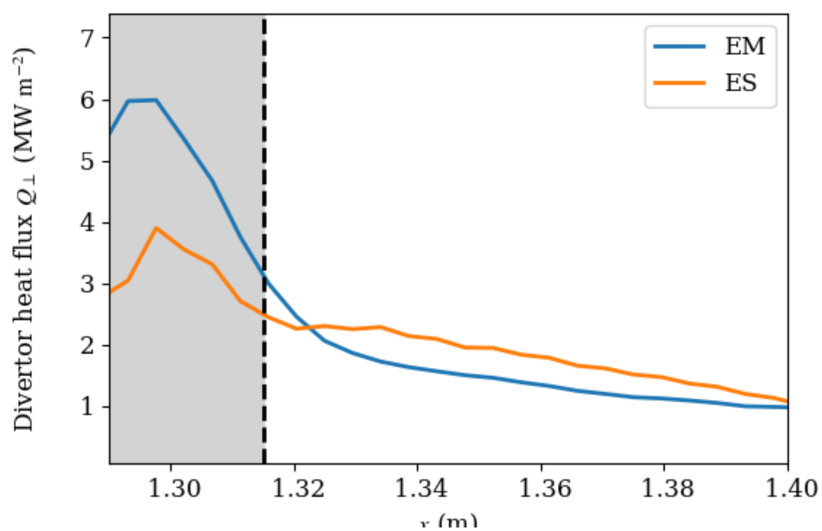
Kurtosis



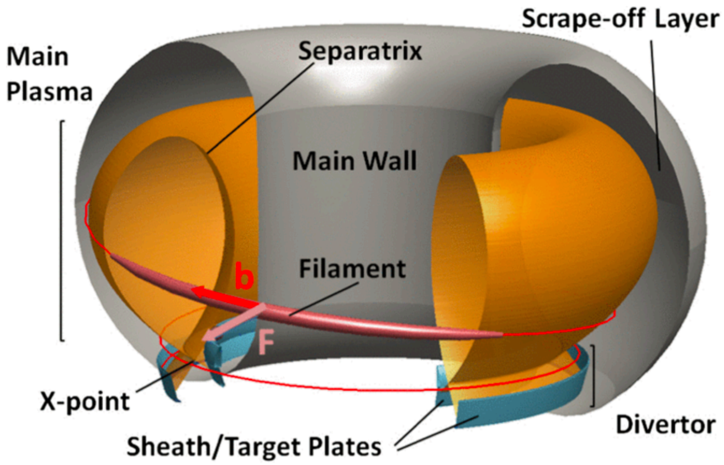
EM has larger, more intermittent density fluctuations

Electrostatic/electromagnetic comparison

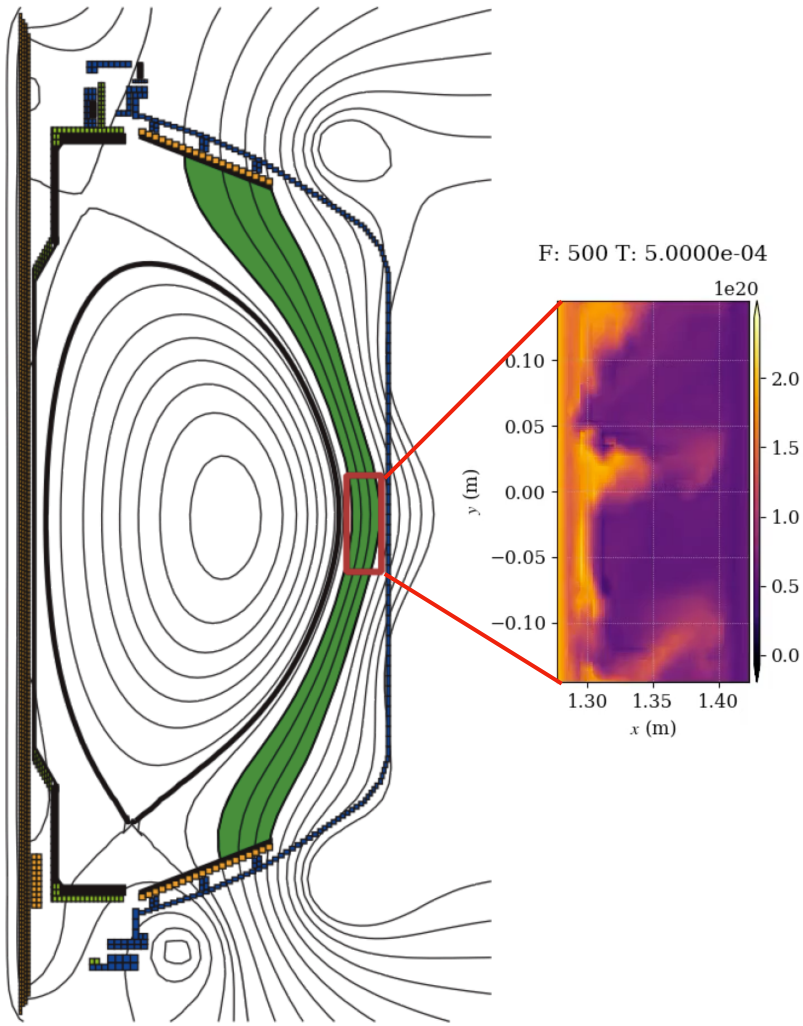




- Radial particle transport reduced in EM case
- Heat flux to divertor is more peaked in EM case

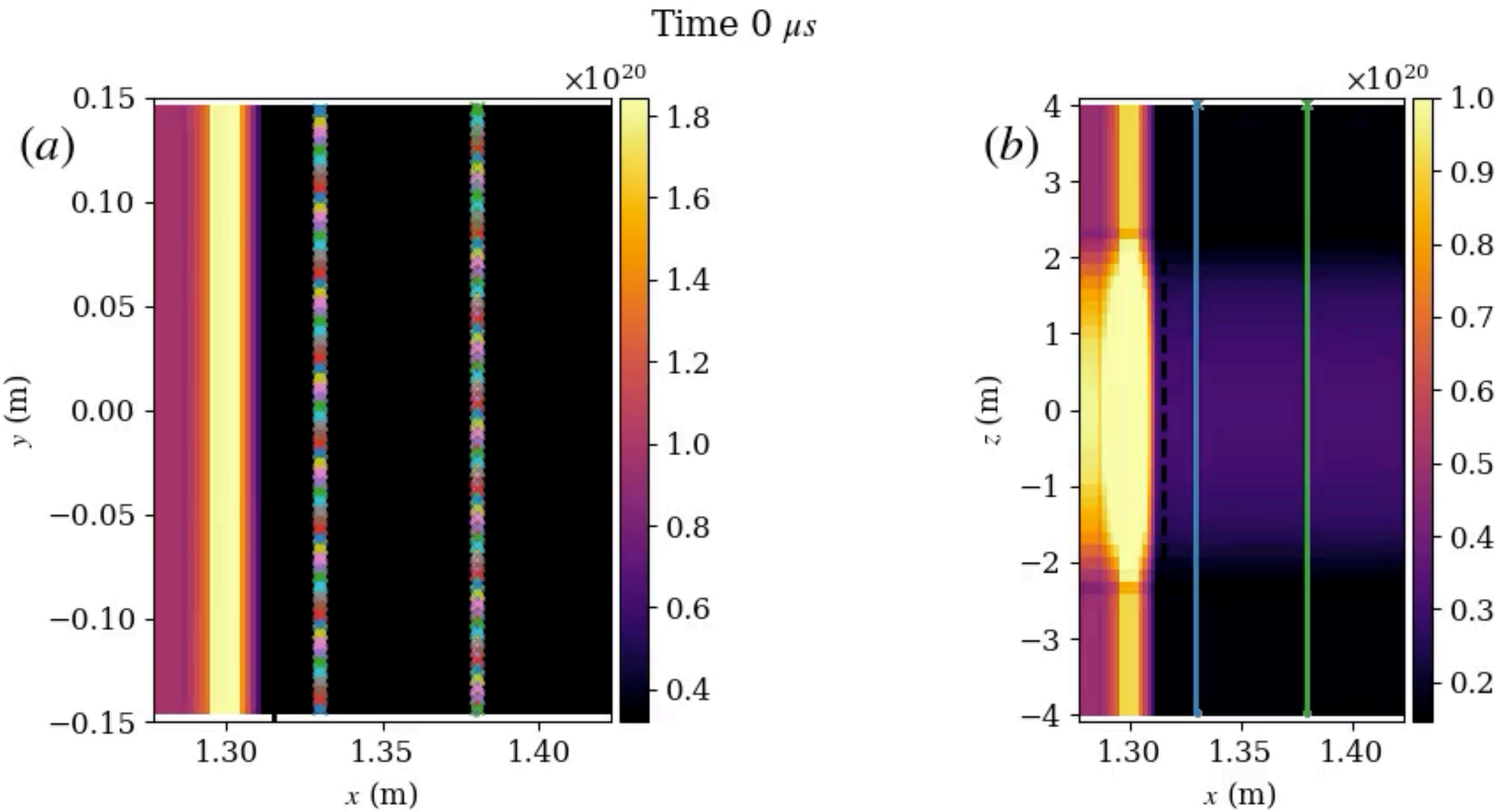


Carralero et al, 2015



Dance of the Field Lines

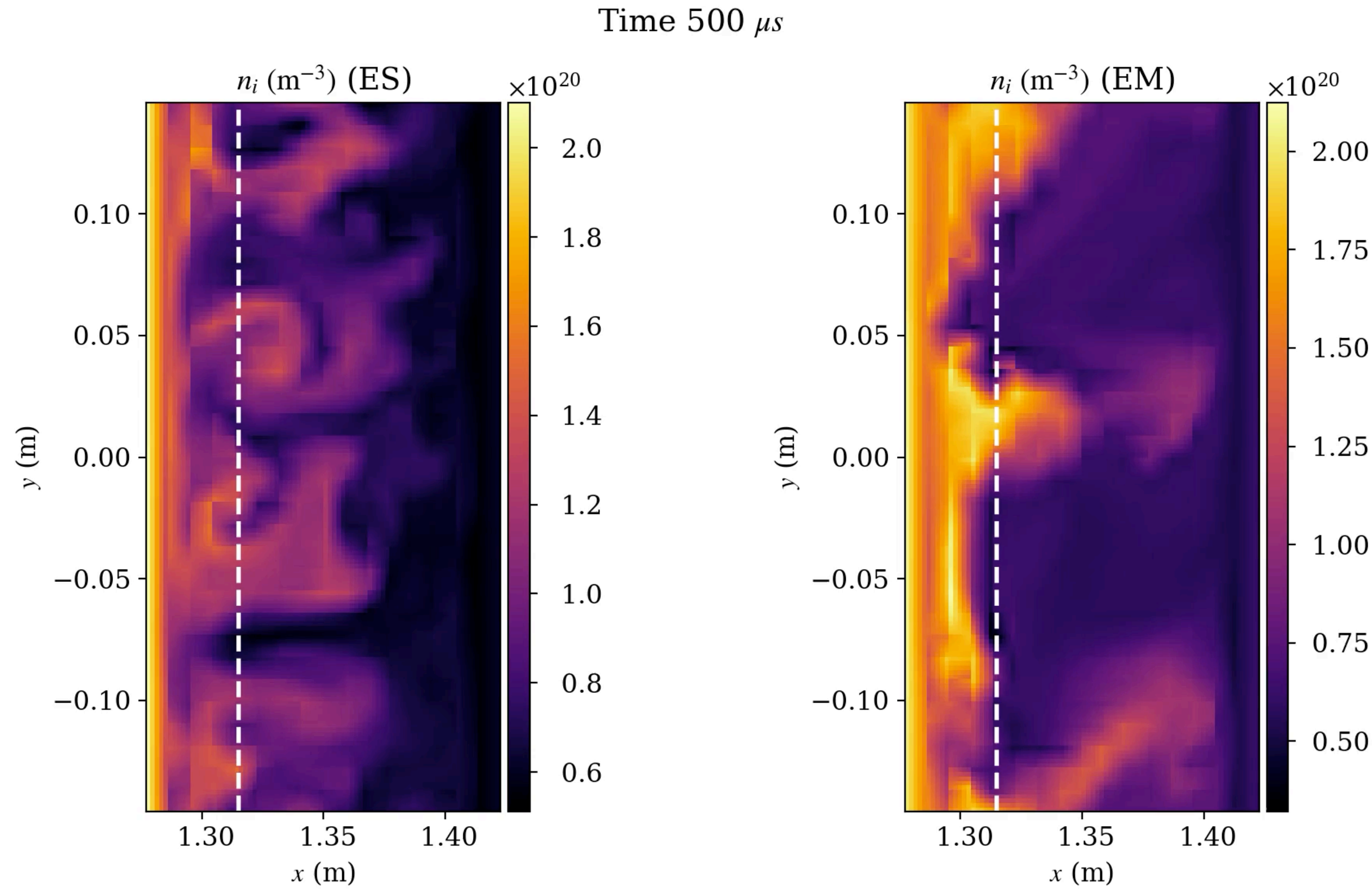
(Electromagnetic GK in SOL)



Blobs ($\beta \sim 1\%$) bend/stretch magnetic field lines ($\delta B/B \sim 0.5\%$)

Footpoints slip some from sheath resistance, also signs of reconnection in plasma.

Modest simulation cost (even for EM!)



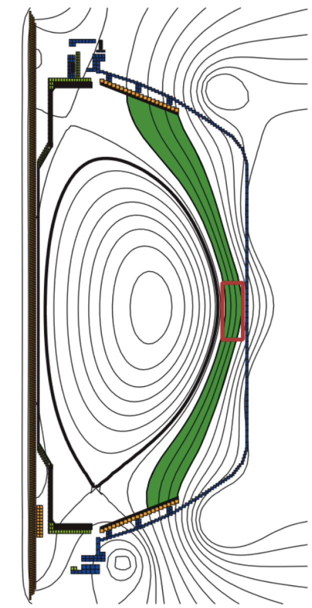
(Nx, Ny, Nz, Nv$_\parallel$, Nμ) ~(32, 64, 20, 20, 10)	Electrostatic	Electromagnetic
Total compute time (128 cores, ~8 CPUs)	8,320 core-hrs (2.7 days)	10,496 core-hrs (3.4 days)
Time/timestep (wall clock)	0.41 s	0.68 s

Summary

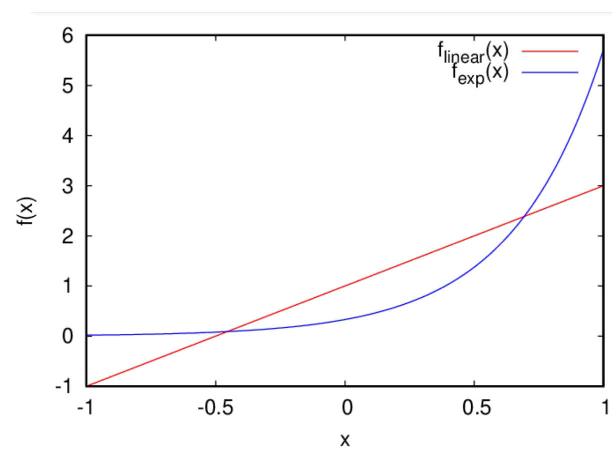
- Edge/SOL region is challenging, requires new codes/methods
- Gkeyll code is a continuum GK code using energy-conserving DG methods
- Gkeyll is being used to study SOL turbulence in tokamaks like NSTX (only handles open field lines right now)
- Gkeyll has produced the first nonlinear electromagnetic gyrokinetic simulations in the SOL

Current/Future Work

- Generalizing the magnetic geometry to include magnetic shear, non-constant curvature, closed field line regions, X-point
  - Non-orthogonal field-aligned coordinate system with magnetic shear now implemented
  - X-point is a singularity in these coordinates, challenging!



- Improving DG algorithms, especially w.r.t. positivity
  - Our previous algorithm did not guarantee $f > 0$
  - Can cause issues with sheath stability, collisions
  - Have developed novel flux-limiter DG algorithm for preserving positivity, working on complete implementation

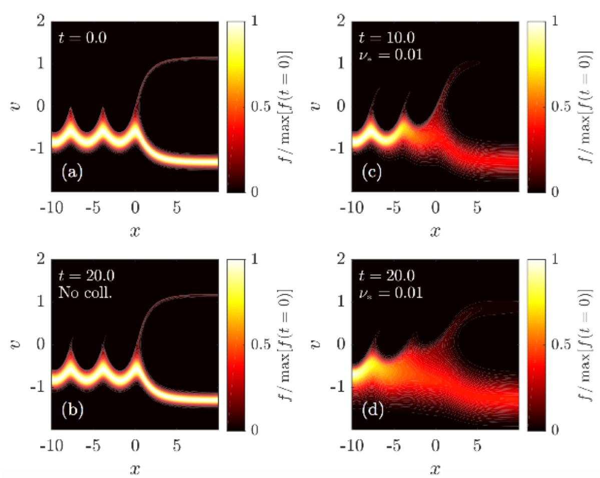


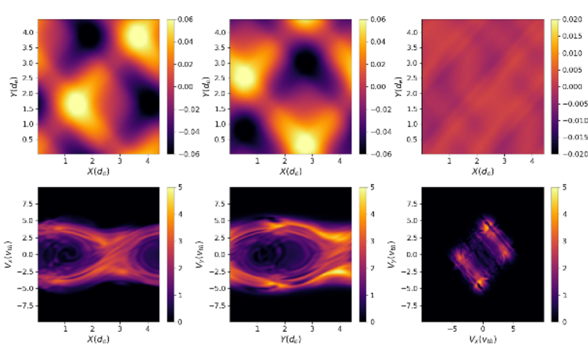
- We have proof-of-concept, but lots more physics to do!

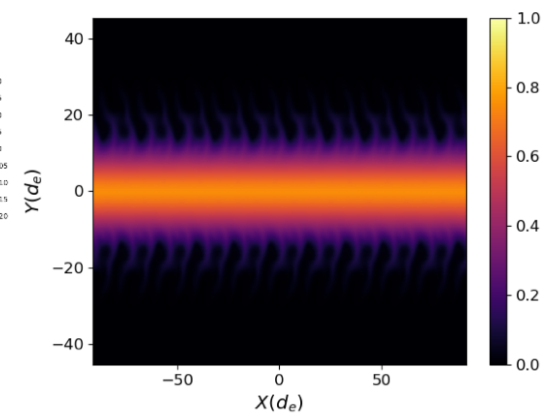
Beyond gyrokinetics: `Gkeyll` Vlasov-Maxwell solvers

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

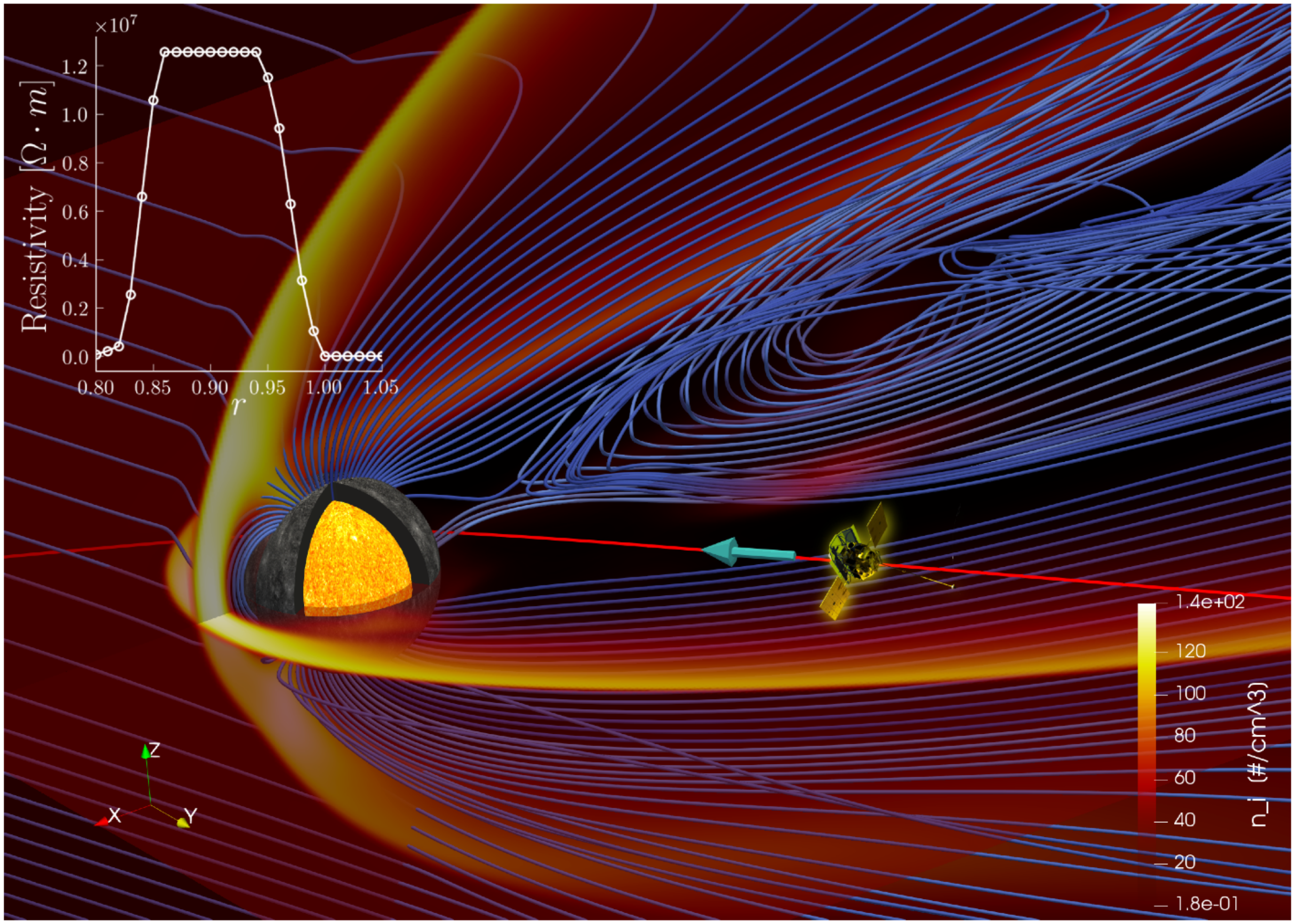






Beyond gyrokinetics: `Gkeyll` Multi-fluid solvers

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.



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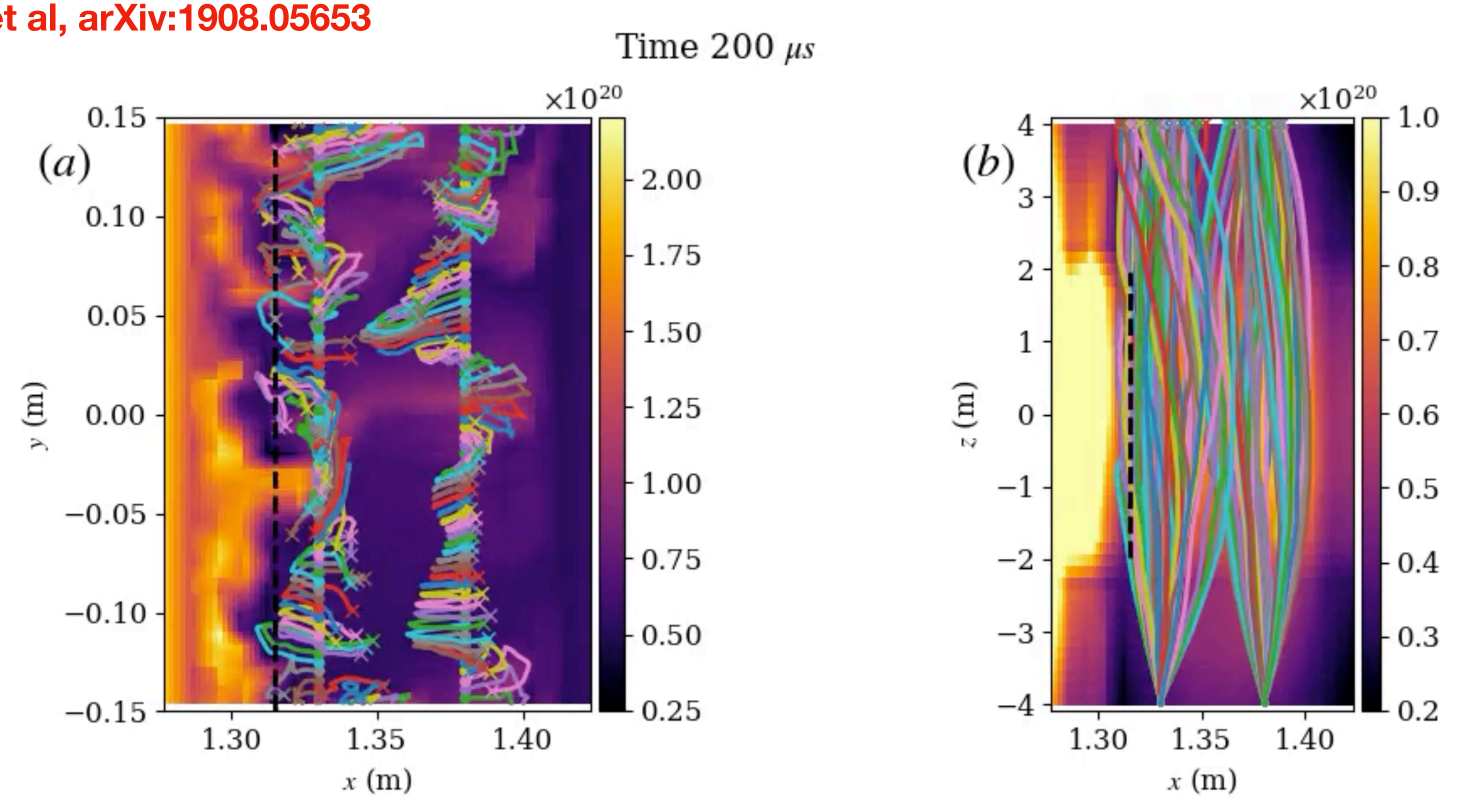
T. Bernard et al, Phys. Plasmas 26 (4) (2019) 042301

A. Hakim et al, arXiv:1908.01814

A. Hakim et al., ArXiv: 1903.08062

N. R. Mandell et al, arXiv:1908.05653



Acknowledgements

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DOE CSGF

Gkeyll team (Gyokinetic+Vlasov):

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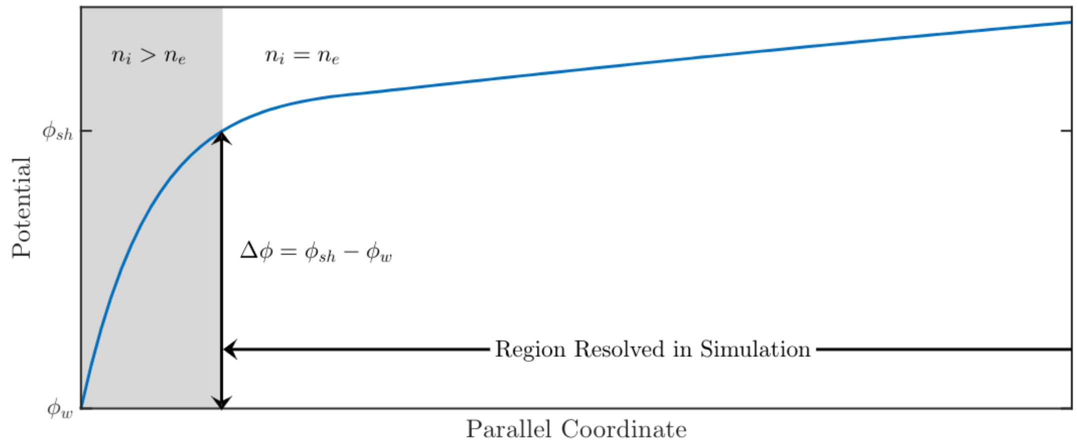
… and others!

https://github.com/ammarhakim/gkyl/

https://gkeyll.readthedocs.io/en/latest/index.html

Back-up slides

Conducting-sheath boundary condition



- Need to model non-neutral sheath using BCs (GK assumes quasi-neutrality, cannot resolve sheath)

- Sheath potential should reflect low energy electrons

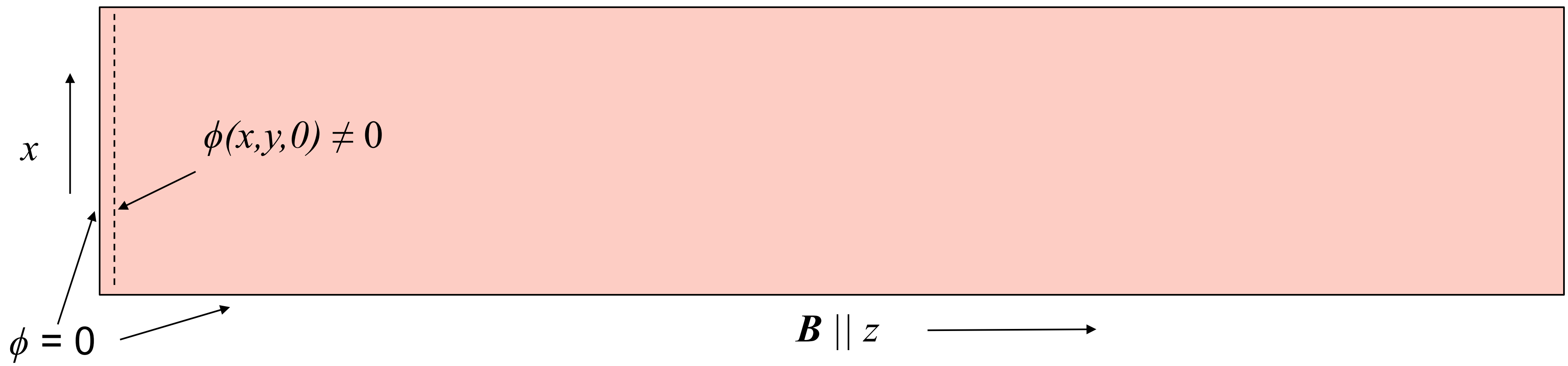
- Solve Poisson equation on z boundary to get $\phi_{sh}(x,y) \doteq \phi(z = z_{sh})$, then use $\Delta\phi = \phi_{sh} - \phi_w$ to reflect electrons with $mv_\parallel^2/2 < |e|\Delta\phi$

$$-\nabla_\perp \cdot \sum_s \frac{m_s n_{0s}}{B^2} \nabla_\perp \phi(z = z_{sh}) = \sum_s q_s \int d^3v \; f_s(z = z_{sh})$$

- Potential self-consistently relaxes to ambipolar-parallel-outflow state, and allows local current fluctuations in and out of wall

Model Sheath Boundary Conditions

$$-\nabla_\perp \cdot (\epsilon_\perp \nabla_\perp \phi) = \sigma_{\rm gc}$$

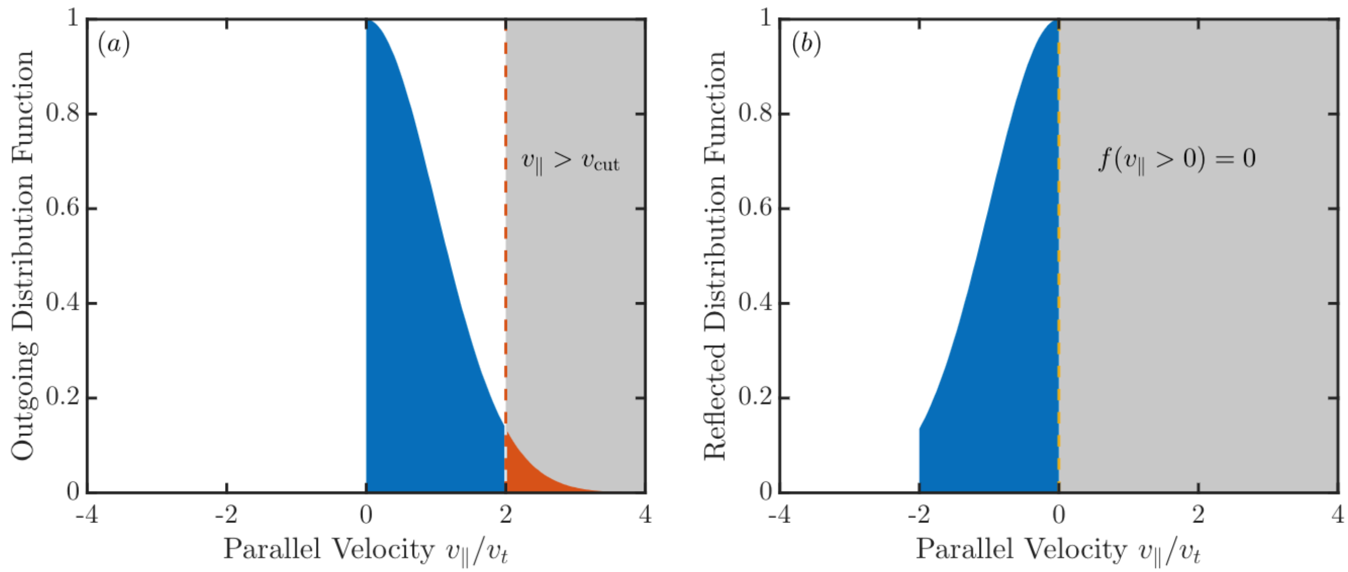


- GK Poisson Eq. solved in 2D planes at fixed z, only needs bcs on side walls (on x or y boundaries). Discontinuous jump between $\phi(x,y,0)$ just inside plasma and $\phi=0$ end plates represents unresolved sheath. Determines reflected electrons:

$$f_e(x,y,0,v_{||},\mu,t) = f_e(x,y,0,-v_{||},\mu,t) \text{ for } 0 < v_{||} < v_c \qquad (1/2)mv_c^2 = q\phi_{\rm sheath}$$
$$f_e(x,y,0,v_{||},\mu,t) = 0 \qquad \text{for } v_c < v_{||}$$

- This is gyrokinetic version of electron sheath boundary condition used in pioneering fluid edge simulations (Ricci, Rogers, et al., Friedman et al.), without assuming Maxwellian f. (Further generalizations possible in future.)
- Unlike some logical sheath models, allows $j_{||} \neq 0$, in which case guiding center charge builds up and ϕ in plasma rises. Allows currents to flow through walls.

Sheath-model boundary condition for electrons



(a) Outgoing electrons with $v_\parallel > v_{cut} = \sqrt{2e\Delta\phi/m}$ are lost into the wall

(b) Rest of outgoing electrons $0 < v_\parallel < v_{cut}$ are reflected back into plasma

Ions: Assuming positive sheath potential (relative to wall), all ions are lost

Ampère cancellation problem

- In $p_\parallel$ formulation, Ampère's law:

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

- "Cancellation problem" arises when there are small errors in the calculation of the integrals, represented by C_n and C_j (which should be exactly 1 in the exact system)

- Recall $v_\parallel$ formulation Ohm's law… same problem…

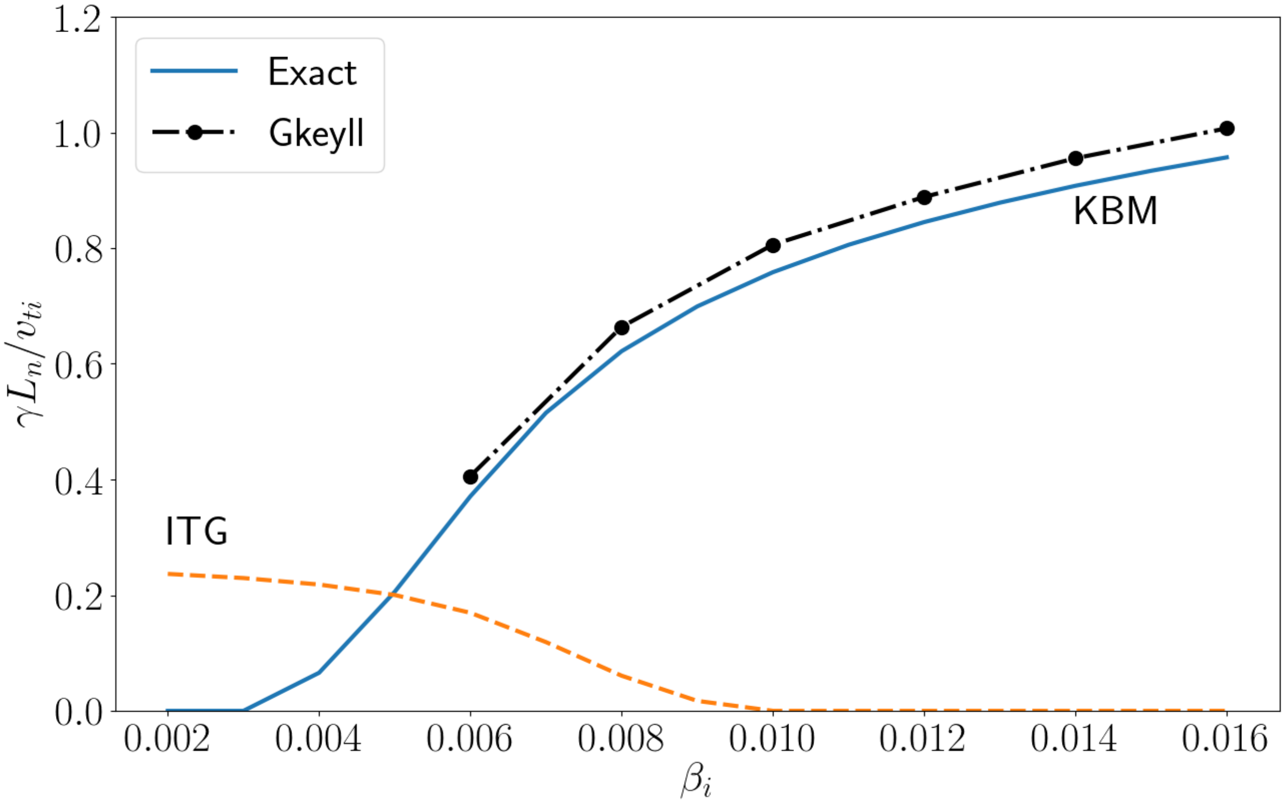
$$\left(-\nabla_\perp^2 + C_n \sum_s \frac{\mu_0 q_s^2}{m_s} \int d^3v\ f_s\right) \frac{\partial A_\parallel}{\partial t} = C_j\ \mu_0 \sum_s q_s \int d^3v\ v_\parallel \frac{\partial f_s}{\partial t}^\star$$

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

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

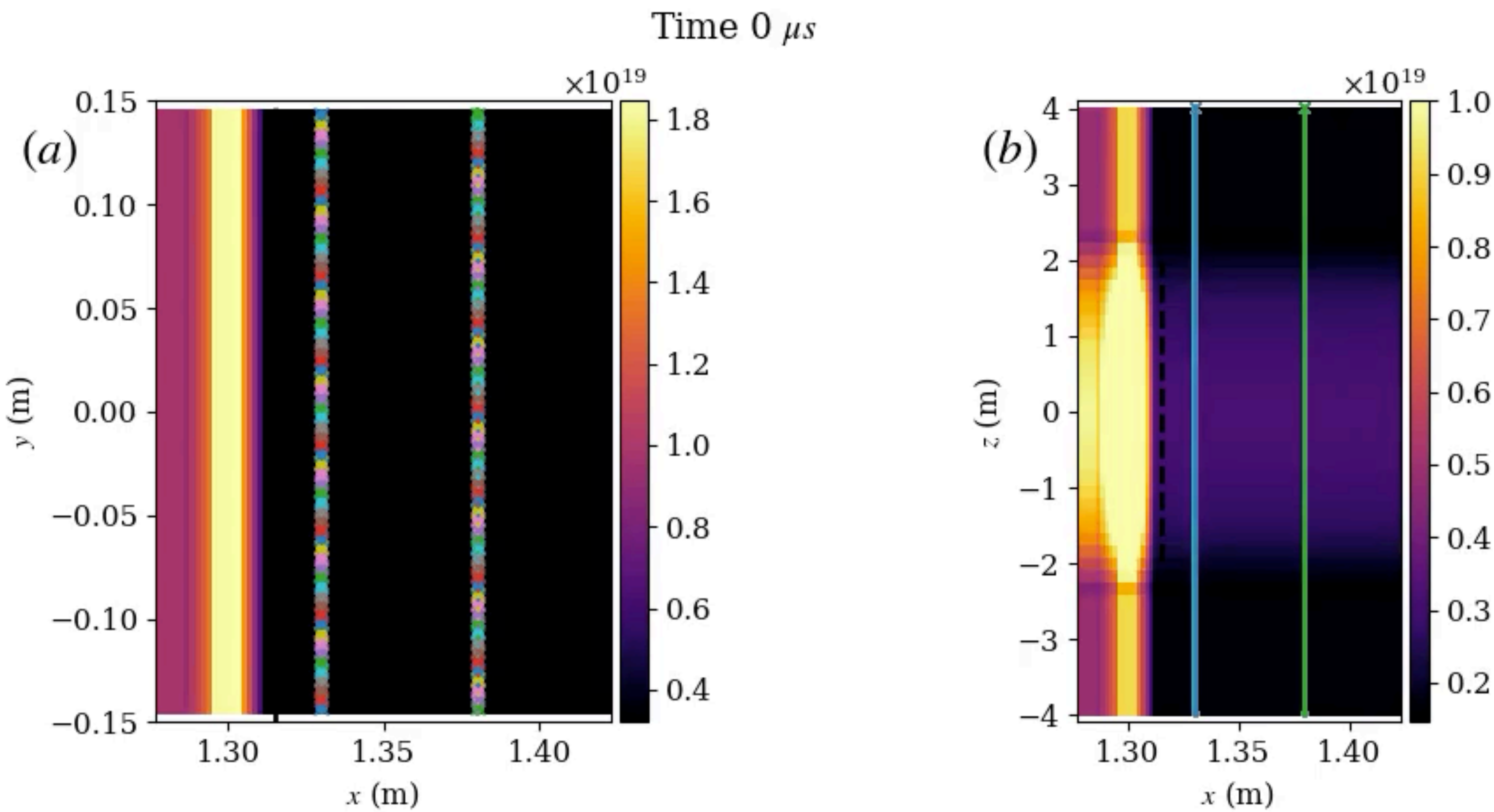
- This reduces to the correct result if integrals calculated consistently, so that $C_n = C_j$, but if not there will be errors $\sim \omega_H$ for modes with $\hat{\beta}/k_\perp^2 \rho_s^2 \gg 1$.

Linear benchmark: KBM instability (local limit)



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

EM in SOL at experimental β



Gkeyll Code: Novel Kinetic Algorithms, Multiple SciDACS

- **Novel version of Discontinuous Galerkin (DG) algorithm, in 5D**
  - Conserves energy for Hamiltonian system even with upwind fluxes [Juno, Hakim, et al. JCP 2018]
  - High-order local algorithms reduce communication costs, helpful for Exascale.
- **New modal version ~30x faster than nodal version**
  - Computer-algebra generated code (w/ Maxima) uses sparseness of modal interactions.
- **Framework: LuaJIT over C++, uses ADIOS, Eigen, MPI.**
- **3 Main Solvers, used in 3 SciDACs:**

1. **Gyrokinetic DG solver** for edge turbulence in fusion,
   in MGK SciDAC project (D. Hatch, PI), pedestal / multiscale work.
   in HBPS SciDAC project (C.S. Chang, PI), scrape-off-layer turbulence work.
2. **Vlasov-Maxwell/Poisson DG solver:** solar wind turbulence (PU/Maryland), plasma-surface interactions in thrusters (AFOSR / Virginia Tech) & tokamak disruption SciDAC (LANL / Virginia Tech)
   - Ran a case with 1 trillion grid points.
3. **Multi-moment multi-fluid (extended MHD) finite-volume solver:** reconnection (Princeton Center for Heliophysics), global magnetosphere simulations (UNH)