Properties of Gyrokinetic Turbulence in Tokamaks, & Discontinuous Galerkin Methods for (Gyro)Kinetics

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(Princeton University, PPPL)

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(slides @ http://w3.pppl.gov/~hammett/talks)

Ask Questions During the Talk!

(Some slides were skipped in presentation)

Properties of Gyrokinetic Turbulence in Tokamaks, & Discontinuous Galerkin Methods for (Gyro)Kinetics

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- **Fusion energy motivation: reducing microturbulence could improve fusion**
- **Intro to properties of gyrokinetic equations and tokamak turbulence**
- **Comprehensive GK sims of core very successful, challenges in edge**

- **Algorithm work:**
  - **Maxwellian-weighted basis functions in DG while preserving conservation properties (see E. Shi's poster)**
  - **Gkeyll, a new code for edge GK using a special energy-conserving version of DG for Hamiltonian systems.**
  - **(Other versions of Gkyell for Vlasov-Poisson, Vlasov-Maxwell, and multi-fluid-Maxwell using various algorithms. See A. Hakim's poster)**
  - **Ampere cancellation problem in gyrokinetics, a subtle fix in DG/FEM**
  - **Multiscale coupling of 5D turbulence and 1D transport: extreme scaling computing for comprehensive tokamak simulations**

Maxwellian-Weighted DG Basis Functions

Standard DG Polynomial Basis Functions:

$$\frac{\partial f(v,t)}{\partial t} = G[f]$$

In each cell Ω_j, expand in basis fcns: $f(v,t) \approx f_h(v,t) = \sum_k f_k(t) b_k(v)$

Choose $\dot{f}_k = df_k/dt$ to minimize error: $\epsilon^2 = \int_{\Omega_j} dv \left(\sum_k \dot{f}_k b_k - G \right)^2$

Error projected into space of $b_k(v)$ is zero: $\int_{\Omega_j} dv\, b_k(v) \left(\dot{f}_h - G \right) = 0$

If $G = -\partial\Gamma/\partial v$, then $b_0(v) = 1$ give density conservation:

$$\int_{\Omega_j} dv\, \dot{f}_h = -\Gamma(v_{j+1/2}) + \Gamma(v_{j-1/2})$$

Standard Maxwellian-Weighted DG Basis Functions:

For many plasma problems of interest, we know Maxwellian-weighted basis functions would be more efficient. (Polynomial basis functions can't integrate to v = ∞, where asymptotic behavior is Maxwellian (sometimes at higher "temperature"), moderate collisions, turbulence driven by gradients of Maxwellians.)

$$f(v,t) \approx f_h(v,t) = \sum_k f_k(t) \underbrace{\exp(-\beta v^2/2) b_k(v)}_{\hat{b}_k(v)}$$

$$\text{Minimizing error leads to: } 0 = \int_{\Omega_j} dv\, \hat{b}_k(v) \left(\dot{f}_h - G \right)$$

But now, $\hat{b}_0 = \exp(-\beta v^2/2)$ does *not* lead to standard particle conservation if $G = -\partial\Gamma/\partial v$

$$\int_{\Omega_j} dv\, \hat{b}_0 \dot{f}_h = - \hat{b}_0(v)\Gamma(v)\Big|_{v_{j-1/2}}^{v_{j+1/2}} + \int_{\Omega_j} dv \frac{\partial \hat{b}_0}{\partial v}\Gamma(v)$$

Standard energy conservation doesn't hold either.

Conservative Maxwellian-Weighted DG Basis Functions:

The trick for preserving conservation properties of DG with Maxwellian-weighted basis functions, $\hat{b}_k(v) = W(v) b_k(v)$, starts by going back to beginning, to the norm defining the error, and introducing a weighting factor:

$$\epsilon^2 = \int_{\Omega_j} dv \, W^{-1}(v) \left(\sum_k \dot{f}_k \hat{b}_k(v) - G \right)^2$$

Choosing $\dot{f}_k$ to minimize error gives:

$$\int_{\Omega_j} dv \, W^{-1}(v) \hat{b}_m(v) \left(\sum_k \dot{f}_k \hat{b} - G \right) = 0$$

$$\int_{\Omega_j} dv \, b_m(v) \left(\sum_k \dot{f}_k \hat{b}_k - G \right) = 0$$

Now $b_0(v) = 1$ gives standard particle conservation. Higher moments give momentum and energy conservation for collision operator (Hamiltonian terms more complicated..., see A. Hakim's poster.)

Weighted DG can be thought of as Petrov-Galerkin, test fncs $\neq$ basis fcns

1D Test problem: Classical Parallel Heat Conduction

$$\frac{\partial f(z, v_{||}, t)}{\partial t} + v_{||}\frac{\partial f}{\partial z} = C[f]$$

Background temperature gradient (w/ force balance), Chapman-Enskog-Braginskii problem locally becomes equivalent to 1D problem:

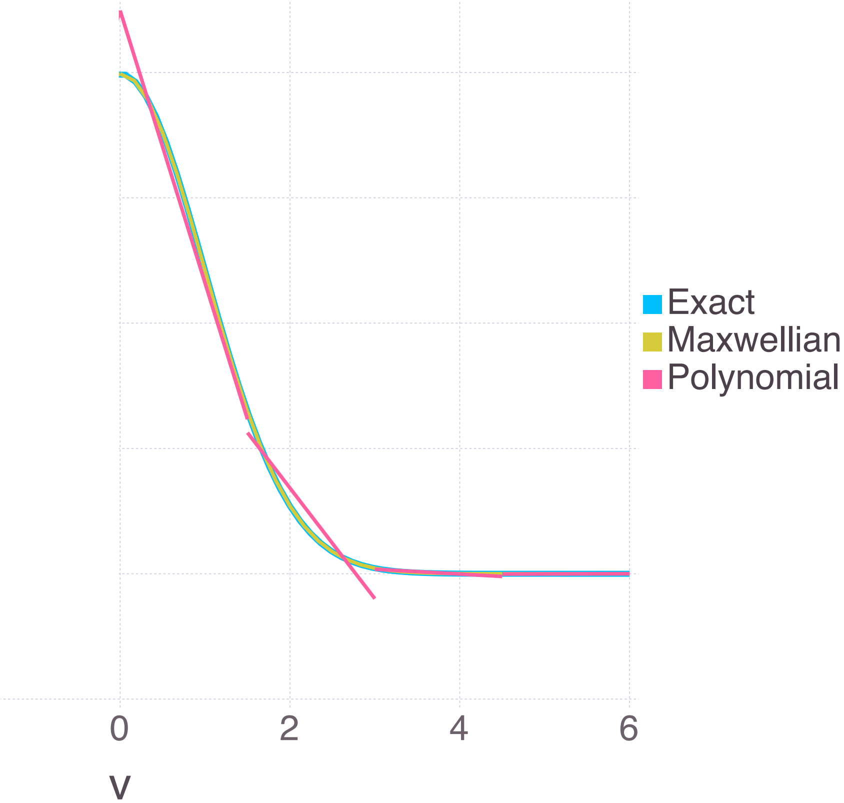
$$\frac{\partial f(v_{||}, t)}{\partial t} = C[f] + \kappa_T \, v_{||} \left(\frac{1}{2} \frac{v_{||}^2}{v_t^2} - c_1 \right) f$$

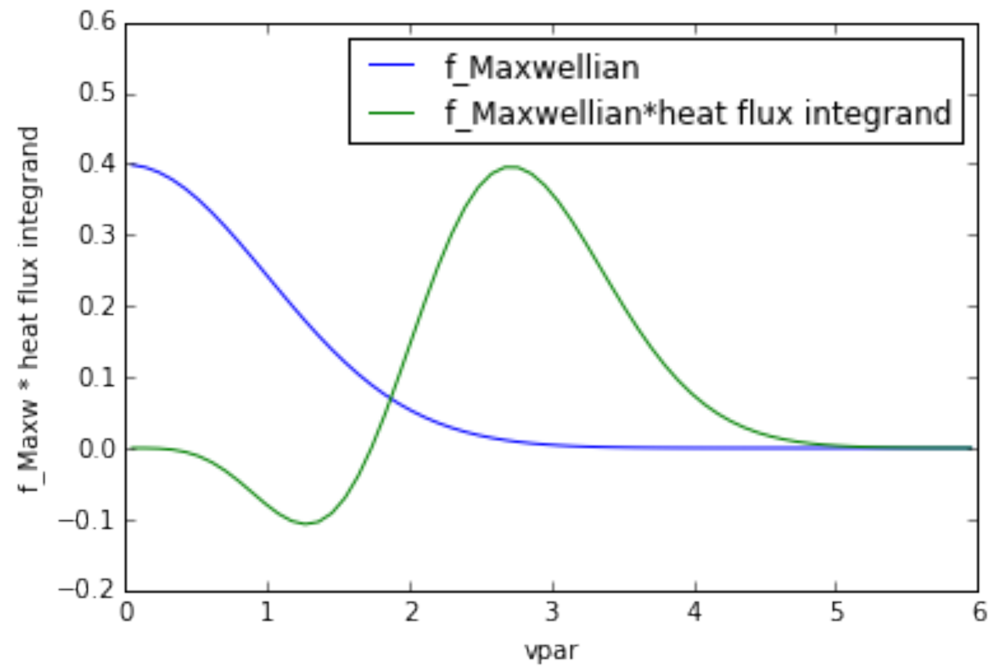
($\kappa_t \ll 1$. c_1 determined by constraint of no momentum injection.)
Lenard-Bernstein Collision model (much better than Krook model for plasmas):

$$C[f] = \frac{\partial}{\partial v_{||}} \left(\nu v_{||} f + \nu v_t^2 \frac{\partial f}{\partial v_{||}} \right)$$

Solve to steady state, calculate heat flux $= \int dv_{||} (1/2) m v_{||}^3 f$.

Maxwellian-weighted basis functions much more efficient



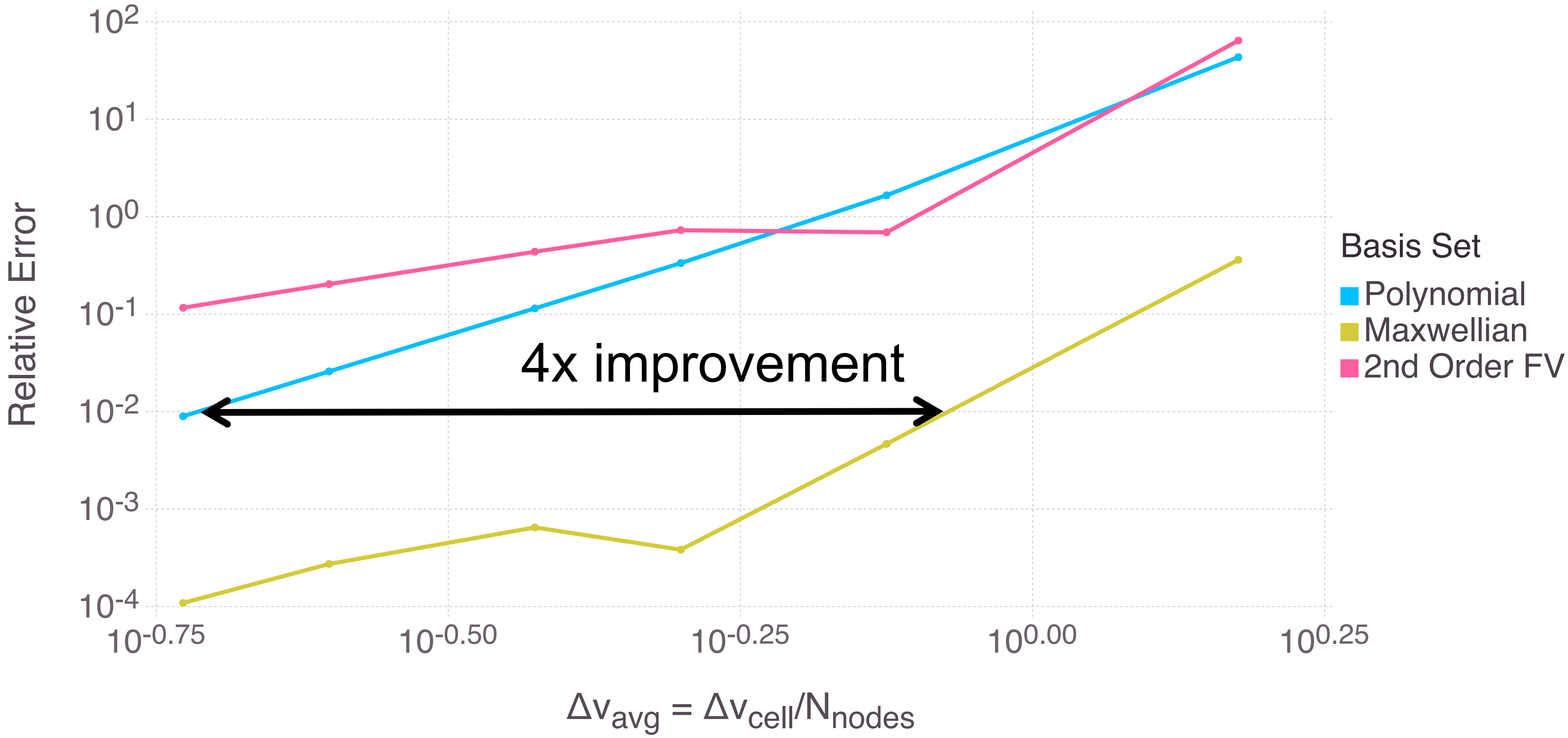


Here, heat flux integrand ~ v^6 $f_{Maxwellian}$, weighted towards tail.

In 3D with $\nu \sim 1/v^3$, get integrand ~ $|v|^{11}$ $f_{Maxwellian}$.

Unweighted polynomial basis functions converge slowly when far out in tail.

Maxwellian-weighted basis functions much more efficient



Combined with 2x improvement in $v_\perp$ → total 8x faster.

(See Eric Shi's poster.)

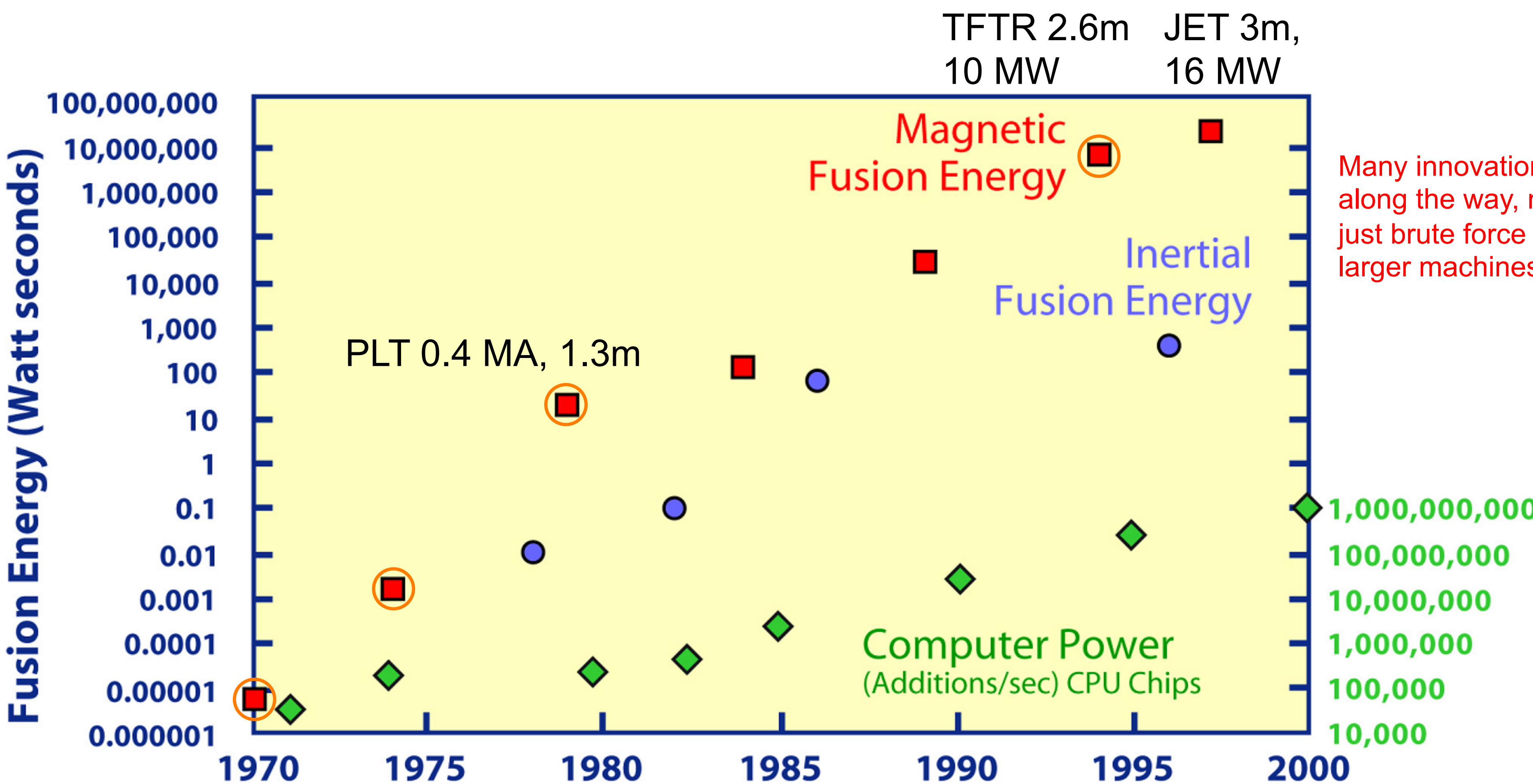
Fusion Intro

My Perspective on Fusion Energy

- Need to pursue many alternative energy sources. All have tradeoffs & uncertainties. Challenging to supply all energy needed in the long term. Energy demand expected to triple throughout the century as poor countries continue to develop.
- Fusion energy is hard, but it's an important problem, we've been making progress, and there are interesting ideas to pursue that could improve it:
  - "advanced tokamak" regimes, spherical torus
  - Liquid metal walls: handle power loads better, "black hole" absorbing wall reduces cold neutral recycling & improves performance. LTX, NSTX, …
  - Recent advances in high-field superconductors: 5.3→9.2 T, $P_{fus} \sim p^2 \sim B^4 \sim$ x 9
  - Stellarators: After 40+ years of research, a hidden symmetry discovered that improves performance
  - other ideas…, robotic manufacturing, …

Progress in Fusion Energy Outpaced Computer Speed

ITER 6.2m
500 MW



Many innovations along the way, not just brute force larger machines.

ITER goal: 200 GJ/pulse (500 MW = 30 x JET's power 16 MW, for 400x longer), 10^7 MJ/day of fusion heat).

Improving Confinement Can Significantly ↓ Size & Construction Cost of Fusion Reactor

Well known that improving confinement & β can lower Cost of Electricity / kWh, at fixed power output.

Even stronger effect if consider smaller power: better confinement allows significantly smaller size/cost at same fusion gain Q ($nT\tau_E$).

Need detailed turbulence simulations to make case for reliable projection to improved confinement.

Caveats: qualitative cost trend, limits on improvements set by blankets, etc., need detailed engineering studies.

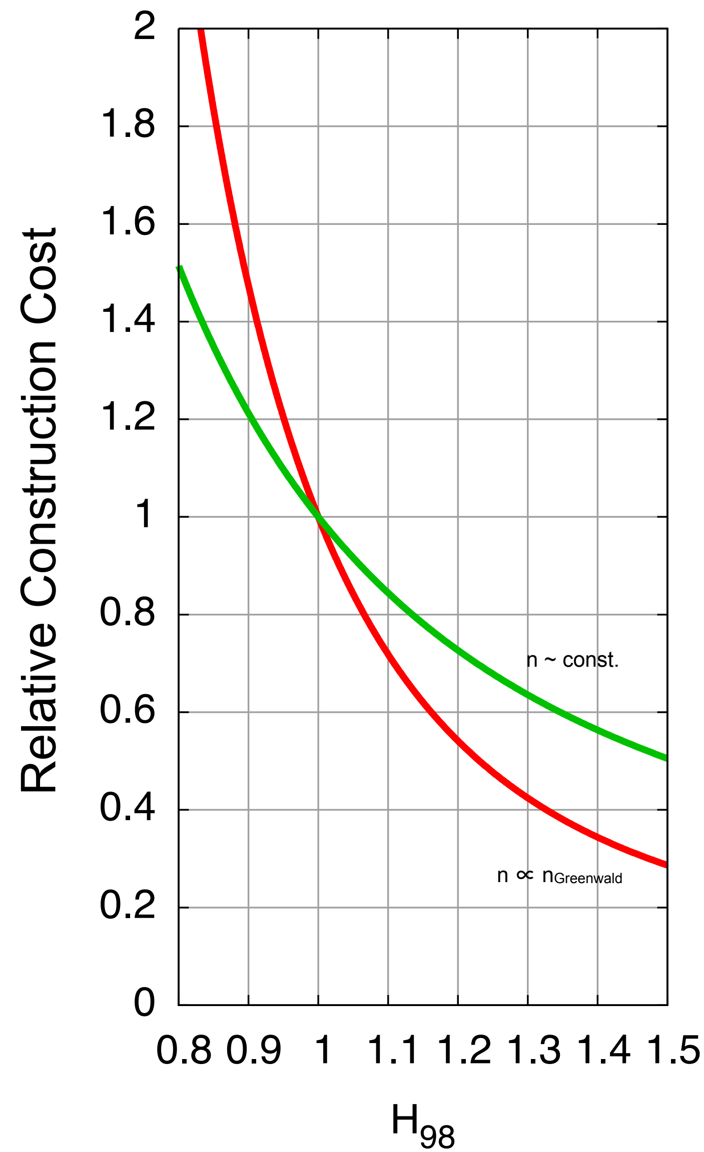
Standard H-mode empirical scaling:

$$\tau_E \sim H\, I_p^{0.93}\, P^{-0.69}\, B^{0.15}\, R^{1.97} \ldots$$

($P = 3VnT/\tau_E$ & assume fixed $nT\tau_E$, q_{95}, β_N, $n/n_{Greenwald}$), get:

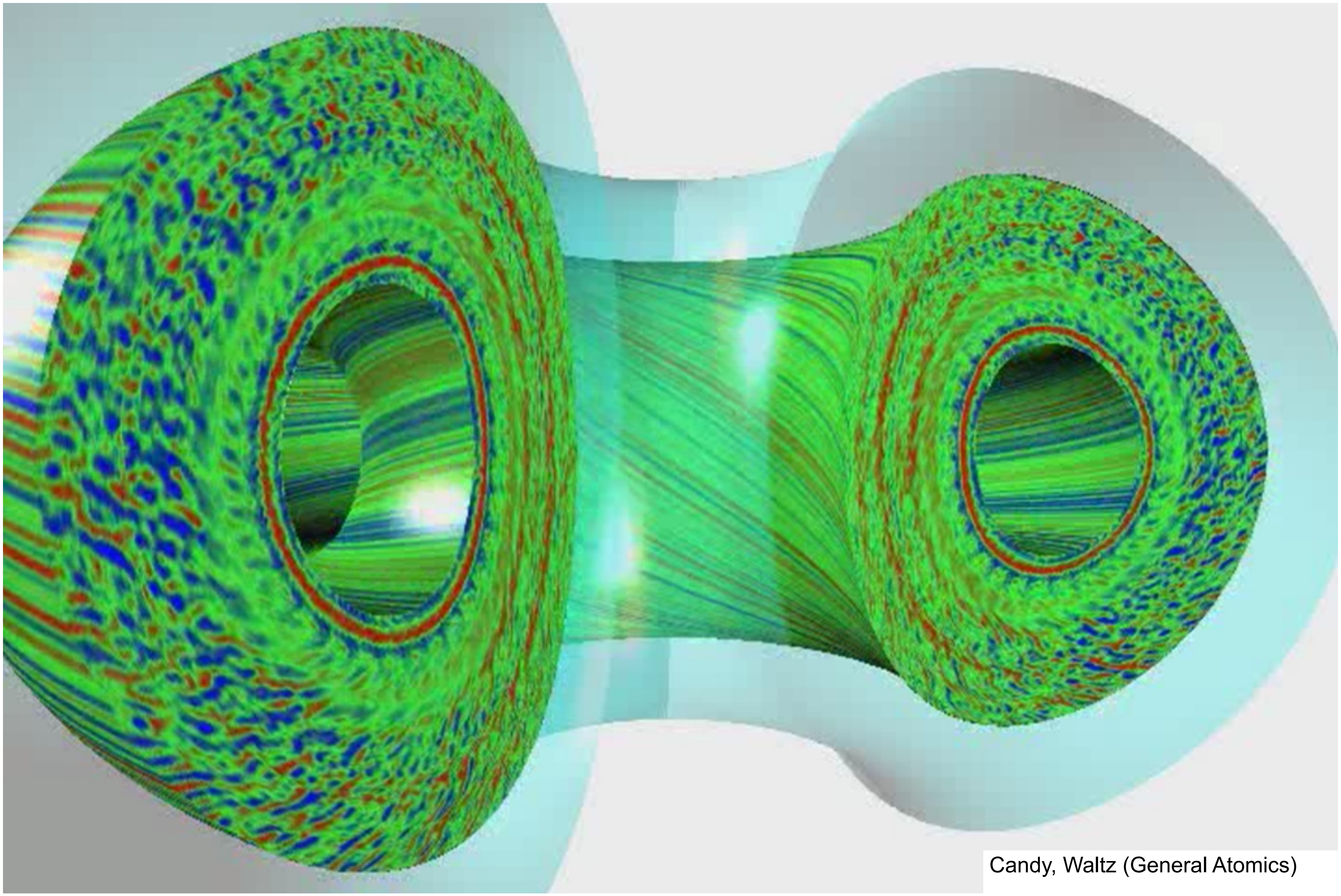
$$R \sim 1 / (H^{2.4}\, B^{1.7})$$

ITER std $H=1$, steady-state $H\sim1.5$
ARIES-AT $H\sim1.5$
MIT ARC (fire.pppl.gov FESAC) $H_{89}/2 \sim 1.4$ (new HTS ~Bx2, $P_{fus} \sim B^4$ at fixed)



(Plots assumes $a/R=0.25$, cost ∝ R^2 roughly. Plot accounts for constraint on B @ magnet with 1.16 m blanket/shield, i.e. $B = B_{mag}\,(R-a-a_{BS})/R$)

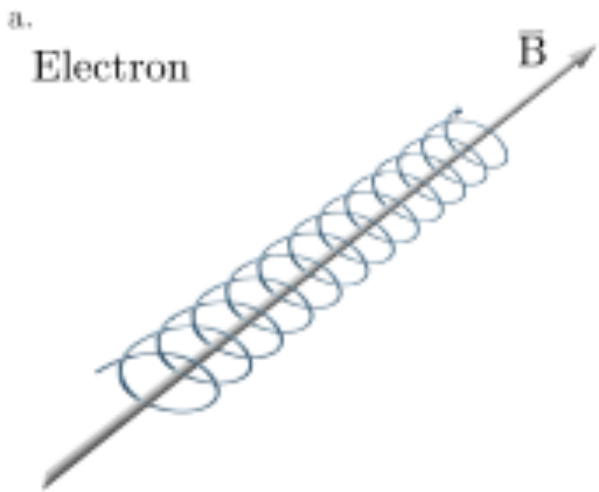
Gyrokinetic Simulation of
Microturbulence in main Tokamak Core

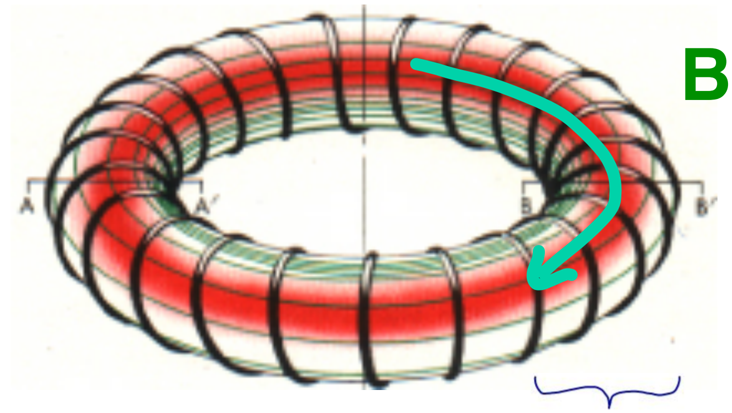


Candy, Waltz (General Atomics)

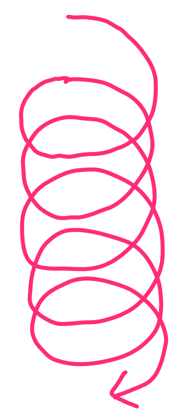
A Crash Course in Magnetic Confinement (in 3 slides)

Particles have helical orbits in B field, not confined along B. Try to fix by wrapping B into a torus.





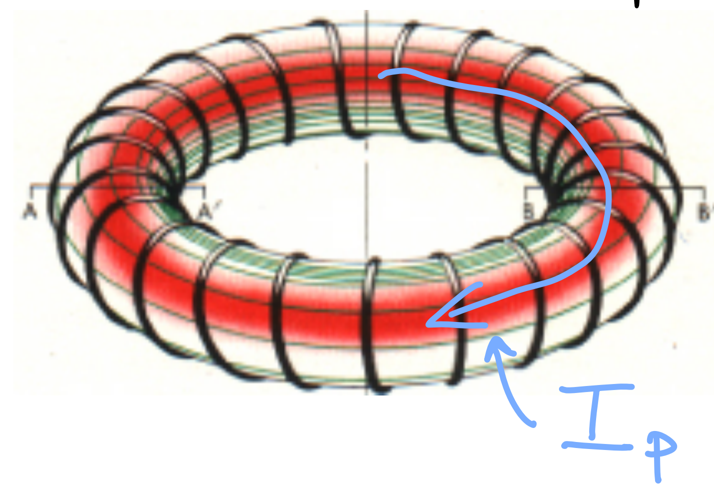
Fermi (~1946): but now
B ~ 1/R, so particles will drift
out:



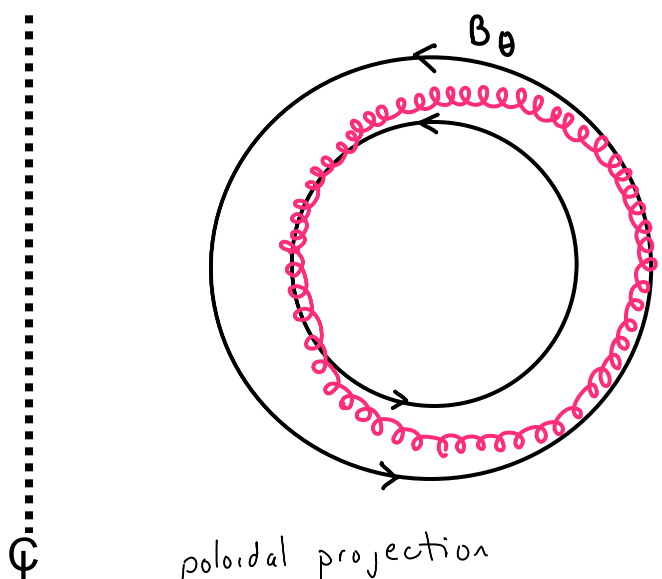
↓ ions drift down

Cure problems by twisting the $\underset{\sim}{B}$ field

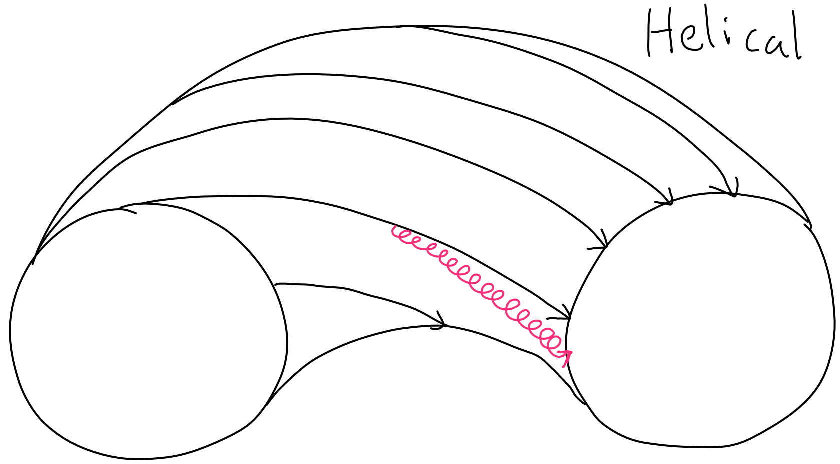
Induce a current in plasma:



Ion motion along twisting $\underset{\sim}{B}$ field + downward drift:



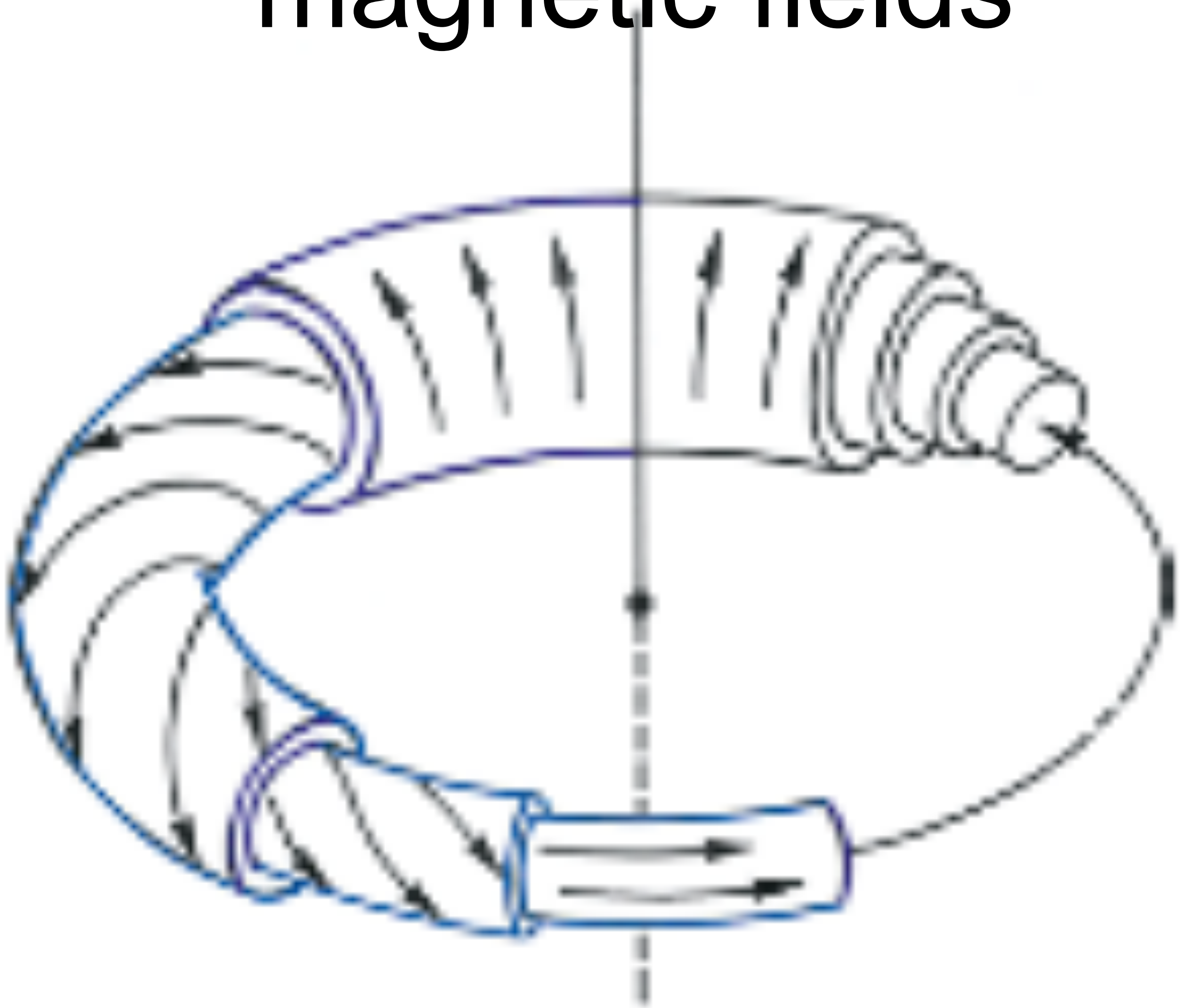
poloidal projection



Helical twist in $\vec{B}$

Perspective view

Torus with sheared helical magnetic fields

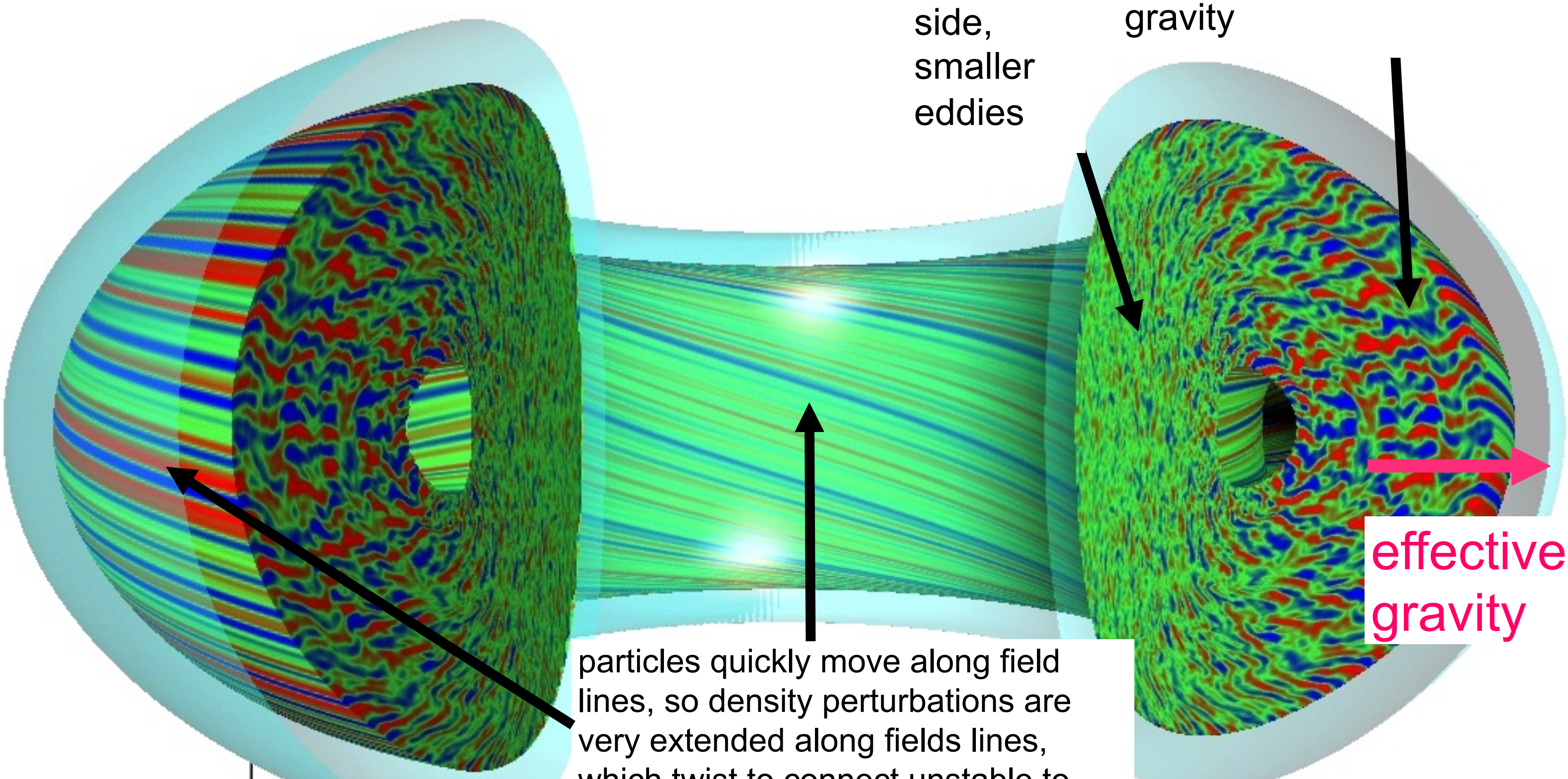


Extreme example, magnetic field is mostly in toroidal direction in standard tokamak.

magnetic shear can help stabilize instabilities
(negative & zero average shear can be better, average ≠ local shear)

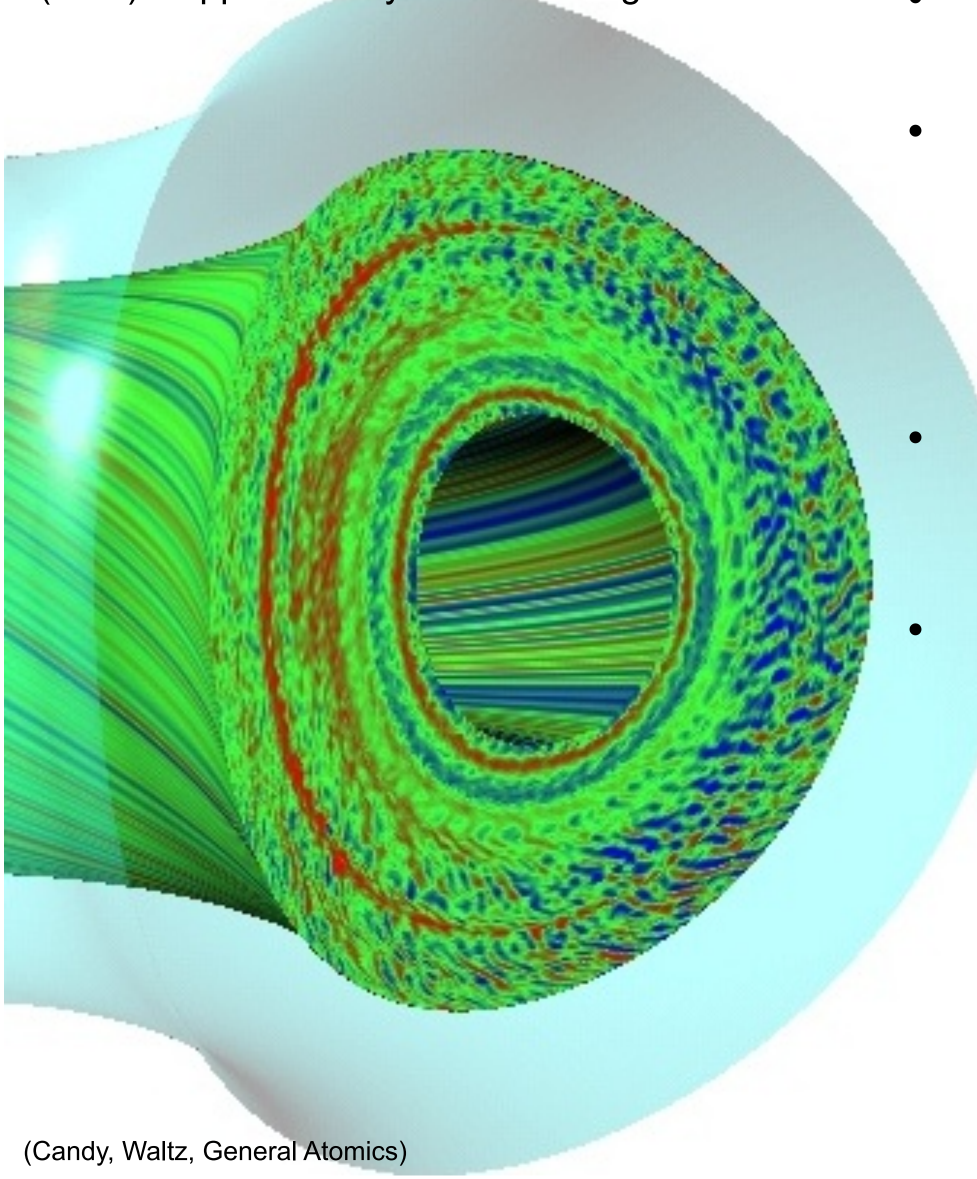
From F.F. Chen, "An Indispensable Truth", 2011

These physical mechanisms can be seen in gyrokinetic simulations and movies



Fairly Comprehensive 5-D Gyrokinetic Turbulence Codes Have Been Developed

small scale, small amplitude density fluctuations (<1%) suppressed by reversed magnetic shear



(Candy, Waltz, General Atomics)

- Solve for the particle distribution function $f(r,\theta,\alpha,E,\mu,t)$ (avg. over gyration: 6D → 5D)
- 500 radii x 32 complex toroidal modes (96 binormal grid points)
  x 10 parallel points along half-orbits
  x 8 energies x 16 $v_{||}/v$
  12 hours on ORNL Cray X1E w/ 256 MSPs
- Realistic toroidal geometry, kinetic ions & electrons, finite-β electro-magnetic fluctuations, full linearized collisions.
- Sophisticated spectral/high-order upwind algorithms. This plot from continuum/ Eulieran code GYRO (Candy & Waltz, SciDAC), GENE (Jenko et al., Garching / UCLA) similar. These and other codes being widely compared with experiments.

Gyrokinetic Eq. Summary

The electrostatic gyrokinetic equation, in a "full-f" drift-kinetic-like form, for the gyro-averaged, guiding-center distribution function $\bar{f}(\vec{R}, v_{||}, \mu, t) = \bar{f}_0 + \delta\bar{f}$:

$$\frac{\partial B\bar{f}}{\partial t} + \nabla \cdot \left(\left(v_{||}\hat{b} + \mathbf{v}_E + \mathbf{v}_d\right) B\bar{f}\right) + \frac{\partial}{\partial v_{||}}\left(\left(-\frac{1}{m}\hat{b}\cdot\nabla(e\bar{\Phi} + \mu B) + v_{||}(\hat{b}\cdot\nabla\hat{b})\mathbf{v}_E\right) B\bar{f}\right) = C[\bar{f}]$$

at long wavelength (the hard part): $-\nabla_\perp \cdot \left(\sum_s \frac{n_s m_s c^2}{B^2}\nabla_\perp \phi\right) = \sum_s q_s \int d^3v\, \bar{f}_s$

magnetic moment $\mu = (m/2)v_\perp^2/B$

$E \times B$ velocity:

$$\mathbf{v}_E = -\frac{c}{B}\nabla\bar{\Phi} \times \hat{b}$$

∇B and curvature drifts:

$$v_d = \frac{v_{||}^2}{\Omega}\hat{b} \times (\hat{b}\cdot\nabla\hat{b}) + \frac{\mu}{\Omega}\hat{b} \times \nabla B$$

With small corrections, can be written in Hamiltonian form $\partial f/\partial t = \{H, f\} + C[f]$.

Derivation refs.: Frieman-Chen, Lee, Dubin, Hahm, Sugama, Brizard, Miyata, Parra, …

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$$-\nabla_\perp\cdot\left(\sum_s \frac{n_s m_s c^2}{B^2}\nabla_\perp\phi\right) = \sum_s q_s \int d^3v\, \bar{f}_s$$

using gyro averaged potential:

$$\begin{aligned}\bar{\phi}(\vec{R}) &= \frac{1}{2\pi}\int d\theta\, \phi(\vec{R} + \vec{\rho}(\theta)) \\ &= \frac{1}{2\pi}\int d\theta \sum_{\vec{k}} \phi_{\vec{k}} \exp(i\vec{k}\cdot(\vec{R} + \vec{\rho}(\theta)) \\ &= \sum_{\vec{k}} J_0(k_\perp\rho)\phi_{\vec{k}} \exp(i\vec{k}\cdot\vec{R})\end{aligned}$$

magnetic moment $\mu = (m/2)v_\perp^2/B$

$E\times B$ velocity:

$$\mathbf{v}_E = -\frac{c}{B}\nabla\bar{\Phi}\times\hat{b}$$

∇B and curvature drifts:

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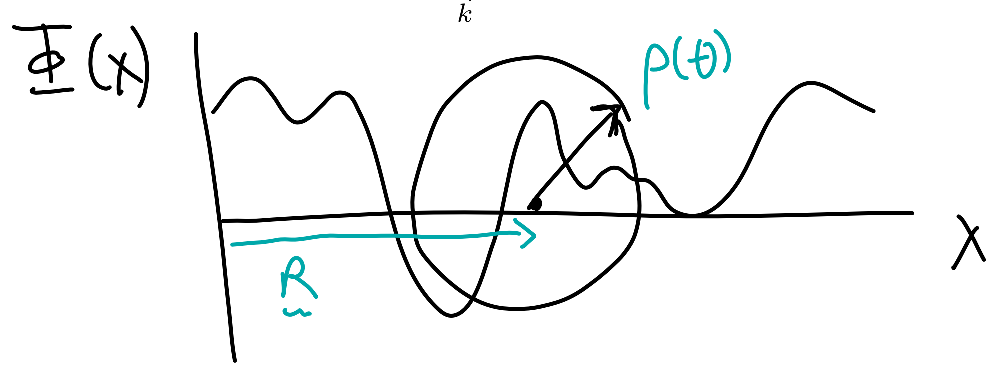

Discontinuous Galerkin Algorithms for Hamiltonian/ Kinetic Problems

(See Ammar Hakim's poster for details)

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Interesting Previous DG for Vlasov-Poisson (VP)

- Ayuso, Carrillo, & Shu 2011: 1D, First DG scheme in literature for which energy conservation can be shown
- Ayuso, Carillo, & Shu 2012: extensions to multi-D, requires multiple (2 x D) Poisson solves
- Ayuso & Hajian 2012: 1D, also requires 2 Poisson solves per step
- Yingda Chen, I. Gamba, P. Morrison, et al., Energy conservation for Vlasov-Maxwell

Special versions of DG for Hamiltonian systems (See A. Hakim's poster & future paper)

- Navier-Stokes fluid eqs. directly represent conservation of particles, momentum, & energy. Finite-Volume methods automatically conserve these also.
- Energy conservation in Vlasov-Poisson and other Hamiltonian systems more subtle: energy conservation an indirect property (integrate by parts, careful treatment of particle-field energy exchange). (Arakawa conserves energy, but standard limiters/upwinding would lose energy conservation.)
- We appear to be first to note a version of DG (based on J.-G. Liu & C.-W. Shu, 2000 for 2D incompressible hydro) can exactly conserve energy for general Hamiltonian problems, $\partial f/\partial t = \{H,f\}$, (for continuous time) with single Poisson solve.
- Interestingly, energy is conserved even with upwind fluxes for f --> limiters (helpful to minimize artificial oscillations & preserve positivity).
- This version requires H to be in a continuous subspace of the basis functions used for f. DG for f, FEM to solve Poisson-type eqs. to find potentials.

Special versions of DG for Hamiltonian systems (See A. Hakim's poster & future paper)

- Hakim's Gkeyll code is using this Hamiltonian DG for gyroknetic studies of tokamak turbulence, and for Vlasov-Poisson (with static B) for plasma thruster simulations.

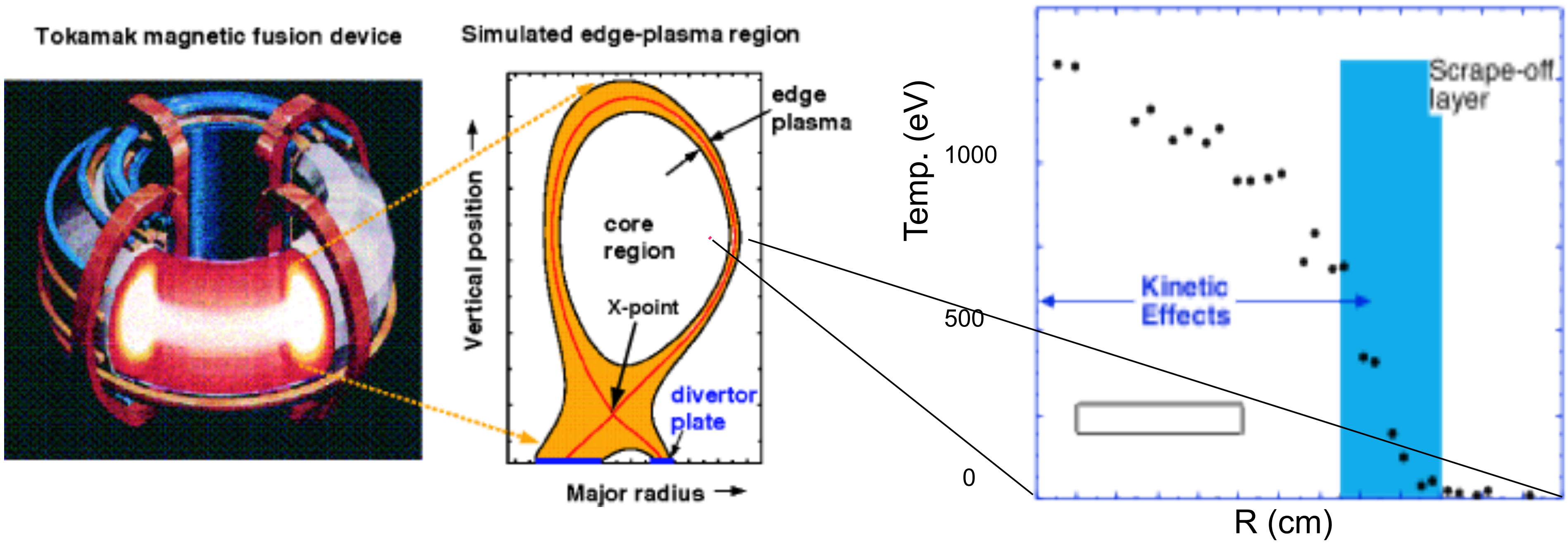
- To preserve the feature of the GK Poisson equation of multiple independent 2D Poisson solves, we discovered a local quasi-projection operator that produces a continouous 3D phi from the 2D solves, while retaining a self-adjoint property so that energy conservation is preserved.

- For Vlasov-Maxwell simulations, using a different energy-conserving treatment.

Simultaneous momentum & energy conservation

- Our scheme can conserve energy or momentum exactly (depending on the basis functions for phi), but not both. Can add a correction term $\sim (\Delta x)^p$ to conserve momentum and energy simultaneously (Finite Volume version: Taitano, Chacon, and Simikov, JCP14)

Edge region very difficult



Edge pedestal temperature profile near the edge of an H-mode discharge in the DIII-D tokamak. [Porter*2000*]. Pedestal is shaded region.

Major extensions to gyrokinetic codes needed to handle additional complications of edge region of tokamaks (& stellarators):

open & closed field lines, steep gradients near beta limit, electric & magnetic fluctuations, strong shear-flow layers, steep-gradients and large amplitude fluctuations, positivity constraints, wide range of collisionality, non-axisymmetric RMP coils, plasma-wall interactions, strong sources and sinks in atomic physics.

A new code with these capabilities might also be useful for a wider range of astrophysics and other applications.

General goal: new robust (gyro)kinetic code benefiting from several advanced continuum algorithms

New continuum code using combination of advanced algorithms that could help it be significantly more efficient and robust, particularly on coarse velocity space grids. Advanced algorithms include:

- certain versions of discontinuous Galerkin (DG) methods that are quite efficient and have good conservation properties (subtle for kinetic Hamiltonian problems), while allowing certain types of limiters (help preserve positivity).

- Maxwellian-weighted (or more general) basis functions,

- subgrid / hypercollision models to model phase-mixing and turbulent mixing to unresolved scales (handles recurrence issues).

DG combines some advantages of Finite Volume (FV) with Finite Element accuracy:
FV interpolates p uniformly-spaced points to get p order accuracy
DG interpolates p optimally-located points to get 2p-1 order accuracy

(DG has lower phase-errors like Finite Elements / Compact Finite Differencing, but calculations are local like FV, explicit code easier to parallelize.)

Ampere Cancellation subleties in DG/ FEM

Simplest Alfven Wave in Gyrokinetics

$$\frac{\partial f_e}{\partial t} + v_{||}\frac{\partial f_e}{\partial z} + \frac{q_e}{m_e}\left(-\frac{\partial \phi}{\partial z} - \frac{\partial A_{||}}{\partial t}\right)\frac{\partial f_e}{\partial v_{||}} = 0$$

$$-n_i k_\perp^2 \rho_{s0}^2 \frac{e\phi}{T_{e0}} = \int dv_{||} f_e - n_i$$

$$k_\perp^2 A_{||} = \mu_0 q_e \int dv_{||}\, f_e v_{||}$$

If $\omega \gg k_{||} v_{te}$, this gives:

$$\omega^2 = \frac{k_{||}^2 v_A^2}{1 + k_\perp^2 \rho_s^2/\hat{\beta}_e}$$

where $\hat{\beta}_e = (\beta_e/2)(m_i/m_e)$. The electrostatic case $A_{||} = 0$ corresponds to the low β limit, where there is an Ω_H mode that is even faster than electrons at low $k_\perp$:

$$\omega^2 = \frac{k_{||}^2 v_{te}^2/\hat{\beta}_e}{1 + k_\perp^2 \rho_s^2/\hat{\beta}_e} \rightarrow \frac{k_{||}^2 v_{te}^2}{k_\perp^2 \rho_s^2}$$

It would seem that finite β should be easier because it limits the fastest wave at low $k_\perp$ to be no faster than the Alfven wave

Handling the $\partial A_{||}/\partial t$ term

$$\frac{\partial f_e}{\partial t} + v_{||}\frac{\partial f_e}{\partial z} + \frac{q_e}{m_e}\left(-\frac{\partial \phi}{\partial z} - \frac{\partial A_{||}}{\partial t}\right)\frac{\partial f_e}{\partial v_{||}} = 0$$

Codes usually eliminate the $\partial A_{||}/\partial t$ term with the substitution $\delta f_e = g + (q_e/m_e)A_{||}\partial F_{e0}/\partial v_{||}$ (or by going to $p_{||} = mv_{||} + q_e A_{||}$ coordinates, which is equivalent linearly). Ampere's law become:

$$\left(k_\perp^2 + \underbrace{C_n \frac{\mu_0 q_e^2}{m_e}\int dp_{||} f_e}_{C_n\,\omega_{pe}^2/c^2}\right) A_{||} = C_j \mu_0 \frac{q_e}{m_e^2}\int dp_{||} f_e\, p_{||}$$

"The Ampere Cancellation Problem": the ratio of the first to second term is very small, $k_\perp^2 \rho_s^2/\hat{\beta} \sim 10^{-5}$, for $k_\perp \rho_s = 0.01$ and $\beta_e \sim 1\%$. Small errors (represented by C_n or $C_j \neq 1$) in large terms can have a large effect:

If $\omega \gg k_{||} v_{te}$:

$$\omega^2 = \frac{k_{||}^2 v_{te}^2}{k_\perp^2 \rho_s^2}\left[\frac{k_\perp^2 \rho_s^2 + (C_n - C_j)\hat{\beta}_e}{k_\perp^2 \rho_s^2 + C_n \hat{\beta}_e}\right]$$

GS2's implicit formulation never had problem. I worked with Jenko in 2001 to fix problem in GENE. Related papers by Candy & Waltz JCP 2003, Y. Chen & S. Parker JCP 2003, B. Cohen 2002, Dannert & Jenko 2004, Belli & Hammett 2005, Bottino et al. IAEA 2010. Latest PIC methods: E. A. Startsev & W.W. Lee 2014 (Double Split Weight), A. Mishchenko et al. Phys. Plasmas 2014 (Pullback method).

Challenge for magnetic fluctuations in DG

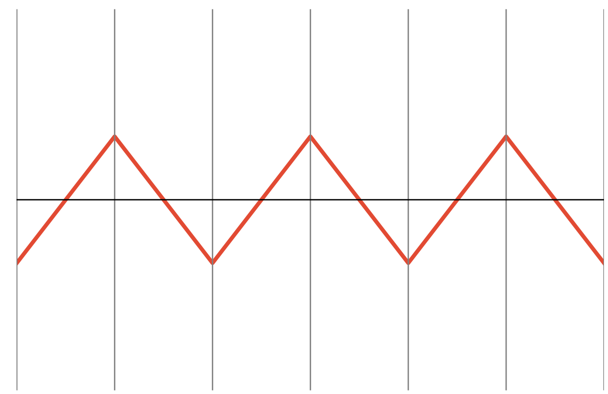
We are using a novel version of the Discontinuous Galerkin (DG) algorithm that can exactly conserve energy for general Hamiltonian problems $\partial f/\partial t = \{H, f\}$. (Based on algorithm by J.-G. Liu and C-W. Shu, 2000.) Requires H (and thus ϕ & $A_{||}$) to be continuous.

In the MHD limit, we need

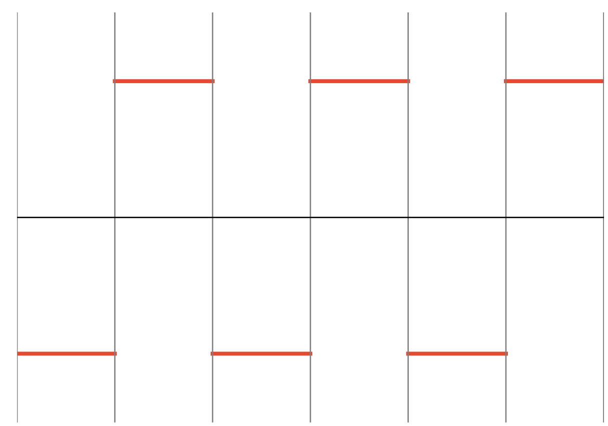
$$E_{||} = -\frac{\partial \phi}{\partial z} - \frac{\partial A_{||}}{\partial t} \approx 0$$

but there is no way for a continuous $A_{||}(z)$ to offset this discontinuous $\partial\phi/\partial z$.

Shortest Wavelength $\phi(z)$



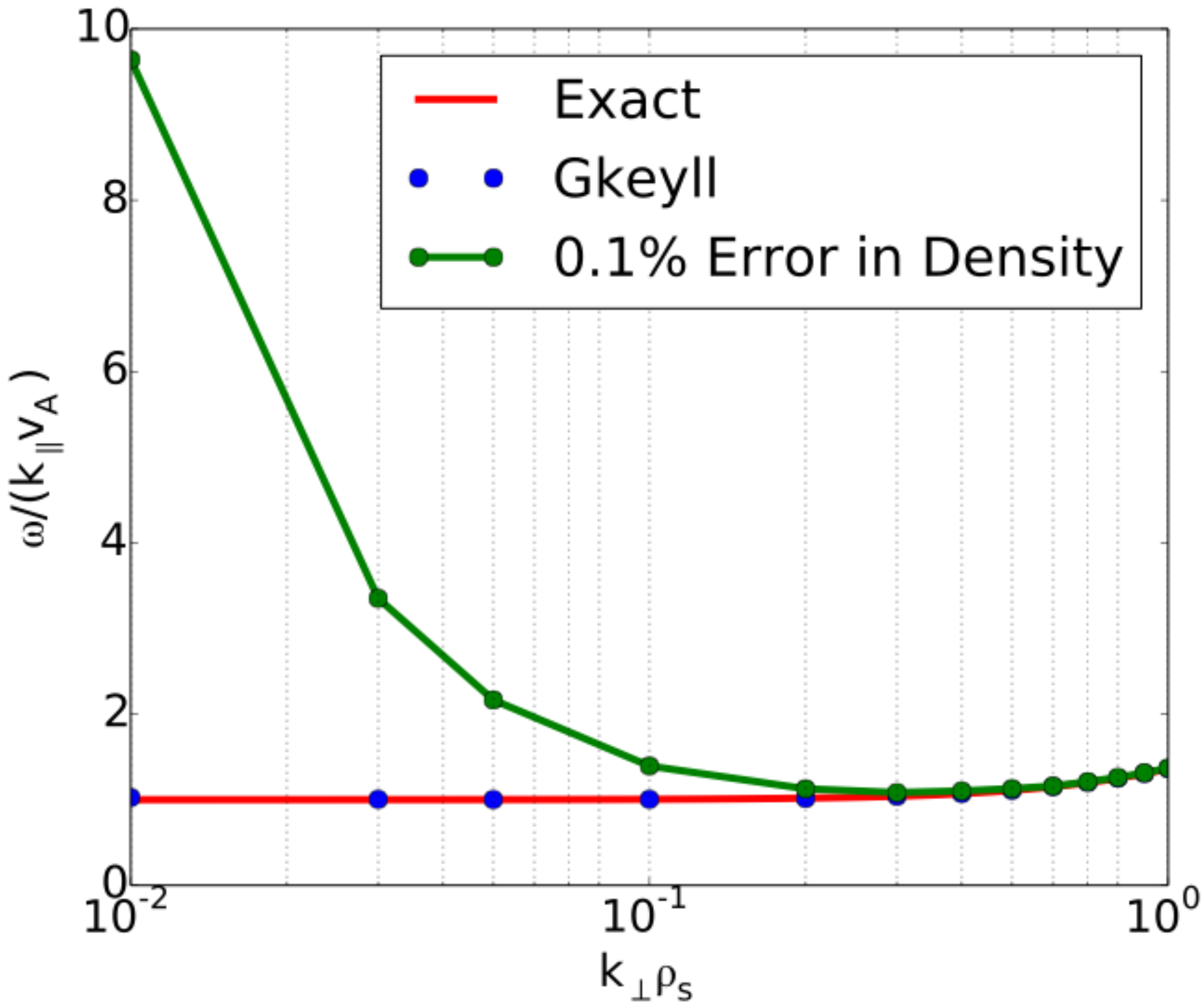
$E_\phi = -\partial\phi(z)/\partial z$



This electrostatic field drives a current that is a square wave, and wants to make a square wave $A_{||}$(z). But projection of this square wave $A_{||}$ onto a continuous subspace gives $A_{||} = 0$, as if $\beta=0$. This gives very high frequency mode at grid scale, requiring a very small time step $\Delta t < k_{||,max}\, v_{te} / (k_{\perp,min}\, \rho_s)$.

Fix for magnetic fluctuations for DG

There are several solutions. One is to project $\phi(z)$ onto a C_1 subspace where ϕ and $\partial\phi/\partial z$ are continuous. (ϕ must be at least piecewise-parabolic in this case.) This allows a C_0 $A_{||}(z,t)$ to better approximate the ideal MHD condition $E_{||} \approx 0 = -\partial\phi/\partial z - \partial A_{||}/\partial t$. Allows Gkeyll to reproduce Alfven wave even at very low $k_\perp \rho_s$ with a normal time step.



In order to conserve energy, the projection operator must be self-adjoint. We have found a local filtering/projection operator that is self-adjoint.

Summary:
Properties of Gyrokinetic Turbulence in Tokamaks, & Discontinuous Galerkin Methods for (Gyro)Kinetics

- **Fusion energy motivation**

- **Gkeyll, a new code for edge GK using a special energy-conserving version of DG for Hamiltonian systems.**
- **(Other versions of Gkyell for Vlasov-Poisson, Vlasov-Maxwell, and multi-fluid-Maxwell using various algorithms. See A. Hakim's poster)**

- **Algorithm work:**
  - **Maxwellian-weighted basis functions in DG while preserving conservation properties (see E. Shi's poster)**
  - **Ampere cancellation problem in gyrokinetics, a subtle fix in DG/FEM**
  - **Multiscale coupling of 5D turbulence and 1D transport: extreme scaling computing for comprehensive tokamak simulations**