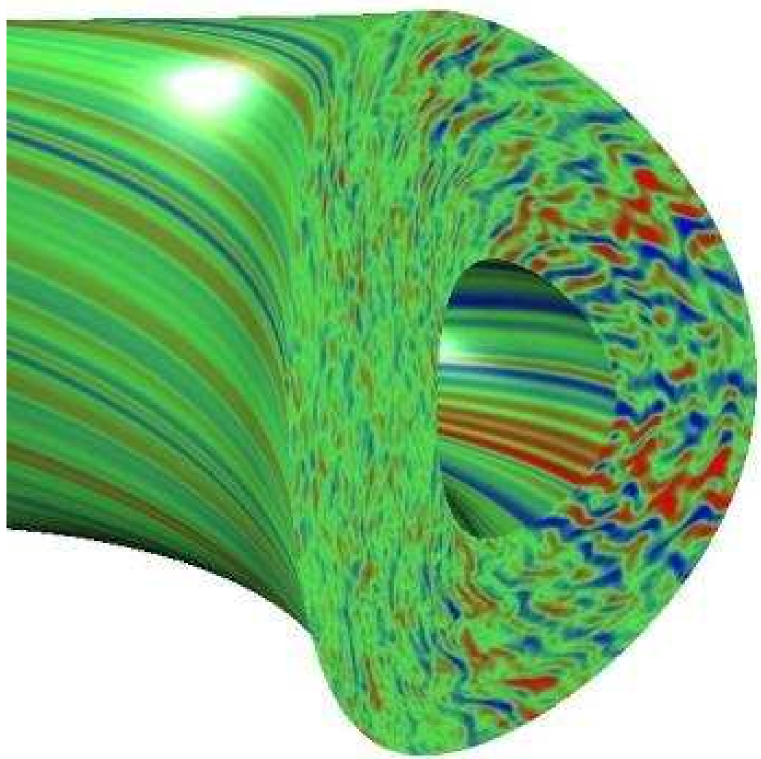
INTRODUCTION TO GYROKINETIC AND FLUID SIMULATIONS OF PLASMA TURBULENCE AND OPPORTUNITES FOR ADVANCED FUSION SIMULATIONS

G.W. Hammett, Princeton Plasma Physics Lab
w3.pppl.gov/∼hammett
Fusion Simulation Project Workshop
San Diego, Sept. 17, 2002

Thanks to Bill Nevins &
the Plasma Microturbulence Project
for many vugraphs. In particular see:

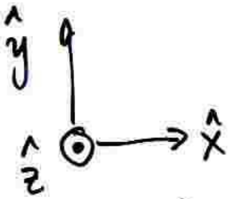
http://www.isofs.info/nevins.pdf
http://fusion.gat.com/theory/pmp

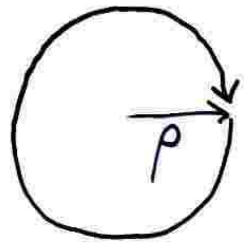
and others working on Braginskii
2-fluid simulations of edge turbulence.
(Collabs. at Univ. Alberta, UCLA,
UCI, Univ. Colorado, Dartmouth, Garching,
General Atomics, LLNL, Univ. Maryland,
MIT, Princeton PPPL, Univ. Texas)



Fundamental Particle Motion in Magnetic & Electric Fields

$$m\frac{d\mathbf{v}}{dt} = q\frac{\mathbf{v}\times\mathbf{B}}{c}$$





$\mathbf{B} \parallel \hat{z} = \hat{b}$

Gyrofrequency $\Omega = \frac{qB}{mc}$

$\Omega_e \sim 10^{11}$ Hz, $\Omega_i \sim 10^{8}$ Hz

Gyroradius $\rho = \frac{v_\perp}{\Omega}$

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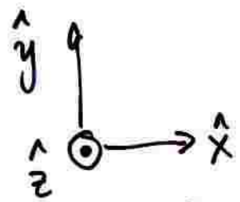

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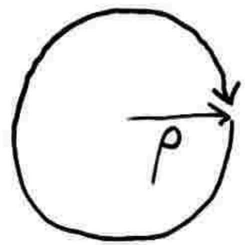

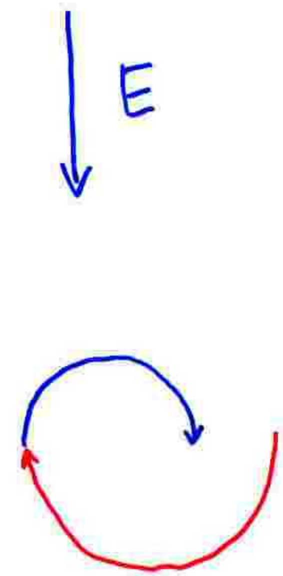

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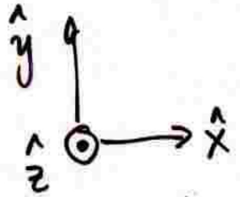

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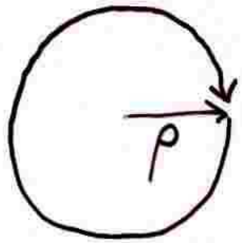

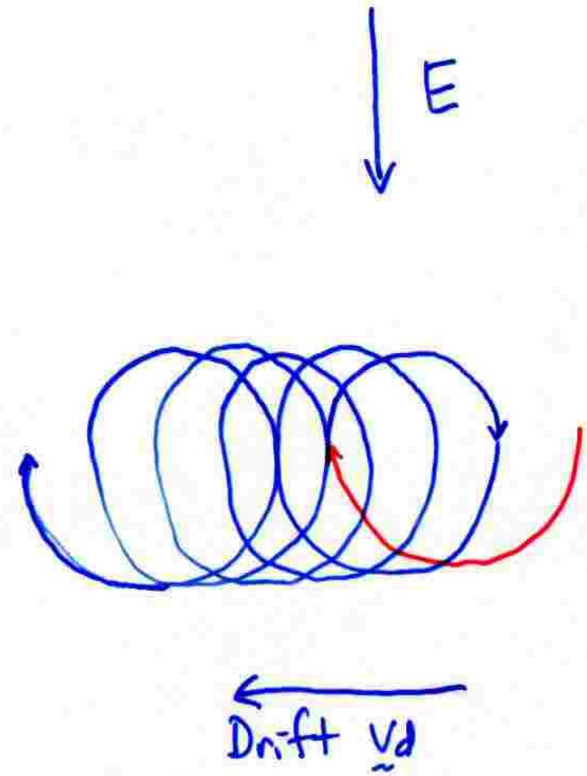

$$= \underset{\sim}{V}_{E\times B} = \frac{c}{B} \underset{\sim}{E} \times \hat{b}$$

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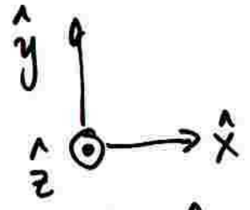

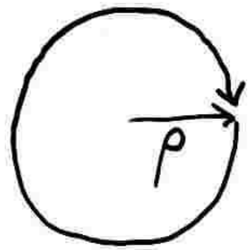

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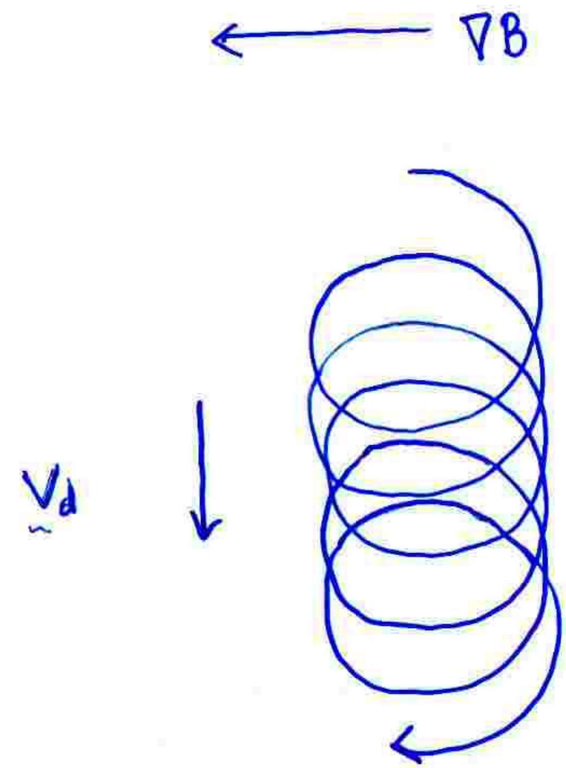
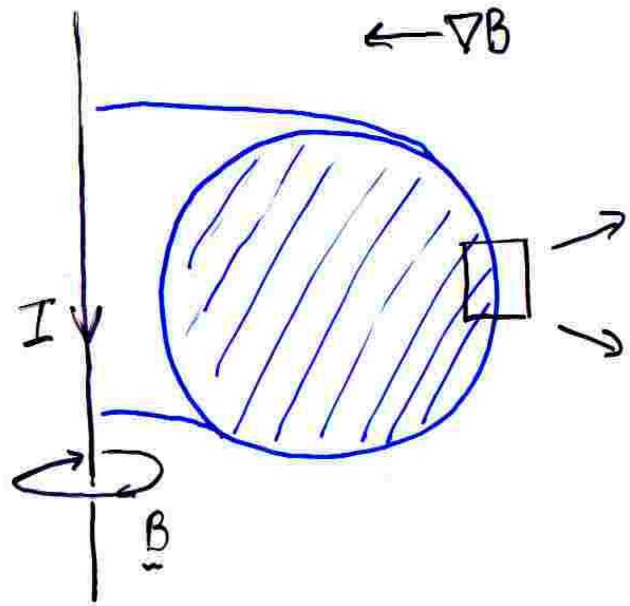
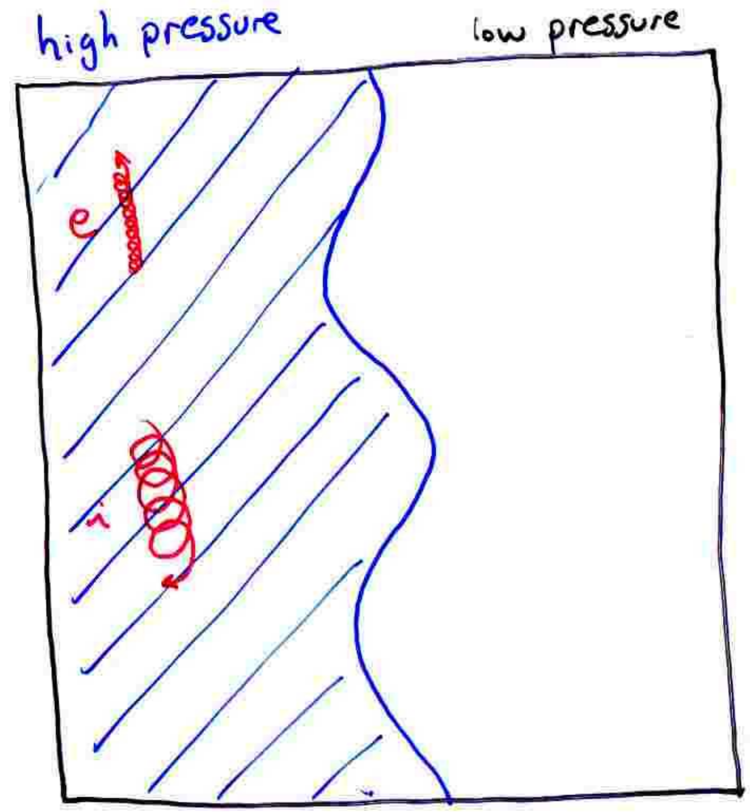


$$\underset{\sim}{V_d} = \frac{v_\perp^2}{2\Omega}\,\hat{b}\times\nabla\ln B$$

"curvature drift" similar

Qualitative Physical Picture of "Bad Curvature" Instabilities (ITG, TEM, ETG, Drift waves, MHD ballooning...)





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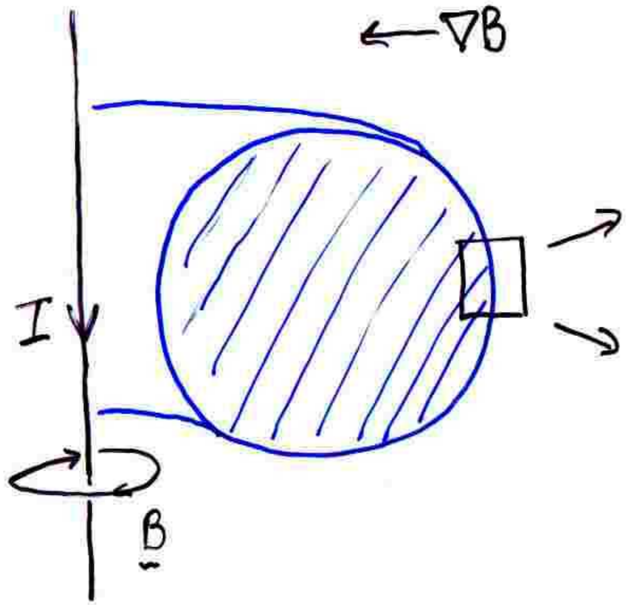

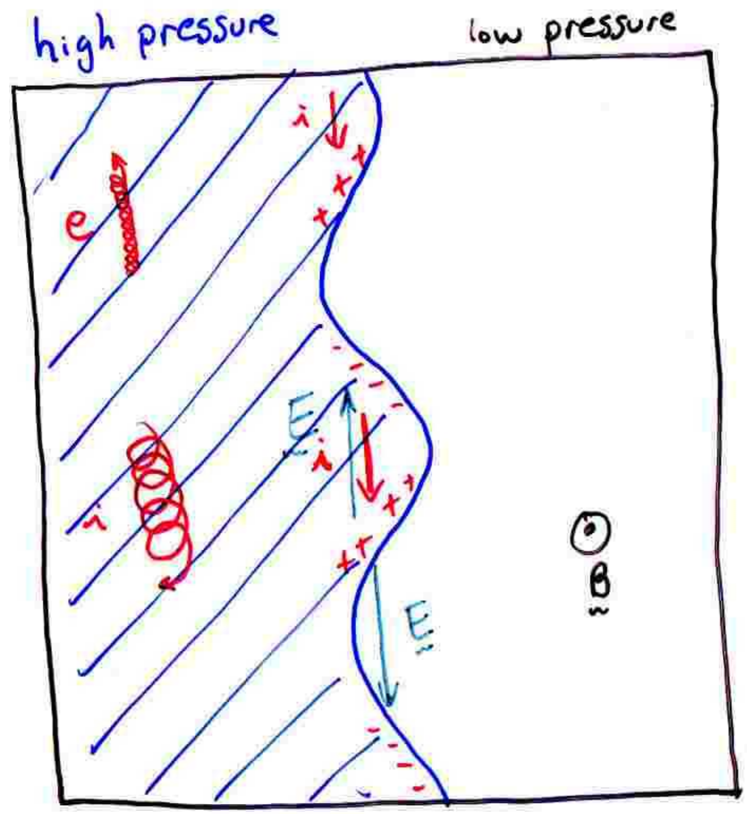

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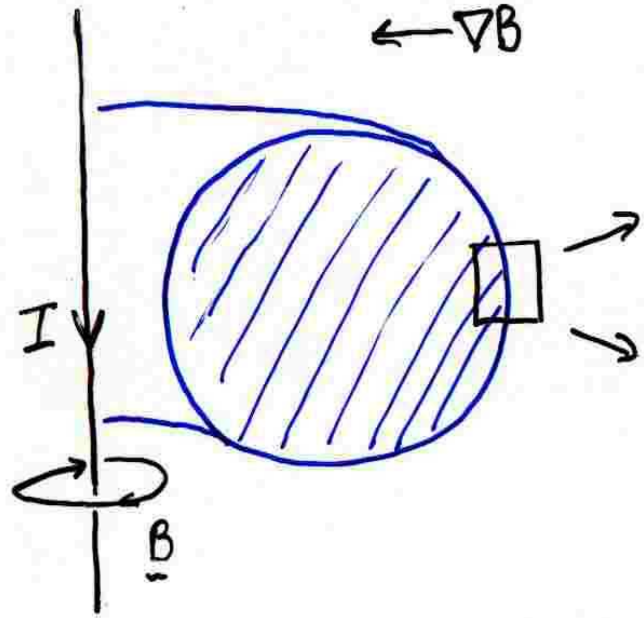
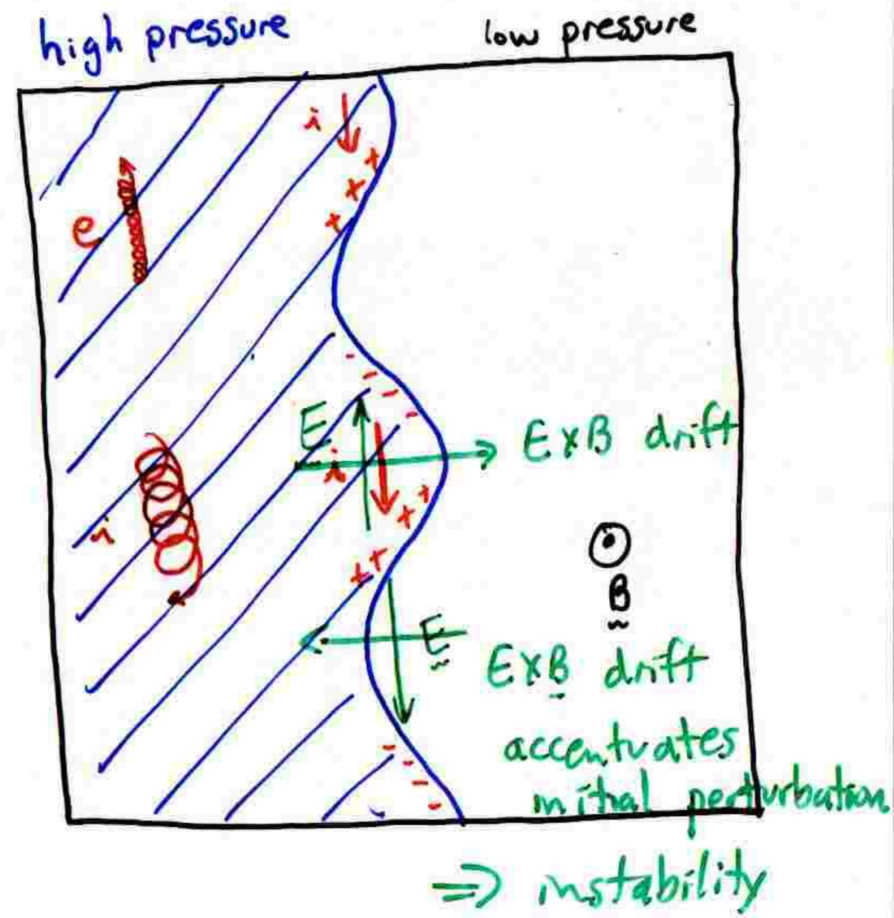
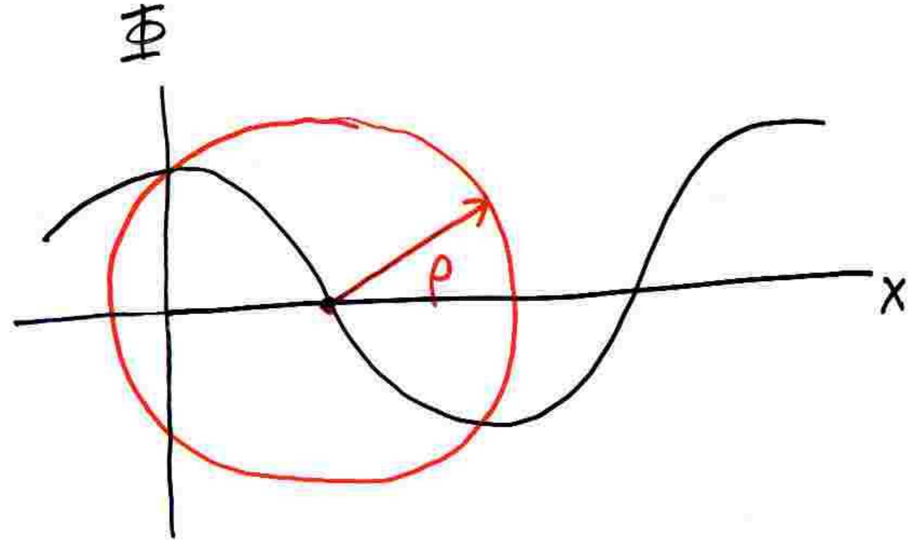




If Electric Field is not uniform, Gyroaverage

$$\underset{\sim}{E} = -\nabla \Phi$$

$$\underset{\sim}{V}_{E\times B} = \frac{c}{B} \hat{b} \times \nabla \langle \Phi \rangle$$



$$\langle \Phi \rangle (\underset{\sim}{x}) = \frac{1}{2\pi} \oint d\underset{\sim}{\rho}\, \Phi(\underset{\sim}{x} + \underset{\sim}{\rho})$$

$$= J_0(k_\perp \rho)\, \Phi$$

A complete description of a plasma

is given by the particle distribution function $F_s(\vec{x}, \vec{v}, t)$, the density of particles at (near) position $\vec{x}$ with velocity $\vec{v}$ and time t, for species s (with charge q_s and mass m_s).

The charge density and current needed for Maxwell's equations to determine the electric and magnetic fields is then:

$$\sigma(\vec{x}, t) = \sum_s q_s \int d^3v F_s(\vec{x}, \vec{v}, t) \qquad \vec{j}(\vec{x}, t) = \sum_s q_s \int d^3v \vec{v} F_s(\vec{x}, \vec{v}, t)$$

F_s **is determined by the Vlasov-Boltzmann equation**

$$\frac{\partial F}{\partial t} + \vec{v} \cdot \frac{\partial F}{\partial \vec{x}} + \frac{q_s}{m_s}\left(\vec{E} + \frac{\vec{v} \times \vec{B}}{c}\right) \cdot \frac{\partial F}{\partial v} = \textbf{Collisions + sources + sinks} \approx 0$$

where sources + sinks includes radiation cooling of electrons, ionization and recombination changes of ion charge state, etc.

Equivalent particle approach

Discrete particle density representation (combined with smoothing and "particle-in-cell" techniques):

$$F_s = \sum_{i=1,N} w_i(t)\delta(\vec{x} - \vec{x}_i(t)\delta(\vec{v} - \vec{v}_i(t)$$

$$\frac{d\vec{x}_i}{dt} = \vec{v}_i \qquad\qquad \frac{d\vec{v}_i}{dt} = \frac{q_i}{m_i}\left(\vec{E}(\vec{x}_i, t) + \frac{\vec{v}_i \times \vec{B}(\vec{x}_i, t)}{c}\right)$$

plus Monte Carlo treatment of collisions, sources and sinks.

Both "continuum" F **and particle descriptions are equivalent (in the limit of a large number of particles, typical fusion particle density** $\sim 10^{14}$**/cm**^{3}**) and are"Exact", but both include an excessive range of time and space scales.**

Most plasma phenomena of interest are slow compared to the electron and ion gyrofrequencies ($\sim 10^{11}$ **Hz and** $\sim 10^8$ **Hz).**

Vlasov, Boltzmann, Liouville Eq:

Particle Distribution

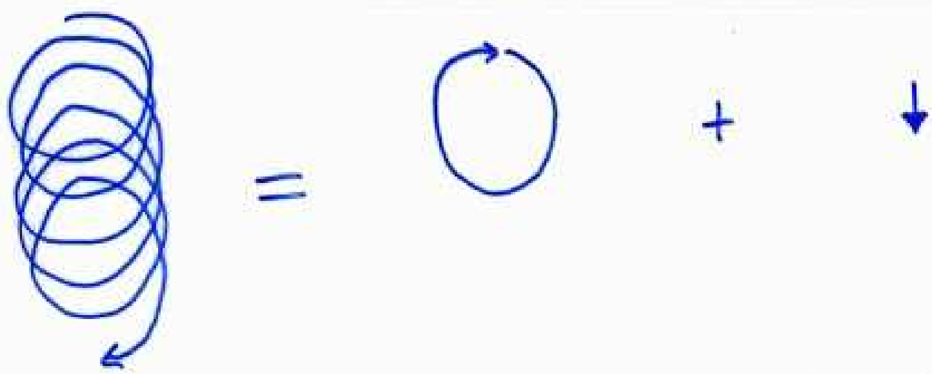
$$\frac{\partial f(\underset{\sim}{x}, \underset{\sim}{v}, t)}{\partial t} + \underset{\sim}{v} \cdot \frac{\partial f}{\partial \underset{\sim}{x}} + \frac{q}{m} \underbrace{\left(\underset{\sim}{E} + \frac{\underset{\sim}{v} \times \underset{\sim}{B}}{c}\right) \cdot \frac{\partial f}{\partial \underset{\sim}{v}}} = C(f)$$

Nonlinear, $\underset{\sim}{E}$ & $\underset{\sim}{B}$ depend on f through Maxwell's Eqs.

Nonlinear Gyrokinetic Eq. 1982–88

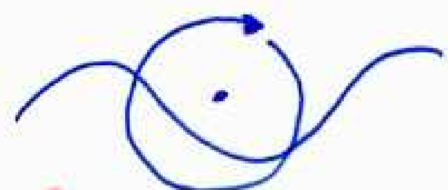
(Frieman & Chen, W.W. Lee, Dubin, Krommes, Hahm, Brizard...)

linear gyrokinetics 1960's & 70's.



$\underset{\sim}{V}_{drift}$

$$\frac{c}{B^2} \langle \underset{\sim}{E} \rangle \times \underset{\sim}{B} + \dots$$



Possible to eliminate fast gyrofrequency time scales & retain nonlinear dynamics & $k_\perp \rho_i \sim 1$

The Nonlinear Gyrokinetic Equation

Guiding center distribution function $F_s(\vec{x}, \vec{v}, t) = F_{0s}(\psi, W) + F_{0s}(\psi, W) q_s \tilde{\phi}/T_s + \tilde{h}_s(\vec{x}, W, \mu, t)$ = **equilibrium + fluctuating components, where the energy** $W = m v_\parallel^2 + \mu B$**, the first adiabatic invariant** $\mu = m v_\perp^2 / B$**, and**

$$\frac{\partial \tilde{h}_s}{\partial t} + \left(\tilde{\vec{v}}_\chi + v_\parallel \hat{b} + \vec{v}_d\right) \cdot \nabla \tilde{h}_s = -\tilde{\vec{v}}_\chi \cdot \nabla F_{0s} - q_s \frac{\partial F_{0s}}{\partial W} \frac{\partial \tilde{\chi}}{\partial t} + \text{Collisions + Sources + Sink}$$

where $\hat{b}$ **points in the direction of the equilibrium magnetic field,** $\vec{v}_d$ **is the curvature and grad B drift,** Ω_s **is the gyrofrequency, and the ExB drift is combined with transport along perturbed magnetic fields lines and the perturbed** ∇B **drift as:**

$$\tilde{\vec{v}}_\chi = \frac{c}{B} \hat{b} \times \nabla \tilde{\chi} \qquad \tilde{\chi} = J_0(\gamma)\left(\tilde{\phi} - \frac{v_\parallel}{c} \tilde{A}_\parallel\right) + \frac{J_1(\gamma)}{\gamma} \frac{m v_\perp^2}{e} \frac{\tilde{B}_\parallel}{B}$$

J_0 **&** J_1 **are Bessel functions with** $\gamma = k_\perp v_\perp / \Omega_s$**, and the fields are from**

$$0 \approx 4\pi \sum_s q_s \int d^3v \left[q_s \tilde{\phi} \frac{\partial F_{0s}}{\partial W} + J_0(\gamma) \tilde{h}_s \right]$$

$$\nabla^2 \tilde{A}_\parallel = -\frac{4\pi}{c} \sum_s q_s \int d^3v\, v_\parallel J_0(\gamma) \tilde{h}_s$$

$$\frac{\tilde{B}_\parallel}{B} = -\frac{4\pi}{B^2} \sum_s \int d^3v\, m v_\perp^2 \frac{J_1(\gamma)}{\gamma} \tilde{h}_s$$

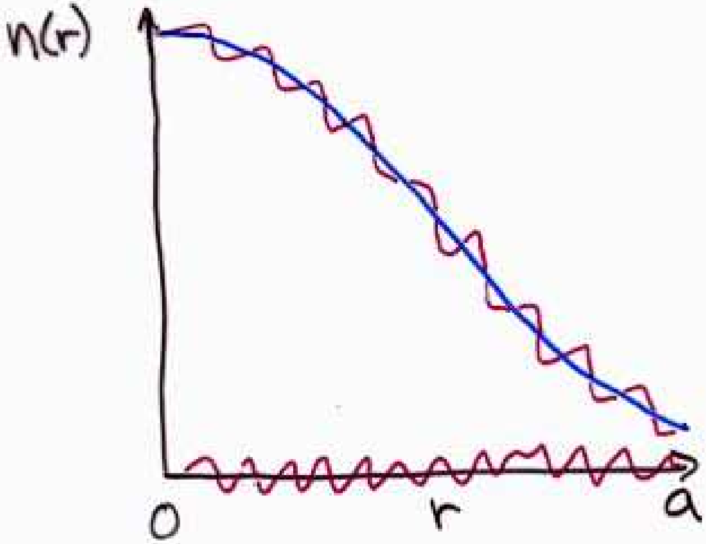
$$\tilde{\vec{E}} = -\nabla\tilde{\phi} - \frac{1}{c}\frac{\partial \tilde{A}_\parallel}{\partial t}\hat{b}$$

$$\vec{B} = \vec{B}_0 + \nabla\tilde{A}_\parallel \times \hat{b} + \tilde{B}_\parallel\hat{b}$$

In a full-torus simulation where plasma variations must be kept

$$J_0(k_\perp v_\perp/\Omega_s)\phi \rightarrow \langle\phi\rangle(\vec{x}) = \frac{1}{2\pi}\int d\vec{\rho}\phi(\vec{x}+\vec{\rho})$$

Microinstabilities are small-amplitude but still nonlinear



$$n = n_0(r) + \tilde{n}(\underset{\sim}{x}, t)$$

$$n_0 \gg \tilde{n}$$

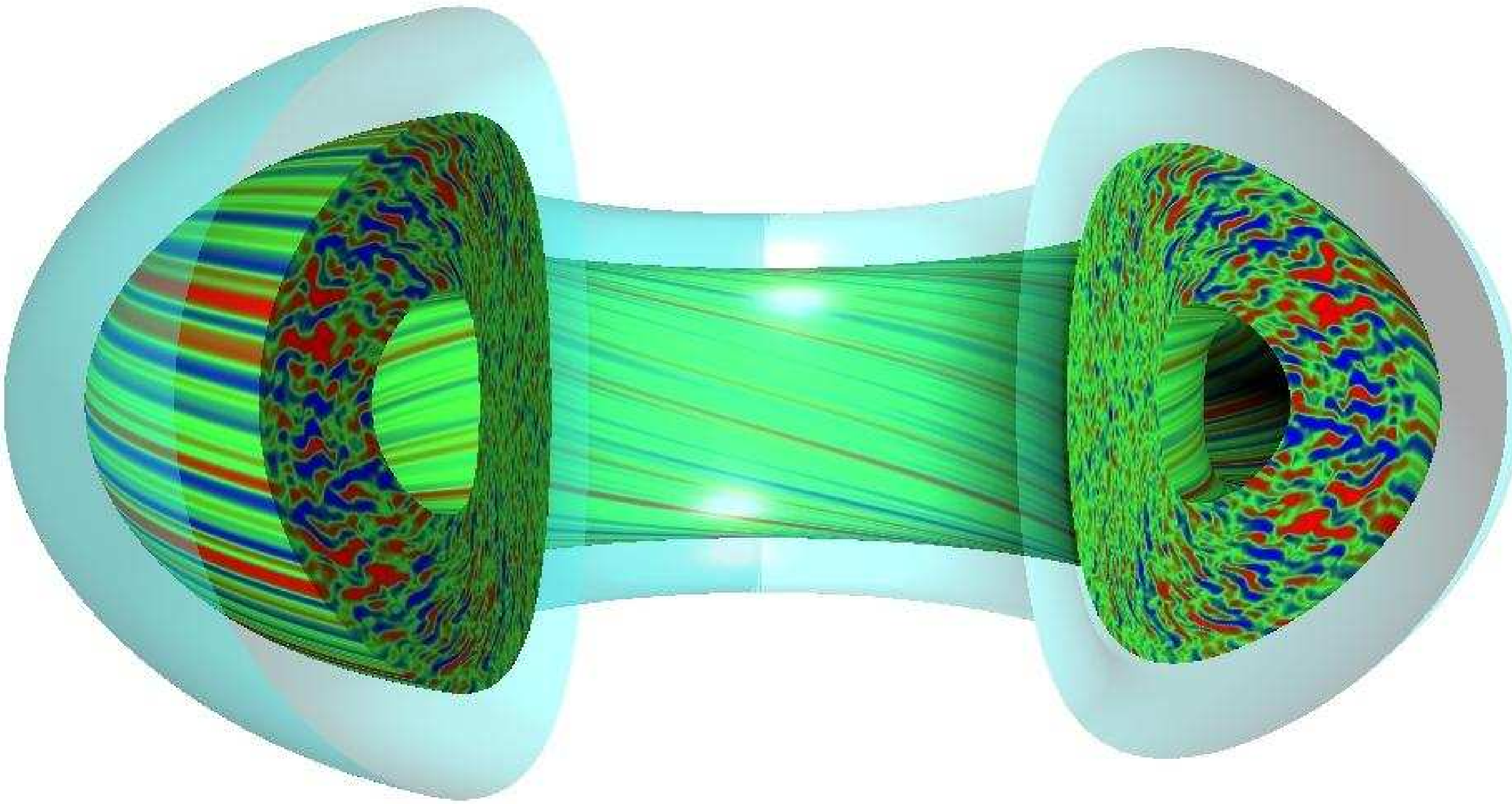
but $\nabla n_0 \sim \nabla \tilde{n}$

Can locally flatten or reverse total gradient that was driving instability.

* Turbulence causes loss of plasma to the wall, but confinement still $\times 10^5$ better than without $\underset{\sim}{B}$.

If no $\underset{\sim}{B}$, loss time $\sim \dfrac{a}{V_t} \sim 1\ \mu\text{sec}$

with $\underset{\sim}{B}$, expts. measure $\sim 0.1 - 1.0$ sec.

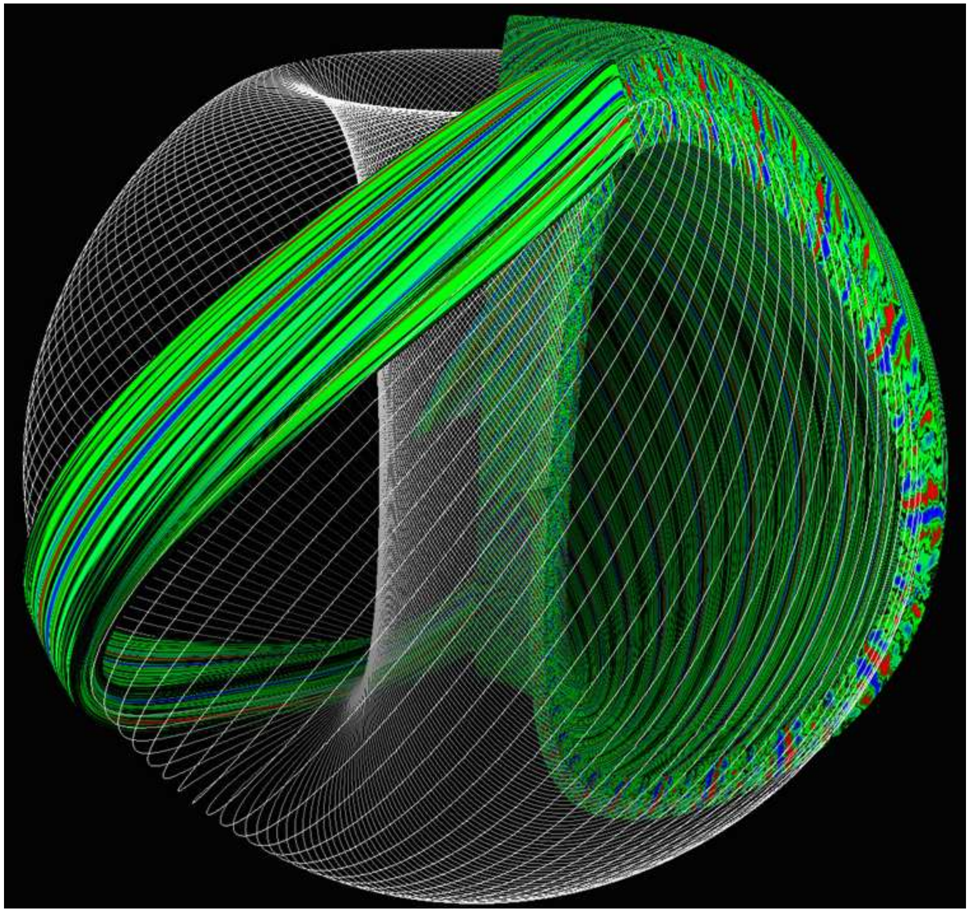


Candy/Waltz movies available at:

http://web.gat.com/comp/parallel/gyro_gallery.html

and other movies can be found from various links starting at:

http://fusion.gat.com/theory/pmp



The Plasma Microturbulence Project supports a 2x2 matrix of codes (geometry x algorithm), each type of code is tuned to optimize in various regimes and so are optimized to study certain types of problems.

Codes using flux-tube geometry (shown here) take advantage of short decorrelation lengths of the turbulence perpendicular to magnetic field lines. Multiple copies of a flux-tube pasted together represent a toroidal annulus.

We Support a 2x2 Matrix of Plasma Turbulence Simulation Codes

	Continuum	PIC
Flux Tube	GS2	SUMMIT
Global	GYRO	GTC

- Why both Continuum and Particle-in-Cell (PIC)?
  - Cross-check on algorithms
  - Continuum currently most developed (already has kinetic e's , $\delta B_\perp$)
  - PIC may ultimately be more efficient
- If we can do Global simulations, why bother with Flux Tubes?
  - Electron-scale (ρ_e, $\delta_e = c/\omega_{pe}$) physics (ETG modes, etc.)
  - Turbulence on multiple space scales (ITG+TEM, TEM+ETG, ITG+TEM+ETG, …)
  - Efficient parameter scans

Current ‘state-of-the-art’

(similar performance achieved in Continuum codes)

Spatial Resolution

- Plasma turbulence is quasi-2-D
  - – Resolution requirement along B–field determined by equilibrium structure
  - – Resolution across B–field determined by microstructure of the turbulence.
  - $\Rightarrow$ ~ $64\times(a/\rho_i)^2$ ~ 2×10^8 grid points to simulate ion-scale turbulence at burning-plasma scale in a global code
  - – Require ~ 8 particles / spatial grid point
  - $\Rightarrow$ ~ 1.6×10^9 particles for global ion-turbulence simulation at ignition scale
  - – ~ 600 bytes/particle
  - $\Rightarrow$ 1 terabyte of RAM

$\Rightarrow$ This resolution is achievable

Temporal Resolution

- Studies of turbulent fluctuations
  - – Characteristic turbulence time-scale
    $\Rightarrow$ c_s/a ~ 1 μs (10 time steps)
  - – Correlation time >> oscillation period
    $\Rightarrow$ τ_c ~ 100× c_s/a ~ 100 μs (10^3 time steps)
  - – Many τ_c’s required
    $\Rightarrow$ $T_{simulation}$ ~ few ms (5×10^4 time steps)
  - – 4×10^{-9} sec/particle-timestep (this has been achieved)
  - $\Rightarrow$ ~90 hours of IBM-SP time/run

☛ Heroic (but within our time allocation)

(Such simulations have been performed, see T.S. Hahm, Z. Lin, APS/DPP 2001)

- Simulations including electrons and δB (short space & time scales) are not yet practical at the burning-plasma scale with a global code

Major Computational and Applied Mathematical Challenges

- **Continuum kernels** solve an advection/diffusion equation on a 5-D grid
  - Linear algebra and sparse matrix solves (LAPAC, UMFPAC, BLAS)
  - Distributed array redistribution algorithms (we have developed or own)
- **Particle-in-Cell kernels** advance particles in a 5-D phase space
  - Efficient “gather/scatter” algorithms which avoid cache conflicts and provide random access to field quantities on 3-D grid
- **Continuum** and **Particle-in-Cell kernels** perform elliptic solves on 3-D grids (often mixing Fourier techniques with direct numerical solves)
- **Other Issues:**
  - Portability between computational platforms
  - Characterizing and improving computational efficiency
  - Distributed code development
  - Expanding our user base

Continuum / Eulerian Codes		*Particle-in-Cell/Lagrangian Codes*	
Flux-tube / thin-annulus	**Full-torus or thin annulus**	**Flux-tube**	**Full-torus**
All now use field-line following coordinate systems, $\Delta x_{\perp}/\Delta x_{\|\|} \sim \rho_i/L \sim 10^{-1}$-$10^{-3}$			
GS2 (Dorland, U. Md., Kotschenreuther)	**Gyro (Candy-Waltz GA)**	**Summit (LLNL, U. Co, UCLA)**	**GTC (Z. Lin et.al. PPPL, UCI)**
$\perp$ Pseudo-spectral linear & nonlinear. **$\|\|$ 2^{cd} order finite-diff. (slight upwind)**	**Toroidal pseudo-spectral** **5^{th}-6^{th} order upwind τ grid to avoid $1/v_{\|\|}$** **collisions w/ direct sparse solver (UMFPACK)**	**Delta-f algorithm reduces particle noise.** **Recent hybrid electron algorithm: fluid with kinetic electron closure.**	
Linear: fully implicit (elegant algorithm) **Nonlinear: 2^{cd} order Adams-Bashforth**	**High accuracy explicit 4^{th} order Runge-Kutta**	**Leap-frog / Predictor-corrector**	
Elliptic solvers easy in Fourier space	**Elliptic solvers with non-uniform coefficients solved by combination of Fourier, iterative, and direct matrix solution**		

Fast time scales hiding in E & B fields: is there a partially-implicit iterative algorithm that can help?

Recommendations (I)

Strengthening PMP Support to Integrated Modeling

(1) Improve the fidelity and performance of Plasma Microturbulence Project codes

(2) Validate these codes against experiment

(3) Expand the user base of the PMP codes

(4) Initiate the development of a kinetic edge turbulence simulation code.

CORE TURBULENT TRANSPORT STILL IMPORTANT

- **Provides most of temperature gradient: 20 keV center $\rightarrow$ 1-4 keV near-edge. Effects of shaping, density peakedness, rotation, impurities, T_i/T_e?**
- **Detailed experimental comparisons possible, fluctuation diagnostics.**
- **Are internal transport barriers possible at reactor scales? $P_{threshold}$? Torque? Controllable?**
- **Electron-scale transport controls advanced reactor performance?**

BUT EDGE TURBULENCE CRITICAL

- **H-mode pedestal (edge transport barrier) greatest source of uncertainty for reactor predictions.**
- **Will divertor melt/erode? Need ELM simulation.**
- **Edge very complicated: Separatrix & divertor geometry matters. Bootstrap current important, second stability regime. Half of power radiated, intense neutral recycling.**
- **High and low collisionality regimes. Present edge codes are collisional fluids, need kinetic extensions.**

3-D Fluid Simulations of Plasma Edge Turbulence BOUT (X.Q. Xu,)

- Braginskii — collisional, two fluid electromagnetic equations
- Realistic ×-point geometry (open and closed flux surfaces)
- BOUT is being applied to DIII-D, C-Mod, NSTX, …
- There is LOTS of edge fluctuation data!

⇒ An Excellent opportunity for code validation

More info:

Plasma Microturbulence Project (PMP):
http://fusion.gat.com/theory/pmp

Nevins presentation on PMP to ISOFS May 2002:
http://www.isofs.info/nevins.pdf

GS2 (Dorland Univ. Md.):
http://gk.umd.edu/GS2/info.html

Useful 2-page gyrokinetic summary:
http://gk.umd.edu/GS2/gs2_back.ps

GTC (Lin PPPL UCI):
http://w3.pppl.gov/~zlin/visualization/

Gyro (Candy/Waltz GA):
http://web.gat.com/comp/parallel/gyro.html

Summit (LLNL/UCLA/U. Co.):
http://www.nersc.gov/scidac/summit