Introduction to Gyrokinetic Theory & Simulations Greg Hammett (Princeton University, PPPL) ITER Summer School, Aix-en-Provence, Aug. 26, 2014 (these slides & handwritten notes @ http://w3.pppl.gov/~hammett/talks/2014/gk\_intro)

- Students, introduce yourselves: where from, what year, main interests.
- Motivation: Reducing microturbulence could help fusion
- Physical picture of turbulent processes in tokamaks
- Brief intro to gyrokinetics concept: average over fast gyromotion.
  - Two main kinds of gyokinetics
    - Iterative/asymptotic, local,  $\delta f$  gyrokinetics
    - Lagrangian/Hamiltonian, global, full-F gyrokinetics
  - Annotated references for suggested reading
  - Handwritten derivation of iterative local gyrokinetics (electrostatic slab)
  - Handwritten gyrokinetic derivation of toroidal ITG instability
- A few slides about algorithms: PIC/continuum, Discontinuous Galerkin.

## Gyrokinetic Simulation of Tokamak Microturbulence



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

Well known that improving confinement &  $\beta$  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  $Q(nT\tau_E)$ .

Standard H-mode empirical scaling:  $\tau_E \sim H I_p^{0.93} P^{-0.69} B^{0.15} R^{1.97} \dots$  $(P = 3VnT/\tau_E$  & assume fixed  $nT\tau_{E,} q_{95}$ ,  $\beta_N$ ,  $n/n_{Greenwald}$ ):

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

ITER std H=1, steady-state  $H\sim 1.5$ ARIES-AT  $H\sim 1.5$ 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  $\propto R^2$  roughly. Plot accounts for constraint on *B* @ magnet with 1.16 m blanket/shield, i.e.  $B = B_{mag} (R-a-a_{BS})/R$ )



## **Interesting Ideas To Improve Fusion**

\* Liquid metal (lithium, tin) films or flows on walls: (1) protects solid wall (2) absorbs incident hydrogen ions, reduces recycling of cold neutrals back to plasma, raises edge temperature & improves global performance. TFTR found: ~2 keV edge temperature. NSTX, LTX: more lithium is better, where is the limit?

\* Spherical Tokamaks (STs) appear to be able to suppress much of the ion turbulence: PPPL & Culham upgrading 1 --> 2 MA to test scaling

\* Advanced tokamaks, alternative operating regimes (reverse magnetic shear or "hybrid"), methods to control Edge Localized Modes, higher plasma shaping. Will beam-driven or spontaneous rotation be more important than previously thought?

\* Tokamaks spontaneously spin: can reduce turbulence and improve MHD stability. Can we enhance this with up-down-asymmetric tokamaks or non-stellarator-symmetric stellarators with quasi-axisymmetry?

\* Many possible stellarator designs, room for further optimization: Quasi-symmetry / quasi-isodynamic improvements discovered relatively recently, after 40 years of fusion research. Stellarators fix disruptions, steady-state, density limit.

\* Robotic manufacturing advances: reduce cost of complex, precision, specialty items

Intuitive picture of tokamak instabilities

-- based on analogy with Inverted Pendulum / Rayleigh-Taylor instability:

-- curved magnetic field lines  $\rightarrow$  effective gravity



#### "Bad Curvature" instability in plasmas ≈ Inverted Pendulum / Rayleigh-Taylor Instability

Top view of toroidal plasma:



Growth rate:

$$\gamma = \sqrt{\frac{g_{eff}}{L}} = \sqrt{\frac{V_t^2}{RL}} = \frac{V_t}{\sqrt{RL}}$$

Similar instability mechanism in MHD & drift/microinstabilities

1/L = |∇p|/p in MHD, ∝ combination of ∇n & ∇T in microinstabilities. The Secret for Stabilizing Bad-Curvature Instabilities

## Twist in **B** carries plasma from bad curvature region to good curvature region:



Similar to how twirling a honey dipper can prevent honey from dripping.



An aside to define some tokamak terminology ( $\iota$  used in stellarator literature):

$$\iota = "rotational transform" (or "twisting rate")$$

$$q = \frac{1}{\iota} = "safety factor" or "inverse rotational transform"$$
(or "inverse twisting rate")
$$q = \# \text{ of times a field line goes around toroidally}$$
in order to go once around poloidally
$$rB_{tm}$$

$$q \approx \frac{7B_{tor}}{RB_{pol}}$$

Note: older stellarator literature (< ~ late 1990s) defined "iota bar":

$$\boldsymbol{t} = \boldsymbol{\iota} \,/ \,(2\pi) = 1 \,/ \,q$$

 $q \approx 1.6$  in the upper right figure 2 slides back.

While MHD works well to lowest order in plasmas,  
there are next-order FLR corrections that defrust  
the magnetic field 
$$\neq$$
 allow  $E_{11} \neq 0 \neq$  allow  
the plasma to more separately from  $\underline{B}$ .  
Still have sound waves that can connect good  $\neq$   
bad convaries region. Unstable if:  
 $\delta \gg connection rate$ 





#### Spherical Torus has improved confinement and pressure limits (but less room in center for coils)



# These physical mechanisms can be seen in gyrokinetic simulations and movies

Stable side, smaller eddies Unstable bad-curvature side, eddies point out, direction of effective gravity

particles quickly move along field lines, so density perturbations are very extended along field lines, which twist to connect unstable to stable side

Microinstabilities are small-amplitude  
but still nonlinear  

$$n(r)$$
  
 $n(r)$   
 $n = n_0(r) + \tilde{n}(x,t)$   
 $n_0 >> \tilde{n}$   
but  $\nabla n_0 \sim \nabla \tilde{n}$   
 $\int C_{on} locally flatten
or reverse total gradient
that was driving instability.
* Turbulence causes loss of plasma to the wall,
but confinement still x10S better than without B.
If no B, loss time ~  $\frac{a}{V_E} \sim 1$  psec  
with B, expts. measure ~ 0.1-1.0 sec.$ 

Note: previous and other figures show color contours of density fluctuations, not of the total density, because if one plotted contours of total density, the tiny fluctuations would not be visible:

$$n_e(\vec{x},t) = n_{e0}(r) + \delta n(\vec{x},t)$$
  
 $\delta n \sim 10^{-3} - 10^{-2} n_{e0}$  in plasma core

For low-frequency fluctuations,  $\omega \ll k_{||} v_{te}$ , electrons have a Boltzmann response to lowest order along a field line:

$$n_{e}(\vec{x},t) = C(r)e^{|e|\phi/T_{e0}}$$

$$\approx n_{e0}\left(1 + \frac{|e|\phi}{T_{e0}}\right)$$

$$\delta n \sim n_{e0}\frac{|e|\phi}{T_{e0}}$$

So contours of density fluctuations are also contours of constant potential, and so represent stream lines for the ExB drift. (Like stream lines in 2D fluid flow.) Can illustrate this with a sketch...

Movie <a href="https://fusion.gat.com/theory-wiki/images/3/35/D3d.n16.2x\_0.6\_fly.mpg">http://fusion.gat.com/theory/Gyromovies</a> shows contour plots of density fluctuations in a cut-away view of a GYRO simulation (Candy & Waltz, GA). This movie illustrates the physical mechanisms described in the last few slides. It also illustrates the important effect of sheared flows in breaking up and limiting the turbulent eddies. Long-wavelength equilibrium sheared flows in this case are driven primarily by external toroidal beam injection. (The movie is made in the frame of reference rotating with the plasma in the middle of the simulation. Barber pole effect makes the dominantly-toroidal rotation appear poloidal..) Short-wavelength, turbulent-driven flows also play important role in nonlinear saturation.



#### Sheared flows can suppress or reduce turbulence



#### Sheared ExB Flows can regulate or completely suppress turbulence (analogous to twisting honey on a fork)



Dominant nonlinear interaction between turbulent eddies and  $\pm \theta$ -directed zonal flows.

Additional large scale sheared zonal flow (driven by beams, neoclassical) can completely suppress turbulence

# Simple picture of reducing turbulence by negative magnetic shear

- Particles that produce an eddy tend to follow field lines.
- Reversed magnetic shear twists eddy in a short distance to point in the ``good curvature direction".
- Locally reversed magnetic shear naturally produced by squeezing magnetic fields at high plasma pressure: ``Second stability'' Advanced Tokamak or Spherical Torus.
- Shaping the plasma (elongation and triangularity) can also change local shear

ŝ=0 No Magnetic Shear ŝ>0 "Normal" Magnetic Shear (in std tokamaks) ŝ<0 Advanced Tokamaks Negative Magnetic Shear "Normal" in stellarators

Fig. from Antonsen, Drake, Guzdar et al. Phys. Plasmas 96 Kessel, Manickam, Rewoldt, Tang Phys. Rev. Lett. 94

#### Fascinating Diversity of Regimes in Fusion Plasmas. What Triggers Change? What Regulates Confinement?



R. Nazikian et al.

## Transition to Enhanced Confinement Regime is Correlated with Suppression of Core Fluctuations in TFTR



 Similar suppression observed on JET (X-mode reflectometer) and DIII-D (FIR Scattering)

Hahm, Burrell, Phys. Plas. 1995, E. Mazzucato et al., PRL 1996.



R. Nazikian et al.

I usually denote the shearing rate as  $\gamma_s$  or  $\gamma_{ExB}$ instead of  $\omega_{ExB}$  because it is a dissipative process and isn't like a real frequency. The shearing rate (in a simple limit of concentric circular flux surfaces) is

$$\gamma_s \approx \frac{d \mathbf{v}_{ExB,\theta}}{dr}$$

## All major tokamaks show turbulence can be suppressed w/ sheared flows & negative magnetic shear / Shafranov shift



Internal transport barrier forms when the flow shearing rate  $dv_{\theta}/dr > \sim$  the max linear growth rate  $\gamma_{lin}^{max}$  of the instabilities that usually drive the turbulence.

Shafranov shift  $\Delta'$  effects (self-induced negative magnetic shear at high plasma pressure) also help reduce the linear growth rate.

Advanced Tokamak goal: Plasma pressure ~ x 2,  $P_{fusion} \propto pressure^2 ~ x 4$ 

Turbulence suppression mechanisms really work: Ion Transport level can be reduced to minimal collisional level in some cases.







⊙ ß  $\leq$ ₽ß



⊙ Ŀ ₽ß

Rosenbluth-Longmire pictuge





G ∇B

Can repeat this analysis on the good curvature side & find it is stable. (Leave as exercise.)

Rosenbluth-Longmire pictuge

Rigorous derivation of ITG growth rate & threshold (in a simple limit) starting from the Gyrokinetic Eq.

(see handwritten notes...)

#### Fairly Comprehensive 5-D Gyrokinetic Turbulence Codes Have Been Developed

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



- Solve for the particle distribution function  $f(r, \theta, \alpha, E, \mu, t)$  (avg. over gyration:  $6D \rightarrow 5D$ )
- 500 radii x 32 complex toroidal modes (96 binormal grid points)
   x 10 parallel points along half-orbits
   x 8 energies x 16 v<sub>||</sub>/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 (SciDAC project), GENE (Garching) similar. These and other codes being widely compared with experiments.

## Major breakthrough: Gyrokinetic predictions now much better than 1990 analytic turbulence theories



Plot made in 1990. Analytic theories disagreed with measured diffusion coefficients by factors of 100-1000. The importance of thresholds for marginal stability not appreciated then. Explains why the edge effects the core so much. (see also S.D. Scott et al., Phys. Fluids B 1990) feasibility of directly coupling gyrokinetic

turbulence codes to long-time-scale

transport codes.

Gyro-Bohm Mixing-length estimate of diffusion caused by microturbulence eddies:

$$\chi \sim \frac{(\Delta x)^2}{\Delta t} \sim (\Delta x)^2 \gamma \sim (\Delta x)^2 \frac{v_t}{\sqrt{RL_T}} k_\theta \rho \sim \rho^2 \frac{v_t}{\sqrt{RL_T}}$$



Peaks at  $r \sim 0$  where T is high. Contradicts expts.

More generally, there is usually a threshold for the instability:

$$\chi = \frac{cT}{eB} \frac{\rho}{R} \left( \frac{R}{L_T} - \frac{R}{L_{T,\text{crit}}} \right) g(q, \hat{s}, T_i/T_e, R/L_T, R/L_n, \dots)$$

Small where T is high, explains  $\chi(r)$  decreasing near axis in expts. (IFS-PPPL transport model, Kotschenreuther, Dorland, Beer, Hammett, Phys. Plasmas 1995, also GLF23, TGLF, and other models)





In cool edge, adding more heating power causes the temperature gradient to increase significantly.



In hot core, no matter how much heating power, you just get (approx.) marginal stability:

$$-\frac{\partial T}{\partial r} = \frac{T}{L_T} = \frac{T}{R} \frac{R}{L_{T,crit}} \quad \Rightarrow \quad T(r) = C \exp\left(-\frac{r}{R} \frac{R}{L_{T,crit}}\right)$$

*C* set by boundary conditions near edge where marginal stability breaks down.

#### Sheldon uses gyrokinetic theory to design a fusion reactor



TV sitcom "The Big Bang Theory", Jan. 31, 2013 "The Cooper/Kripke Inversion". Equation for critical-gradient plasma turbulence from gyrokinetic/gyrofluid simulations based on work by Dorland, Kotschenreuther, Hammett, Beer, Waltz, Biglari et al., see slide #34 of <u>http://w3.pppl.gov/~hammett/talks/2005/kitp-fusion-status.pdf</u>. Gyro orbit picture from Krommes 2012, <u>http://dx.doi.org/10.1146/annurev-fluid-120710-101223</u>.

# Gyrokinetic-based TGLF transport model compares well with core of many experiments



Biggest gap: doesn't predict edge region (r/a>0.8).

#### Motivation: Need comprehensive simulations of edge, because pedestal temperature has big effect on fusion gain Q



Because of marginal stability effects, the edge boundary condition strongly affects the core: the edge is the tail that wags the dog.

Need an edge code to answer many important questions:

height of the pedestal, conditions for Hmode transport barrier formation, effect of RMP coils to suppress ELMs, divertor power handling, improvements with lithium walls...

#### Edge region very difficult



Present core gyrokinetic codes are highly optimized for core, need new codes to handle additional complications of edge region of tokamaks (& stellarators):

open & closed field lines, plasma-wall-interactions, large amplitude fluctuations, positivity constraints, atomic physics, non-axisymmetric RMP / stellarator coils, magnetic fluctuations near beta limit...

Hard problem: but success of core gyrokinetic codes makes me believe this is tractable, with a major initiative

if low frequencies  $\omega \ll cyclotron$  frequency  $(\Omega_c)$ ,  $\rightarrow$  average over particle gyration, treat particles as rings of charge in spatially varying fields



potential averaged around particle orbit, even if  $k_{\perp}\rho_i$  large



When calculating charge at point Q, have to sum over all particles whose guiding centers are on the dashed line, & have to include small variation of particle density around gyro-orbit ( $\rightarrow$ polarization shielding)

Development of nonlinear gyrokinetics was a major breakthrough

### Development of & physics in Gyrokinetic Eqs.

Development of gyrokinetic equations one of the triumphs of high-power theoretical plasma physics and applied math (asymptotic analysis)

Interesting pre-history and history of gyrokinetics...

Key advance: Frieman & Chen (79-82) show nonlinear gyrokinetics possible, used an iterative local approach

Another version of gyrokinetics: Hamiltonian / Lagrangian Field-Theory derivations (Hahm, Brizard, Qin, Sugama, ...), insures conservation properties for global codes, easier to go to higher order

Chew-Goldberger-Low (1956) MHD-ordered Drift-Kinetic Eq.:

$$\epsilon \sim \frac{\rm frequency}{\rm gyrofrequency} \sim \frac{\omega}{\Omega_c} \sim \frac{\rm gyroradius}{\rm gradient\ Length} \sim \frac{\rho}{L} \ll 1$$

Later recognized MHD ordering demonstrates stability only for fast instabilities, with growth rates  $\gamma \sim \epsilon \Omega_c$ , and misses slow drift instabilities with  $\gamma \sim \epsilon^2 \Omega_c$ :

$$rac{\omega_*}{\Omega_c}\sim k_y
horac{
ho}{L}\sim\epsilon^2$$

Extensions of CGL to higher  $\mathcal{O}(\epsilon^2)$ , but very complicated

Deriviation of MHD-Drift-Kinetic Eq.:

\* R. M. Kulsrud, in *Proc. International School of Physics Enrico Fermi, Course XXV, Advanced Plasma Theory*, edited by M. N. *Rosenbluth, Varenna, Italy, 1962.* 

\* R. M. Kulsrud, in *Handbook of Plasma Physics*, edited by M. N. Rosenbluth & R. Z. Sagdeev, 1983.

## Big Breakthrough: *Nonlinear* Gyrokinetics

- Long, interesting history of linear gyrokinetics, 1960's, 1970's.
- E. A. Frieman & L. Chen 79-82, showed it is possible to gyro-average nonlinear terms and keep full FLR-effects for arbitrary k<sub>⊥</sub>ρ, & get rigorous solution w/o closure problem. Very impressive. Triumph of asymptotic analysis and theoretical insight. <sub>Guided by expts., µwave scattering, physics insights</sub>
- (usually, averaging nonlinear terms → closure problems, such as fluid equation closures, statistical turbulence theories,...
   Perhaps some understood, or in retrospect: J.B. Taylor '67 showed adiabatic invariant still exists at arbitrary k<sub>⊥</sub>ρ, for small amplitude perturbations...)
- GK ordering allows capture of drift/micro-instabilities & much of MHD at just order ε & not ε<sup>2</sup>

$$\mathcal{E} \sim \frac{\omega}{s_{1}} \sim \frac{f}{t_{0}} \sim \frac{f}{f_{0}} \sim \frac{e\Phi}{T_{0}}$$
 but  $h_{1}\rho \sim O(1)$   
 $\sim \frac{h_{11}}{h_{1}}$ 

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

$$\frac{\partial \tilde{f}}{\partial t} + (v_{\parallel}\hat{\mathbf{b}} + \mathbf{v}_{E} + \mathbf{v}_{d}) \cdot \nabla \tilde{f} + \left(\frac{q}{m}E_{\parallel} - \mu\nabla_{\parallel}B + v_{\parallel}(\hat{\mathbf{b}}\cdot\nabla\hat{\mathbf{b}})\cdot\mathbf{v}_{E}\right)\frac{\partial \tilde{f}}{\partial v_{\parallel}} = 0$$

$$\bigvee_{\tilde{e}} = -\frac{c}{b}\nabla\langle\Phi\rangle\times\hat{b} \qquad \tilde{e}_{\parallel} = -\hat{b}\cdot\nabla\langle\Phi\rangle\times\hat{\mathbf{b}} + v_{\parallel}(\hat{\mathbf{b}}\cdot\nabla\hat{\mathbf{b}})\cdot\mathbf{v}_{E}$$

$$\text{using gyroaveraged potential:} \quad \langle\phi\rangle(\vec{R}) = \frac{1}{2\pi}\int d\theta\,\phi(\vec{R} + \vec{\rho}(\theta))$$

$$= \frac{1}{2\pi}\int d\theta\sum_{\vec{k}}\phi_{\vec{k}}\,e^{i\vec{k}\cdot\vec{R}} = J_{0}\phi$$

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

$$\underbrace{\Phi}(\mathbf{x}) \qquad \underbrace{\Phi}(\mathbf{x}) = \frac{1}{b}\nabla(\mathbf{x}) + \frac{\rho(\theta)}{b}\nabla(\mathbf{x}) + \frac{\rho(\theta)}{b}\nabla(\mathbf{$$

phase-space conservation for global codes.)

$$f(\underline{x}, \underline{v}, t)$$
  
Catto Guiding center coordinates:  

$$\underline{x} = R_{gc} + f(\theta)$$
  

$$f_{gc} (R_{gc}, V_{ii}, N, t)$$
  
Independent of gyro-angle  $\theta$  to lawest order  
eliminates high gyro frequency dynamics.  
But to calculate physical density:  

$$n(\underline{x}) = \int d^{3}v \quad f_{gc} (\underline{x} - f(\theta), V_{ii}, t) \quad (+ p darization piece)$$
  

$$\propto \int d\theta \sum_{\underline{k}} \hat{f}_{\underline{k}} e^{\underline{x}} \underline{h} \cdot (\underline{x} - f(\theta))$$
  

$$\propto \sum_{\underline{k}} \hat{f}_{\underline{k}} e^{\underline{x}} \underline{h} \cdot \underline{x} \quad J_{0}(\underline{h}, p)$$

#### The Meaning of Gyrokinetics

• low frequencies  $\omega \ll \Omega_c = eB/mc$  for each species



- reduced response: "gyroaveraging"
- reaction to fields, polarisation density:

"gyroscreening"

#### **Polarization Density Plays Key Role in Gyrokinetic Poisson / Quasineutrality Eq.**

At long wavelengths (neglecting higher-order FLR corrections to polarization density):

$$-\nabla_{\perp} \cdot \left(\frac{\sum_{s} 4\pi n_s m_s c^2}{B^2} \nabla_{\perp} \phi\right) = \sum_{s} 4\pi e_s \int m_s B_{||}^* dv_{||} d\mu d\theta \ \bar{f}(\vec{x} - \vec{\rho}(\mu, \theta), \mu, v_{||})$$

-(Polarization charge density) = guiding center charge density (including gyroaveraging)

Looks like a Poisson equation, but actually is a statement of quasineutrality:

$$0 = \sigma = \sigma_{\rm gc} + \sigma_{\rm pol}$$

Because the polarization density depends on the potential, this is how the potential gets determined. The polarization density can be shown to be related to the higher-order polarization drift:

$$rac{\partial \sigma_{
m pol}}{\partial t} = - 
abla \cdot ec{j}_{
m pol} \propto 
abla \cdot rac{\partial ec{E}}{\partial t}$$

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In order for a non-local/global gyrokinetic code to have a conserved energylike quantity using just the lowest order drifts (ExB, grad(B) and curvature) from the first order Hamiltonian  $H_1 \sim (\rho/L) T$ , the density on the LHS must be replaced by a time-independent  $n_{s0}$ . Okay for short time scales.

In order to allow a time varying  $n_s$ , and conserve the energy properly, one must include drifts from the second order Hamiltonian  $H_2 \sim (\rho/L)^2 T$ . Natural consequence of Lagrangian field theory approach.

(Local gyrokinetics also satisfies energy conservation,  $H_2$  effects incorporated in the higher-order transport equations.)

Density calculation for Poisson Eq. includes Important  
Polarization shielding  

$$n(\underline{x}) = n_{gc} + n_{poe}$$
  
 $n_{gc}(\underline{x}) = \int d^{3}v \quad \overline{f}(\overline{x} - \overline{p}(\theta), V_{11}, N)$   
 $n_{poe}(\underline{x}) = n_{o}(\overline{f_{o}} - 1) \stackrel{e}{=} \stackrel{e}{=} \frac{\overline{f}}{T_{o}} \approx -n_{o}h_{1} \stackrel{2}{p_{i}} \stackrel{e}{=} \stackrel{e}{=} \frac{\overline{f}}{T_{o}}$   
 $n_{poe}$  arises from gyro-phase dependent part:

$$\widetilde{f}_{\theta} = -F_{\theta} \stackrel{e}{=} \left[ \underbrace{\Phi}(\vec{R} + \vec{\rho}(\theta)) - \langle \underline{\Phi} \rangle (\vec{R}) \right]$$

Particles have an adiabatic response around their gyro-ring

alternative derivation: next order correction to adiabatic invariant mu

#### First Gyrokinetic PIC code

- Frieman & Chen had first derivation, but very complicated. (Nonlinearities in ballooning/field-aligned coordinates clarified in Beer, Cowley, Hammett, '95.)
- W.W. Lee '83 & '87 derivations somewhat clearer, used Catto transformation to guiding center coordinates, & then asymptotic expansion. Made clearer the role of the polarization density (higher order polarization drift dropped from gyrokinetic equation, but resulting polarization density contributes to the gyrokinetic Poisson equation (because even small charge densities lead to large forces in plasmas)).
- Lee made clearer that GK polarization density eliminates small Debye scale and high frequency plasma oscillations, making simulations much more tractable. Demonstrates first GK PIC simulations (slab, electrostatic, 2-D on early 1980's computers).

### Two main types of gyrokinetics

- Original local " $\delta f$ " iterative/asymptotic gyrokinetics, directly expands Vlasov Eq. and  $F = F_0 + \varepsilon F_1$  (Frieman and Chen). Rigorous for small  $\rho_* = \rho/L$  gyroBohm limit, important limit to study. Eddy size  $L_{eddy} \sim \rho \ll L$ . Simulate small-scale turbulence in a local region where radial variation of parameters ( $\omega_*(r), v(r)$ , etc.) can be neglected. (I.e., both  $n_0$  and  $dn_0/dr$  are treated as constant, as in Hasegawa-Mima eq.) The most complete derivations, including both gyrokinetic turbulence equation & next order transport equations:
  - Ian Abel, Rep. Prog. Phys. 76 (2013) 116201 (69 pp)
  - Sugama and Horton, Phys. Plasmas 5 (1998) 2560 (14 pp)
- Global "full *F*" Lagrangian/Hamiltonian gyrokinetics. Does not break up  $F = F_0 + \delta f$ . Does not assume eddy sizes  $L_{eddy} << L$ , and so includes effect of radial variation of parameters and possible non-gyroBohm regimes. (Probably important near plasma edge and near transport barriers.) Maybe consistent only in some case:
  - $\rho \sim L_{eddy} \ll L$ , (gyroBohm regime) or
  - $\rho \ll L_{eddy} \sim L$ , (i.e.,  $k_{\perp} \rho \ll l$ , Bohm regime) but not
  - $\rho \sim L_{eddy} \sim L$  (but perhaps generalizations exist for SOL, ...)
  - First derivation in Lagrangian field theory approach that gave particle+field energy conservation consistently is Sugama (2000), followed quickly by Brizard (2000) and others.

### Two main types of gyrokinetics (part 2)

- Note: both the local delta-f approach and the global full-F approaches are "multiscale":  $\omega \ll \Omega$ .
- There is also some mixture of techniques. Parra and Catto 2008 (PPCF 50, 065014) shows how to derive a set of global full-F gyrokinetic equations using an iterative technique directly on the Vlasov equation.
- There are many gyrokinetic papers, with some variation in assumed orderings (for example, with strong equilibrium ExB flows or not), the physical effects included (for example, simple vs. general geometry, electrostatic,  $\delta A_{||}$ ,  $\delta B_{||}$ , ...), order of accuracy, the degree of energy and momentum conservation or accuracy.
- Some derivations are more general than their apparent stated assumptions. The frequency ordering (in the plasmas frame) is more fundamental than spatial orderings.

#### **Outline of Iterative local gyrokinetics**

- Original "2-scale" local "delta f" gyrokinetics with direct iterative/asymptotic expansion of Vlasov eq. and  $F = F_0 + \varepsilon F_1$  (or  $\delta f$ )
- Involves 4 orders of expansion to go through transport time scale (Sugama 98, Barnes 08, Plunk09, Abel 13):
- $\varepsilon^{-1}$ :  $F_0$  independent of gyro-angle:

- $\varepsilon^{1}$ : standard GK equation on  $\omega_{*}$  turbulence time scale
- $\epsilon^2$ : transport equations for slow variation of  $F_0$  on transport time scale.

$$\frac{q}{m}\frac{\vec{v}\times\vec{B}}{c}\cdot\nabla_{v}F_{0}=\Omega\frac{\partial F_{0}}{\partial\theta}=0$$

$$\tilde{F}_1 = -\frac{q(\phi - \langle \phi \rangle)}{T} F_0$$
$$\frac{\partial F_1}{\partial t} = \dots$$

$$\frac{\partial n_0}{\partial t} = \dots$$

## Suggested Refs for iterative local gyrokinetics

- Original "2-scale" local "δf" gyrokinetics (Frieman and Chen, '83). However, very complicated. (Nonlinearity in ballooning/field-line coordinates clarified in Beer, Cowley Hammett, '95.)
- Lee '83 (Phys. Fluids 26, 556), used Catto coordinate transformation. (Lee '83 is iterative, but writes things in full-F global form. Keeps higher-order terms in Poisson eq. that aren't necessary... Energy & momentum conservation subtleties.)
- Linear papers by Catto '78, and by Antonsen & Lane '80 are instructive.
- My 20-page handwritten notes on a complete derivation of gyrokinetics in δf slab electrostatic limit. Tried to show all steps. (Based on (and fixes some typos in) Dorland Thesis (1993), Appendix C tutorial, which summarizes Lee '83.) (handwritten notes at <u>http://w3.pppl.gov/~hammett/talks/2014/gk\_intro</u>)
- Cowley Vienna notes, 2008
- Howes 2006, Gyrokinetics for Astrophysics tutorial paper. Complete, systematic derivation in slab limit. (Dorland thesis and Howes '06 available at <a href="http://w3.pppl.gov/~hammett/papers">http://w3.pppl.gov/~hammett/papers</a>)
- The most complete, systematic derivations in general geometry, including next order transport equations:
  - Ian Abel, Rep. Prog. Phys. 76 (2013) 116201 (69 pp)
  - Sugama and Horton, Phys. Plasmas 5 (1998) 2560 (14 pp).
- Derivation of a global gyrokinetics, but w/ traditional iterative asymptotic approach:
  - Parra and Catto 2008

## Lagrangian/Hamiltonian Lie-Perturbation methods

Advantage:  $\partial f/\partial t = \{H, f\}$ , make approximations to Hamiltonian/Lagrangian, but preserve important Hamiltonian properties: exact conservation for a global code of an energy *H*, phase-space, symplectic etc., easier to extend to full *f* instead of breaking up  $f=f_0+f_1$ , easier to extend to higher-order terms that may be important in some regimes (perhaps in edge turbulence where  $f_1 << f_0$  assumption weak), etc.

(Energy conservation in local iterative gyrokinetics is also correct, handled in higher order transport equations. See Abel '13)

Dubin, Krommes, Oberman, & Lee '83 built on Littlejohn, Hamiltonian, slab, electrostatic

Hahm '88: Lagrangian approach advantages, extended to toroidal geometry &  $\delta B_{\perp}$ 

Brizard: Lagrangian, extended to full  $\delta B_{\perp}$  and  $\delta B_{\parallel}$ , nonlinear properties

Dimits & Lodestro generalization of ordering

- Qin: Various extensions and tests. Linear benchmarks with PEST MHD code, including kink mode. Higher-order extensions that may be useful near edge. Extensions to general frequency for RF resonant heating, etc.
- Sugama (2000), Brizard (2000) Lagrangian field theory for particles and fields together. Second order drifts from  $H_2 \sim \varepsilon^2 T$  required to get exact energy conservation with polarization density that is linear in phi.

Brizard-Hahm RMP 2007

#### Suggested References for Learning Lagrangian Field-Theory Approaches to Gyrokinetics

- I (and many others) find this topic very difficult (but I appreciate it's usefulness and importance).
- Start with Krommes' 2012 Annual Rev. of Fluid Mechanics, "The Gyrokinetic Description of Microturbulence in Magnetized Plamsas", <u>http://dx.doi.org/10.1146/annurev-fluid-120710-101223</u>. Nice review article that surveys the big picture without trying to do the gory derivation.
- Next do background textbook reading reminding yourself of the basics of Lagrangian/ Hamiltonian mechanics. (Concise summaries: Miyamoto's textbook, Steven's "The Six Core Theories of Modern Physics", errata at <u>http://w3.pppl.gov/~hammett/courses/physics-summaries/core-theories-errata.pdf</u>).)
- Helander & Sigmar's book has a nice review of Lagrangian mechanics, and a nice Lagrangian variational derivation of single particle drifts.
- Parra & Calvo PPCF 2011, a Lagrangian Field-Theory derivation of gyrokinetics but without relying on the language of differential geometry. Don't need to know what "differential form", "one form", "two form", "wedge product", "Lie transform" mean. Would start with the slab limit. (Recent 2014 paper on arxiv.org with Burby showing equivalence with differential geometric approaches.)
- Sugama 2000, PoP 7, 466, \*key paper\*, first paper on Lagrangian field theory for gyrokinetics, to get field equations on an equal footing with particle drifts, particle-field energy conservation. Some use of Lie transforms but not differential forms.

#### Suggested References for Learning Lagrangian Field-Theory Approaches to Gyrokinetics With More Differential Geometry

- Littlejohn, J. Plasma Physics 29 (1983), 111 "Variational principles of guiding center motion". Introduced Lagrangian variational methods to particle drift calculations. (I think there is an error in the ordering of a certain term that requires him to go to higher order than necessary, but this pioneering paper is still important for the concepts.)
- Cary and Littlejohn, Annals of Physics 151, 1 (1983), "Noncanonical Hamiltonian Mechanics and Its Application to Magnetic Field Line Flow". Has a nice tutorial on differential forms and Lie transforms used in some GK. See also Littlejohn, J. Math. Phys. 23, 742 (1982).
- Kikuchi's textbook, "Frontiers in Fusion Research" (2011). Interesting textbook, with highlights of interesting physics and current research in various parts of fusion. First textbook I think that tries to present gyrokinetics using Lie transforms (though he glosses over the gyrokinetic field equation). Fairly readable, but there are some typos to watch for.
- Krommes & Hammett 2013 (<u>http://bp.pppl.gov/pub\_report//2014/PPPL-4945-abs.html</u>) on momentum transport ordering difficulties pointed out by Parra & Catto. Krommes included an extensive tutorial on Lagrangian differential geometry approaches to gyrokinetics.
- Series of geometrical Lagrangian papers: Brizard, Qin, B.Scott, J. Squire, J. Burby, Brizard-Hahm Rev. Mod. Phys. 2007, Cary-Brizard Rev. Mod. Phys. 2009, Idomura, Miyato & Scott, Brizard & Tronko, ...
- Good gyrokinetics & turbulence tutorials by Jenko, by Bottino, and others: <u>http://www2.ipp.mpg.de/~fsj/tutorial.html</u>

#### Parra & Catto pointed out challenges of momentum transport

In a series of papers, Parra & Catto pointed out challenges of momentum transport in a standard regime (gyroBohm ordering, axisymmetric, up-down symmetric, slow flows of order the diamagnetic velocity  $v_* \sim \varepsilon v_t$ ). In particular, they showed that the standard Lagrangian gyrokinetic approach would require the third order Hamiltonian  $H_3$  to deal with momentum transport accurately in this low flow ordering. They advocate supplementing with a separate equation for directly solving for toroidal momentum evolution, then need only  $H_2$ . (See Krommes & Hammett, PPPL report 4945, 2013. <u>http://bp.pppl.gov/pub\_report//2014/PPPL-4945-abs.html</u>)

Our report gives some straightforward ordering arguments (originally due to P&C) demonstrating their point. One should understand the implications in a balanced way. Slow flows in this regime are so slow that usually they would not significantly affect the turbulence, though they might still be important for MHD stability. Flows are usually more important in regimes that break some of these assumptions (like non-gyroBohm scaling near the edge or near transport barriers), but then still need a second order Hamiltonian. P&C deserve credit for pointing out these subtle issues and helping people realize the importance of even  $H_2$  for a complete treatment in other regimes. (Many codes at present neglect  $H_2$ .)

## PIC & Continuum algorithm comparisons

Both PIC & continuum codes need comparable spatial resolution to represent electromagnetic/gravitational fields. But use different methods to do velocity integrals to calculate charge/current densities needed to find fields.

Convergence rates for d-dimensional integral, where  $N = N_1^d$ :

2cd order (midpoint) Eulerian:  $\epsilon \sim (\Delta x)^2 \sim \frac{C_2}{N^2} \sim \frac{C_2}{N^{2/d}}$ 

Monte Carlo sampling:

$$\epsilon \sim \frac{C_{\rm MC}}{N_{\rm particles}^{1/2}}$$



Continuum methods appear competitive/better for d <= 4.

Caveats:

(1) coefficients highly problem-dependent

(2) Don't need same resolution in all directions,

(3) Modern continuum codes use higher-order/spectral methods.

(4) Focused here on velocity integration methods, but algorithms also differ in how they solve particle motion or solve for distribution function. PIC particles ~move to where needed...

## PIC & Continuum algorithm comparisons

- Very different algorithms with different numerical properties.
  - -PIC: Lagrangian / Monte-Carlo random sampling
  - Continuum: Eulerian (or semi-Lagrangian) / optimized integration
- Essential to have independent algorithms to cross check each other, particularly for the types of difficult problems we study.
- Modern Continuum codes use range of advanced CFD algorithms (pseudo-spectral, high-order upwind, discontinuous Galerkin, Arakawa,...) not just simple grid.
- Error vs. N (# particles/cell or velocity grid points):



- PIC may be better for problems with large "signal" where larger noise can be tolerated. Continuum may be better for problems where low noise is needed (e.g. near marginal stability).
- Continuum appears asymptotically more efficient for gyrokinetics and even full Vlasov (d=2 and d=3 velocity space)

# PIC & Continuum algorithm comparisons: details

- Some PIC simulations of reconnection or tokamak edge plasmas now use 1000 particles/cell --> 5000 quantities/cell (3x & 2v for each particle).
- "finite-size-particles" smooth fields over ~3 adjacent cells in each direction (similarly, "force-softening" in N-body tree codes)
- Equivalent continuum code would have ~ 520x260 in  $(v_{\parallel}, v_{\perp})$  (or ~ 55<sup>3</sup> in 3V) per resolved region. (GYRO, GENE, & GS2 often converge very well with just 8  $\mu$  and 16  $v_{\parallel}$ ).
- Because collisions enter as ~  $v v_t^2 \partial^2 / \partial v^2$ , continuum codes don't need much velocity resolution at moderate collisionality to be fully resolved.

With Ammar Hakim & grad student Eric Shi, working on new continuum gyrokinetic code for the challenging edge region, using Discontinuous Galerkin & other advanced algorithms

• Several advanced algorithms to significantly improve efficiency:

Discontinuous Galerkin (DG) algorithms, improved conservation properties for Hamiltonian systems, optimized (Maxwellian-weighted) basis functions, sub-grid turbulence models in phase space, efficient use of massively parallel computers.

- A version of DG (based on C.-W. Shu & Liu, 2000) can exactly conserve energy for general Hamiltonian problems,  $\partial f/\partial t = \{H, f\}$ . Interestingly, does so even with upwind fluxes for *f*--> limiters (helpful to minimize artificial oscillations & preserve positivity).
- Efficient Gaussian integration --> ~ twice the accuracy / interpolation point:
  - Standard interpolation: p uniformly-spaced points to get p order accuracy
     DG interpolates p optimally-located points to get 2p-1 order accuracy
- Kinetic turbulence very challenging, benefits from all tricks we can find. Potentially big win: Factor of 2 reduction in resolution --> 64x speedup in 5D gyrokinetics

Goal: a robust code capable of relatively fast simulations at low velocity resolution, but with qualitatively-good gyro-fluid-like results, or fully converged kinetic results at high velocity resolution w/ massive computing.

#### Discontinuous Galerkin (DG) Combines Attractive Features of Finite-Volume & Finite Element Methods



Standard finite-volume (FV) methods evolve just average value in each cell (piecewise constant), combined with interpolations

DG evolves higher-order moments in each cell. I.e. uses higher-order basis functions, like finite-element methods, but, allows discontinuities at boundary like shock-capturing finite-volume methods --> (1) easier flux limiters like shock-capturing finite-volume methods (preserve positivity, important for large amplitude fluctuations in edge) (2) calculations local so easier to parallelize.

Hot topic in CFD & Applied Math: >1000 citations to Cockburn & Shu JCP/SIAM 1998. 64

#### Discontinuous Galerkin (DG) Combines Attractive Features of Finite-Volume & Finite Element Methods



Don't get hung up on the word "discontinuous". Simplest DG is piecewise constant: equivalent to standard finite volume methods that evolve just cell averaged quantities. Can reconstruct smooth interpolations between adjacent cells when needed.

Going to at least piecewise linear allows energy conservation (even with upwinding).

DG has ~twice the accuracy per point of FV, by optimal spacing of points within cell.

Introduction to Gyrokinetic Theory & Simulations Greg Hammett (Princeton University, PPPL) ITER Summer School, Aix-en-Provence, Aug. 26, 2014 (these slides & handwritten notes @ http://w3.pppl.gov/~hammett/talks/2014/gk\_intro)

- Students, introduce yourselves: where from, what year, main interests.
- Motivation: Reducing microturbulence could help fusion
- Physical picture of turbulent processes in tokamaks
- Brief intro to gyrokinetics concept: average over fast gyromotion.
  - Two main kinds of gyokinetics
    - Iterative/asymptotic, local,  $\delta f$  gyrokinetics
    - Lagrangian/Hamiltonian, global, full-F gyrokinetics
  - Annotated references for suggested reading
  - Handwritten derivation of iterative local gyrokinetics (electrostatic slab)
  - Handwritten gyrokinetic derivation of toroidal ITG instability
- A few slides about algorithms: PIC/continuum, Discontinuous Galerkin.