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A primer on gyrokinetic theory and simulation

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Some introductory remarks

My lecture series will cover three interrelated topics:

- A primer on gyrokinetic theory and simulation
- Features of linear and nonlinear gyrokinetics
- Recent progress towards a numerical tokamak

I will attempt to present the material in an accessible way

Please feel free to interrupt me if you have a question

Why invent gyrokinetics?

ITER and plasma turbulence

ITER is one of the most challenging scientific projects

Plasma turbulence determines its energy confinement time



Turbulent fluctuations are quasi-2D



Use field-aligned coordinates and minimize the simulation volume

Turbulent mixing in a tokamak

ExB drift velocity

$$\tilde{\mathbf{v}}_E = \frac{c}{B^2} \mathbf{B} \times \nabla \tilde{\phi}$$

$$\mathbf{Q} \equiv \frac{3}{2} \langle \tilde{p} \, \tilde{\mathbf{v}}_E \rangle = -n \chi \nabla T$$





Typical heat and particle diffusivities are of the order of 1 m²/s.

Gyrokinetic theory: A brief guided tour

What is gyrokinetic theory?

Dilute and/or hot plasmas are almost collisionless.

Thus, if kinetic effects (finite Larmor radius, Landau damping, magnetic trapping etc.) play a role, MHD is not applicable, and one has to use a kinetic description!

 $\left[\frac{\partial}{\partial t}\right]$

Vlasov-Maxwell equations

$$+\mathbf{v}\cdot\frac{\partial}{\partial\mathbf{x}}+\frac{q}{m}\left(\mathbf{E}+\frac{\mathbf{v}}{c}\times\mathbf{B}\right)\cdot\frac{\partial}{\partial\mathbf{v}}\left[f(\mathbf{x},\mathbf{v},t)=0\right]$$

Removing the fast gyromotion leads to a dramatic speed-up

 $\omega \ll \Omega$



Charged rings as quasiparticles; gyrocenter coordinates; keep kinetic effects



Details may be found in: Brizard & Hahm, Rev. Mod. Phys. 79, 421 (2007)

The gyrokinetic ordering

- The gyrokinetic model is a Vlasov-Maxwell on which the GK ordering is imposed:
- \Rightarrow Slow time variation as compared to the gyro-motion time scale:

$$\omega/\Omega_i \sim \epsilon_g \ll 1$$

 \Rightarrow Spatial equilibrium scale much larger than the Larmor radius:

$$ho/L_n \sim
ho/L_T \equiv \epsilon_g \ll 1$$

 \Rightarrow Strong anisotropy, i.e. only perpendicular gradients of the fluctuating quantities can be large ($k_{\perp}\rho \sim 1$, $k_{\parallel}\rho \sim \epsilon_g$):

$$k_\parallel/k_\perp\sim\epsilon_g\ll 1$$
 .

⇒ Small amplitude perturbations, i.e. energy of perturbation much smaller than the thermal energy:

$$e\phi/T_e \sim \epsilon_g \ll 1$$

A. Bottino

A brief historical review

• The word "Gyrokinetic" appeared in the literature in the late sixties. Rutherford and Frieman, Taylor and Hastie [1968].

Goal: Provide a adequate formalism for the linear study of kinetic drift-waves in general magnetic configurations, including finite Larmor radius effects.

- First nonlinear set of equations for the perturbed distribution function δF.
 Frieman and Liu Chen [1982].
 → Gyrokinetic ordering.
- Littlejohn [1979], Dubin [1983], Hahm[1988], Brizard [1989], ...

Firm and more transparent theoretical foundation for GK:

GK equations based on Hamiltonian or Lagrangian variation methods.

Lagrangian ↓ remove gyro-angle dependency in Lagrangian (change of coordinate system) ↓ equation of motion

A Lagrangian approach

If the Lagrangian of a dynamical system is known...

Example: charged particle motion, in non canonical coordinates (\vec{x}, \vec{v}) :

$$\begin{split} L &= \left(\frac{e}{c}\vec{A}(\vec{x},t) + m\vec{v}\right) \cdot \dot{\vec{x}} - H(\vec{x},\vec{v}) \\ H &= \frac{m}{2}v^2 + e\phi(\vec{x},t) \end{split}$$
 with $\vec{B} = \nabla \times \vec{A}$ and $\vec{E} = -\nabla \phi - \partial_t \vec{A}/c$.

...the equation of motion are given by the Lagrange equations: $\frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = 0 \quad \text{with } i = 1, \dots, 6$

Lagrange equation of motion for a charged particle:

$$\vec{v} \Rightarrow -\frac{\partial L}{\partial \vec{v}} = 0 \Rightarrow \dot{\vec{x}} = \vec{v}$$

$$\vec{x} \Rightarrow \frac{d}{dt} \frac{\partial L}{\partial \vec{v}} - \frac{\partial L}{\partial \vec{v}} = 0 \Rightarrow \dot{\vec{v}} = \frac{e}{m} \left(\vec{E} + \frac{\vec{v}}{c} \times \vec{B} \right)$$

Guiding center coordinates

GK ordering, but $k_{\perp}\rho \simeq 1 \Rightarrow k_{\perp}\rho \ll 1$ $\Rightarrow \vec{B}(\vec{x})$, static magnetic field.

• Single particle Lagrangian:

$$L = \left(\frac{e}{c}\vec{A}(\vec{x}) + m\vec{v}\right) \cdot \dot{\vec{x}} - \frac{m}{2}v^2 + e\phi(\vec{x},t)$$

Change of coordinates:

particle coordinates $(\vec{x}, \vec{v}) \Rightarrow$ guiding center coordinates $(\vec{R}, v_{\parallel}, \mu, \varphi)$

$$\begin{aligned} \vec{x} &= \vec{R} + \vec{\rho} \equiv \vec{R} + \frac{v_{\perp}}{\Omega} \hat{a}(\vec{R}, \varphi) \\ \mu &= v_{\perp}^2 / 2B(\vec{R}) \\ v_{\parallel} &= \vec{v} \cdot \vec{b} \\ \varphi &= \tan^{-1} \left(\frac{\vec{v} \cdot \vec{e}_1}{\vec{v} \cdot \vec{e}_2} \right) \end{aligned}$$

 \vec{R} guiding center position; $\Omega \equiv eB/mc$ gyrofrequency. $\hat{a} \equiv \cos(\varphi) \ \vec{e_1} + \sin(\varphi) \ \vec{e_2}$ $\vec{e_1}(\vec{R}, \varphi), \ \vec{e_2}(\vec{R}, \varphi)$ orthogonal unity vectors in the plane perpendicular to $\vec{b} \equiv \vec{B}/B$.

Guiding center coordinates (cont'd)

$$L_{DK} = \left(m v_{\parallel} \vec{b} + \frac{e}{c} \vec{A}(\vec{R}) \right) \cdot \dot{\vec{R}} + \frac{\mu B}{\Omega} \dot{\varphi} - H_{DK}$$
$$H_{DK} = \frac{m}{2} v_{\parallel}^2 + \mu B + q \phi(\vec{R})$$

Lagrange equations:

$$\begin{split} \dot{\vec{R}} &= v_{\parallel} \vec{b} + \frac{B}{B_{\parallel}^*} \left(\vec{v}_{E \times B} + \vec{v}_{\nabla B} + \vec{v}_C \right) \\ \dot{v_{\parallel}} &= \left(-\mu \nabla B + e\vec{E} \right) \cdot \frac{\dot{\vec{R}}}{mv_{\parallel}} \quad ; \quad \dot{\mu} = 0 \quad ; \quad \dot{\varphi} = \Omega \end{split}$$

$\vec{v}_{E \times B} \equiv$	$rac{c}{B^2} ec{E} imes ec{B}$	$E \times B$ drift
$\vec{v}_{\nabla B} \equiv$	$\frac{\mu}{m\Omega} \vec{b} \times \nabla B$	∇B drift
	$rac{v_{\parallel}^2}{\Omega}ec{b} imes(ec{b}\cdot abla)ec{b}$	Curvature drift

with $\vec{B^*} \equiv \vec{B} + (mc/e)v_{\parallel} \nabla \times \vec{b} = B(1 + \mathcal{O}(\rho_{\parallel}/L_B)).$

Including fluctuating fields



Resulting Lagrangian 1-form

Eliminate explicit gyrophase dependence via near-identity (Lie) transforms to gyrocenter coordinates:

$$\Gamma = \left(m v_{\parallel} \mathbf{b}_0 + \frac{e}{c} \,\bar{A}_{1\parallel} \,\mathbf{b}_0 + \frac{e}{c} \,\mathbf{A}_0 \right) \cdot d\mathbf{X} + \frac{mc}{e} \,\mu \,d\theta - \\ - \left(\frac{m}{2} v_{\parallel}^2 + \mu B_0 + \mu \bar{B}_{1\parallel} + e \,\bar{\phi}_1 \right) \,dt$$

$$\bar{\phi}_1 \equiv I_0(\lambda) \phi_1, \quad \bar{A}_{1||} \equiv I_0(\lambda) A_{1||}, \quad \bar{B}_{1||} \equiv I_1(\lambda) B_{1||}$$

Euler-Lagrange equations

$$\dot{\mathbf{X}} = v_{\parallel} \mathbf{b} + \frac{B}{B_{\parallel}^*} \left(\frac{v_{\parallel}}{B} \bar{\mathbf{B}}_{1\perp} + \frac{c}{B^2} \bar{\mathbf{E}}_1 \times \mathbf{B} + \frac{\mu}{m\Omega} \mathbf{b} \times \nabla (B + \bar{B}_{1\parallel}) + \frac{v_{\parallel}^2}{\Omega} (\nabla \times \mathbf{b})_{\perp} \right)$$

$$\dot{v}_{\parallel} = \frac{\dot{\mathbf{X}}}{mv_{\parallel}} \cdot \left(e\bar{\mathbf{E}}_1 - \mu\nabla(B + \bar{B}_{1\parallel}) \right) \qquad \qquad \dot{\mu} = 0$$

$$f = f(\mathbf{X}, v_{\parallel}, \mu; t)$$
$$\frac{\partial f}{\partial t} + \dot{\mathbf{X}} \cdot \frac{\partial f}{\partial \mathbf{X}} + \dot{v}_{\parallel} \frac{\partial f}{\partial v_{\parallel}} = 0$$

Gyroaveraged potentials



- Full Lorentz dynamics
- Gyrokinetic approx.: $\phi^{\text{eff}}(\vec{x},\rho) = \frac{1}{2\pi} \int_0^{2\pi} d\varphi \Phi(\vec{x}+\vec{\rho})$ $= \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} d\vec{k} \, e^{i\vec{k}\vec{x}} \phi(\vec{k}) J_0(|\vec{k}|\rho)$

Appropriate field equations

Reformulate Maxwell's equations in gyrocenter coordinates:

$$\begin{split} \nabla_{\perp}^{2}\phi_{1} &= -4\pi\sum en_{1}, \quad \frac{n_{1}}{n_{0}} = \frac{\bar{n}_{1}}{n_{0}} - \left(1 - \|I_{0}^{2}\|\right)\frac{e\phi_{1}}{T} + \|xI_{0}I_{1}\|\frac{B_{1\|}}{B}, \\ \nabla_{\perp}^{2}A_{1\|} &= -\frac{4\pi}{c}\sum \bar{J}_{1\|}, \\ \frac{B_{1\|}}{B} &= -\sum \epsilon_{\beta} \left(\frac{\bar{p}_{1\perp}}{n_{0}T} + \|xI_{1}I_{0}\|\frac{e\phi_{1}}{T} + \|x^{2}I_{1}^{2}\|\frac{B_{1\|}}{B}\right), \end{split}$$

Nonlinear integro-differential equations in **5 dimensions**...

Major theoretical speedups

relative to original Vlasov/pre-Maxwell system on a naïve grid, for ITER $1/\rho_* = a/\rho \sim 1000$

- Nonlinear gyrokinetic equations
 - □ eliminate plasma frequency: $\omega_{pe}/\Omega_i \sim m_i/m_e$ x10³
 - □ eliminate Debye length scale: $(\rho_i / \lambda_{De})^3 \sim (m_i / m_e)^{3/2}$ x10⁵
 - □ average over fast ion gyration: $\Omega_i / \omega \sim 1 / \rho_*$ x10³

Field-aligned coordinates

□ adapt to elongated structure of turbulent eddies: $\Delta_{\mu}/\Delta_{\perp} \sim 1/\rho_{*}$ x10³

Reduced simulation volume

- \Box reduce toroidal mode numbers (i.e., 1/15 of toroidal direction) x15
- \Box L_r ~ a/6 ~ 160 ρ ~ 10 correlation lengths x6

Total speedup

- For comparison: Massively parallel computers (1984-2009) x10⁷
- **x10**¹⁶

Status quo in gyrokinetic simulation

- over the last decade or so, GK has emerged as the standard approach to plasma turbulence
- a variety of nonlinear GK codes is being used and (further) developed
- these codes differ with respect to their numerics, physics, parallel scalability, and public availability



Extreme computing in support of ITER: The GENE code

The gyrokinetic Vlasov code GENE

http://gene.rzg.mpg.de

GENE is a physically comprehensive Vlasov code:

- allows for kinetic electrons & electromagnetic fluctuations, collisions, and external ExB shear flows
- is coupled to various MHD equilibrium codes and two transport codes
- can be used as initial value or eigenvalue solver



Concepts for efficiency & flexibility

Field-aligned (Clebsch-type) coordinates to exploit the high anisotropy of plasma turbulence

parallel (z) derivatives taken to be small compared to perpendicular (x,y) ones





Numerical methods – Time stepping scheme

Method of Lines:

- turn PDEs into ODEs by discretizing the spatial derivative first
- solve for the continuous time coordinate



Numerical methods – Time stepping scheme (cont'd)

Time Solver:

(Full) Nonlinear system: $\frac{\partial g}{\partial t} = \mathcal{V}[g] = Z + \mathcal{L}[g] + \mathcal{N}[g]$ • Several *ERK* methods, e.g. 4th order $g_{n+1} = g_n + \frac{\Delta t}{6} (k_1 + 2k_2 + 2k_3 + k_4)$ $k_1 = \mathcal{V}(t_n, g_n),$ $k_2 = \mathcal{V}(t_n + \Delta t/2, g_n + k_1 \Delta t/2),$ $k_3 = \mathcal{V}(t_n + \Delta t/2, g_n + k_2 \Delta t/2),$ $k_4 = \mathcal{V}(t_n + \Delta t, g_n + k_3 \Delta t).$

 Optimum linear time step can be precomputed using iterative EV solver

Adaptive CFL time step adaption for nonlinearity

Linear stability regions for low-order ERK schemes



Phase space discretization

GENE is a *Eulerian* code, representing the 5D distribution function on a fixed grid in (**x**, v_{||},μ)





radial direction x: toroidal direction y: parallel direction z: v_{\parallel} -velocity space: μ -velocity space:

equidistant grid (either configuration or Fourier space) equidistant grid in Fourier space

- equidistant grid points
- equidistant grid
 - Gauss-Legendre or Gauss-Laguerre knots

Phase space discretization (cont'd)

$$\frac{\partial f_{\sigma}}{\partial t} + \dot{\mathbf{X}} \cdot \nabla f_{\sigma} + \dot{v}_{\parallel} \frac{\partial f_{\sigma}}{\partial v_{\parallel}} = 0$$

$$\frac{\partial f}{\partial z} \rightarrow \frac{f(z_{(k-2)}) - 8f(z_{(k-1)}) + 8f(z_{(k+1)}) - f(z_{(k+2)})}{12\Delta z}$$

- 4th order finite differences are basic choice
- however, the more elaborate Arakawa-scheme is employed, if possible [A. Arakawa, JCP 135, 103 (1997), reprint]

Exception: spectral methods are employed in the y direction - always x direction - depends on the type of operation (local/global)

Local vs. global GENE

- Local: in the radial direction
 - □ Simulation domain small compared to machine size;

thus, constant temperatures/densities and fixed gradients

Periodic boundary conditions; allows application of spectral methods



- **<u>Global</u>**: adding nonlocal features in the *radial* direction
 - □ Consider full temperature & density profiles; radially varying metric
 - □ Dirichlet or v. Neumann boundary conditions
 - Heat sources & sinks

Local vs. global GENE: Numerics



Gyro-averaging procedure in more detail

$$\bar{f}(\mathbf{x}) \equiv \frac{1}{2\pi} \oint \mathrm{d}\theta \, f(\mathbf{x} + \mathbf{r}(\theta))$$

- discretize gyro-angle integration
- coordinate transform

c (1

- interpolation between grid-cells required
 - here: 1-dimensional problem (y remains in Fourier space)
 - use "finite-elements" which allows easy extraction of gyroaveraged quantities at original grid points (~ Hermite polynomial interpol.)

$$f(x) = \mathbf{\Lambda}(x) \cdot \mathbf{f} = \sum_{m=0}^{(p-1)/2} \mathbf{P}_m(x) \mathcal{D}^m \mathbf{f}$$

$$\frac{\partial^u}{\partial x^u} P_{n,m}(x) \Big|_{x=x_{(i)}} = \delta_{in} \delta_{um}$$

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$$\mathcal{G}_{in}(k_y, z, \mu) = \frac{1}{2\pi} \int_0^{\infty} d\theta \Lambda_n(x_{(i)} + r^*) e^{-iyt} d\theta \int_0^{-1} \frac{1}{0} e^{-iyt} d$$



μ-velocity space: Not required (if collisions are neglected)

Source and sink models in GENE

Full domain:

Radially dependent heat source/sink in whole domain (density and parallel momentum are unaffected)

$$\frac{df_{1}}{dt} = -\gamma_{h} \left[\langle f_{1}(\vec{X}, |\mathbf{v}_{\parallel}|, \mu) \rangle - \langle f_{0}(\vec{X}, |\mathbf{v}_{\parallel}|, \mu) \rangle \frac{\langle \int d\vec{v} \langle f_{1}(\vec{X}, |\mathbf{v}_{\parallel}|, \mu) \rangle \rangle}{\langle \int d\vec{v} \langle f_{0}(\vec{X}, |\mathbf{v}_{\parallel}|, \mu) \rangle \rangle} \right]$$

Localized sources:

- Krook operator, $\frac{df_1}{dt} = -\nu_{\rm K}(x)f_1$, to damp fluctuations close to the boundaries
- Heat source model (cmp. Grandgirard et al., PPCF '07)

$$\frac{\mathrm{d}f_1}{\mathrm{d}t} = \mathcal{S}_H = \mathcal{S}_0 \mathcal{S}_x \mathcal{S}_E$$

$$\mathcal{S}_E = \frac{2}{3} \frac{1}{p_{0\sigma}(x)} \left(\frac{v_{\parallel}^2 + \mu B_0}{T_{0\sigma}(x)/T_{0\sigma}(x_0)} - \frac{3}{2} \right) f_{0\sigma}$$

$$\mathcal{S}_x = \mathcal{S}_{x,in}(x) / \int \mathrm{d}^3 x \, \mathcal{S}_{x,in}(x) J(x, z)$$

$$\mathcal{S}_x = \mathcal{S}_{x,in}(x) / \int \mathrm{d}^3 x \, \mathcal{S}_{x,in}(x) J(x, z)$$

and floating boundary conditions



 $S_{x,in}(x)$

0.8

0.9

Magnetic geometry

- arbitrary flux-surface shapes can be considered as long as the metric $g = (g^{ij}) = (\nabla u^i \cdot \nabla u^j)$ is provided to compute expressions like $\frac{1}{B_0^2} (\mathbf{B}_0 \times \nabla \zeta) \cdot \nabla = \frac{1}{\mathcal{C}} \frac{g^{1i}g^{2j} g^{2i}g^{1j}}{\gamma_1} \partial_i \zeta \partial_j$
- simple choice: circular concentric flux surfaces



 others can be read in via interfaces to TRACER/GIST (field line tracer) and the equilibrium code CHEASE

Input: GENE Launcher

	4		GENE Launcher			_ O X
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Jobs =>	1	2	3	4	5	
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Global Gyrokinetic Simulation of Turbulence in ASDEX Upgrade



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Summary and outlook

Some outroductory remarks

Goal of this first lecture: Introduction to gyrokinetic theory and simulation

More info: Review by Brizard & Hahm, 2007 http://gene.rzg.mpg.de

Topic of next lecture:

Linear and nonlinear gyrokinetics "in action"