Discontinuous Galerkin methods, positivity, exponential reconstruction, and initial simulations of gyrokinetic turbulence in a model tokamak scrape-off-layer

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(with minor modifications after talk)

Summary / References

Gkeyll apparently is the first successful *continuum* gyrokinetic code doing turbulence on open field lines with sheath boundary conditions (XGC was only other code, PICbased GK):

E.L. Shi, G.W. Hammett, T. Stoltzfus-Dueck, A. Hakim, J. Plasma Physics (2017) http://dx.doi.org/10.1017/S002237781700037X

That was with straight field lines, LAPD-like case. First extension to a helical model of a tokamak SOL including bad-curvature drive, for NSTX-type parameters:

"Gyrokinetic Continuum Simulation of Turbulence in Open-Field-Line Plasmas", Eric L. Shi, Ph.D. Dissertation, Princeton University, (Arxiv, 2017). <u>https://arxiv.org/abs/1708.07283</u>

Collaborated with Q. Pan, who extended a version of GENE to full-F for open field line systems and did LAPD simulations: Q. Pan, D. Told, E. Shi, G. Hammett, F. Jenko (revised paper subm. to PoP, 2018)

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.

Stronger effect if consider smaller power: better confinement allows smaller size & capital cost at same fusion gain $Q(nT\tau_E)$.

Standard ITER 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 $nT\tau_{E, q_{95}, \beta_N, n/n_{Greenwald})$:

Capital Cost \$ ~ $R^2 \sim 1 / (H^{4.8} B^{3.4})$

ITER std H=1, steady-state $H\sim 1.6$ ARIES-AT $H\sim 1.5$ MIT ARC $H_{89}/2 \sim 1.4$

Comprehensive simulations, validated with experiments, can help make case for extrapolating improved H to reactors.

(Plots assumes cost $\propto R^2$ roughly. Includes constraint on *B* @ magnet with ARIES-AT 1.16 m blanket/shield, a/R=0.25, i.e. $B = B_{mag} (R-a-a_{BS})/R$. Neglects current drive issues.)

Hammett & Dorland, White Paper 2017, https://sites.google.com/site/usmfrstrategicdirections/view-whitepapers



Interesting Ideas To Improve Fusion

* New high-field superconductors (MIT). Dramatic reduction in size & cost (x1/5 ?)

* Liquid metal (lithium, tin) coatings/flows on walls or vapor shielding: (1) protects solid wall (2) absorbs 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 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 regimes (reverse magnetic shear / "hybrid"), methods to control ELMs, higher plasma shaping, advanced divertors.

* Tokamaks spontaneously spin: reduce turbulence & improve MHD stability. ITER spins more than previously expected? Up-down-asymmetric tokamaks/stellarators?

* New stellarator designs, room for further optimization: Hidden symmetry discovered after 35+ years of fusion research. Fixes disruptions, steady-state, density limit.

* More speculative concepts, but potentially big payoff: FRCs, RFPs, ...

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

Pedestal Temperature Has a Big Effect on Fusion Performance



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

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, non-Maxwellian full-F), atomic physics, non-axisymmetric RMP / stellarator coils, magnetic fluctuations near beta limit, stable sheath model...

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

Gkeyll using novel algorithms, has multiple spinoffs

Novel version of Discontinuous Galerkin algorithm, conserves energy for Hamiltonian system even with upwinding. High-order algorithms that reduce communication costs helpful for Exascale computers.

- 4 Main Versions / spinoffs (consolidating kinetic versions some):
- Gyrokinetic DG version for edge turbulence in fusion LAPD results: E. Shi, Hammett, Stoltzfus-Dueck. Hakim, J. Plasma Physics (2017), Shi et al. PoP 2015, Shi Ph.D. 2017.
- Vlasov/Poisson DG version for plasma thrusters (AFOSR/Virginia Tech) Cagas et al. Phys. Plasmas (2017)
- Vlasov/Maxwell DG version for solar wind turbulence (U. Maryland, NSF) J. TenBarge, Sherwood Inv. Talk (2017), J. Juno et al., JCP 2017, Shocks in Laser-Plasma Interaction: Pusztai et al., Arxiv (2017)
- Multi-moment multi-fluid (~extended MHD) finite-volume version, studying reconnection (Princeton Center for Heliophysics). Also coupled with OpenGGCM global magnetosphere code (UNH) J. Ng PoP 2015, L. Wang PoP 2015

Also, modeled Lithium Vapor Box ideas by adding evaporation/condensation b.c.s to finite-volume fluid version. Co-authors on Goldston et al. 2017 Nucl. Mat. & Energy

Gkeyll: First Continuum 5D Gyrokinetic Simulations of Turbulence in SOL with sheath model boundary conditions



XGC is only gyrokinetic turbulence code that can handle separatrix at present.

E. Shi Ph.D. 2017 LAPD: E. Shi, A. Hakim, T. Stolzfus-Dueck, J. Plasma Physics (2017)

x (m)

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(movie) 9

Gkeyll: First Continuum 5D Gyrokinetic Simulations of Turbulence in SOL with sheath model boundary conditions



Various simplifications at present, such as helical model of SOL (toroidal + vertical B field). XGC is only gyrokinetic turbulence code that can handle separatrix at present.

E. Shi Ph.D. 2017 LAPD: E. Shi, A. Hakim, T. Stolzfus-Dueck, J. Plasma Physics (2017)

1.35

x (m)

1.4

1.3

First Gkeyll Simulation of 3D+2v Gyrokinetic Turbulence in Scrape Off Layer (SOL).





 $\times 10^{17}$

8

6

4

2

Worried about difficulties in gyrokinetic-sheath interactions and other edge ٠

computation that drove h (working on

Present mod

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becial algorit arge amplitud o positivity e

an into & fixed several problems Now appears fairly robust 5.

eath) more general than simple

logical sheath, allows currents into and out of walls.

- Gyrokinetic extension of pioneering fluid work (Rogers & Ricci, Umansky, Friedman et al.) ٠
- Simple helical SOL at present (like Torpex, Helimak expts.), no separatrix, but have bad-٠ curvature drive, have done simulations of NSTX-like case. E. L. Shi, G. Hammett, T. Stoltzfus-Dueck, A. Hakim, JPP 2017

Toroidal case (left) vs. Slab case (right)



Clearly shows bad curvature enhances instability drive

Divertor heat flux broadens ~ theta ~ 1/B_pol



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



Larger amplitude & more intermittent blobs in far SOL

Figure 5.13: Electron density fluctuation statistics (top row) and potential fluctuation statistics (bottom row) computed near the z = 0 m plane for three cases with different magnetic field line incidence angle θ . The potential fluctuations are notably less intermittent than the density fluctuations. The shaded area indicates the region in which the source is concentrated.

Initially worried about complications in interactions between sheaths (10¹¹ Hz) & gyrokinetics (~10⁵ Hz)

- In a gyrokinetic code, don't want to directly resolve tiny Debye-scale sheath (~10⁻³ cm), evolves on extremely rapid time scale.
- "Logical sheath": adjust phi at boundary to reflect most electrons and let through just enough electrons to match ion flux, $j_{||} = 0$ (Parker, Procassini, Birdsall, Cohen 1993)
- Used in our 1D SOL ELM heat-pulse tests (Shi, Hakim, Hammett 2015), compares well with full PIC code, but how to interface with multi-dimensional GK?
- Eventually implemented gyrokinetic equivalent of sheath boundary conditions in early fluid edge simulations (Ricci, Rogers, GBS; Umansky, Friedman, BOUT++):
- Use GK Poisson eq. to determine potential everywhere in simulation, use jump between that at edge & $\phi = 0$ plates to determine what fraction of electrons to reflect. Allows currents to flow in/out walls, steady state gives usual $\phi_s \sim 3 T_e$.
- Tried to increase side wall potential to avoid sharp gradients with sheath potential, was like biasing system with a power supply, drove huge potential oscillations.
- Forgot collisions at first (because of previous ELM work), drives ultra-high frequencies
- Initially started with too much density near side walls, drove huge potentials.

Gyrokinetic Equations in a simple limit

For simplicity, consider long-wavelength full-F gyrokinetics, curvature drifts turned off, and time-independent dielectric coefficient $\varepsilon_{\perp 0}(x) = c^2/v_A^2 = c^2 4\pi \Sigma_s n_0(x) m/B^2$:

$$\frac{\partial}{\partial t}f(x,y,z,v_{||},\mu,t) + \frac{\partial}{\partial z}\left(v_{||}f\right) + \nabla \cdot \left(\vec{v}_E f\right) + \frac{\partial}{\partial v_{||}}\left(\frac{q}{m}E_{||}f\right) = C[f] + S$$

$$-\nabla_{\perp} \cdot (\epsilon_{\perp 0} \nabla_{\perp} \phi) = \sigma_{\rm gc} = \sum_{s} q \left(\frac{2\pi B}{m}\right) \int dv_{||} d\mu f$$

(guiding center charge + polarization charge = 0)

$$\vec{v}_E = \frac{1}{B}\hat{z} \times \nabla\phi$$

 $E_{||} = -\partial\phi/\partial z$

Can write this GK equation in Hamiltonian form with $H = \frac{1}{2}mv_{||}^2 + q\phi$

Model Sheath Boundary Conditions

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



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

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

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

Sheath-Model Boundary Conditions for Electrons



Figure: Illustration of sheath-model boundary condition. (a) Outgoing electrons with $v_{\parallel} > v_c = \sqrt{2e\Delta\phi/m} = 2$ are lost into the wall, where $\Delta\phi = \phi_{sh} - \phi_w$, ϕ_s is determined from the GK Poisson equation, and $\phi_w = 0$ for a grounded wall. (b) The rest of the outgoing particles $(0 < v_{\parallel} < v_c)$ are reflected back into the plasma.

Appear to be the first continuum gyrokinetic simulations of SOL turbulence

- There have been a few pioneering explorations in past, but they were not continued, apparently because of various numerical difficulties
 - Pioneering work with finite-difference TEMPEST code (LLNL, ~2006), focused on 4D axisymmetric neoclassical calc. Switched to finite-volume COGENT code with better conservation & numerical properties (not yet 5D).
 - COGENT doing pioneering work on full collision operator and 4th order accuracy on general mapped grids. Axisymmetric neoclassical at present.
 - "Use of the FEFI nonlocal gyrokinetic model is planned but a sheath model compatible with violent shear Alfvén dynamics in front of the divertor plate remains to be found." (Zweben, Scott, et al., 2009)
 "Comparison of scrape-off layer turbulence in Alcator C-Mod with three dimensional gyrofluid computations", PoP, http://dx.doi.org/10.1063/1.3191721
- Numerical challenges of edge:
 - Large amplitude fluctuations, need f>0 (sheath instabilities if f<0 ?)
 - Conservation properties (small charge imbalances drive large potentials)
 - Stable interaction of gyrokinetics w/ sheath
 - High frequency " Ω_H " mode / "Ampere cancellation problem"?
 - Complications, but not main roadblocks: Coordinate singularies, collisions, ...



• Left: Collisionless simulation, ϕ vs. time near simulation center, for a case with spatially uniform source. The potential is initially at a normal sheath level of ~3 T_e, but get huge, very-high-frequency oscillations after an ion connection time $L_{||}/v_{ti} \sim 0.7 ms$.

- Right: Collisions included, density vs. time. Normal sheath & turbulence level.
- Sheath potential confines most electrons. Essential to have some collisions to scatter some electrons over the sheath barrier.

Gkeyll Software Structure

- Gkeyll is a framework for kinetic and fluid plasma simulations.
- Core code in C++, with Lua scripting language on top, mpi parallelization, python for postprocessing & plots. Cmake and modern build system. Many modern packages: hdf5→adios, eigen, (PETSc), gsl, boost, blitz.
 - Core framework infrastructure created by A. Hakim (PPPL)
 - Similarities with BOUT++ and Dedalus frameworks
 - New grid-based algorithms and models can be rapidly added and tested
 - Individual simulations are written by users in Lua scripting language
 - Applications: fluid and kinetic magnetic reconnection, planetary and satellite magnetospheres, sheath physics
- E. Shi wrote a large amount of new C++ code for tokamak gyrokinetic version:
 - Eventually extended Gkeyll kinetic capabilities from 1D1V to 3D2V
 - Examples: 2D to 5D Serendipity basis functions, gyrokinetic equation solver, drag/diffusion collision operator, sheath-model BCs, positivity-adjustment algorithm,
 - Lua simulation scripts by themselves are 3000 lines.
- A. Hakim added domain-decomposition capabilities and gyrokinetic-Poissonequation solver for gyrokinetic version.

Why consider Discontinuous Galerkin (DG) Algorithms for (Gyro)kinetics at Exascale?

- Higher order methods do more FLOPS to extract more out of data, need fewer data points, reduce communications that can be a bottleneck on exascale computers.
- DG allows use of limiters / upwinding to avoid negative density overshoots, which can be a major problem in the edge region of fusion devices.
- We found a version of DG that can conserve energy exactly for Hamiltonian systems like gyrokinetics, even with upwinding / limiters (for continuous time)
- Novel version of DG conserves energy with exponential basis functions, exp(p(x))
- Locality of DG means it should scale well like other continuum codes (GENE continuum code has demonstrated excellent strong scaling to 262,000 cores)
- DG: 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 New ideas about using sparse quadratures in DG (~10x fewer grid points)
- 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

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



Standard finite-volume (FV) methods evolve cell averages + 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) (2) calculations local so easier to parallelize.

Hot topic in CFD & Applied Math: >1500 citations to Cockburn & Shu JCP/SIAM 1998

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.

Need at least piecewise linear DG for energy conservation (conserves energy even with upwinding). Standard Finite Volume methods do not conserve energy exactly for Vlasov-type problems (except Arakawa method, which can have artificial oscillations). Unlike Navier-Stokes fluid eqs., energy conservation in kinetic/Vlasov-Boltzmann equations is indirect, involving integration-by-parts and particle-field energy exchange.

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: $f(v,t) \approx f_h(v,t) = \sum_{i} f_k(t) b_k(v)$

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

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:

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

(This is the essence of DG, combined with efficient evaluation of integrals & Godunov approach to calculating upwind fluxes at discontinuous boundaries with an (approximate) Riemann solver.)

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 are ill-behaved at high v, can't integrate to $v = \infty$, where asymptotic behavior is Maxwellian (perhaps w/ higher "temperature"). Helps handle moderate collision frequencies of edge region.

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

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 $G = -\partial\Gamma/\partial v$

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

Standard energy conservation doesn't hold either.

Conservative Maxwellian-Weighted DG Basis Functions:

The trick for preserving conservation properties of DG with Maxwellianweighted 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

Collision Operator Benchmark

Compare Maxwellian-weighted and polynomial basis functions by solving the equation (Lenard-Bernstein collision operator)



Example Using Local Maxwellian Parameters



Figure: The local Maxwellian parameter calculation is applied to discretize a function including a non-monotonic bump to demonstrate the ability to handle strongly non-Maxwellian functions.

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:

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

 $(\kappa_t \ll 1. c_1 \text{ determined by constraint of no momentum injection.})$ 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 = $\int dv_{||}(1/2)mv_{||}^3 f$.

Maxwellian-weighted basis functions much more efficient



Figure: Relative error in heat flux calculation for cases of varying cell width, keeping $v_{\text{max}} = 8v_T$.

Future Work

- Have demonstrated feasibility/practicality of continuum gyrokinetic edge simulations, but more work needed for detailed comparisons with experiments:
- Better magnetic Geometry. 1st step: shaping in closed *or* open field lines, 2nd step: separatrix and X-point. Have ideas for dealing with challenges near X-point. (Dorf et al., worked on this with Cogent code in 2D.)
- Only have a simple Lenard-Bernstein collision operator at present. Need better operator for accuracy in collisional edge, to get thermal forces, perp. viscosity, etc. (Pan & Ernst recent work relevant: gyroaveraged full linearized collision operator including field-particle terms and FLR effects, in conservative self-adjoint form.)
- Super-time stepping or other implicit treatment for collisions, high-frequency Ω_H mode
- Better recycling models, atomic physics (charge exchange, ionization, radiation), want to study improved confinement with reduced recycling by lithium.
- Further improvement to sheath boundary conditions
- Compare w/ wider range experiments (LAPD, NSTX-U, Helimak, Cmod, MAST-U, ...)
- Algorithm development possibilities: Switching nodal DG to modal DG, faster for our form of equations, More robust positivity (almost finished), Maxwellian-weighted basis functions, Sparse grids

Summary

- Motivation: raising the pedestal can help fusion a lot, but simulating edge is hard.
- First successful *continuum* gyrokinetic code doing turbulence on open field lines with sheath boundary conditions (only other code: XGC, PIC GK) LAPD-like case with straight field lines:
 E.L. Shi, G.W. Hammett, T. Stoltzfus-Dueck, A. Hakim, J. Plasma Physics (2017) http://dx.doi.org/10.1017/S002237781700037X
- First extension to a helical model of a tokamak SOL including bad-curvature drive: "Gyrokinetic Continuum Simulation of Turbulence in Open-Field-Line Plasmas", Eric L. Shi, Ph.D. Dissertation, Princeton University, 2017. <u>https://arxiv.org/abs/1708.07283</u>
- Using model sheath boundary conditions that allow currents into & out of wall
- Algorithm development possibilities, higher order methods with reduced communication costs good for Exascale computer architectures.
 - Maxwellian-weighted basis functions
 - Sparse grids