Recent Results from the Gkeyll Discontinuous Galerkin Kinetic Code

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Gkeyll Overview

- Prototype code to explore advanced algorithms for continuum edge gyrokinetic simulation (e.g. edge plasma turbulence)
- Main code is written in C++ with Lua scripts to drive simulations
- DG algorithm (an extension of the work of Liu and Shu[1]) conserves energy exactly for general Hamiltonian systems and is stable in the L_2 norm of the distribution function f
  - Allow distribution function to be discontinuous
  - Hamiltonian must be in the continuous subset of space used for f

Goal

A robust code capable of running very quickly at coarse velocity space resolution while preserving all conservation laws of gyrokinetic/gyrofluid equations and giving fairly good results.

[1] J.-G. Liu and C.-W. Shu. "A High-Order Discontinuous Galerkin Method for 2D Incompressible Flows". In: *J. Comp. Phys.* 160.2 (2000), pp. 577 –596. ISSN: 0021-9991.

Recent Progress

- Studied ELM heat-pulse problem with gyrokinetics in a simplified scrape-off-layer geometry, Demonstrated good agreement with full PIC and Vlasov codes while being many orders of magnitude faster because gyrokinetics doesn't have to resolve the Debye length.
- Discovered and fixed subtle issues with our DG algorithm when including magnetic fluctuations, which had required very small time steps for stability at low $k_\perp \rho_s$.
- Extended Gkeyll's Poisson bracket solve capabilities to handle general Hamiltonian systems in $2x + 2v$ and $3x + 2v$ and performed initial simulations of $2x + 2v$ ETG turbulence

Discontinuous Galerkin Solutions

Discontinuous Galerkin schemes use discontinuous function spaces (usually made of polynomials) to represent the solution.

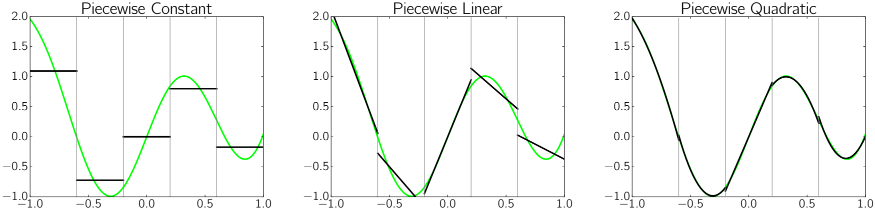


Figure: The best L_2 fit of $x^4 + \sin(5x)$ (green) using piecewise constant (left), linear (center), and quadratic (right) polynomials.

Hybrid Discontinuous/Continuous Galerkin Scheme

Introduce a phase-space mesh $\mathcal{T}$ with cells $K_j \in \mathcal{T}$, $j = 1, \ldots, N$ and introduce the following piecewise polynomial approximation space for the distribution function $f(t, \mathbf{z})$

$$\mathcal{V}_h^p = \{v : v|_K \in \mathbf{P}^p, \forall K \in \mathcal{T}\}$$

where $\mathbf{P}^p$ is (some) space of polynomials. To approximate the Hamiltonian, on the other hand, we introduce the space

$$\mathcal{W}_{0,h}^p = \mathcal{V}_h^p \cap C_0(\mathbf{Z})$$

Essentially, we allow the distribution function to be discontinuous, while requiring that the Hamiltonian is in the continuous subset of the space used for the distribution function

Discretization of the Evolution Equation

- Find f_h in the space of discontinuous piecewise polynomials such that for all basis functions ϕ_k, we have

$$f_h(x, y, v_\parallel, \mu, t) = \sum_k f_k(t)\phi_k(x, y, v_\parallel, \mu)$$

$$\int_{K_j} \mathcal{J}_h \phi_k \frac{\partial f_h}{\partial t} d\mathbf{z} = \int_{K_j} \mathcal{J}_h \nabla\phi_k \cdot \boldsymbol{\alpha}_h f_h d\mathbf{z} - \oint_{\partial K_j} \mathcal{J}_h \phi_k^- \mathbf{n} \cdot \boldsymbol{\alpha}_h \widehat{F}\, dS$$

- Here, $\widehat{F} = \widehat{F}(f_h^+, f_h^-)$ is the consistent numerical flux on surface ∂K_j and $\mathcal{J}_h$ has been taken to be time independent.
- The notation g^- (g^+) indicates that the function is evaluated just inside (outside) on the location on the surface ∂K_j.

Evolution Equation

The Poisson bracket operator is defined as

$$\{f, g\} = \frac{\partial f}{\partial z^i} \Pi^{ij} \frac{\partial g}{\partial z^j}.$$

We are interested in solving conservative equations of the form

$$\frac{\partial (\mathcal{J} f)}{\partial t} + \nabla \cdot (\mathcal{J} \boldsymbol{\alpha} f) = 0,$$

where ∇ is the phase-space gradient operator and $\boldsymbol{\alpha}$ is the phase space velocity vector whose components are defined as

$$\alpha_i = \dot{z}^i = \{z^i, H\} = \Pi^{ij} \frac{\partial H}{\partial z^j}.$$

ETG Test Problem Description

- Model problem involves curvature-driven ETG instabilities and turbulence in a local 2D (2x+2v) limit
- Simulation domain is a small box of size $\Delta R \times \Delta R$ on the outer midplane of a tokamak
- Axisymmetry in toroidal direction
- Parallel gradients of f are ignored
- Use set of coordinates $(x, y, v_{\|}, \mu)$, where
    - x is the radial coordinate
    - y is the vertical coordinate
- Goals are to reproduce linear growth rate of instability and produce 2D turbulent nonlinear saturation

Physical Parameters Based on Cyclone Base Case[2]

Symbol	Expression	Value
ΔR	$32\rho_s$	1.819×10^{-3} m
ρ_s	c_s/Ω_{ci}	5.683×10^{-5} m
B_0		1.91 T
a		0.4701 m
R_0		1.313 m
R	$R_0 + 0.5a$	1.548 m
L_T	R/10	0.1548 m
n_0		4.992×10^{19} m^{-3}
$T_{i0} = T_{e0}$		2.072 keV

[2] A. M. Dimits et al. "Comparisons and physics basis of tokamak transport models and turbulence simulations". In: *Phys. Plasmas* 7.3 (2000), pp. 969–983.

Test Problem Equations

$$H_s = \frac{1}{2} m_s v_\parallel^2 + \mu B + q_s \phi$$

$$\mu = \frac{m v_\perp^2}{2B}$$

$$\Omega_s = \frac{q_s B}{m_s}$$

$$\mathbf{\Pi} = \begin{pmatrix} 0 & -\frac{1}{q_s B_\parallel^*} & 0 & 0 \\ \frac{1}{q_s B_\parallel^*} & 0 & \frac{B_y^*}{m_s B_\parallel^*} & 0 \\ 0 & -\frac{B_y^*}{m_s B_\parallel^*} & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

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

$$\mathbf{B}^* = \mathbf{B} + \frac{B v_\parallel}{\Omega_s} \nabla \times \mathbf{b} \Rightarrow \mathbf{B} - \frac{m_s v_\parallel}{q_s x} \hat{y}$$

$$B_\parallel^* = \mathbf{b} \cdot \mathbf{B}^* \Rightarrow B$$

$$\mathcal{J} = m_s B_\parallel^* \Rightarrow m_s B$$

Potential solved for by assuming adiabatic ions and using quasineutraility:

$$-n_{i0}(x_0) \frac{q_i}{T_{i0}} \phi(x, y, t) = n_e(x, y, t) - n_{i0}(x),$$

where $n_{i0}(x_0)$ is the value of the ion density in the center of the simulation

Grid Resolution and Boundary Conditions

- Initial simulations represent solution using piecewise linear basis functions
  - Plan to investigate use of higher-order polynomials, Maxwellian-weighted basis functions in future
- Boundary conditions:
  - Zero flux BCs in $v_{\|}$ and μ on f
  - Periodic BCs in x and y on fluctuating components of ϕ and f

Coordinate	Number of Cells	Minimum	Maximum
x	N_x	R	$R + \Delta R$
y	N_y	$-\Delta R/2$	$\Delta R/2$
$v_{\|}$	$N_{v_{\|}}$	-$\min\left(4, 2.5\sqrt{\frac{N_{v_{\|}}}{4}}\right) v_{Te}$	$\min\left(4, 2.5\sqrt{\frac{N_{v_{\|}}}{4}}\right) v_{Te}$
μ	$N_\mu = N_{v_{\|}}/2$	0	$\min\left(16, 4\sqrt{\frac{N_\mu}{2}}\right) \frac{m v_{Te}^2}{2B_0}$

Initial Conditions

$$f_e(x, y, v_\parallel, \mu) = \frac{n_e(x, y)}{[2\pi T_{e0}(x)/m]^{3/2}} \exp\left[-\frac{m v_\parallel^2}{2 T_{e0}(x)}\right] \exp\left[-\frac{\mu B(x)}{T_{e0}(x)}\right]$$

$$T_{e0}(x, y) = T_{e0}\left(1 - \frac{x - R}{L_T}\right)$$

$$n_{i0}(x) = n_0$$

$$T_{i0}(x) = T_{i0}$$

For linear simulations, we initialize a perturbation with a single k_y mode:

$$n_e(x, y) = n_0\left[1 + 10^{-3}\frac{\rho_e}{L_T}\cos(k_{y,min} y)\right].$$

For nonlinear simulations, a spectrum of k_x modes are included:

$$n_e(x, y) = n_0\left\{1 + 10^{-2}\frac{\rho_e}{L_T}\cos(k_{y,min} y)\exp\left[\frac{(x - x_0)^2}{2\sigma^2}\right]\right\}, \quad \sigma = \Delta R/4.$$

Linear Dispersion Relation for ITG/ETG in Local ($k_\parallel = 0$) Toroidal Limit

The dispersion relation for the system can be derived as[3]

$$
\begin{aligned}
-n_{0a}\frac{q_a\phi}{T_a} &= -n_{0s}\frac{q_s\phi}{T_s}\int d^3v\, F_0 \frac{\omega-\omega_*^T}{\omega-\omega_{dv}} \\
&= -n_{0s}\frac{q_s\phi}{T_s}\left[R_0\left(\frac{\omega}{\omega_d}\right)+\frac{R}{L_n}R_1\left(\frac{\omega}{\omega_d}\right)+\frac{R}{L_T}R_2\left(\frac{\omega}{\omega_d}\right)\right],
\end{aligned}
$$

where $\omega_*^T = \omega_*[1+(L_n/L_T)(v_\parallel^2/2v_t^2+\mu B/v_t^2-3/2)]$, $\omega_{dv} = \omega_d(v_\parallel^2+\mu B)/v_t^2$, $\omega_d = k_y\rho_e v_t/R$.

Here, the subscript a refers to the adiabatic species and the subscript s refers to the kinetic species.

[3] M. A. Beer and G. W. Hammett. "Toroidal gyrofluid equations for simulations of tokamak turbulence". In: *Phys. Plasmas* 3.11 (1996), pp. 4046–4064.

Linear Dispersion Relation for ITG/ETG in Local ($k_\parallel = 0$) Toroidal Limit

Neglecting FLR effects, the three parts of the ion response function can be written in terms of the plasma dispersion function[4]:

$$R_0(x) = 1 - \frac{x}{2} Z^2 \left(\sqrt{\frac{x}{2}} \right)$$

$$R_1(x) = \frac{1}{2} Z^2 \left(\sqrt{\frac{x}{2}} \right)$$

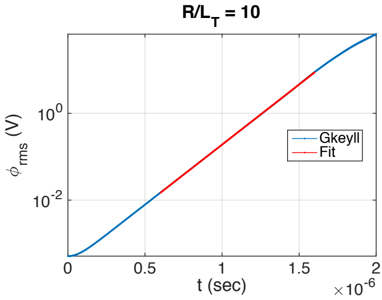
$$R_2(x) = \left(\frac{x}{2} - \frac{1}{2} \right) Z^2 \left(\sqrt{\frac{x}{2}} \right) + \sqrt{\frac{x}{2}} Z \left(\sqrt{\frac{x}{2}} \right).$$

Using $n_{0a} = n_{0s}$, and $q_a/q_s = -1$, the dispersion relation is

$$0 = D(\omega) = R_0 \left(\frac{\omega}{\omega_d} \right) + \frac{R}{L_n} R_1 \left(\frac{\omega}{\omega_d} \right) + \frac{R}{L_T} R_2 \left(\frac{\omega}{\omega_d} \right) + \frac{T_s}{T_a}.$$

[4] H. Biglari, P. H. Diamond, and M. N. Rosenbluth. "Toroidal ion pressure gradient driven drift instabilities and transport revisited". In: *Phys. Fluids B* 1.1 (1989), pp. 109–118.

Linear Growth Rate Tests



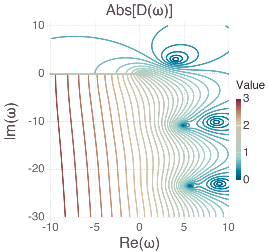


Figure: A linear growth rate for the ETG instability can be extracted from the ϕ_{rms} vs. t plot and compared with the exact value.

For $R/L_n = 0$ using $N_x = 4$, $N_y = 8$, $N_{v_\parallel} = 16$, and $N_\mu = 8$:

R/L_T	$\gamma_{sim}/\gamma_{exact}$
20	1.045
10	1.095
5	1.435

Linear Growth Rate: Convergence

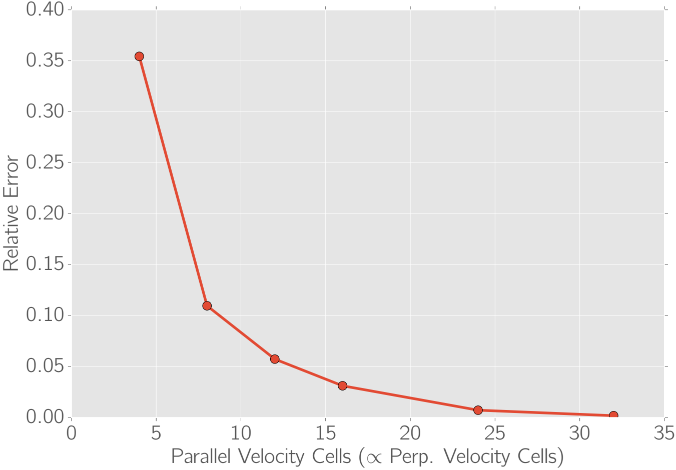


Figure: Convergence of numerical linear growth rate for $R/L_T = 20$ as the number of cells in $v_\parallel$ and μ is increased. $N_\mu = N_{v_\parallel}/2$. Convergence is expected to improve greatly when Maxwellian-weighted basis functions are implemented.

Nonlinear Turbulent Saturation

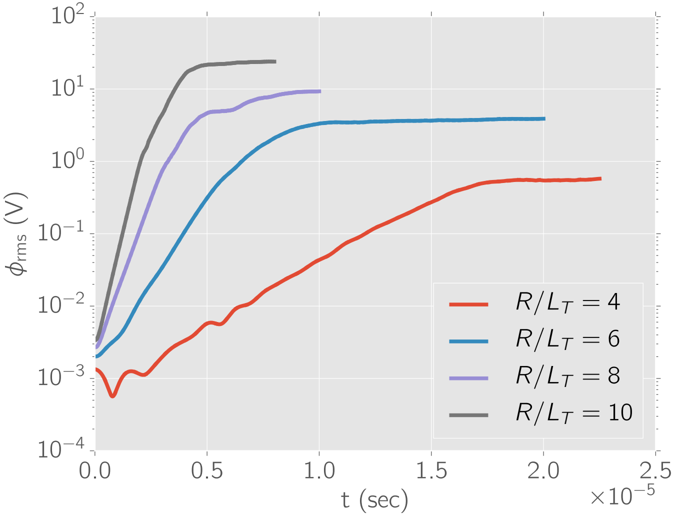


Figure: Plot of ϕ_{rms} vs t for simulations performed at various R/L_T values using $N_X = 8$, $N_Y = 8$, $N_{v_\parallel} = 4$, $N_\mu = 2$.

Nonlinear Turbulent Saturation ($R/L_T = 8$)

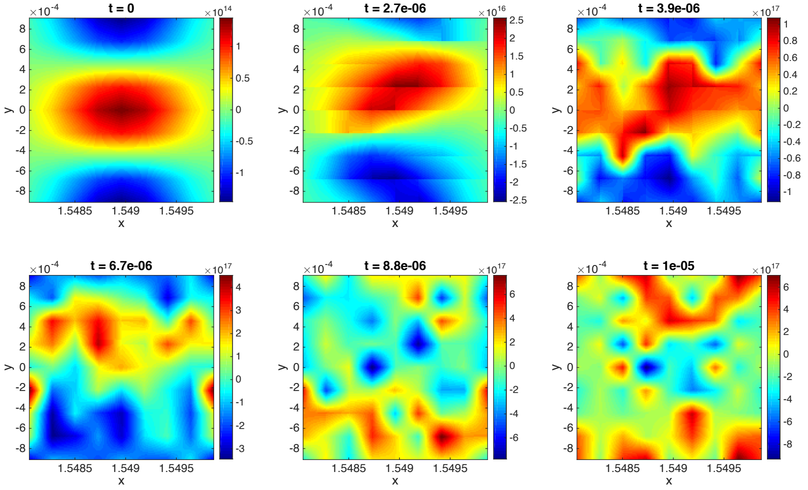


Figure: Plot of $n_e - n_{e0}$ at various times. $N_X = 8$, $N_Y = 8$, $N_{v_\parallel} = 4$, $N_\mu = 2$.

Simplest Alfvén Wave in Gyrokinetics

Electromagnetic fluctuations have been challenging for some formulations of gyrokinetics

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

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

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

After linearization and taking the limit $\omega \gg k_\| v_{te}$, we have

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

where $\hat{\beta}_e = (\beta_e/2)(m_i/m_e)$. The electrostatic case $A_\| = 0$ corresponds to the $\beta_e \to 0$ limit, in which there is a Ω_H mode that is even faster than electrons, for $k_\perp \ll 1$:

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

It would seem that including a finite beta term should be numerically easier, as at low $k_\perp$ the fastest wave would be no faster than the Alfvén wave.

Handling the $\partial A_\parallel/\partial t$ term

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

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

$$\left(k_\perp^2 + C_n \frac{\mu_0 q_e^2}{m_e}\int dp_\parallel\, f_e\right) A_\parallel = C_j \mu_0 \frac{q_e}{m_e^2}\int dp_\parallel\, f_e p_\parallel$$

"Ampere Cancellation Problem": the ratio of the first to the second term is very small, $k_\perp^2 \rho_s^2/\hat{\beta}_e \approx 10^{-5}$, for $k_\perp \rho_s = 0.01$ and $\hat{\beta}_e = 10$ (1% plasma beta). C_n and C_j represent small errors (for the exact system both should be exactly 1.0). After linearizing and taking $\omega \gg k_\parallel v_{te}$, we get

$$\omega^2 = \frac{k_\parallel^2 v_A^2}{C_n + k_\perp^2 \rho_s^2/\hat{\beta}_e}\left[1 + (C_n - C_j)\frac{\hat{\beta}_e}{k_\perp^2 \rho_s^2}\right]$$

Note that if $C_n = C_j = 1$, this reduces to the Alfvén wave dispersion relation on the previous slide. However, if $C_n - C_j \neq 0$, then there will be large errors for modes with $k_\perp^2 \rho_s^2 \ll 1$.

Gkeyll can reproduce the Alfvén wave dispersion relation

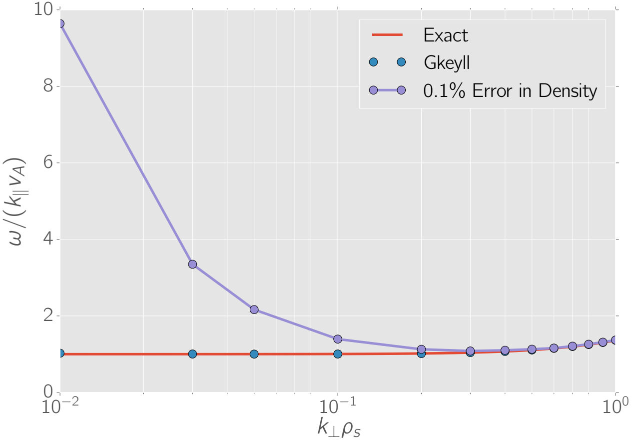


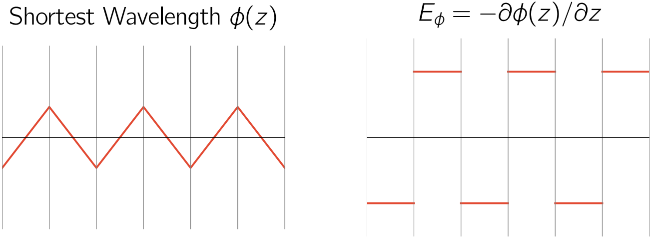
Figure: Frequency for shear Alfvén waves with $\beta_e = 1\%$. The simulation results from Gkeyll agree with the exact result to at least two significant figures. The purple curve is the result if there are just 0.1% errors in the C_n term in the modified Ampere's law.

Magnetic Fluctuations in DG

In the MHD limit, we need

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

but there is no way for a *continuous* $A_{\parallel}(z)$ to offset the discontinuous $\partial\phi/\partial z$. To achieve energy conservation, our DG algorithm requires H (and thus ϕ and $A_{\parallel}$) to be in a continuous subspace of f.



This results in $A_{\parallel} = 0$ (as if $\beta = 0$) and a very small time step is required to resolve this grid-scale mode ($\Delta t < k_{\parallel,\max} v_{te}/(k_{\perp,\min}\rho_s)$).

Magnetic Fluctuations in DG

- We resolve this issue by projecting $\phi(z)$ onto a C_1 subspace so ϕ and $\partial\phi/\partial z$ are continuous (ϕ must be at least piecewise parabolic in this case). This allows a continuous $A_\parallel(z,t)$ to better approximate the ideal MHD condition $E_\parallel \approx 0 = -\partial\phi/\partial z - \partial A_\parallel/\partial t$.
- In order to conserve energy, the projection operator must be self-adjoint.
- We have found a local self-adjoint smoothing operator that allows Gkeyll to reproduce the correct frequency of the Alfvén wave even at very low $k_\perp \rho_s$ with a normal time step

Conclusions

- Demonstrated ability to handle magnetic fluctuations in an efficient way
- For initial ETG simulations, we are able to observe linear growth rates that converge to the correct values
  - Nonlinear runs look qualitatively reasonable and reach turbulent saturated states
- Future plans:
  - Implement Maxwellian-weighted basis functions in μ and $v_\parallel$
  - Solve Poisson equation for potential in $2x + 2v$ and $3x + 2v$ simulations
  - Add support for more complicated geometries e.g. non-rectangular and non-uniform meshes
  - Run tests with a third spatial dimension $(3x + 2v)$