Nonlinear Fokker-Planck-like collisions in discontinuous Galerkin full-f kinetics

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Need a model for collisions in Gkeyll's kinetic solvers

Vlasov-Maxwell:

$$\frac{\partial f_s}{\partial t} + \nabla_{\mathbf{z}} \cdot \boldsymbol{\alpha} f_s = C[f_s] + S_s \qquad \boldsymbol{\alpha} = (\mathbf{v}, q_s(\mathbf{E} + \mathbf{v} \times \mathbf{B})/m_s)$$

collision term

See → P3.007 A. Hakim → P3.012 J. Juno
→ P3.011 V. Skoutnev → P3.013 J. TenBarge

Long wave length full-f gyrokinetics:

$$\frac{\partial \mathcal{J} f_s}{\partial t} + \boldsymbol{\nabla} \cdot \mathcal{J} \dot{\mathbf{R}} f_s + \frac{\partial}{\partial v_\parallel} \mathcal{J} \dot{v}_\parallel f_s = \mathcal{J} C[f_s] + \mathcal{J} S_s$$

See → P3.006 T. Bernard → P3.007 A. Hakim
→ P3.008 N. Mandell → P3.010 G. Hammett

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Use a Fokker-Planck-like model of collisions

Recall the (Rosenbluth) Fokker-Planck operator:

$$C[f_s] = -\frac{\partial}{\partial v_i}\left(\langle \Delta v_i \rangle_s f_s\right) + \frac{1}{2}\frac{\partial^2}{\partial v_i v_j}\left(\langle \Delta v_i \Delta v_j \rangle_s f_s\right)$$

For now consider the Dougherty limit

$$\langle \Delta v_i \rangle_s = -\nu_{ss}\left(v_i - u_{s,i}\right) - \sum_{r \neq s} \nu_{sr}\left(v_i - u_{sr,i}\right)$$

$$\langle \Delta v_i \Delta v_j \rangle_s = 2\nu_{ss} v_{t,s}^2 \delta_{ij} + \sum_{r \neq s} 2\nu_{sr} v_{t,sr}^2 \delta_{ij}$$

The operator remains nonlinear and full-f given that (in 1D)

$$M_{0s} u_s = M_{1s}$$

$$M_{0s} v_{ts}^2 = M_{2s} - M_{1s} u_s$$

where $M_{ks} = \int_{-\infty}^{\infty} v^k f_s(x, v, t)\, \mathrm{d}v$

u_{sr} and $v_{t,sr}^2$ defined later.

Self-collisions are conservative + have an H-theorem

Dougherty like-particle collisions conserve particles, momentum and energy.

Momentum conservation, for example, follows from (assume $\nu_{ss} \neq \nu_{ss}(v)$)

$$\begin{aligned}\int_{-\infty}^{\infty} vC[f_s] &= \int_{-\infty}^{\infty} \nu_{ss} v \frac{\partial}{\partial v}\left[(v-u_s)\, f_s + v_{t,s}^2 \frac{\partial f_s}{\partial v}\right] \mathrm{d}v, \\ &= \left\{\nu_{ss} v \left[(v-u_s)\, f_s + v_{t,s}^2 \frac{\partial f_s}{\partial v}\right] - \nu_{ss} v_{t,s}^2 f_s\right\}_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \nu_{ss}\,(v-u_s)\, f_s \,\mathrm{d}v, \\ &= -\nu_{ss}\,(M_{1s} - u_s M_{0s}) = 0\end{aligned}$$

One can also show that this (self-collisions) operator is self-adjoint and has an H-theorem[1]:

$$\frac{\partial \mathcal{S}}{\partial t} \geq 0$$

where $\mathcal{S}$ is the entropy.

[1]Hakim, Francisquez, Juno, Hammett (2019), *Conservative Discontinuous Galerkin Schemes for Nonlinear Fokker-Planck Collision Operators*. arXiv:1903.08062.

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Variety of multi-species Dougherty collisions exist

$$C[f_s, f_r] = \nu_{sr} \frac{\partial}{\partial v} \left[(v - u_{sr}) f_s + v_{t,sr}^2 \frac{\partial f_s}{\partial v} \right],$$

- $u_{sr} = [m_r n_r / (m_s n_s)] u_r$ used to study universal instability[2].
  $v_{t,sr} = v_{t,s}$
- $u_{sr} = [\nu_{rs} m_r / (\nu_{sr} m_s)] u_s$ used to study ion acoustic waves[3].
  $v_{t,sr} = v_{t,s}$
- $u_{sr} = u_s$ used to study drift waves with varying collisionality[4].
  $v_{t,sr} = v_{t,s}$
- $u_{ei} = u_i$ used in simulations of LAPD and NSTX[5].
  $v_{t,ei}^2 = v_{t,e}^2 + (u_i - u_e)^2$

[2]Ong, et. al. PoP 4 (1970).
[3]Ong, et. al. PoP 7 (1973).
[4]Jorge, et. al. PRL 121 (2018).
[5]Pan, et. al. PoP 25 (2018).
Shi, et. al. PoP 26 (2019).

Instead compute u_{sr} & $v_{t,sr}^2$ as done for BGK operator

Greene[6] combined conservation with momentum and energy relaxation rates[7] (for distributions near Maxwellians) for the operator $C[f_s, f_r] = \nu_{sr}\left(f_{M,sr} - f_s\right)$

The cross-species thermal speed, for example, is

$$v_{t,ie}^2 = \frac{1}{m_i + m_e}\left[m_e\left(v_{t,e}^2 + v_{t,i}^2\right) + \beta\left(m_e v_{t,e}^2 - m_i v_{t,e}^2\right) + \frac{1-\beta^2}{6} m_e\left(u_e - u_i\right)^2\right] - \frac{(1+\beta)^2}{12}\frac{m_i - m_e}{m_i + m_e}\left(u_e - u_i\right)^2$$

$\beta > -1$ is arbitrary.

Note that at $\beta = 1$ and large relative flows, negative cross-temperature is possible.

[6]Greene, Phys. Fluids 16 (1973).

[7]Morse, Phys. Fluids 6 (1963).

Demand conservation + relaxation rates[7] $\Longrightarrow$ u_{sr} & $v_{t,sr}^2$

conservation

$$\sum_{\substack{s \\ r\neq s}} \int_{-\infty}^{\infty} m_s v\, \nu_{sr} \frac{\partial}{\partial v}\left[(v-u_{sr})\, f_s + v_{t,sr}^2 \frac{\partial f_s}{\partial v}\right] \mathrm{d}v = 0$$

$$\sum_{\substack{s \\ r\neq s}} \int_{-\infty}^{\infty} \frac{1}{2} m_s v^2\, \nu_{sr} \frac{\partial}{\partial v}\left[(v-u_{sr})\, f_s + v_{t,sr}^2 \frac{\partial f_s}{\partial v}\right] \mathrm{d}v = 0$$

relaxation rates
(for near-Maxwellians)

$$\frac{\partial}{\partial t} m_s M_{1s} = m_s \nu_{sr} \delta_s \left(1+\beta\right)\left(M_{1r} - M_{1s}\right)$$

$$\frac{\partial}{\partial t} \frac{1}{2} m_s v_{t,s}^2 M_{0s} = \frac{m_s \nu_{sr}}{m_s + m_r} \delta_s \frac{1+\beta}{2} M_{0s} \left[m_r v_{t,r}^2 - m_s v_{t,s}^2 + m_r \left(u_r - u_s\right)^2\right]$$

$$\beta > -1 \qquad \delta_s^2 = \frac{m_r n_r \nu_{rs}}{m_s n_s \nu_{sr}}$$

This is a linear system for the unknowns u_{sr}, $v_{t,sr}^2$, u_{rs} and $v_{t,rs}^2$.

[7]Morse, Phys. Fluids 6 (1963).

Demand conservation + relaxation rates[7] $\Longrightarrow u_{sr}$ & $v_{t,sr}^2$

For the Dougherty operator these cross-velocities and cross-temperatures are

$$u_{sr} = u_s - \delta_s \frac{1+\beta}{2}\left(u_s - u_r\right)$$

$$v_{t,sr}^2 = v_{t,s}^2 + \frac{\delta_s}{2}\frac{1+\beta}{1+\frac{m_s}{m_r}}\left[v_{t,r}^2 - \frac{m_s}{m_r}v_{t,s}^2 + \left(u_s - u_r\right)^2\right]$$

As $\left(u_s - u_r\right)^2$ increases, there is no risk of negative temperature (compare with BGK case on slide 6)

[7]Morse, Phys. Fluids 6 (1963).

Multi-species Dougherty collisions are conservative

With this choice of u_{sr} and $v_{t,sr}^2$ the operator

$$C[f_s, f_r] = \nu_{sr} \frac{\partial}{\partial v} \left[(v - u_{sr}) f_s + v_{t,sr}^2 \frac{\partial f_s}{\partial v} \right],$$

is conservative by construction.

Interested in δf ? the linearized form of this operator is also conservative

H-theorem of multi-species Dougherty collisions proven for special cases

$$C[f_s, f_r] = \nu_{sr} \frac{\partial}{\partial v} \left[\underbrace{(v - u_{sr})\, f_s + v_{t,sr}^2 \frac{\partial f_s}{\partial v}}_{F_{sr}} \right],$$

One can show the entropy $\mathcal{S}$ satisfies

$$\frac{\partial \mathcal{S}}{\partial t} = \sum_{\substack{s \\ r \neq s}} \frac{\nu_{sr}}{v_{t,sr}^2} \int_{-\infty}^{\infty} \frac{1}{f_s} \left[F_{sr}^2 - F_{sr} \cdot (v - u_{sr})\, f_s \right] \mathrm{d}v$$

Although we have not shown this is in general ≥ 0, we can prove:

- $\dot{\mathcal{S}} \geq 0$ if $f_{s,r}$ are Maxwellian.
- $-\sum_{\substack{s \\ r \neq s}} \frac{\nu_{sr}}{v_{t,sr}^2} \int_{-\infty}^{\infty} F_{sr} \cdot (v - u_{sr})\, \mathrm{d}v \geq 0$ for arbitrary $f_{s,r}$ when $\begin{cases} u_s = u_r, \ \delta_s = 1, \ \beta \leq 1 \\ T_s = T_r, \ \beta \leq 0 \end{cases}$ and a range of δ_s.

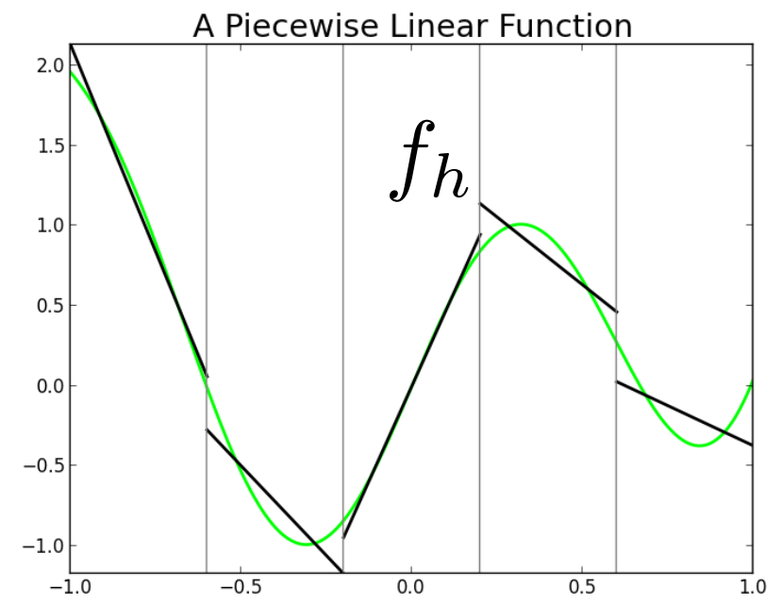
Discontinuous Galerkin operator uses 3 key methods[1]

Seek discrete solutions with the modal representation

$$f_h = \sum_k f_k \psi_k$$

e.g. for 1x2v, piecewise linear

$$\psi_k \in \sqrt{\frac{3}{8}} \left\{ \frac{1}{\sqrt{3}}, x, v_x, v_y, \sqrt{3} x v_x, \sqrt{3} x v_y, \sqrt{3} v_x v_y, 3 x v_x v_y \right\}$$



1. **Weak equalities:** In the interval I, weak equality of two functions is defined as

$$f \doteq g \quad \Longleftrightarrow \quad \int_I (f - g)\, \psi_k \, \mathrm{d}x = 0$$

e.g. given $M_0,\ M_1$ compute the flow velocity via $u M_0 \doteq M_1$

$$\Rightarrow \sum_m u_m \int_I M_0 \psi_k \psi_m \, \mathrm{d}x = \int_I M_1 \psi_k \, \mathrm{d}x$$

Invert this linear system to get the u_m expansion coefficients.

[1]Hakim, Francisquez, Juno, Hammett (2019), *Conservative Discontinuous Galerkin Schemes for Nonlinear Fokker-Planck Collision Operators*. arXiv:1903.08062.

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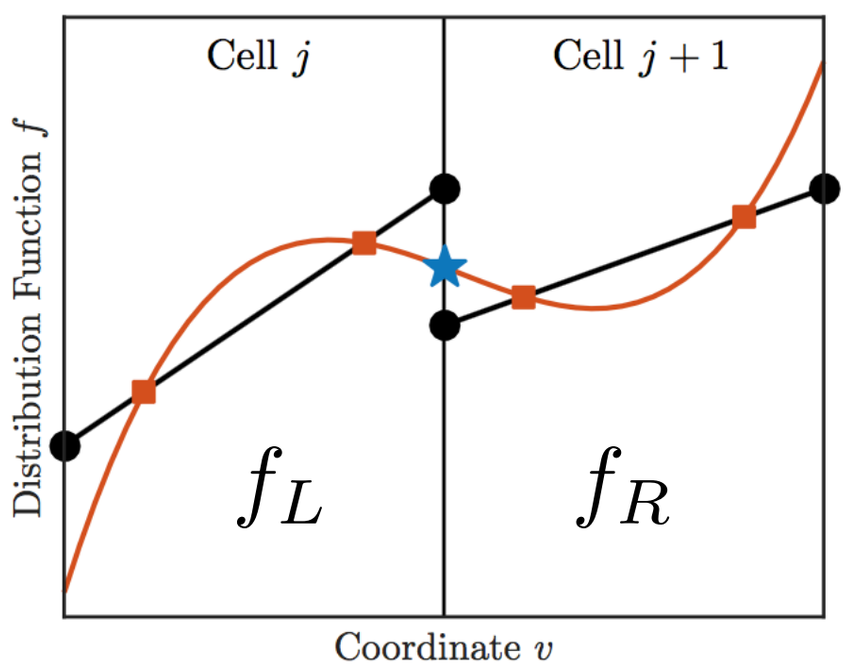
Discontinuous Galerkin operator uses 3 key methods

2. **Recovery DG:** After 2 integrations by parts our scheme is

$$\int_{\Omega_{i,j}} \psi_k \frac{\partial f_h}{\partial t}\,\mathrm{d}x\,\mathrm{d}v = \int_{x_{i-1/2}}^{x_{i+1/2}} \left\{ \psi_k \left[(v-u)\, f_h + v_t^2 \frac{\partial f_h}{\partial v} \right] - \frac{\partial \psi_k}{\partial v} v_t^2 f_h \right\}_{v_{j-1/2}}^{v_{j+1/2}} \mathrm{d}x$$
$$- \int_{\Omega_{i,j}} \left[\frac{\partial \psi_k}{\partial v} (v-u)\, f_h - \frac{\partial^2 \psi_k}{\partial v^2} v_t^2 f_h \right] \mathrm{d}x\,\mathrm{d}v$$

Need derivatives of f_h at cell boundaries, but f_h is discontinuous there.

Consider two adjacent cells



E. Shi, PhD thesis 2017.

Given adjacent solutions, f_L and f_R, of order p, construct the recovery polynomial

$$\hat{f} = \sum_{m=0}^{2p-1} \hat{f}_m x^m \quad \text{with} \quad \begin{aligned} \hat{f} &\doteq f_L \\ \hat{f} &\doteq f_R \end{aligned}$$

which is continuous at cell boundaries. It can be replaced for f_h in the discrete scheme.

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Discontinuous Galerkin operator uses 3 key methods

3. **Boundary corrections:** In a finite velocity space, momentum conservation is seen by setting $\psi_k = v$ in our discrete scheme and summing over all the cells:

$$\sum_{i,j} \int_{\Omega_{i,j}} v \frac{\partial f_h}{\partial t} \, \mathrm{d}x \, \mathrm{d}v = \sum_{i,j} \int_{x_{i-1/2}}^{x_{i+1/2}} \left\{ v \left[(v-u) \, f_h + v_t^2 \frac{\partial \hat{f}_h}{\partial v} \right] - v_t^2 \hat{f}_h \right\}_{v_{j-1/2}}^{v_{j+1/2}} \mathrm{d}x - \sum_{i,j} \int_{\Omega_{i,j}} (v-u) \, f_h \, \mathrm{d}x \, \mathrm{d}v$$

use a continuous-across-cells form of this flux and zero-flux BC.

$$\sum_i \int_{x_{i-1/2}}^{x_{i+1/2}} \left(\left\{ -v_t^2 \hat{f}_h \right\}_{v_{\min}}^{v_{\max}} \mathrm{d}x - M_1 + u M_0 \right) \mathrm{d}x = 0$$

Incorporating energy conservation reveals one must compute u & v_t^2 via

$$\left\{ v_t^2 \hat{f}_h \right\}_{v_{\min}}^{v_{\max}} + M_1 - u M_0 \doteq 0$$

$$\left\{ v v_t^2 \hat{f}_h \right\}_{v_{\min}}^{v_{\max}} + M_2 - u M_1 - v_t^2 M_0 \doteq 0$$

a linear system inverted in every cell.

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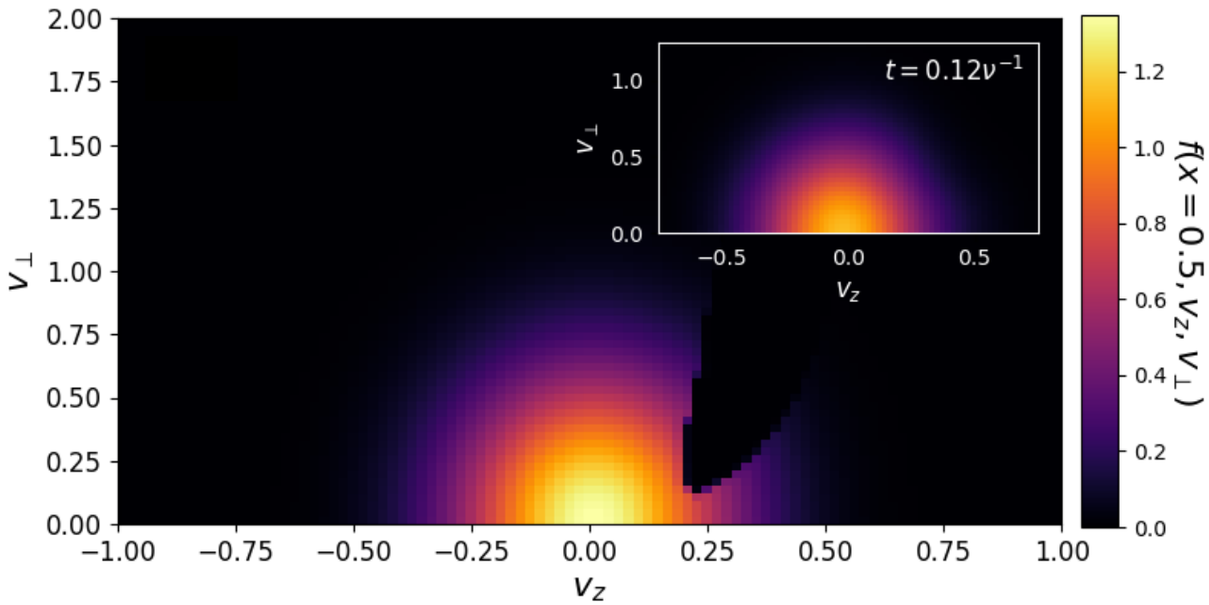
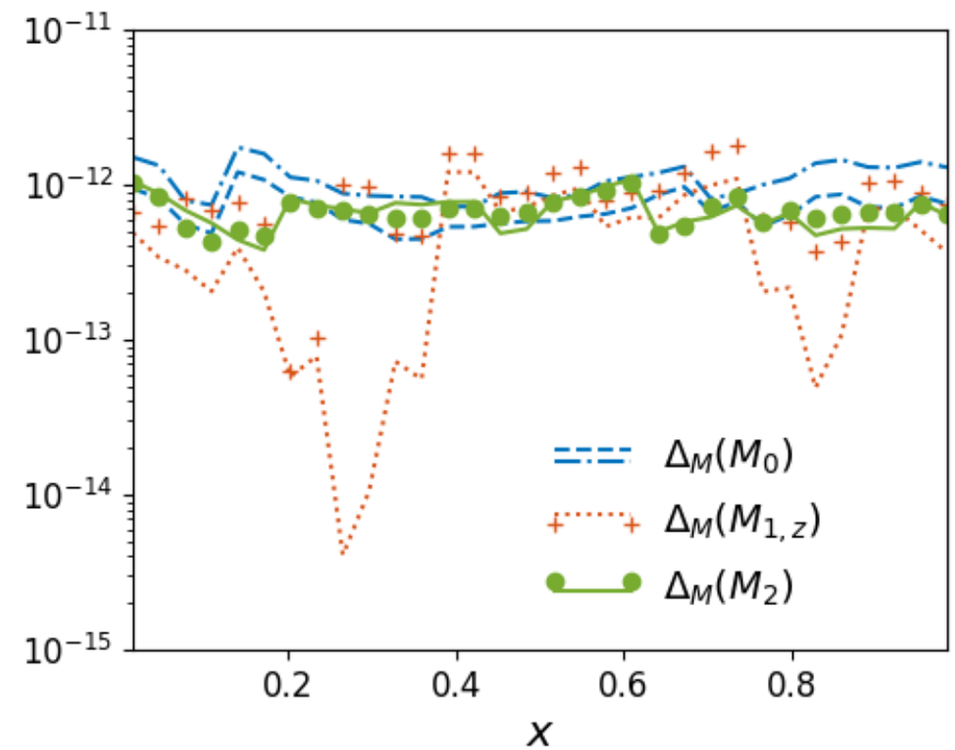
Benchmarks show exact discrete conservation

1X3V loss cone relaxation with piecewise linear basis and 16x32³ cells.





$$\Delta_M(M_j) = \left| \frac{M_j(t_{\text{final}}) - M_{j,M}}{M_j(t=0)} \right|$$

Number, momentum and energy density errors are machine precision.

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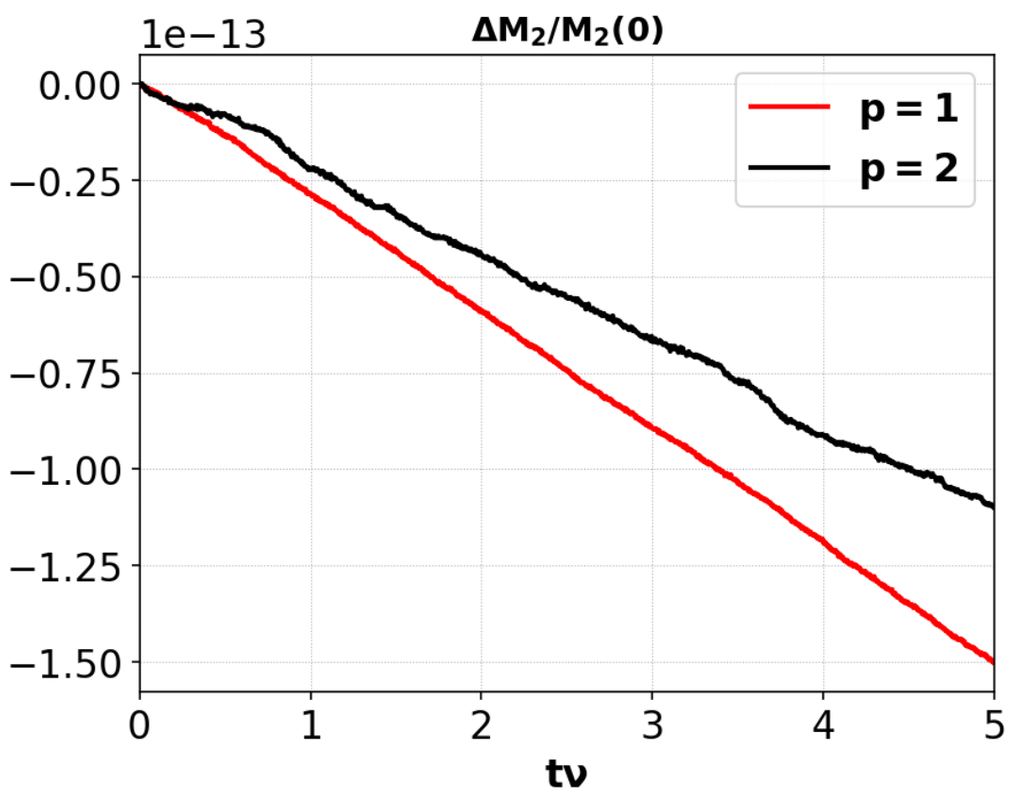
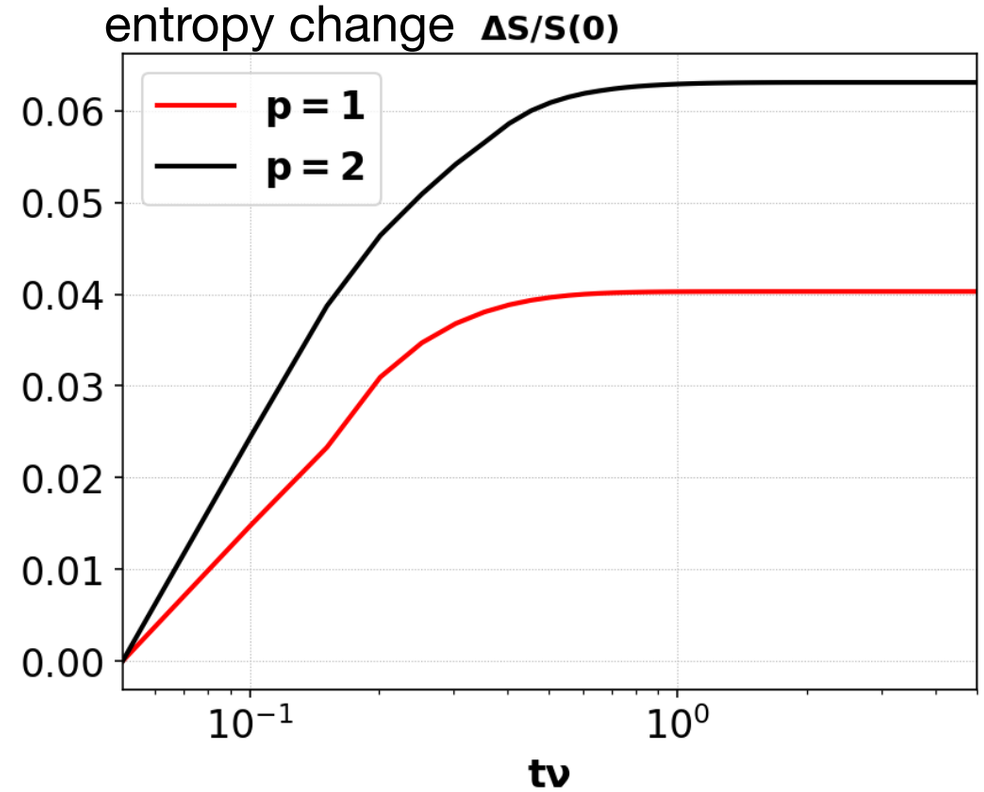
Benchmarks show exact discrete conservation[1]

1X1V uniform distribution $f(x,v) = \begin{cases} 1/(2v_0) & |v| < v_0 \\ 0 & |v| \geq v_0 \end{cases}$ with 16 (piecewise linear) or 8 (piecewise quadratic) cells.





Energy density errors remain machine precision, and entropy monotonically increases. **This is also true for piecewise linear basis!**

[1]Hakim, Francisquez, Juno, Hammett (2019), *Conservative Discontinuous Galerkin Schemes for Nonlinear Fokker-Planck Collision Operators*. arXiv:1903.08062.

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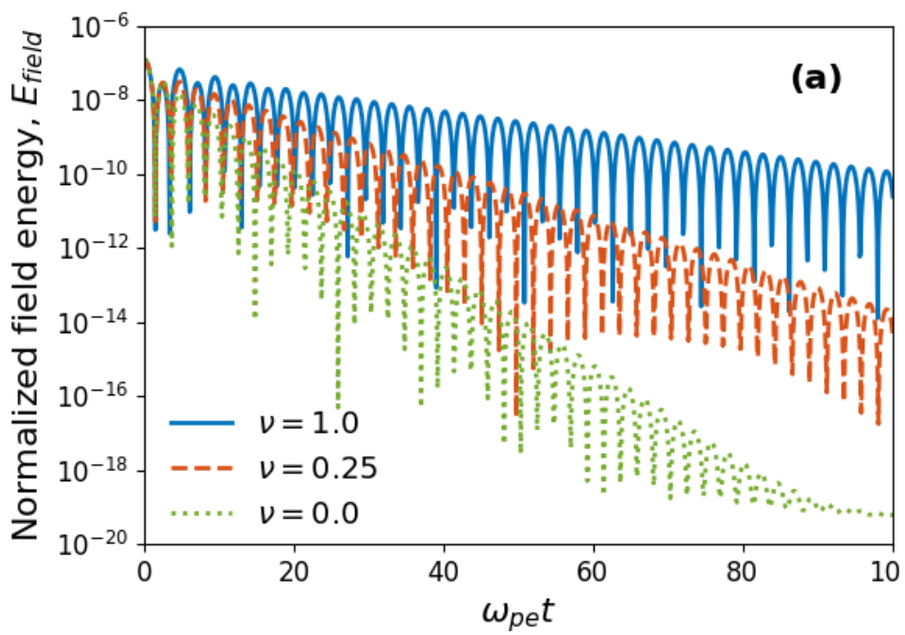
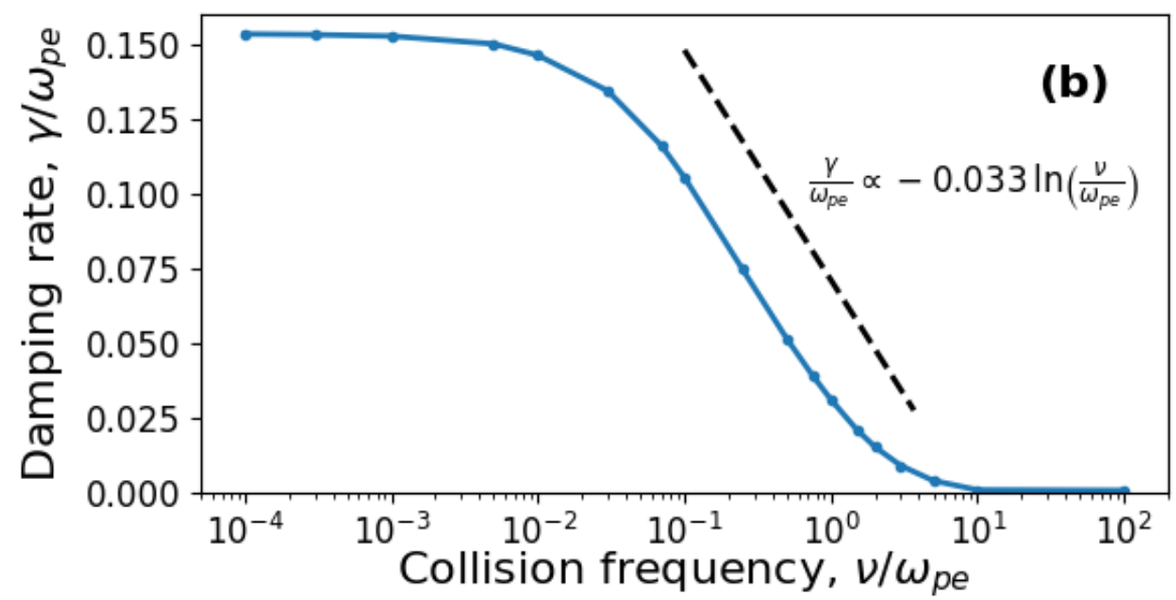
Vlasov-Dougherty solver validated with analytics

Here we show Landau damping of a Langmuir wave initialized with

$$f_e(x,v,0) = \frac{1}{\sqrt{2\pi v_{te}^2}} \exp\left[-v^2/\left(2v_{te}^2\right)\right]\left[1+\alpha\cos\left(kx\right)\right]$$





Scaling of damping rate with collisionality follows analytic theory[8].

→ see P3.013 J. TenBarge: magnetic pumping benchmark.

[8]Anderson, PoP 14 (2007).

[1]Hakim, Francisquez, Juno, Hammett (2019), *Conservative Discontinuous Galerkin Schemes for Nonlinear Fokker-Planck Collision Operators*. arXiv:1903.08062.

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Discrete multi-species Dougherty has similar subtleties

In finite velocity space there is no closed form solution for u_{sr} , $v^2_{t,sr}$.

One must include velocity boundary corrections and invert the linear system

$$
\begin{aligned}
&m_e\nu_{ei}M_{0e}u_{ei} - m_e\nu_{ei}v^2_{tei}\left\{f_e\right\}_{v_{e,min}}^{v_{e,max}} \\
&+m_i\nu_{ie}M_{0i}u_{ie} - m_i\nu_{ie}v^2_{tie}\left\{f_i\right\}_{v_{i,min}}^{v_{i,max}} \doteq m_e\nu_{ei}M_{1e} + m_i\nu_{ie}M_{1i}.
\end{aligned}
$$

$$
\begin{aligned}
&m_e\nu_{ei}M_{1e}u_{ei} + m_e\nu_{ei}\left(d_vM_{0e} - \left\{vf_e\right\}_{v_{e,min}}^{v_{e,max}}\right)v^2_{tei} \\
&+m_i\nu_{ie}M_{1i}u_{ie} + m_i\nu_{ie}\left(d_vM_{0i} - \left\{vf_i\right\}_{v_{i,min}}^{v_{i,max}}\right)v^2_{tie} \doteq m_e\nu_{ei}M_{2e} + m_i\nu_{ie}M_{2i}.
\end{aligned}
$$

$$
\begin{aligned}
&m_e\nu_{ei}M_{0e}u_{ei} - m_e\nu_{ei}v^2_{tei}\left\{f_e\right\}_{v_{e,min}}^{v_{e,max}} \\
&-m_i\nu_{ie}M_{0i}u_{ie} + m_i\nu_{ie}v^2_{tie}\left\{f_i\right\}_{v_{i,min}}^{v_{i,max}} \doteq m_e\nu_{ei}M_{1e} - m_i\nu_{ie}M_{1i} - m_e\nu_{ei}\delta_e\left(1+\beta\right)\left(M_{1e} - M_{1i}\right)
\end{aligned}
$$

$$
\begin{aligned}
&m_e\nu_{ei}\left(M_{1e} - u_eM_{0e}\right)u_{ei} + m_e\nu_{ei}\left(d_vM_{0e} - \left\{\left(v-u_e\right)f_e\right\}_{v_{e,min}}^{v_{e,max}}\right)v^2_{tei} \\
&- m_i\nu_{ie}\left(M_{1i} - u_iM_{0i}\right)u_{ie,i} - m_i\nu_{ie}\left(d_vM_{0i} - \left\{\left(v-u_i\right)f_i\right\}_{v_{i,min}}^{v_{i,max}}\right)v^2_{tie} \\
&\doteq m_e\nu_{ei}\left(M_{2e} - u_eM_{1e}\right) - m_i\nu_{ie}\left(M_{2i} - u_iM_{1i}\right) \\
&\quad - m_e\nu_{ei}\delta_e\frac{1+\beta}{m_i+m_e}\left[m_e\left(M_{2e} - u_eM_{1e}\right) - m_i\left(M_{2i} - u_iM_{1i}\right) + \frac{1}{2}\left(m_e - m_i\right)\left(u_e - u_i\right)\left(M_{1e} - M_{1i}\right)\right]
\end{aligned}
$$

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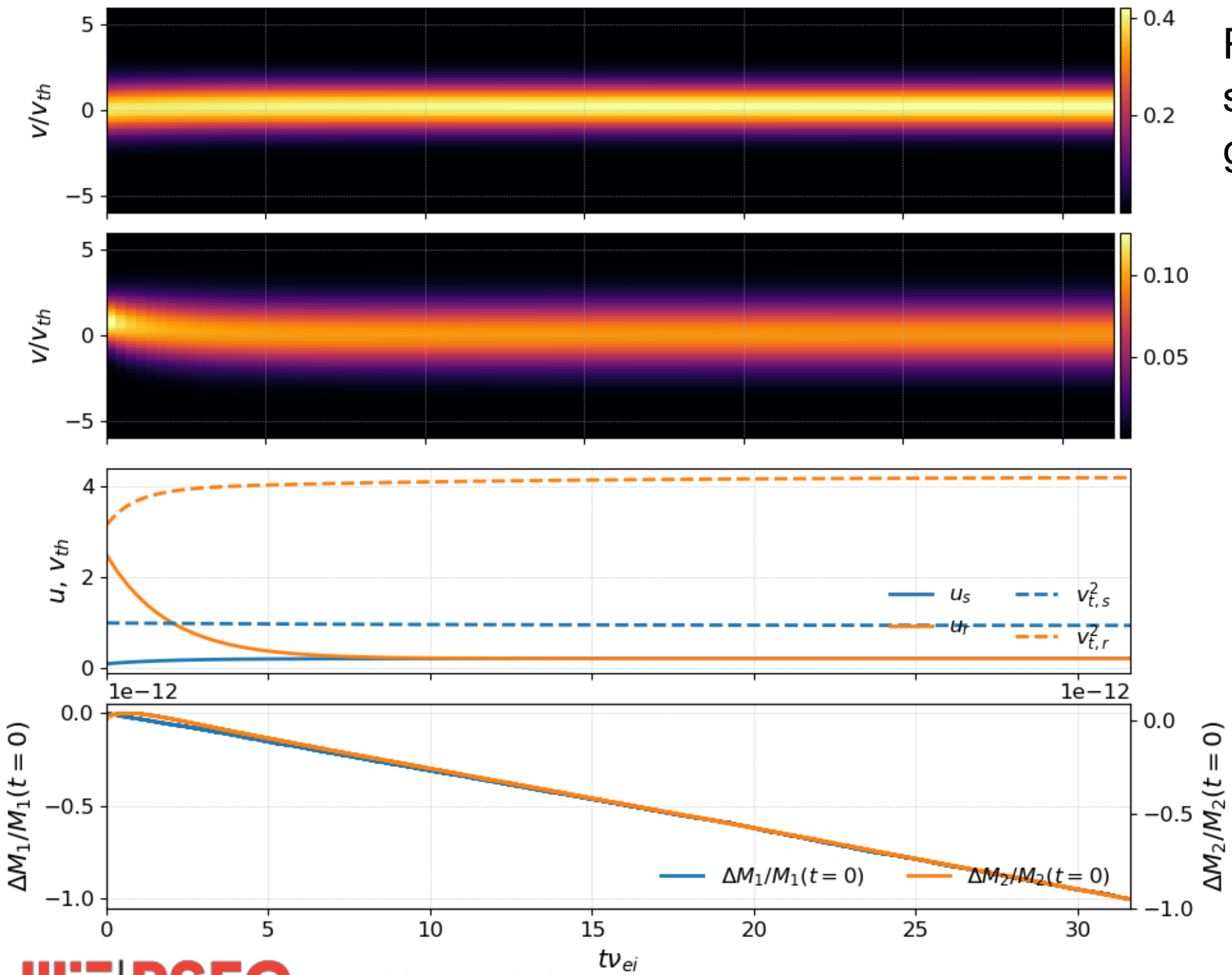
Relaxation between two species remains conservative



Relaxation of two species on a 32^2 grid.

$$\frac{u_r}{u_s} = 25 \quad \frac{m_r}{m_s} = 20$$

$$\frac{T_r}{T_s} = 2$$

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Thanks for reading! Here's a recap:

- Conservative implementation of self-species and multi-species collisions with a Dougherty operator is accomplished in Gkeyll's discontinuous Galerkin scheme.
- A suite of weak equalities, recovery DG, and boundary corrections needed to achieve desired properties.
- Benchmarks and comparison with analytic theory show a satisfactory implementation of self-species collisions.
- Work is ongoing further exploring the H-theorem and physical properties of the multi-species Dougherty collision operator.