PPPL seminar, July 8, 2020

Learning long division: weak operations in a discontinuous Galerkin kinetic solver

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Extended edge turbulence modeling capabilities with GDB[1,2]

At Dartmouth College we[1,2] developed a code, GDB, to study tokamak edge turbulence, transport and profile evolution using 3D drift-ordered two-fluid Braginskii equations:

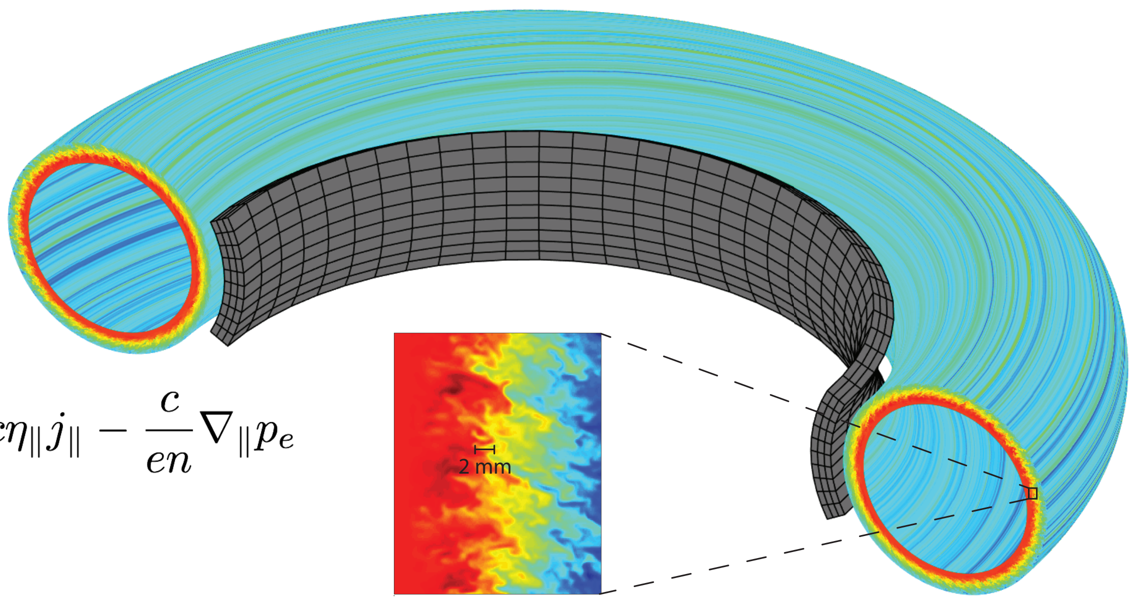
$$\frac{d^i n}{dt} = \frac{2cn}{B}\left[C(\phi) - \frac{C(p_e)}{en}\right] + \frac{1}{e}\nabla_\parallel j_\parallel - n\nabla_\parallel v_{\parallel i}$$

$$\nabla_\perp \cdot \frac{nc}{B\omega_{ci}}\frac{d^i}{dt}\left(\nabla_\perp\phi + \frac{\nabla_\perp p_i}{en}\right) = -\frac{2c}{eB}C(p_e+p_i) + \frac{1}{e}\nabla_\parallel j_\parallel - \frac{1}{3m_i\omega_{ci}}C(G)$$

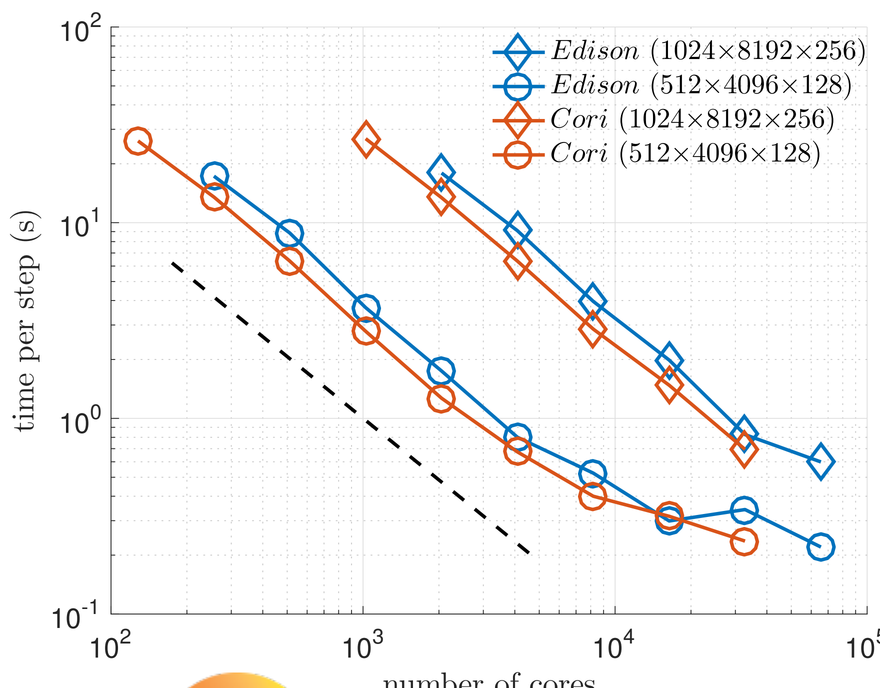
$$\frac{d^i v_{\parallel i}}{dt} = -\frac{1}{m_i n}\left[\nabla_\parallel(p_e+p_i) + \frac{2}{3}\nabla_\parallel G\right] + \frac{2T_i}{m_i\omega_{ci}}C(v_{\parallel i})$$

$$\frac{\partial}{\partial t}\left(1 - d_e\nabla_\perp^2\right)\psi = \frac{m_e c}{e}\left\{\frac{c}{B}\left[\phi, \frac{j_\parallel}{en}\right] + v_{\parallel e}\nabla_\parallel\left(\frac{j_\parallel}{en}\right)\right\} + c\nabla_\parallel\phi + c\eta_\parallel j_\parallel - \frac{c}{en}\nabla_\parallel p_e$$

$$\frac{d^s T_s}{dt} = \frac{2T_s}{3n}\left[\frac{d^s n}{dt} + \frac{1}{T_s}\nabla_\parallel \kappa_\parallel^s \nabla_\parallel T_s - \frac{5cn}{eB}C_{(T_s)}\right]$$



GDB numerics:
- Centered finite-differences.
- Flux-coordinate independent approach.
- Subcycle parabolic terms, i.e. $\propto \nabla_\parallel \kappa_\parallel^s \nabla_\parallel T_s$
- Multigrid for field equations, e.g. $\psi - d_e^2\nabla_\perp^2\psi = \Psi$
- 3D (asynchronous) MPI domain decomposition.



[1]B. Zhu, M. Francisquez, B. N. Rogers, Comp. Phys. Comm. 232 (2018) 46–58.
[2]M. Francisquez, B. Zhu, B. N. Rogers, Comp. Phys. Comm. 236 (2019) 104–117.

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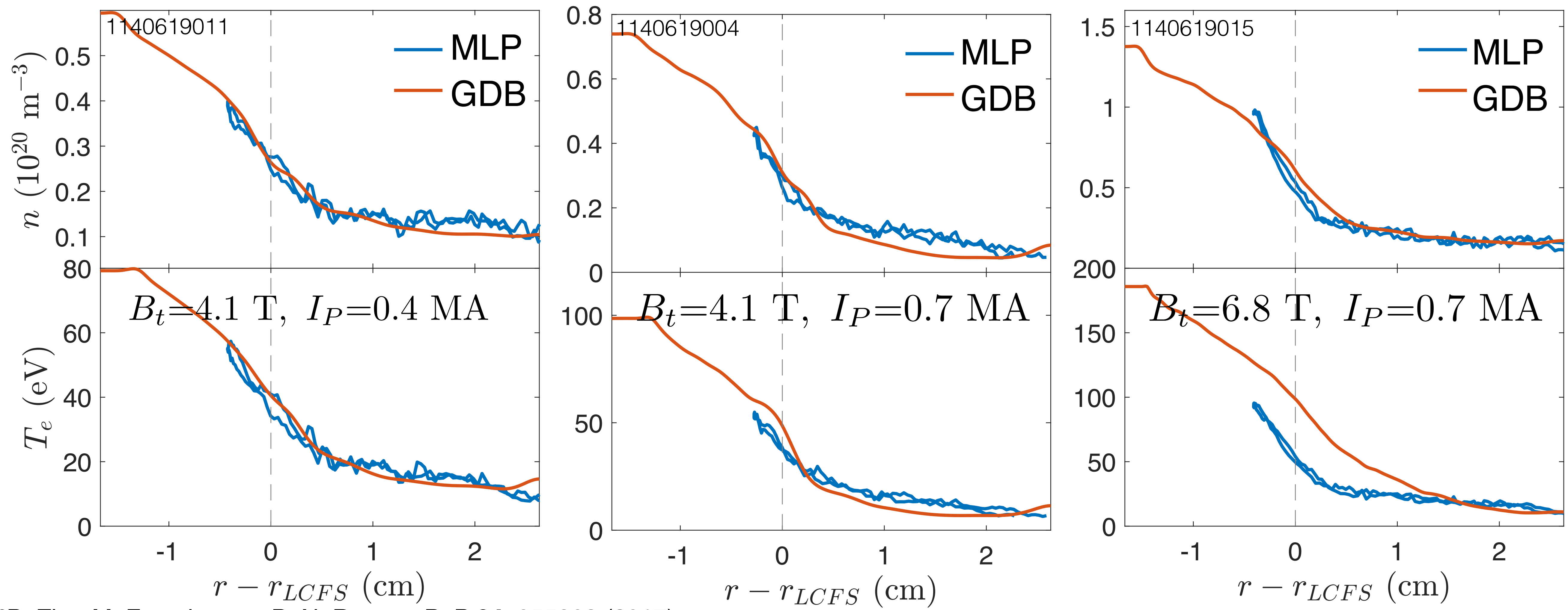
Used GDB to study $E\times B$ profile evolution & compare with C-Mod

1. Term-by-term analysis of the simulations
   $\Rightarrow$ develop criteria setting $E\times B$ profiles when n or T_s increases[3,4].

2. Examined turbulence statistics[4] & compared SOL profiles against mirror Langmuir probe (MLP) data from Alcator C-Mod:



[3]B. Zhu, M. Francisquez, B. N. Rogers, PoP **24**, 055903 (2017).
[4]M. Francisquez, B. Zhu, B. N. Rogers, NF **57** (2017) 116049.

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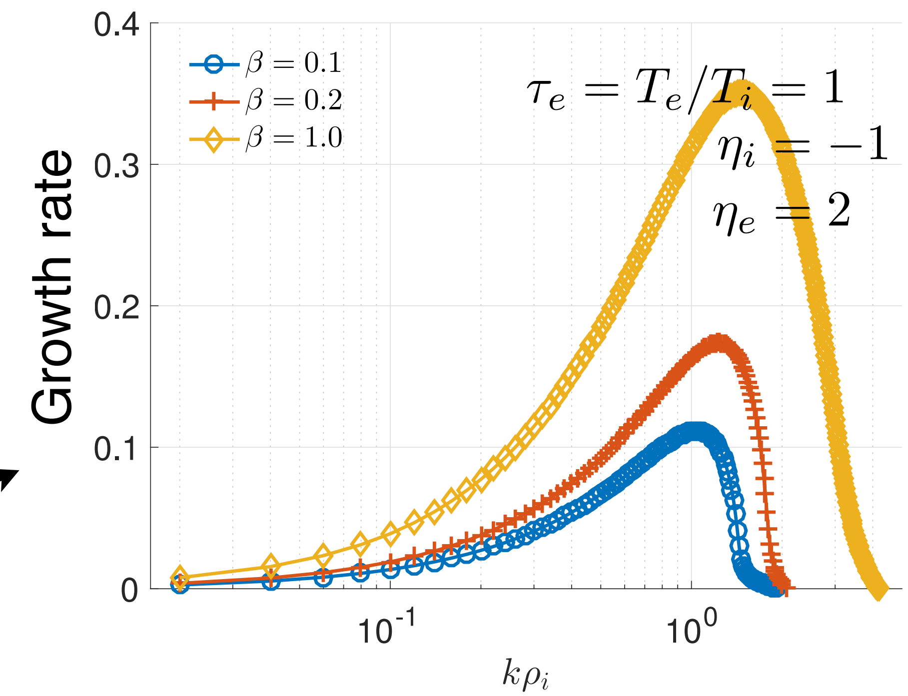
Beyond fluids, an interesting exercise in gyrokinetics: the $\delta B_{\|}$ universal mode

[5,6] Gyrokinetic study of slab universal modes with $\delta B_{\|}$

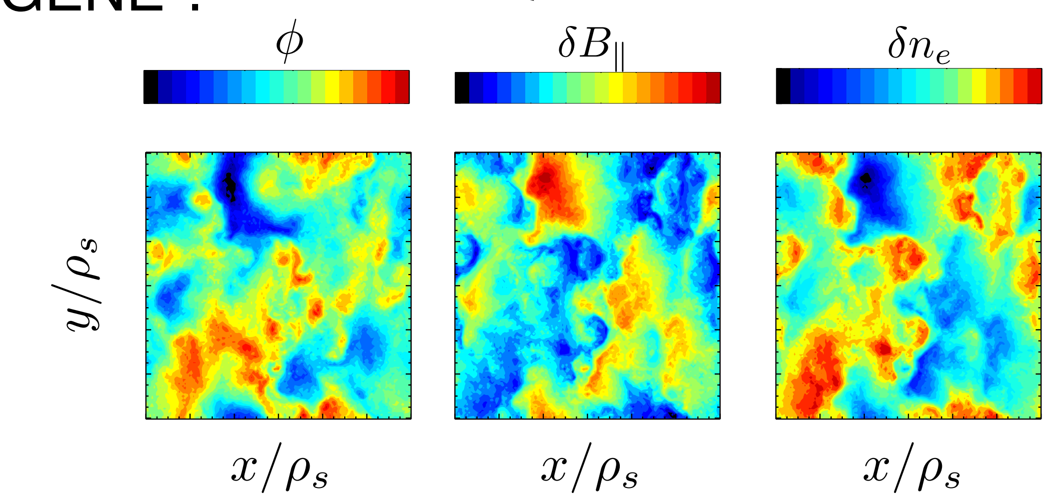
- No field-aligned variation ($k_{\|} = 0$).
- Gradient in density (L_n) and/or temperatures ($\eta_{i,e}$).
- Equilibrium pressure balance $\beta/(2L_p) + 1/L_B = 0$



1. Obtain a linear dispersion relation
   $\Rightarrow$ Instability requires $\eta_i < 0$ or $\eta_e < 0$.

2. Instability vanishes if $\eta_s \geq 0$ and $\beta/(2L_p) + 1/L_B = 0$
   $\Rightarrow$ Equilibrium pressure balance makes the GDC instability[7] unlikely.

3. Performed some preliminary nonlinear simulations with GENE[6].



4. There's been more recent study of the GDC and $\delta B_{\|}$ universal instabilities, this time for pair plasmas[8,9].

[5]B. N. Rogers, B. Zhu, M. Francisquez, PoP 25, 052115 (2018).
[6]M. Francisquez, APS DPP invited talk (2018).
[7]M. J. Pueschel, et al., PoP 22 (2015).
[8]M. J. Pueschel, et al., submitted to PoP (2020).
[9]B. Zhu, M. Francisquez, B. N. Rogers, submitted to PoP (2020).

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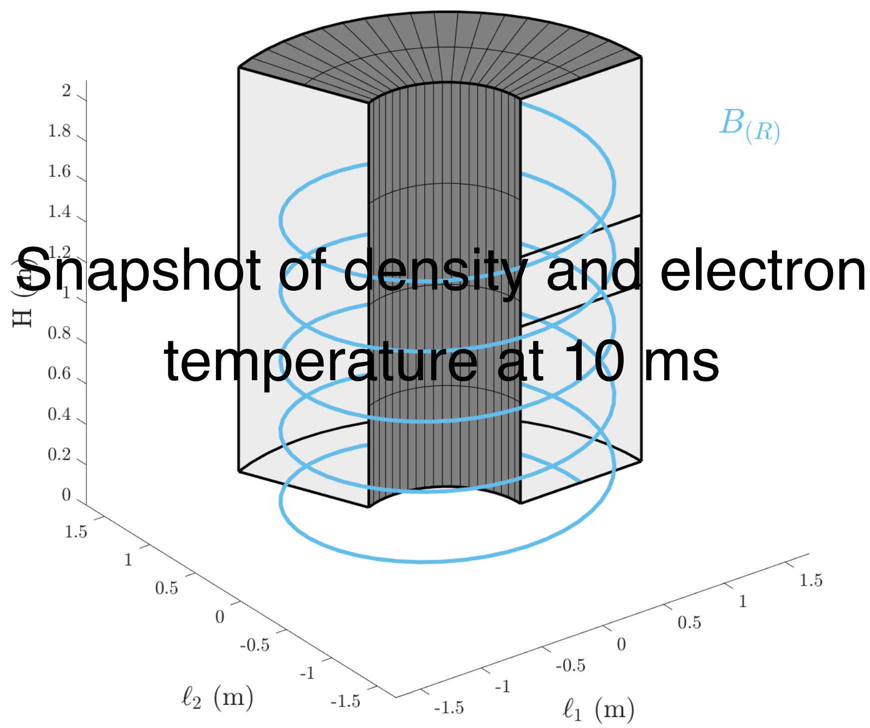
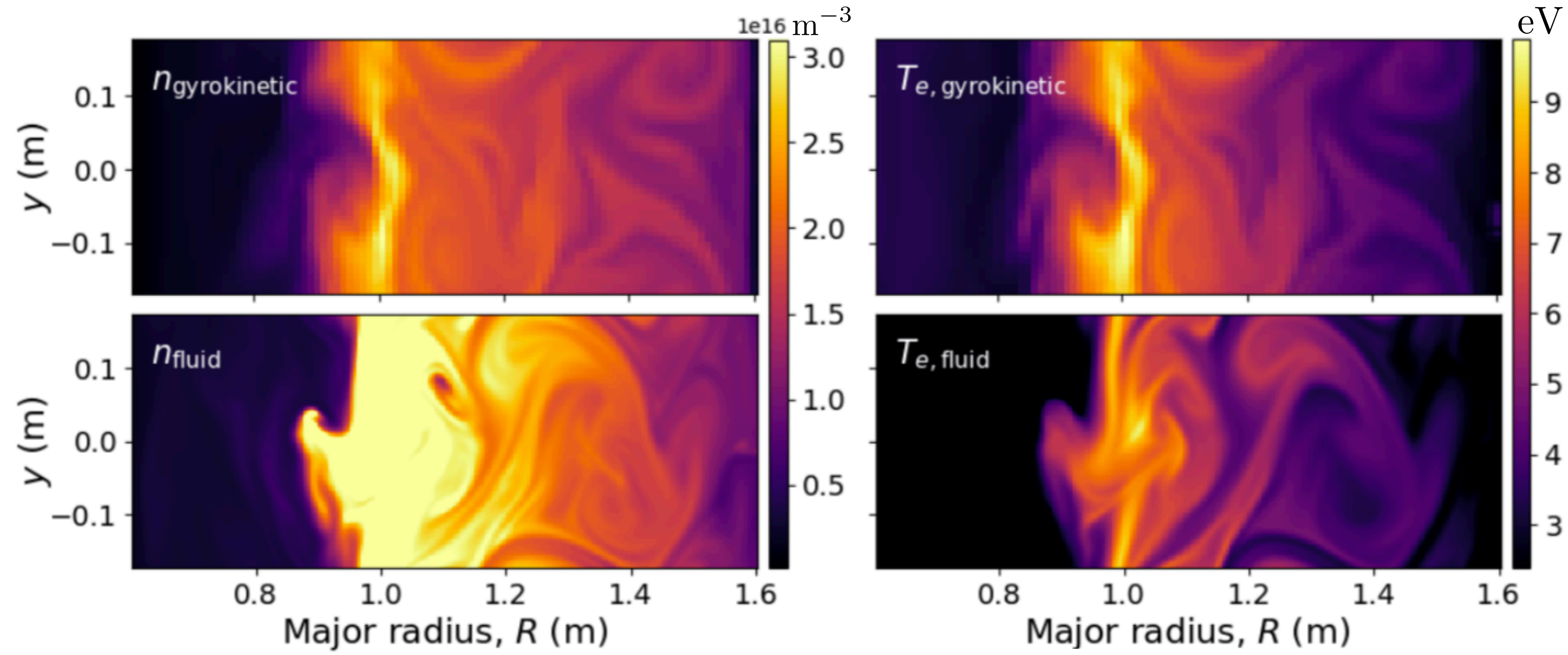
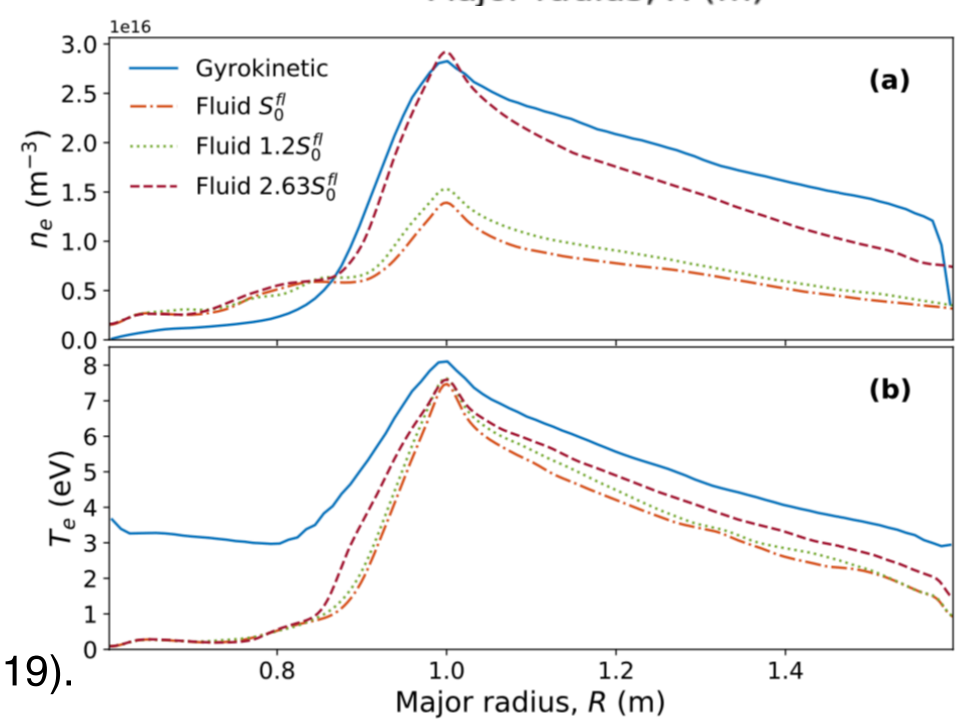
How do GDB results compare with gyrokinetic ones?

We simulated the Texas Helimak device with both Gkeyll* and GDB[10]



Snapshot of density and electron temperature at 10 ms





Lessons & observations from this comparison:[10]

1. GDB's geometric simplifications and non-conservative implementation leads to significant particle loss.
2. Significant qualitative and some quantitative agreement in several diagnostics.
3. Improved realism in both GDB and Gkeyll is called for.

*1st version of Gkeyll (gyrokinetic solver). See T. N. Bernard, et al. PoP 26, 042301 (2019).

[10]M. Francisquez, et al. PoP (2020), accepted.

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Striving to improve Gkeyll*, we# made several contributions leveraging the concept of weak equality

- GKEYLL aims to model plasmas at all scales.
- Provide fluid, gyrokinetic, and kinetic models for **arbitrary dimensions** under the same framework.
- Use state-of-the-art high-order **discontinuous Galerkin** methods.

rock opera band (https://spoti.fi/38FenTw)

*Gkeyll was re-written in 2018-2019.
#M. Francisquez & the Gkeyll team.

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Weak operations in a discontinuous Galerkin solver

- Weak division
- Collision operators
- Hermite transforms
- Poisson solvers
- Multiblock geometry

*Gkeyll was re-written in 2018-2019.
#M. Francisquez & the Gkeyll team.

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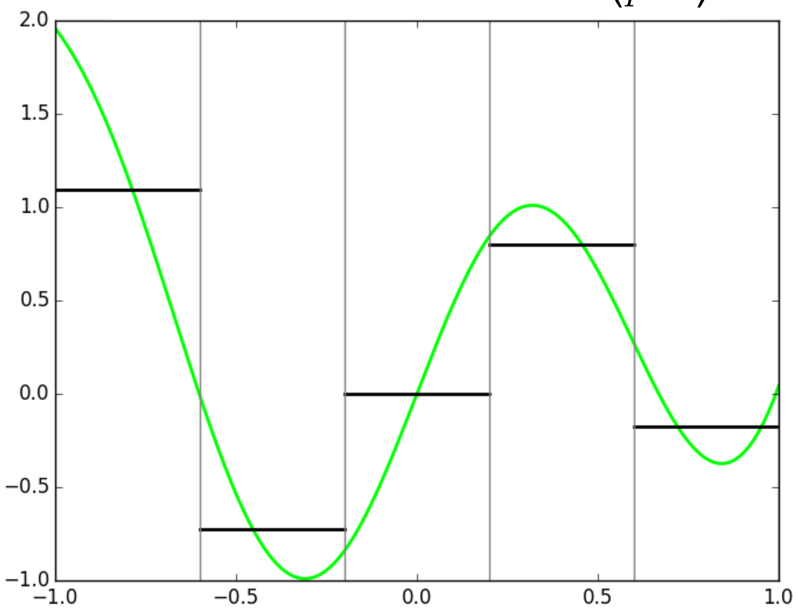
Discontinuous Galerkin (DG) refresher

A 1D function, $f = f(x)$, expanded in a cell-wise discontinuous basis.

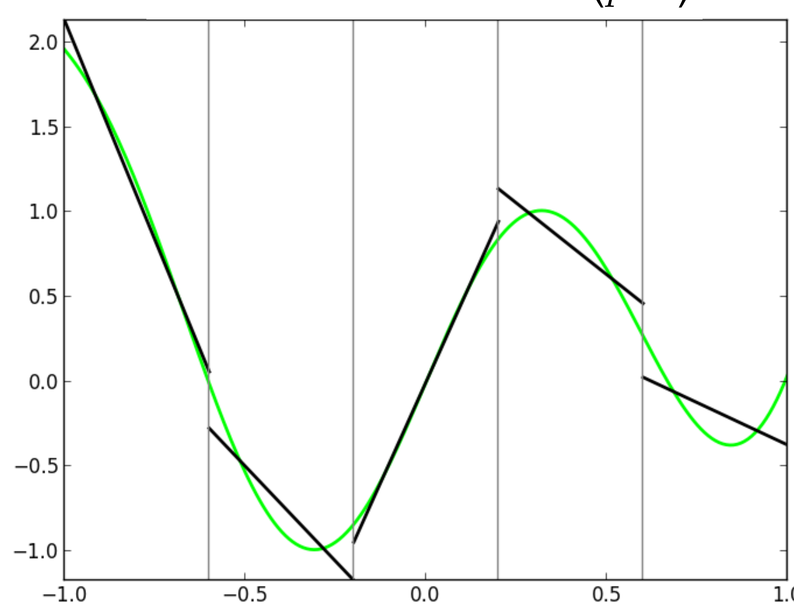
In a single cell: $$f = \sum_k f_k \psi_k$$

Piecewise constant basis ($p=0$)



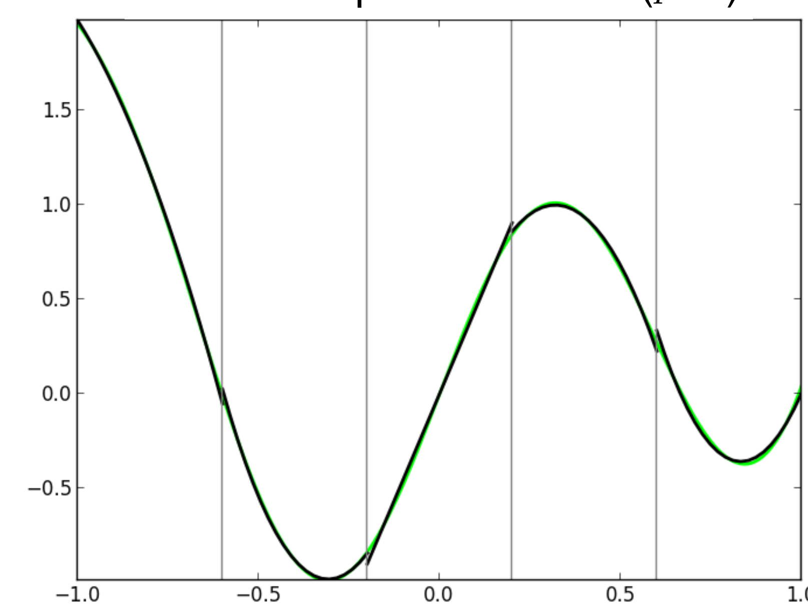
$$\psi_k \in \{1\}$$

Piecewise linear basis ($p=1$)



$$\psi_k \in \left\{ \frac{1}{\sqrt{2}}, \sqrt{\frac{3}{2}}x \right\}$$

Piecewise quadratic basis ($p=2$)



$$\psi_k \in \left\{ \frac{1}{\sqrt{2}}, \sqrt{\frac{3}{2}}x, \frac{3}{2}\sqrt{\frac{5}{2}}\left(x^2 - \frac{1}{3}\right) \right\}$$

Discontinuous Galerkin (DG) refresher

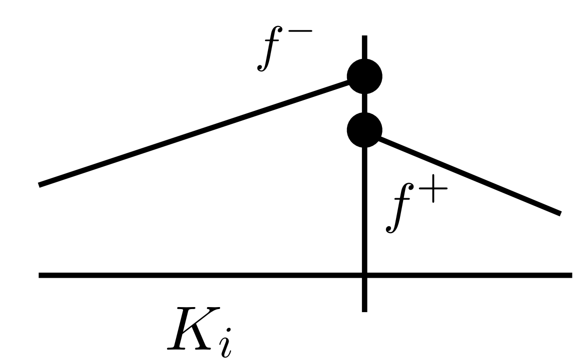
A 1D function, $f = f(x)$, expanded in a cell-wise discontinuous basis.

In a single cell: $f = \sum_k f_k \psi_k$

Suppose we wish to solve $\dfrac{\partial f}{\partial t} + \nabla_{\mathbf{z}} \cdot (\boldsymbol{\alpha} f) = 0$

Project onto the basis **in one cell** K_i. Obtain the discrete (or weak) form

$$\int_{K_i} \mathrm{d}\mathbf{z}\, \psi_k \frac{\partial f}{\partial t} + \oint_{\partial K_i} \mathrm{d}S\, \psi_k^- \hat{\mathbf{n}} \cdot \mathbf{F} - \int_{K_i} \mathrm{d}\mathbf{z}\, \nabla_{\mathbf{z}} \psi_k \cdot \boldsymbol{\alpha} f = 0$$



numerical flux

$\mathbf{F} = \mathbf{F}\left(\boldsymbol{\alpha}^- f^-, \boldsymbol{\alpha}^+ f^+\right)$

$\hat{\mathbf{n}}$: unit vector normal to ∂K_i

What are these equations $\dfrac{\partial f}{\partial t} + \nabla_{\mathbf{z}} \cdot (\boldsymbol{\alpha} f) = 0$?

Fluid equations:

$$\frac{\partial n}{\partial t} + \nabla \cdot n\mathbf{u} = 0,$$
$$\frac{\partial n\mathbf{u}}{\partial t} + \nabla \cdot \frac{P}{m} = \frac{q}{m} n \left(\mathbf{E} + \mathbf{u} \times \mathbf{B}\right),$$
$$\vdots$$

Vlasov equation:

$$\frac{\partial f}{\partial t} + \nabla \cdot \mathbf{v} f + \nabla_{\mathbf{v}} \cdot \frac{q}{m} \left(\mathbf{E} + \mathbf{v} \times \mathbf{B}\right) f = 0$$

Gyrokinetics:

$$\frac{\partial \mathcal{J} f}{\partial t} + \nabla \cdot \mathcal{J} \dot{\mathbf{R}} f + \frac{\partial}{\partial v_{\|}} \mathcal{J} \dot{v}_{\|} f = 0$$

I will focus on these

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What are these equations $\dfrac{\partial f}{\partial t} + \nabla_{\mathbf{z}} \cdot (\boldsymbol{\alpha} f) = 0$?

Fluid equations:

$$\frac{\partial n}{\partial t} + \nabla \cdot n\mathbf{u} = 0,$$
$$\frac{\partial n\mathbf{u}}{\partial t} + \nabla \cdot \frac{P}{m} = \frac{q}{m} n \left(\mathbf{E} + \mathbf{u} \times \mathbf{B}\right),$$
$$\vdots$$

discontinuous Galerkin

Suppose DG is used to evolve number and momentum densities:

$$n = M_0 = \sum_k M_{0,k} \psi_k$$

$$nu_x = M_{1x} = \sum_k M_{1x,k} \psi_k$$

How do we compute the DG expansion of the velocity $u_x = \dfrac{M_{1x}}{M_0}$?

Weak operations in discontinuous Galerkin solvers

- Weak division
- Collision operators
- Hermite transforms
- Multigrid Poisson solvers
- Mapped multiblock geometry

Learning to divide in a discontinuous Galerkin (DG) solver

$$\mathbf{u} = \frac{\mathbf{M_1}}{M_0}$$

Recall these two have a DG (polynomial) expansion

distribution function

$$M_0 = \int f\left(\mathbf{x}, \mathbf{v}, t\right) \mathrm{d}\mathbf{v}$$

$$\mathbf{M_1} = \int \mathbf{v} f(\mathbf{x}, \mathbf{v}, t)\, \mathrm{d}\mathbf{v}$$

DG division needs to yield a DG expansion, i.e. in 1D $u = \sum_k u_k \psi_k$

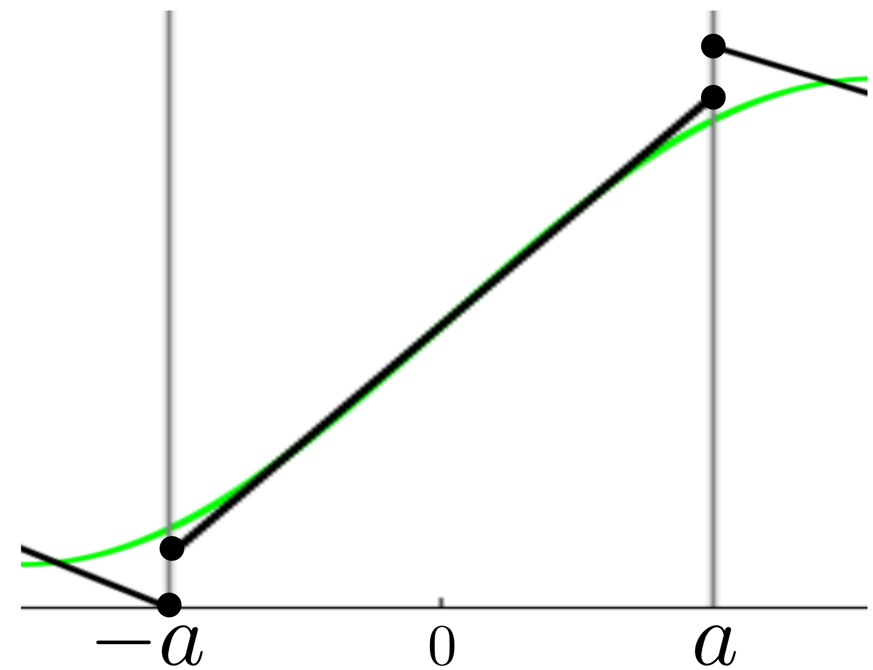
Two “naive” forms of DG division:

1. Nodal division: Given $M_1(x = \pm a)$ and $M_0(x = \pm a)$,

$$\Rightarrow u_{(x=\pm a)} = \frac{M_1(x = \pm a)}{M_0(x = \pm a)}$$

$$\Rightarrow u = \frac{u_{(x=a)} + u_{(x=-a)}}{2} + x\frac{u_{(x=a)} - u_{(x=-a)}}{2}$$

2. Project $\frac{M_1}{M_0}$ onto the basis: $u_k = \int \psi_k \frac{\sum_\ell \psi_\ell M_{1,\ell}}{\sum_\ell \psi_\ell M_{0,\ell}}\, \mathrm{d}x$



¡ In general these can lead to aliasing & non-conservation !

DG (weak) division leads to small linear problems

Use the concept of weak equality from finite element theory:

distribution function

$$M_0 = \int f(x,v,t)\,\mathrm{d}v$$

$$M_1 = \int v f(x,v,t)\,\mathrm{d}v$$

$$f \doteq g \quad \Rightarrow \quad \int_{K_i} \psi_k (f-g)\,\mathrm{d}\mathbf{x} = 0$$

Pose calculation of u as $uM_0 \doteq M_1$

$$\int \psi_k \left(\sum_l u_l \psi_l\right)\left(\sum_m M_{0,m}\psi_m\right)\mathrm{d}x = \int \psi_k \sum_l M_{1,l}\psi_l\;\mathrm{d}x$$

Can write this as $(T \cdot \mathcal{M}_0)\cdot u = M \cdot \mathcal{M}_1$

vectors of expansion coefficients

$$T_{klm} = \int \psi_k \psi_l \psi_m\,\mathrm{d}x$$

$$M_{kl} = \int \psi_k \psi_l\,\mathrm{d}x$$

A small linear problem for the coefficients u_l, to be solved in each configuration-space cell.

1st Gkeyll contribution: Ability to perform weak operations $g \cdot h$, g/h, $\mathbf{v}/g$, $\mathbf{v}\cdot\mathbf{w}$.

¡for any dimensionality and polynomial basis!

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Weak operations in discontinuous Galerkin solvers

- Weak division
- Collision operators
- Hermite transforms
- Multigrid Poisson solvers
- Mapped multiblock geometry

Weak division is needed for a conservative Dougherty collision operator

Some plasmas of interest have finite collisionality. Introduce a collision operator

Vlasov equation: $$\frac{\partial f}{\partial t} + \nabla\cdot\mathbf{v}f + \nabla_{\mathbf{v}}\cdot\frac{q}{m}\left(\mathbf{E}+\mathbf{v}\times\mathbf{B}\right)f = \boxed{C[f]}$$

Gyrokinetics: $$\frac{\partial \mathcal{J}f}{\partial t} + \nabla\cdot\mathcal{J}\dot{\mathbf{R}}f + \frac{\partial}{\partial v_\parallel}\mathcal{J}\dot{v}_\parallel f = \boxed{\mathcal{J}\mathcal{C}[f]}$$

For simplicity, affordability, and as a learning exercise we chose the Dougherty operator:

$$C[f] = \nu\frac{\partial}{\partial\mathbf{v}}\cdot\left[\left(\mathbf{v}-\mathbf{u}\right)f + v_t^2\frac{\partial f}{\partial\mathbf{v}}\right]$$

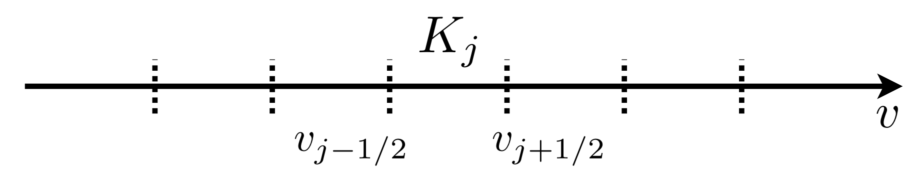
$$\mathcal{J}\mathcal{C}[f] = \nu\frac{\partial}{\partial v_\parallel}\left[\left(v_\parallel - u_\parallel\right)\mathcal{J}f + v_t^2\frac{\partial\mathcal{J}f}{\partial v_\parallel}\right] + \nu\frac{\partial}{\partial\mu}\left[2\mu\mathcal{J}f + 2\frac{mv_t^2}{B}\mu\frac{\partial\mathcal{J}f}{\partial\mu}\right]$$

computed through **weak division**

Dougherty collisions can be formulated conservatively[11]

In 1 velocity dimension: $$C[f] = \nu \frac{\partial}{\partial v}\left[(v-u)\,f + v_t^2 \frac{\partial f}{\partial v}\right] \qquad \nu \neq \nu(v)$$

Its weak form (projection onto the basis in one cell) is



$$\int_{K_j} \psi_k \frac{\partial f}{\partial t}\,\mathrm{d}\mathbf{z} = \int_{\partial K_j} \left\{ \psi_k \left[(v-u)\,f + v_t^2 \frac{\partial f}{\partial v}\right] - \frac{\partial \psi_k}{\partial v} v_t^2 f \right\}_{v_{j-1/2}}^{v_{j+1/2}} \mathrm{d}\mathbf{z}$$
$$- \int_{K_j} \left[\frac{\partial \psi_k}{\partial v}(v-u)\,f - \frac{\partial^2 \psi_k}{\partial v^2} v_t^2 f\right] \mathrm{d}\mathbf{z}$$

Sum over all cells and…

- Set $\psi_k = 1$ $\;\rightarrow\;$ $\displaystyle\sum_j \int_{K_j} \frac{\partial f}{\partial t}\,\mathrm{d}\mathbf{z} = 0$
- Set $\psi_k = v$ $\;\rightarrow\;$ $\displaystyle\sum_j \int_{K_j} v\frac{\partial f}{\partial t}\,\mathrm{d}\mathbf{z} = 0$ if $uM_0 \doteq M_1$
- Set $\psi_k = v^2$ $\;\rightarrow\;$ $\displaystyle\sum_j \int_{K_j} v^2\frac{\partial f}{\partial t}\,\mathrm{d}\mathbf{z} = 0$ if $uM_1 + v_t^2 M_0 \doteq M_2$

$$M_2 = \int v^2 f(x,v,t)\,\mathrm{d}v$$

[11]A. Hakim, M. Francisquez, J. Juno, G. W. Hammett, JPP (2020), accepted.

Dougherty collisions can be formulated conservatively[11]

In summary:

1. Requiring the discrete form

$$\int_{K_j} \psi_k \frac{\partial f}{\partial t}\,\mathrm{d}\mathbf{z} = \int_{\partial K_j} \left\{\psi_k \left[(v-u)\,f + v_t^2 \frac{\partial f}{\partial v}\right] - \frac{\partial \psi_k}{\partial v} v_t^2 f\right\}_{v_{j-1/2}}^{v_{j+1/2}} \mathrm{d}\mathbf{z} - \int_{K_j} \left[\frac{\partial \psi_k}{\partial v}\,(v-u)\,f - \frac{\partial^2 \psi_k}{\partial v^2} v_t^2 f\right] \mathrm{d}\mathbf{z}$$

   to conserve momentum leads to a natural definition of weak division as

$$uM_0 \doteq M_1$$

   in order to compute u. Likewise, energy conservation defines v_t^2 through

$$uM_1 + v_t^2 M_0 \doteq M_2$$

2. **Not shown**: the definition of boundary derivatives $\left.\dfrac{\partial f}{\partial v}\right|_{v_{j-1/2}}^{v_{j+1/2}}$ (recall f is discontinuous at cell boundaries) is also inherited from the concept of weak equality.

[11]A. Hakim, M. Francisquez, J. Juno, G. W. Hammett, JPP (2020), accepted.

Also implemented a gyro-averaged Dougherty collision operator[12]

Gkeyll's (long-wavelength) gyrokinetic solver

$$\frac{\partial \mathcal{J} f}{\partial t} + \nabla \cdot \mathcal{J}\dot{\mathbf{R}} f + \frac{\partial}{\partial v_\parallel}\mathcal{J} \dot{v}_\parallel f - \frac{\partial}{\partial v_\parallel}\mathcal{J}\frac{q}{m}\frac{\partial A_\parallel}{\partial t} f = \mathcal{J}\mathcal{C}[f]$$

$$\mathcal{J}\mathcal{C}[f] = \nu \frac{\partial}{\partial v_\parallel}\left[\left(v_\parallel - u_\parallel\right)\mathcal{J} f + v_t^2 \frac{\partial \mathcal{J} f}{\partial v_\parallel}\right] + \nu \frac{\partial}{\partial \mu}\left[2\mu \mathcal{J} f + 2\frac{m v_t^2}{B}\mu \frac{\partial \mathcal{J} f}{\partial \mu}\right]$$

Conservation leads to similar weak definitions

$$u_\parallel M_0 \doteq M_1$$
$$u_\parallel M_1 + v_t^2 M_0 \doteq M_2$$

This (electromagnetic) gyrokinetic-Dougherty system was used to examine profile evolution and turbulent fluctuations in an NSTX-like scrape-off layer.[13]

[12] M. Francisquez, T. N. Bernard, N. R. Mandell, G. W. Hammett, A. Hakim, NF (2020), accepted.

[13] N. R. Mandell, A. Hakim, G. W. Hammett, M. Francisquez, JPP 86 (2020), 905860109 .

Benchmarks demonstrate exact conservation (not shown) & agree with analytic theory[11,12]

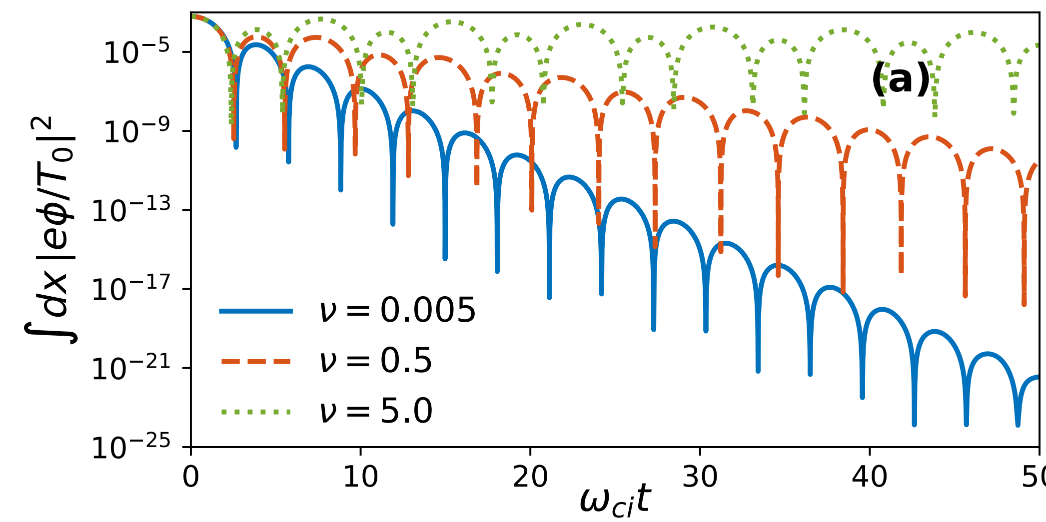
Benchmark 1: Collisional Landau damping of ion acoustic waves[14,15]

Initialize an ion sound wave, use adiabatic electrons, and evolve $f_i(x, v_\parallel, \mu, t)$ via

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

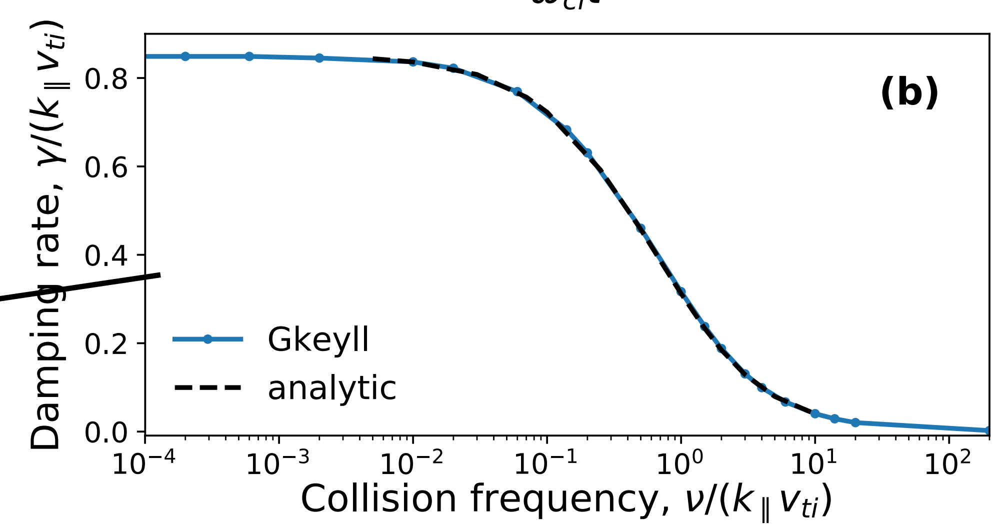
in 3D $(x, v_\parallel, \mu)$ with $\mathcal{J} = B = \hat{\mathbf{b}} \cdot \mathbf{B} = \hat{\mathbf{z}} \cdot \mathbf{B}$.

See wave damping through the electrostatic energy:



Following earlier works[14,15], one can obtain a linear dispersion relation by expanding the perturbed distribution function in a Hermite-Laguerre basis, and truncating the Hermite spectrum.

$\Rightarrow$ Implementation in Gkeyll agrees with this analytic dispersion relation across several decades of the collision frequency[12].



[11] A. Hakim, M. Francisquez, J. Juno, G. W. Hammett, JPP (2020), accepted.

[12] M. Francisquez, T. N. Bernard, N. R. Mandell, G. W. Hammett, A. Hakim, NF (2020), accepted.

[14] C. S. Ng, A. Bhattacharjee, F. Skiff, PRL 83 (1999), No. 10, 1974-1977.

[15] M. W. Anderson, T. M. O'Neil, PoP **14**, 112110 (2007).

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Benchmarks demonstrate exact conservation (not shown) & agree with analytic theory[11,12]

Benchmark 2: Heating via magnetic pumping[11]. Evolve electrons and ions solving

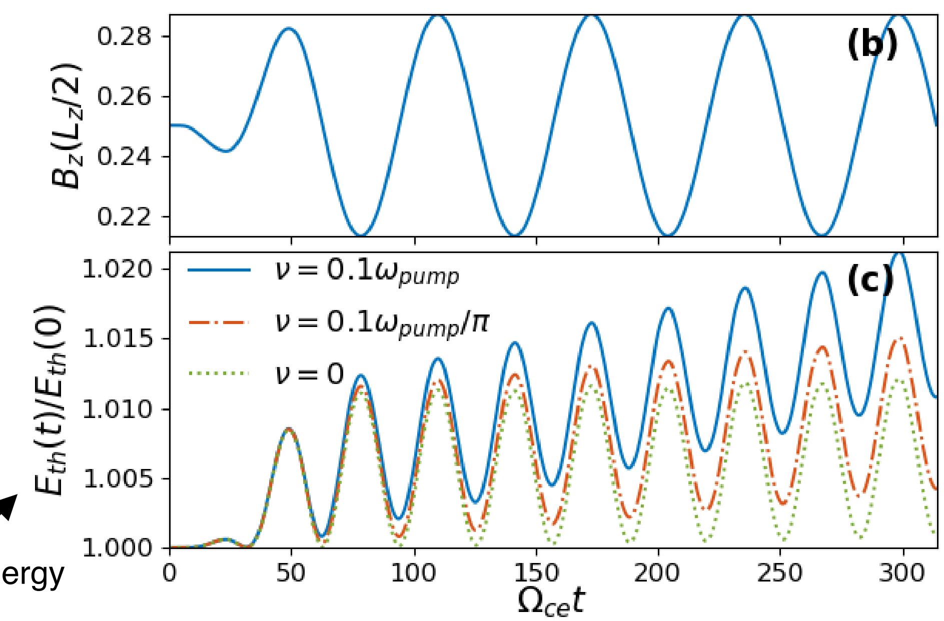
$$\frac{\partial f_s}{\partial t} + v_x \frac{\partial f_s}{\partial x} + \frac{q_s}{m_s}\left(\mathbf{E} + \mathbf{v}\times\mathbf{B}\right)\cdot\frac{\partial f_s}{\partial \mathbf{v}} = \nu_s \frac{\partial}{\partial \mathbf{v}}\cdot\left[\left(\mathbf{v}-\mathbf{u}_s\right) f_s + v_{ts}^2 \frac{\partial f_s}{\partial \mathbf{v}}\right] \qquad \nabla\times\mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \qquad \nabla\times\mathbf{B} = \mathbf{J} + \frac{\partial \mathbf{E}}{\partial t}$$

where the current density

$$\mathbf{J} = \sum_s q_s \mathbf{M_1}^s + \hat{\mathbf{y}}\tilde{J}_0 \sin\left(\omega_{\mathrm{pump}} t\right)\left[\exp\left(-\frac{\left(x-x_1\right)^2}{2\sigma_J^2}\right) - \exp\left(-\frac{\left(x-x_2\right)^2}{2\sigma_J^2}\right)\right]$$

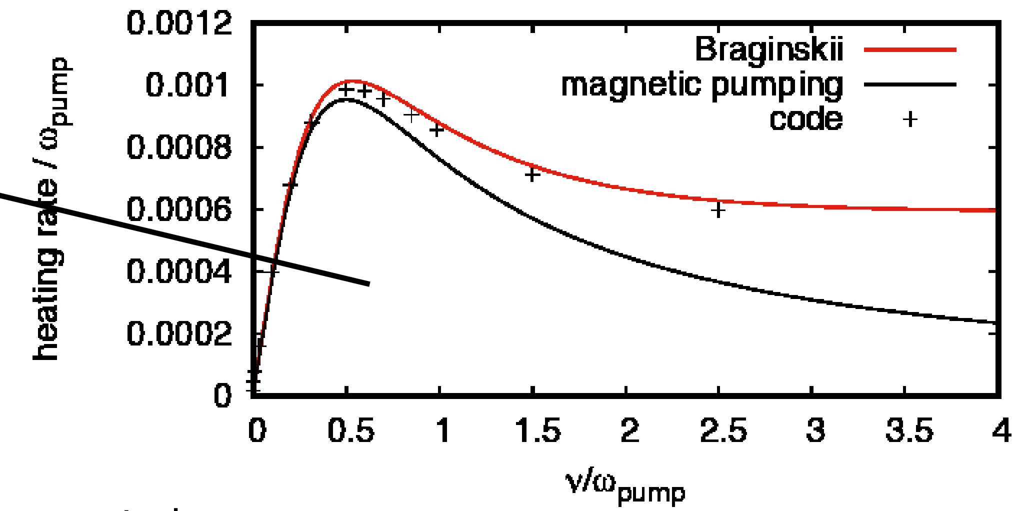
drives an oscillating B-field, on top of $\mathbf{B_0} = \hat{\mathbf{z}}B_0$.

A similar system was studied with PIC simulations to explore particle heating in the solar wind.[16]



E_{th} : thermal energy

$\Rightarrow$ At low ν, simulations agree with standard magnetic pumping theory. Gkeyll also recovers the high ν scaling, in which (for the parameters used) one must account for viscous heating .



[11] A. Hakim, M. Francisquez, J. Juno, G. W. Hammett, JPP (2020), accepted.

[12] M. Francisquez, T. N. Bernard, N. R. Mandell, G. W. Hammett, A. Hakim, NF (2020), accepted.

[16] E. Lichko, J. Egedal, W. Daughton, J. Kasper, ApJ 850:L28, (2017).

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Weak operations in discontinuous Galerkin solvers

- Weak division
- Collision operators
- Hermite transforms
- Multigrid Poisson solvers
- Mapped multiblock geometry

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Hermite transforms of DG data formulated via weak equality[12]

Previous diagnostics & benchmarks show fields & moments of f behave correctly.

But what about the distribution function itself?

Consider a Hermite expansion of f: $$f(v) = \sum_{m=0}^{m_{\max}} f_m \frac{1}{\sqrt{2^m \pi\, m!}} \mathrm{H}_m(v) e^{-v^2}$$

It simplifies the Dougherty collision operator into $$\frac{\partial f_m}{\partial t} = -\nu\, m\, f_m \quad \Rightarrow \quad f_m(t) = f_m(t=0) e^{-\nu m t}$$

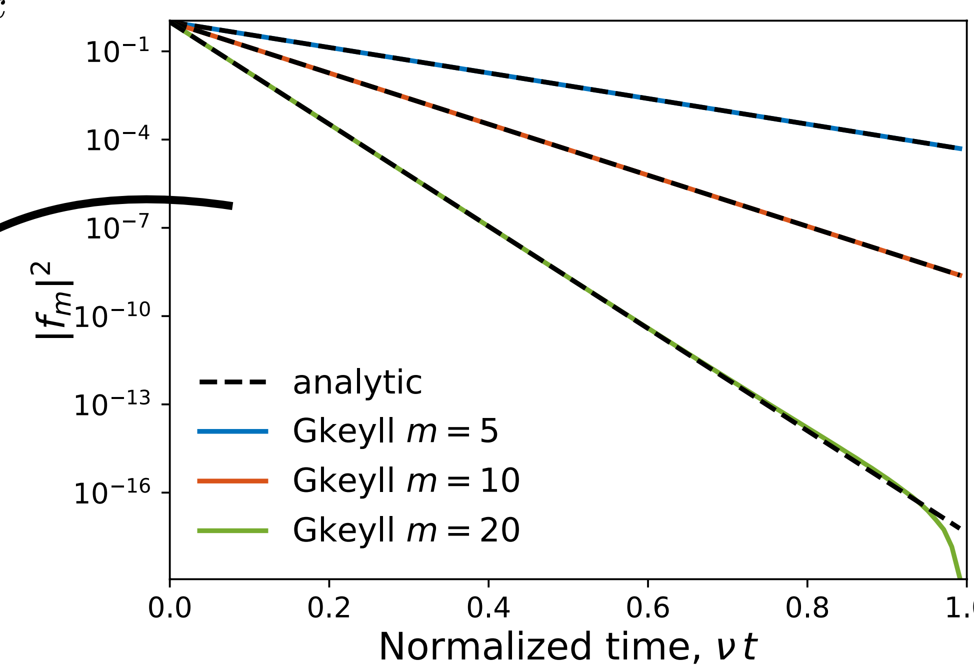
For a DG expansion, perform a Hermite transform to compute f_m via the weak equivalence:

$$\sum_{m=0}^{m_{\max}} f_m \frac{1}{\sqrt{2^m \pi\, m!}} \mathrm{H}_m(v) e^{-v^2} \doteq \sum_k f_k \psi_k(v) \longleftarrow \text{a large linear problem}$$

Initialize $f_{m=0} = f_{m=5} = f_{m=10} = f_{m=20} = 1$
else $f_m = 0$, and evolve f with

$$\frac{\partial f}{\partial t} = \nu \frac{\partial}{\partial v}\left[(v-u)\, f + v_t^2 \frac{\partial f}{\partial v}\right]$$

Time evolution of Hermite moments in DG follows theory



[12]M. Francisquez, T. N. Bernard, N. R. Mandell, G. W. Hammett, A. Hakim, NF (2020), accepted/to appear.

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Aside: multi-species Dougherty collisions also supported in Gkeyll[18]

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

The cross species velocities and thermal speeds, u_{sr} and $v_{t,sr}$, now require more complicated weak operations. For example, conservation requires:

$$m_e \nu_{ei} M_{0e} u_{ei} + m_i \nu_{ie} M_{0i} u_{ie} \doteq m_e \nu_{ei} M_{1e} + m_i \nu_{ie} M_{1i}$$

$$m_e \nu_{ei} \left(u_{ei} M_{1e} + v_{t,ei}^2 M_{0e} \right) + m_i \nu_{ie} \left(u_{ie} M_{1i} + v_{t,ie}^2 M_{0i} \right) \doteq m_e \nu_{ei} M_{2e} + m_i \nu_{ie} M_{2i}$$

This multi-species collision operator has been used, for example, in studying the generation of magnetic fields in 6D kinetic dynamo simulations.[17]

[17] I. Pusztai, J. Juno, A. Brandenburg, J. M. TenBarge, A. Hakim, M. Francisquez, A. Sundstrom, PRL 124, 255102 (2020).

[18] M. Francisquez, J. Juno, A. Hakim, G. W. Hammett, D. R. Ernst (in preparation).

Weak operations in discontinuous Galerkin solvers

- Weak division
- Collision operators
- Hermite transforms
- Multigrid Poisson solvers (work in progress)
- Mapped multiblock geometry

Rosenbluth-Fokker-Planck collisions demand solution to Poisson problems

Rosenbluth FPO: $C[f] = -\frac{\partial}{\partial v_i} a_i f + \frac{1}{2}\frac{\partial^2}{\partial v_i \partial v_j} D_{ij} f$ $\qquad a_i = \frac{\partial h}{\partial v_i} \qquad D_{ij} = \frac{\partial^2 g}{\partial v_i \partial v_j}$

$$-\nabla_{\mathbf{v}}^2 h = f \qquad \nabla_{\mathbf{v}}^2 g = h$$

Goal: design + implement a robust, highly accurate and efficient FPO algorithm*.

Discrete form of 1D Poisson $\partial_{xx}\phi = -\rho$:

$$\int_{K_i} \mathrm{d}x\, \psi_k \frac{\partial^2 \phi}{\partial x^2} = -\int_{K_i} \mathrm{d}x\, \psi_k\, \rho,$$

$$\left[\psi_k \frac{\partial \phi}{\partial x} - \frac{\partial \psi_k}{\partial x}\phi\right]_{\partial K_i} + \int_{K_i} \mathrm{d}x\, \frac{\partial^2 \psi_k}{\partial x^2}\phi = -\int_{K_i} \mathrm{d}x\, \psi_k\, \rho,$$

As in the Dougherty operator, compute define boundary derivatives $\left.\frac{\partial \phi}{\partial x}\right|_{\partial K_i}$ via weak recovery.

This is different from established approaches via lower order equations or penalty forms[19,20]

$\Rightarrow$ More accurate and does not have adjustable/undetermined coefficients.

* Work lead by P. Cagas (VT), A. Hakim (PPPL), B. Srinivasan (VT).

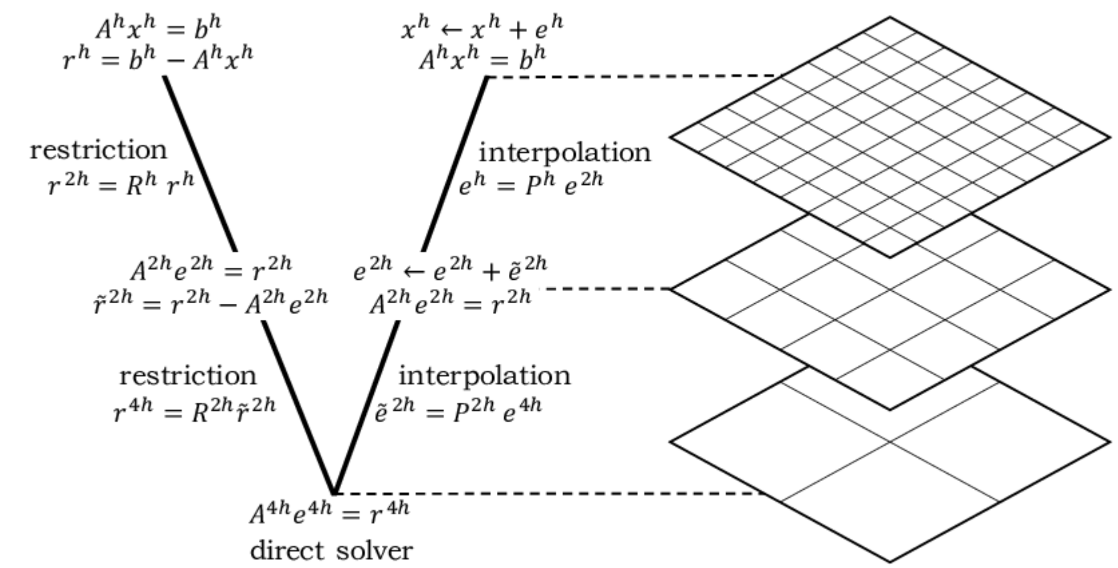
[19] B. Cockburn, B. Dong, J. Guzman, 77, Math. Comput. 264 (2008), 1887–1916.

[20] M. F. Wheeler, SIAM J. Numer. Anal. 15 No 1 (1978).

A (recovery) DG multigrid solver may provide optimal computational scaling

Consider a multigrid solution of $A\,x = b$

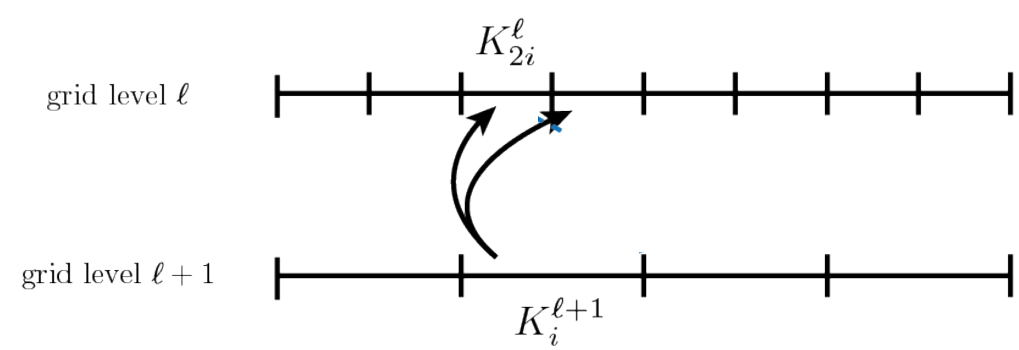
Conceptually, it requires transferring fields between different grids and performing (linear) operations on each grid.



Taken from [21].

How to transfer DG fields between two grids?

Answer: weak equality provides natural inter-grid operators



$$f_{2i}^{\ell} \doteq f_i^{\ell+1} \quad \underset{\xi_i^{\ell+1} = \frac{\xi_{2i}^{\ell}-1}{2}}{\Rightarrow} \quad \int_{K_{2i}^{\ell}} \mathrm{d}\xi_{2i}^{\ell}\; \psi_m\left(\xi_{2i}^{\ell}\right) \sum_k f_{2i,k}^{\ell} \psi_k\left(\xi_{2i}^{\ell}\right) = \int_{K_{2i}^{\ell}} \mathrm{d}\xi_{2i}^{\ell}\; \psi_m\left(\xi_{2i}^{\ell}\right) \sum_k f_{i,k}^{\ell+1} \psi_k\left(\xi_i^{\ell+1}\right)$$

$\Rightarrow$ for piecewise linear basis: $$\begin{bmatrix} f_{2i,0}^{\ell} \\ f_{2i,1}^{\ell} \end{bmatrix} = \begin{bmatrix} 1 & \sqrt{3}/2 \\ 0 & 1/2 \end{bmatrix} \begin{bmatrix} f_{i,0}^{\ell+1} \\ f_{i,1}^{\ell+1} \end{bmatrix}$$

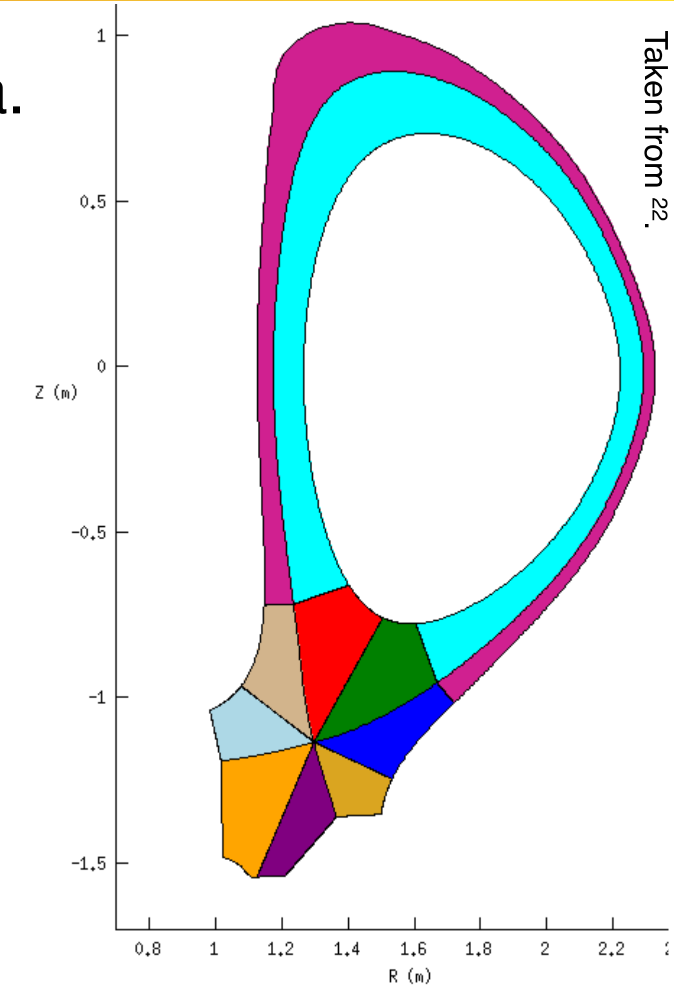
[21] H. Ibeid, L. Olson, W. Gropp, "FFT, FMM, and Multigrid on the Road to Exascale" (2018), https://arxiv.org/abs/1810.11883.

Weak operations in discontinuous Galerkin solvers

- Weak division
- Collision operators
- Hermite transforms
- Multigrid Poisson solvers
- Mapped multiblock geometry (future work)

We are evaluating the use of mapped multi blocks for complex geometries

For example, COGENT[22] uses 10 blocks for a diverted edge plasma.



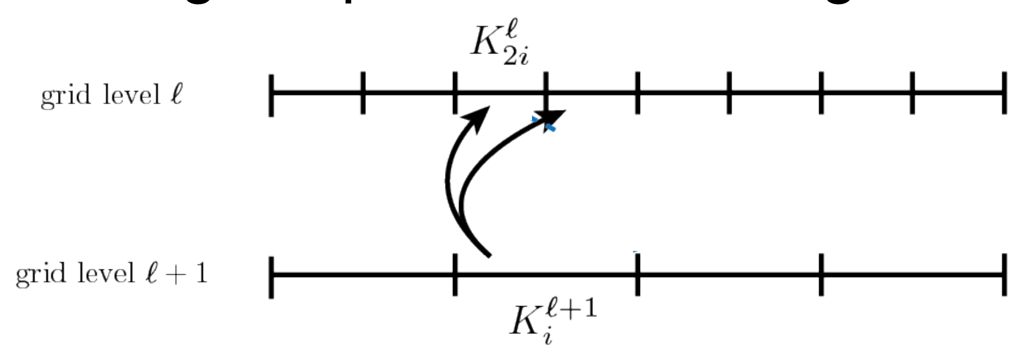
Taken from [22].

Blocks have different grids with:

- different mappings between computational and physical space.
- different resolutions.

Initial tests* suggest that if coordinate mappings between two blocks are the same (i.e. similar metric) but resolutions are different, the weak equality formulation of intergrid operators for multigrid

$$f_{2i}^{\ell} \doteq f_i^{\ell+1} \quad \Rightarrow$$



may also work for exchanging fields between two blocks.

Future work: test current inter-block transfers (same metric), formulate transfers between blocks with different metric, explore more complicated geometries.

* In collaboration with R. Mukherjee (PPPL).

[22]M. R. Dorr, et al. "High-order Discretization of a Gyrokinetic Vlasov Model in Edge Plasma Geometry" (2017), https://arxiv.org/abs/1712.01978.

Summary

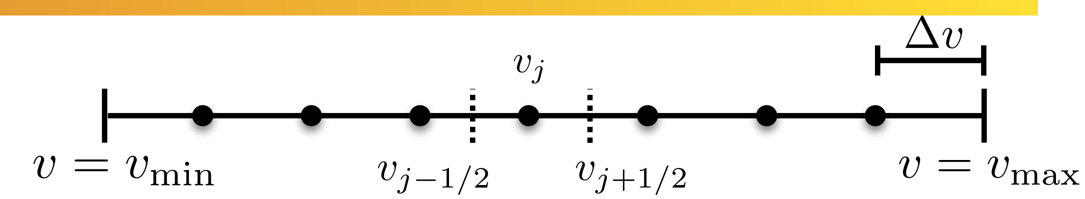
Gkeyll provides a platform for fluid and kinetic studies of plasmas. In its development we have made several contributions (to the code and to DG literature) which leverage weak equalities:

- Weak division gets defined by the (kinetic) equation and the physics constraints (conservation). Yields an alias-free and conservative DG division.
- The conservative weak form of a Dougherty operator has been implemented in both Vlasov and gyrokinetic solvers of Gkeyll (including multispecies). Benchmarks show that conservation is obeyed, and that physics results agree with theoretical expectations.
- Weak equality provides the means to formulate a useful Hermite transform diagnostic. This diagnostic suggests that the time evolution of f is also described accurately.
- We formulated and implemented a multigrid algorithm for the (recovery) DG discretization of the Poisson equation (aimed at Rosenbluth-Fokker-Planck collisions).
- Lessons from inter-grid transfers in multigrid are informing our understanding of potential approaches to DG mapped multiblocks in Gkeyll.

Supplementary slides

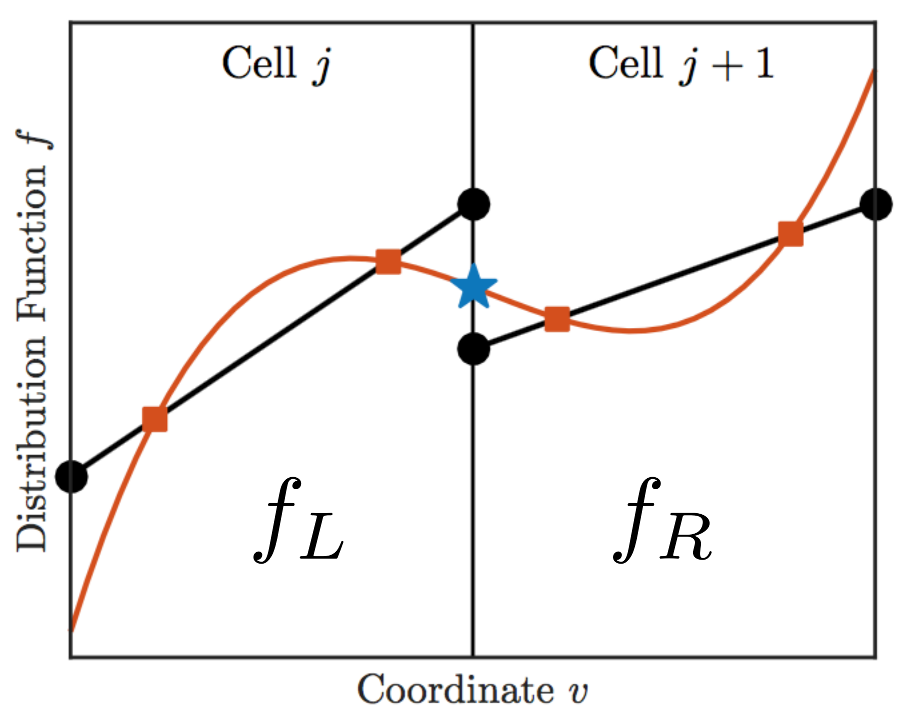
Recovery DG for Dougherty collisions

Dougherty weak form in 1 velocity dimension:



$$\int_{K_j} \psi_k \frac{\partial f}{\partial t}\, \mathrm{d}\mathbf{z} = \int_{\partial K_j} \left\{ \psi_k \left[(v-u)\, f + v_t^2 \frac{\partial f}{\partial v} \right] - \frac{\partial \psi_k}{\partial v} v_t^2 f \right\}_{v_{j-1/2}}^{v_{j+1/2}} \mathrm{d}\mathbf{z}$$
$$- \int_{K_j} \left[\frac{\partial \psi_k}{\partial v} (v-u)\, f - \frac{\partial^2 \psi_k}{\partial v^2} v_t^2 f \right] \mathrm{d}\mathbf{z}$$

Consider two adjacent cells



E. Shi, PhD thesis 2017.

Given the solution in two adjacent cells, f_L and f_R, each an expansion of order p, we can construct the recovery polynomial

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