Tools for Plasma Kinetics Simulation in PETSc

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Collaborators

Plasma Collaboration

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Projection and Discrete Gradients

Joe Pusztay

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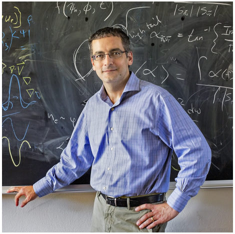
Collaborators

Metriplectic
Simulation

Eero Hirvijoki

Runaway
Electrons



Dylan Brennan

Outline

Structure-Preserving Evolution

Collisions

Vlasov Equation

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{x}} + \frac{d\mathbf{v}}{dt} \cdot \frac{\partial f}{\partial \mathbf{v}} = 0$$

We will need

- Particle discretization
- Symplectic integrators

Vlasov-Poisson Equation

$$
\begin{aligned}
\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{x}} - \frac{q \nabla \phi}{m} \cdot \frac{\partial f}{\partial \mathbf{v}} &= 0 \\
-\Delta \phi &= \rho
\end{aligned}
$$

We will need

- FEM discretization
- FEM-Particle map

Weak Equivalence

$$f_{FEM} = \sum_i \phi_i \mathrm{f}_i \qquad f_{PM} = \sum_p \delta(\mathbf{x} - \mathbf{x}_p)\delta(\mathbf{v} - \mathbf{v}_p)\mathrm{w}_p$$

Require that moments are preserved

$$\int \phi_i f_{FEM} = \int \phi_i f_{PM}$$

$$M\mathrm{f} = M_P \mathrm{w}$$

where M is the mass matrix, and

$$\begin{aligned}[M_P]_{ip} &= \int \phi_i \, \delta(\mathbf{x} - \mathbf{x}_p) \\ &= \phi_i(\mathbf{x}_p)\end{aligned}$$

Projections

Particle $\rightarrow$ FEM (deposition)

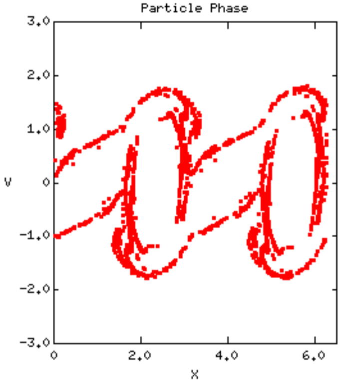
$$\begin{aligned} M\mathrm{f} &= M_P\mathrm{w} \\ \mathrm{f} &= M^{-1}M_P\mathrm{w} \end{aligned}$$

FEM $\rightarrow$ Particle

$$\mathrm{w} = M_P^{+}M\mathrm{f}$$

Examples

Two stream instability test in PETSc



(**MollenAdamsKnepleyHagerChang2021**)

Vlasov-Poisson-Landau Equation

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{x}} - \frac{q\nabla\phi}{m} \cdot \frac{\partial f}{\partial \mathbf{v}} = C(f)$$

$$-\Delta\phi = \rho$$

We will need

- Action of the Landau operator
- Metriplectic integrator

Long Time Evolution

Symmetries must be present in the discrete system:

- Conservation of mass
- Conservation of momentum
- Conservation of energy
- Monotonicity of entropy

Long Time Evolution

Tools we will need:

- Symplectic integrator will preserve moments
- Projection will preserve moments
- Discrete Landau must preserve moments
- DG integrator to preserve monotonic entropy
- Splitting should not destroy these properties

Discrete Gradients

Discrete Gradient integrators

$$\frac{f^{n+1} - f^n}{\Delta t} = S(f^n, f^{n+1}) \nabla F(f^n, f^{n+1})$$

satisfy a secant condition

$$\left(f^{n+1} - f^n\right) \cdot \nabla F(f^n, f^{n+1}) = F(f^{n+1}) - F(f^n).$$

Monotonicity of entropy means monotonicity of free energy:

$$\begin{aligned} S(f^{n+1}) - S(f^n) &= \left(E(f^{n+1}) - F(f^{n+1})\right) - \left(E(f^n) - F(f^n)\right) \\ &= -\left(F(f^{n+1}) - F(f^n)\right) \\ &= -\left(f^{n+1} - f^n\right) \cdot \nabla F \\ &= -\Delta t \nabla F \cdot S \cdot \nabla F \\ &\geq 0 \end{aligned}$$

since our S is symmetric negative semi-definite.

Outline

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Landau Operator

Strong Form

$$C_\alpha(f)$$
$$= \sum_\beta \nu_{\alpha\beta} \frac{m_0}{m_\alpha} \nabla \cdot \int d\mathbf{v}' \, \mathbf{U}(\mathbf{v}, \mathbf{v}') \left(\frac{m_0}{m_\alpha} f_\beta(\mathbf{v}') \nabla f_\alpha(\mathbf{v}) - f_\alpha(\mathbf{v}) \nabla' f_\beta(\mathbf{v}') \frac{m_0}{m_\beta} \right)$$

$$\mathbf{U}(\mathbf{v}, \mathbf{v}') = \frac{1}{|\mathbf{v} - \mathbf{v}'|} \mathbf{I} - \frac{(\mathbf{v} - \mathbf{v}') \otimes (\mathbf{v} - \mathbf{v}')}{|\mathbf{v} - \mathbf{v}'|^3}$$

$$\nu_{\alpha\beta} = \frac{e_\alpha^2 e_\eta^2 \ln \Lambda_{\alpha\beta}}{8\pi m_0^2 \epsilon_0^2}$$
$$m_0 = \text{reference mass}$$

Landau Operator

Weak Form

$$\sum_{\beta} \nu_{\alpha\beta} \frac{m_0^2}{m_\alpha} \int d\mathbf{v}' \, \nabla' \psi(\mathbf{v}') \cdot \left(\frac{1}{m_\alpha} \mathbf{K}(f_\beta, \mathbf{v}') \phi(\mathbf{v}') + \frac{1}{m_\beta} \mathbf{D}(f_\beta, \mathbf{v}') \cdot \nabla' \phi(\mathbf{v}') \right)$$

$$\mathbf{K}(f, \mathbf{v}) = \int d\mathbf{v}' \, \mathbf{U}(\mathbf{v}, \mathbf{v}') \cdot \nabla' f(\mathbf{v}')$$

$$\mathbf{D}(f, \mathbf{v}) = \int d\mathbf{v}' \, \mathbf{U}(\mathbf{v}, \mathbf{v}') f(\mathbf{v}')$$

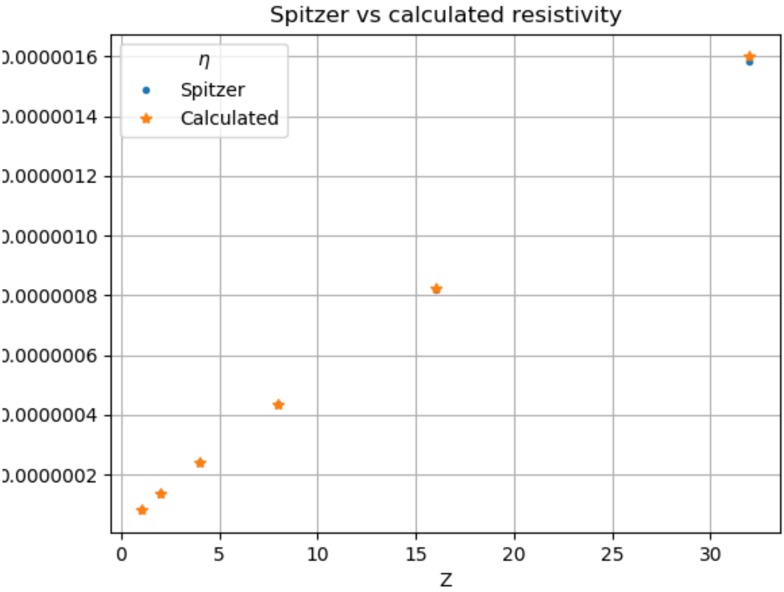
(**Hirvijoki2017**)

- Conservative projection to/from FEM
- Constant order Q_k
- Adaptive p4est grid

(**AdamsHirvijokiKnepleyBrownIsaacMills2017**)

Spitzer Resistivity

(AdamsKnepleyBrennan2021)



Outline

Particle Landau

(Hirvijoki2021)

If we ignore position, we have

$$\frac{d\mathbf{v}_p}{dt} = \frac{\nu}{m} \sum_{p'} w_{p'} \mathbf{Q}\left(\mathbf{v}_p - \mathbf{v}_{p'}\right) \Gamma(S, p, p')$$

where $\mathbf{Q}$ is the Landau tensor,

$$\mathbf{Q}(\mathbf{v}) = \frac{1}{\|\mathbf{v}\|}\mathbf{I} - \frac{\mathbf{v} \otimes \mathbf{v}}{\|\mathbf{v}\|^3}$$

and

$$\Gamma(S, p, p') = \frac{1}{w_p} \frac{\partial S}{\partial \mathbf{v}_p} - \frac{1}{w_{p'}} \frac{\partial S}{\partial \mathbf{v}_{p'}}$$

$$S = -\int d\mathbf{v} f(\mathbf{v}) \ln f(\mathbf{v})$$

Particle Landau

(Hirvijoki2021)

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$$S = -\sum_p w_p \ln w_p$$

Particle Landau

(Hirvijoki2021)

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$$\frac{d\mathbf{v}_p}{dt} = \frac{\nu}{m}\sum_{p'} w_{p'}\mathbf{Q}\left(\mathbf{v}_p - \mathbf{v}_{p'}\right)\Gamma(S,p,p')$$

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$$S_\epsilon = -\int d\mathbf{v}\sum_p w_p\psi_\epsilon(\mathbf{v}-\mathbf{v}_p)\ln\left(\sum_{p'} w_{p'}\psi_\epsilon(\mathbf{v}-\mathbf{v}_{p'})\right)$$

Particle Landau

(Hirvijoki2021)

$$\frac{\mathbf{v}_p^{n+1} - \mathbf{v}_p^n}{\Delta t} = \frac{\nu}{m} \sum_{p'} w_{p'} \mathbf{Q} \left(\mathbf{v}_p^{n+1/2} - \mathbf{v}_{p'}^{n+1/2} \right) \Gamma(S_\epsilon^n, p, p')$$

where $\mathbf{Q}$ is the Landau tensor,

$$\mathbf{Q}(\mathbf{v}) = \frac{1}{\|\mathbf{v}\|} \mathbf{I} - \frac{\mathbf{v} \otimes \mathbf{v}}{\|\mathbf{v}\|^3}$$

and

$$\Gamma(S, p, p') = \frac{1}{w_p} \frac{\partial S}{\partial \mathbf{v}_p} - \frac{1}{w_{p'}} \frac{\partial S}{\partial \mathbf{v}_{p'}}$$

$$S_\epsilon = -\int d\mathbf{v} \sum_p w_p \psi_\epsilon(\mathbf{v} - \mathbf{v}_p) \ln \left(\sum_{p'} w_{p'} \psi_\epsilon(\mathbf{v} - \mathbf{v}_{p'}) \right)$$

Future Work

- Prove that splitting preserves structure
- Scalability tests
- Higher order Discrete Gradients
- Mixed-Poisson FEM

References I