#### Tools for Plasma Kinetics Simulation in PETSc

#### Matthew Knepley, Joseph Pusztay, Mark Adams

Computer Science and Engineering University at Buffalo

SIAM Computational Science and Engineering, Cyberspace March 1, 2021





### Collaborators

# Plasma Collaboration

# Projection and Discrete Gradients



#### Mark Adams



Joe Pusztay

Dan Finn

Collaborators

# Metriplectic Simulation

Runaway Electrons



#### Eero Hirvijoki



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

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

We will need

- FEM discretization
- ► FEM-Particle map

#### Weak Equivalence

$$f_{FEM} = \sum_{i} \phi_{i} \mathbf{f}_{i}$$
  $f_{PM} = \sum_{p} \delta(\mathbf{x} - \mathbf{x}_{p}) \delta(\mathbf{v} - \mathbf{v}_{p}) \mathbf{w}_{p}$ 

Require that moments are preserved

$$\int \phi_i f_{FEM} = \int \phi_i f_{PM}$$
$$Mf = M_P w$$

where M is the mass matrix, and

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

# Projections

# Particle $\rightarrow$ FEM (deposition)

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

 $\text{FEM} \rightarrow \text{Particle}$ 

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

## Examples





(Mollén et al. 2021)

# Vlasov-Poisson-Landau Equation

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

# We will need

- Action of the Landau operator
- Metriplectic integrator

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

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

Monotonicity of entropy means monotonicity of free energy:

$$S(f^{n+1}) - S(f^n) = (E(f^{n+1}) - F(f^{n+1})) - (E(f^n) - F(f^n))$$
$$= -(F(f^{n+1}) - F(f^n))$$
$$= -(f^{n+1} - f^n) \cdot \nabla F$$
$$= -\Delta t \nabla F \cdot S \cdot \nabla F$$
$$\ge 0$$

since our S is symmetric negative semi-definite.

# Outline

Structure-Preserving Evolution

Collisions Collisions in the FE Basis Collision in the Particle Basis

# Outline

#### Collisions Collisions in the FE Basis Collision in the Particle Basis

#### Landau Operator Strong Form

 $\alpha$  ( $\alpha$ )

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

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

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

 $m_0$  = reference mass

#### Landau Operator Weak Form

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

(Hirvijoki and Adams 2017)

# Landau Operator

Implementation

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

(Adams, Hirvijoki, et al. 2017)

# Spitzer Resistivity

#### (Adams, Knepley, and Brennan 2021)



# Outline

#### Collisions Collisions in the FE Basis Collision in the Particle Basis

# Particle Landau

(Hirvijoki 2021)

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,

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

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

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

# Particle Landau

(Hirvijoki 2021)

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,

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

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

$$S = -\sum_{p} w_p \ln w_p$$

# Particle Landau

(Hirvijoki 2021)

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,

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

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

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

#### Particle Landau (Hirvijoki 2021)

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

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

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

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

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

## Future Work

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

# References I



Ē.

```
Mollén, Albert, Mark F. Adams, Matthew G. Knepley, Robert Hager, and C. S. Chang (2021).

Implementation of higher-order velocity mapping between marker particles and grid in the particle-in-cell code XGC.

arXiv: 2012.11764 [plasm-ph].
```



- Adams, Mark F., Eero Hirvijoki, Matthew G. Knepley, Jed Brown, Tobin Isaac, and Richard Mills (2017). "Landau Collision Integral Solver with Adaptive Mesh Refinement on Emerging Architectures". In: <u>SIAM Journal on Scientific Computing</u> 39.6, pp. C452–C465. DOI: 10.1137/17M1118828. eprint: 1702.08880.
- Adams, Mark F., Matthew G. Knepley, and Dylan Brennan (2021). Runaway Electron Generation with High-Performance, Structure Preserving Discretization of Fokker-Plank-Landau.
- Hirvijoki, Eero (2021). "Structure-preserving marker-particle discretizations of Coulomb collisions for particle-in-cell codes". In: Plasma Phys. Control. Fusion. in press. DOI: 10.1088/1361-6587/abe884.