LANDAU COLLISIONS IN THE PARTICLE BASIS WITH PETSC-PIC

PETSc 2023

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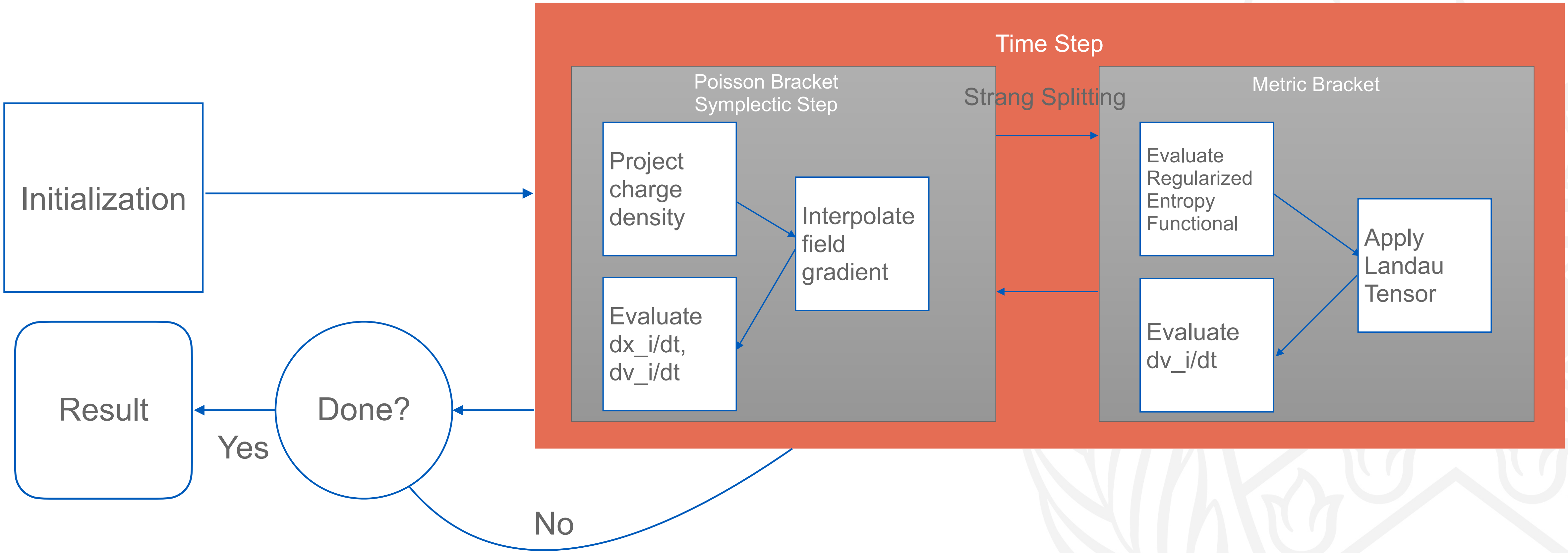
Metriplectic Formulation

$$\frac{dU}{dt} = (U, F) + \{U, F\}$$

Morrison, P. J. (1986). A Paradigm for Joined Hamiltonian and Dissipative Systems. Physica D
Kraus, Hirvijoki (2017). Metriplectic Integrators for the Landau Collision Operator. PoP
Hirvijoki, Kraus, Burby (2018). Metriplectic particle in cell integrators for the Landau Collision Operator.

The Process


Initialization
Time Step
Poisson Bracket
Symplectic Step
Strang Splitting
Metric Bracket
Project charge density
Interpolate field gradient
Evaluate dx_i/dt, dv_i/dt
Evaluate Regularized Entropy Functional
Apply Landau Tensor
Evaluate dv_i/dt
Result
Done?
Yes
No

Landau Collision Integral

- Represent transfer of momentum in the grazing limit
  - Non relativistic particles
- Conservative in the continuum
  - Conservative FE discretization in PETSc by Adams et al
    - PETSc implmentation in plexlandau/ex1 and ex2
  - Particle discretizations remained challenging

$$\frac{df_\alpha}{dt} = \sum_\beta C_{\alpha\beta}[f_\alpha, f_\beta]$$

$$C_{\alpha\beta} = \nu_{\alpha\beta}\frac{m_0}{m\alpha}\nabla\cdot\int_{\bar{\Omega}} d\bar{v}U(v,\bar{v})\cdot(\frac{m_0}{m_\alpha}\bar{f}_\beta\nabla f_\alpha - \frac{m_0}{m_\beta}f_\alpha\bar{\nabla}\bar{f}_\beta)$$

$$U(\vec{v},\bar{v}) = \frac{1}{|\vec{v}-\bar{v}|^3}(|\vec{v}-\bar{v}|^2 I - (\vec{v}-\bar{v})(\vec{v}-\bar{v}))$$

Grid Approach

- FE implementation by Adams et al
- High order elements, non conforming adaptive mesh refinement
- Conservative
- Works at exascale
- Well verified (stationary Maxwellian, effective reproduction of Spitzer model of plasma friction)
- Supports multiple species per grid

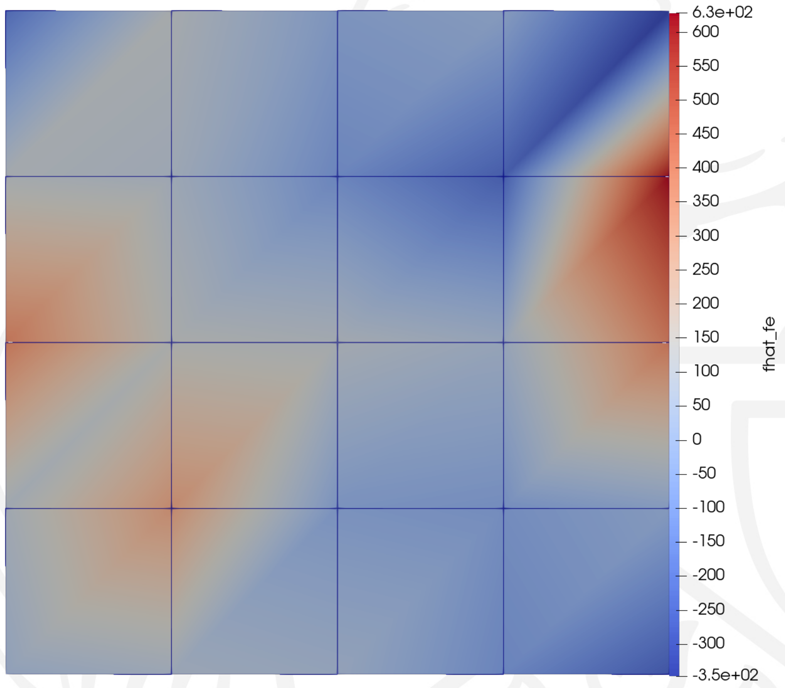


Fig: Arbitrary field projected to the grid from the particle basis

$$f_{FE} = \sum_i \phi_i \hat{f}$$

Adams, Wang, Merson, Knepley (2022). A performance portable, fully implicit Landau collision operator with batched linear solvers
Adams, Hirvijoki, Knepley, Brown, Isaac, Mills (2017). Landau Collision Integral Solver with Adaptive Mesh Refinement on Emerging Architectures
Adams, Brennan, Knepley, Wang (2022) Landau collision operator in the CUDA programming model applied to thermal quench plasmas

Basis Projection

- Incompatible representations
- Compare continuous functions with radon measure
- Need to transition between representations
- Enforce weak equivalence

$$\int f_{FE} = \int f_p$$

$$\int v f_{FE} = \int v f_p$$

$$\int_\Omega \phi_i \, f_{FE} = \int_\Omega \phi_i \, f_P \quad \forall \phi_i \in \mathscr{V}$$

$$\int_\Omega \phi_i \sum_j f_j \phi_j = \int_\Omega \phi_i \sum_p w_p \delta(\hat{x} - \hat{x}_p)$$

$$\sum_j f_j \int_\Omega \phi_i \phi_j = \sum_p w_p \int_\Omega \phi_i \delta(\hat{x} - \hat{x}_p) \longrightarrow M\hat{f} = M_P \hat{w}$$

Projection Operator

- Particle-Mesh interaction required
- Deposit particles to grid to calculate charge density/potential fields
- Synthesize particles from mesh to evaluate changes in weighting
- Deposition - Mass Matrix inversion (easy!)
- Synthesis - Pseudo Inverse of particle mass matrix (not as easy :( )
    - KSPLSQR (no PC, heavy)
    - preconditioned KSPLSQR w/ normal equations and ASM/icc or BJacobi/LU

$$\int_\Omega \phi_i \sum_j \hat{f}_j \phi_j = \int_\Omega \phi_i \sum_p \hat{w}_p \delta(x - x_p)$$

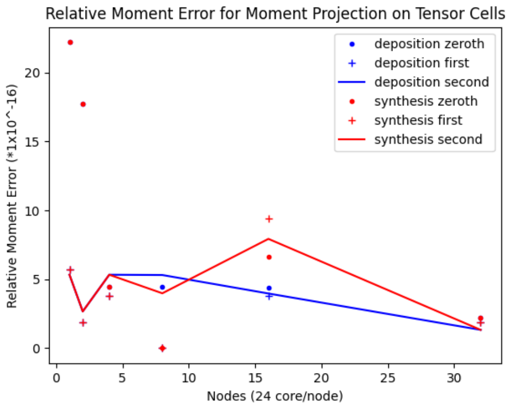
$$\sum_j \hat{f}_j \int_\Omega \phi_i \phi_j = \sum_p \hat{w}_p \int_\Omega \phi_i \delta(x - x_p)$$

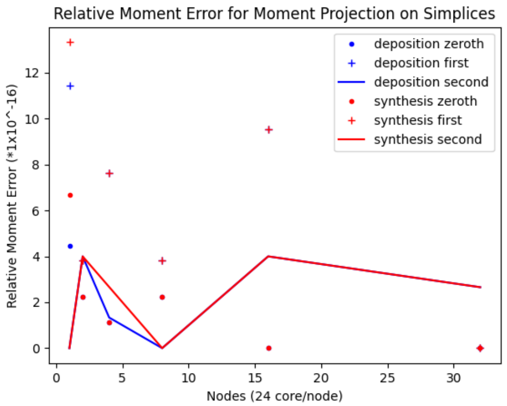
$$M\hat{f} = V\hat{w}$$

$$\hat{f} = M^{-1} M_P \hat{w} \qquad \hat{w} = M_P^\dagger M \hat{f}$$

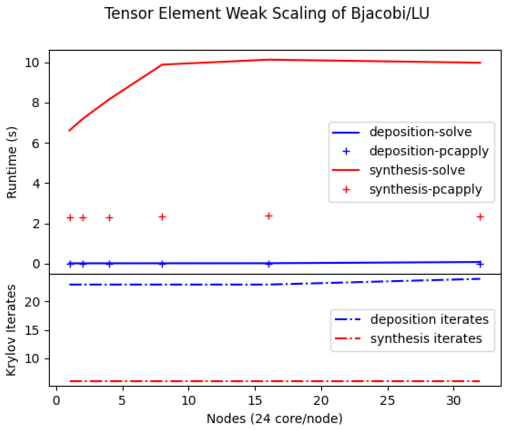
Pusztay, Knepley, Adams (2022). *Conservative Projection between FEM and Particle Bases*, SISC

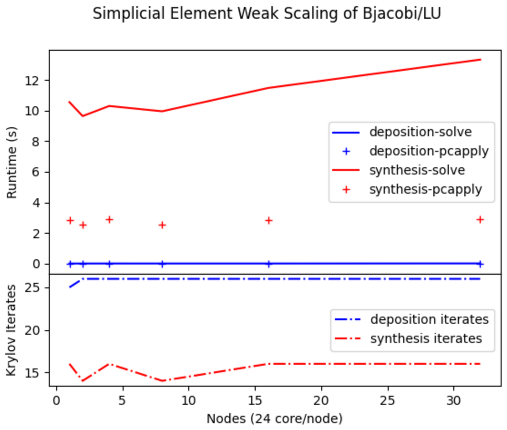
Projection Operator





Relative Error



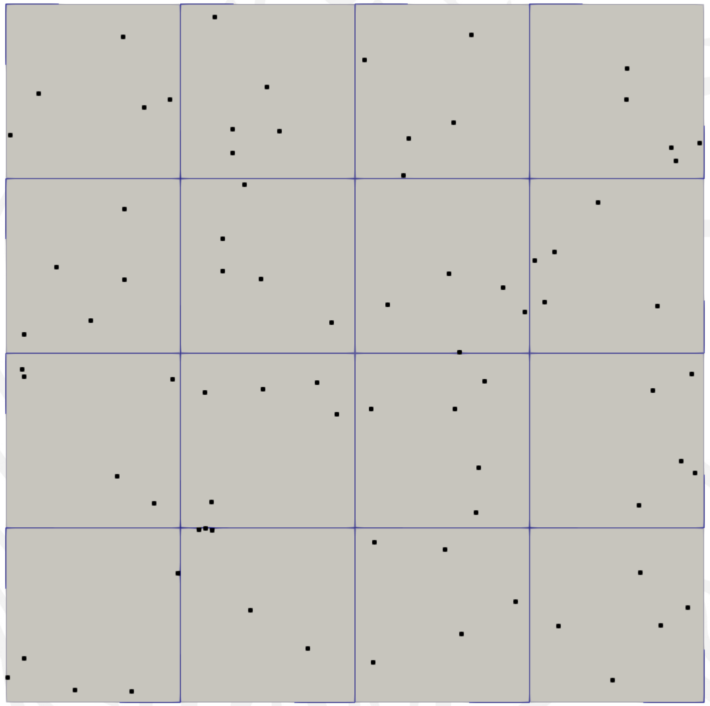


Cost (scaling)

Particle Approach

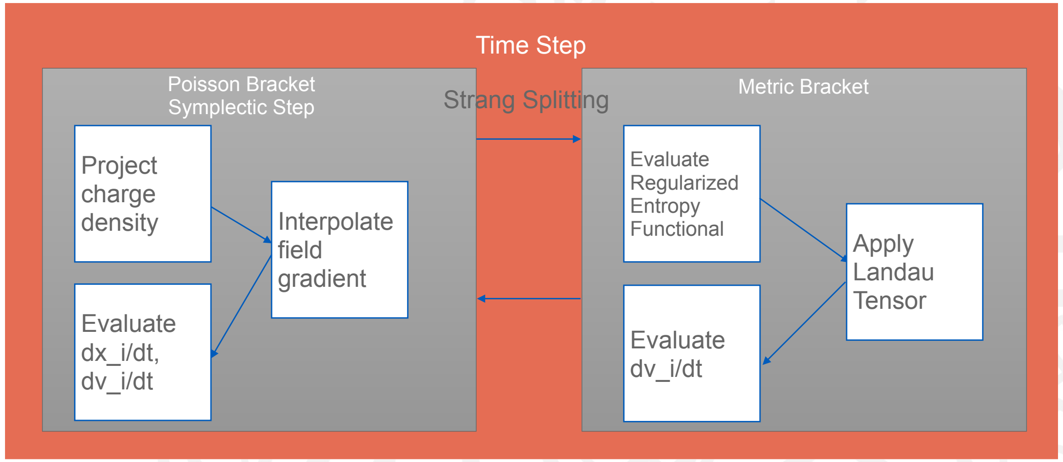
- Say we have no velocity grid…

$$f_P = \sum_i w_i \delta(x - x_p)$$



Metriplectic Formulation

- Notion of Metriplectic structure, two brackets
  - Poisson, Metric
- Demonstrably conserve symplectic structure in the Poisson bracket
- Metric bracket guarantees Hamiltonian as a Casimir of the bracket (mass, momentum, energy conservation)
- Monotonic entropy production



$$\frac{dU}{dt} = (U, F) + \{U, F\}$$

$$C_{\alpha\beta} = \nu_{\alpha\beta}\frac{m_0}{m\alpha}\nabla \cdot \int_{\bar{\Omega}} d\bar{v}U(v,\bar{v}) \cdot (\frac{m_0}{m_\alpha}\bar{f}_\beta \nabla f_\alpha - \frac{m_0}{m_\beta} f_\alpha \bar{\nabla}\bar{f}_\beta)$$

Collisions in the Particle Basis

- Carillo et. al demonstrate Maxwellian steady state of the particle representation of the collision operator
  - Interpret Landau collision integral as gradient flow over set of probability measures
  - Cast in terms of entropy functional
  - velocity evolution determined as variational derivative of the entropy functional
  - Regularize Entropy
    - Mollification procedure

$$f_p = \sum_p w_p \delta(v - v_p)$$

$$S = \int f ln f$$

$$U_\epsilon = -\int Q(\xi)(\nabla_v \frac{\delta S}{\delta f} - \nabla_{\bar{v}} \frac{\delta S}{\delta \bar{f}}) d\bar{v}$$

[1] Carillo et al, A particle method for the homogeneous Landau equation
[2] Hirvijoki, Structure-preserving marker-particle discretizations of Coulomb collisions for particle-in-cell codes
[3] Zonta et al, Multispecies structure-preserving particle discretization of the Landau collision operator

Mollification

- Integrate distribution against smooth function
  - Gaussians
- Essentially perform a convolution with smooth set of functions
  - Generate smooth, differentiable representation of the basis of delta functions
- This is not carried out in application
  - Just replace delta function with gaussian at particle coordinate

$$\psi_\epsilon = \frac{1}{2\pi\epsilon} e^{\frac{-(v^2)}{2\epsilon}}$$

$$S \rightarrow S_\epsilon = -\int \psi * f ln \psi * f$$

$$S = -\int_\Omega \sum_p w_p \psi_\epsilon (v - v_p) ln \sum_k w_k \psi_\epsilon (v - v_k)$$

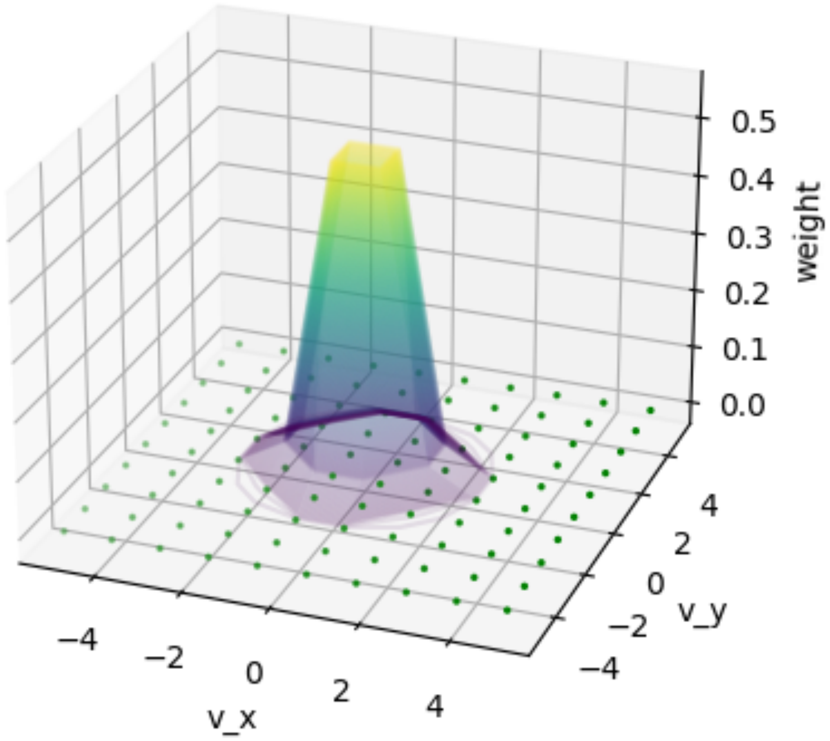
$$\frac{dv_p}{dt} = \sum_{\bar{p}} \nu_{p\bar{p}} 1(p, \bar{p}) Q(\xi) \Gamma(S_\epsilon, p, \bar{p})$$

$$\Gamma(S_\epsilon, p, \bar{p}) = \frac{\partial S}{m \partial v_p} - \frac{\partial S}{m \partial v_{\bar{p}}}$$

[1] Carillo et al, A particle method for the homogeneous Landau equation
[2] Hirvijoki, Structure-preserving marker-particle discretizations of Coulomb collisions for particle-in-cell codes

Initialization

- Convergence of the method only guaranteed for sufficiently regular particle spacing
  - Lay particles out in a grid
  - Calculate weight based on initial conditions in that region of velocity space
- Regularization parameter limits particle irregularity
  - Prohibits QMC methods (ie Sobol sequence Quiet Starts)
  - Uniformly weighted particles under investigation
    - regularization parameter in terms of discrepency of the set



Stepping

- Precompute entropy functional gradients for each species
- Form the Jacobian
  - Approximated either Finite Difference or Matrix Free
  - SNESFD (Heavy)
  - SNESMF (Less heavy)
- Compute residual over all pairs
- Copy back to Swarm

$$\frac{v^{n+1} - v^n}{\Delta t} = \sum_{\bar{p}} 1(p, \bar{p}) Q(\xi^{n+1/2}) \Gamma(S^n, p, \bar{p})$$

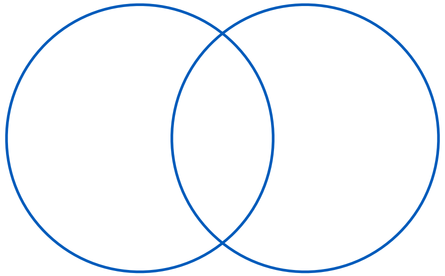
Entropy Functional Gradient

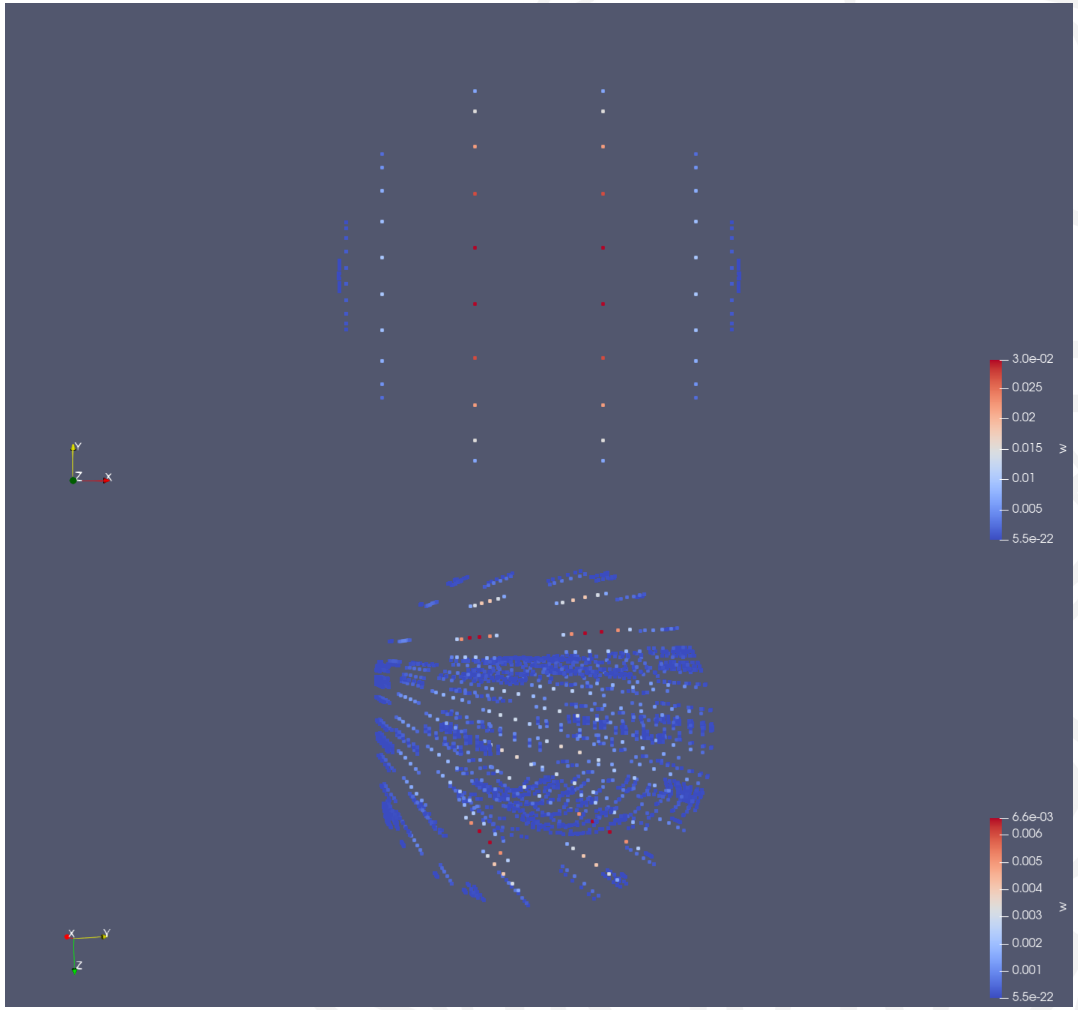
$$\frac{\partial S_\epsilon}{\partial v_p} = -\int \nabla_{v_p} \sum_p w_p \psi_\epsilon(v - v_p) ln \sum_k w_k \psi_\epsilon(v - v_k)$$

$$= -\int w_p \psi'(v - v_p)(1 + ln \sum_k w_k \psi(v - v_k))$$

Evaluation of the Entropy Functional Gradient

- Gauss-Hermite Quadrature
- AlgoIM - High order quadrature over implicitly defined domains
  - Can generate high order quadrature of complex domains including cusps and intersections of arbitrary polynomial functions
  - Trimmed quadrature space can be leveraged to increase speedup



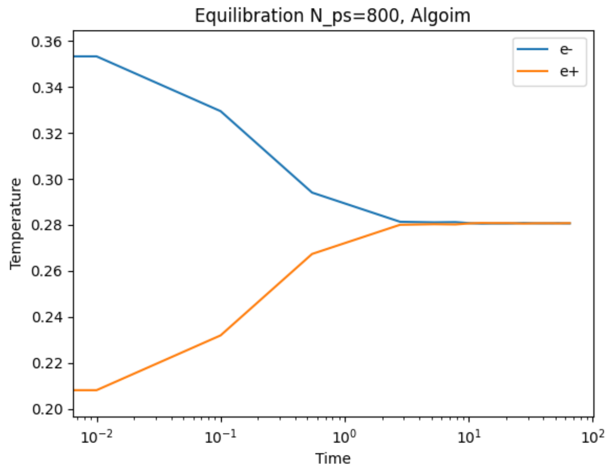


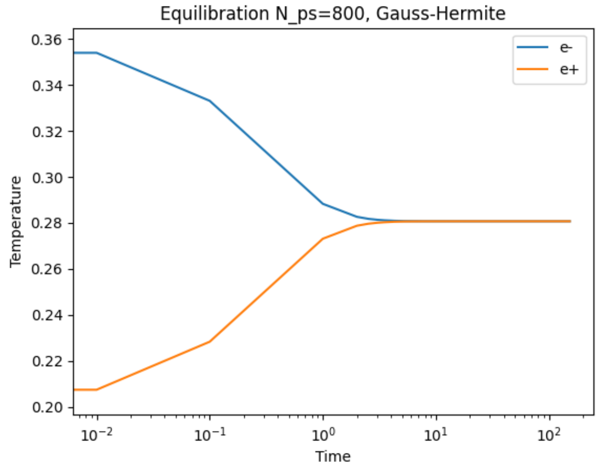
R. I. Saye, *High-order quadrature on multi-component domains implicitly defined by multivariate polynomials*, Journal of Computational Physics, 448, 110720 (2022).

Particle Basis Landau

- Recent theoretical work makes evaluation of the integral in the particle basis possible with proof of conservative properties
- Initial implementation non due to time discretization conservative
- Hirvijoki proposed new time discretization
- Implicit midpoint like time stepping
    - TSTHETA w/ theta = 0.5

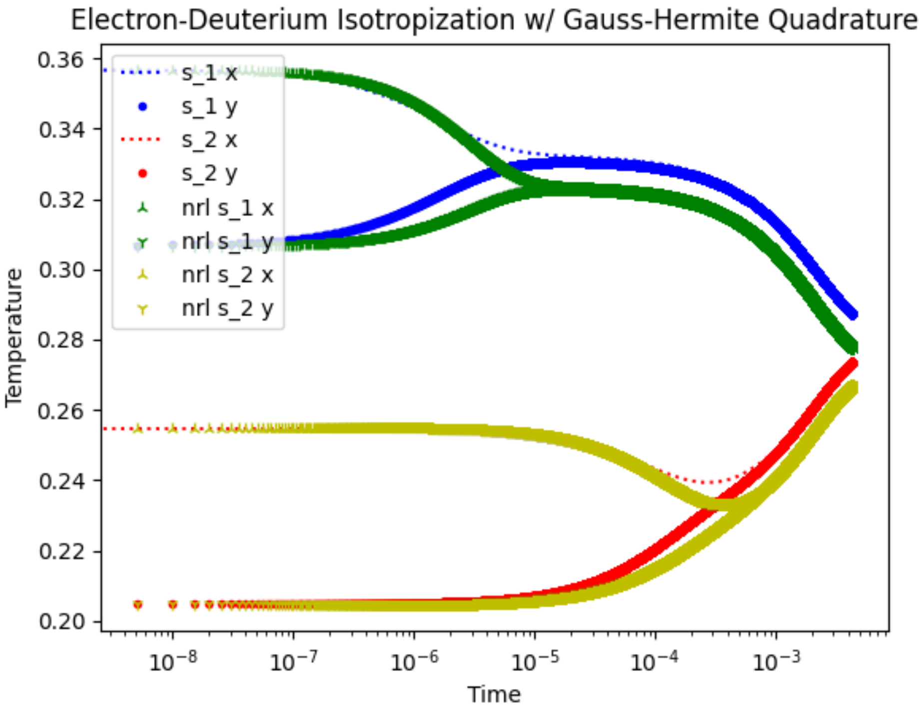
$$\frac{v^{n+1} - v^n}{\Delta t} = \sum_{\bar{p}} 1(p, \bar{p}) Q(\xi^{n+1/2}) \Gamma(S^n, p, \bar{p})$$

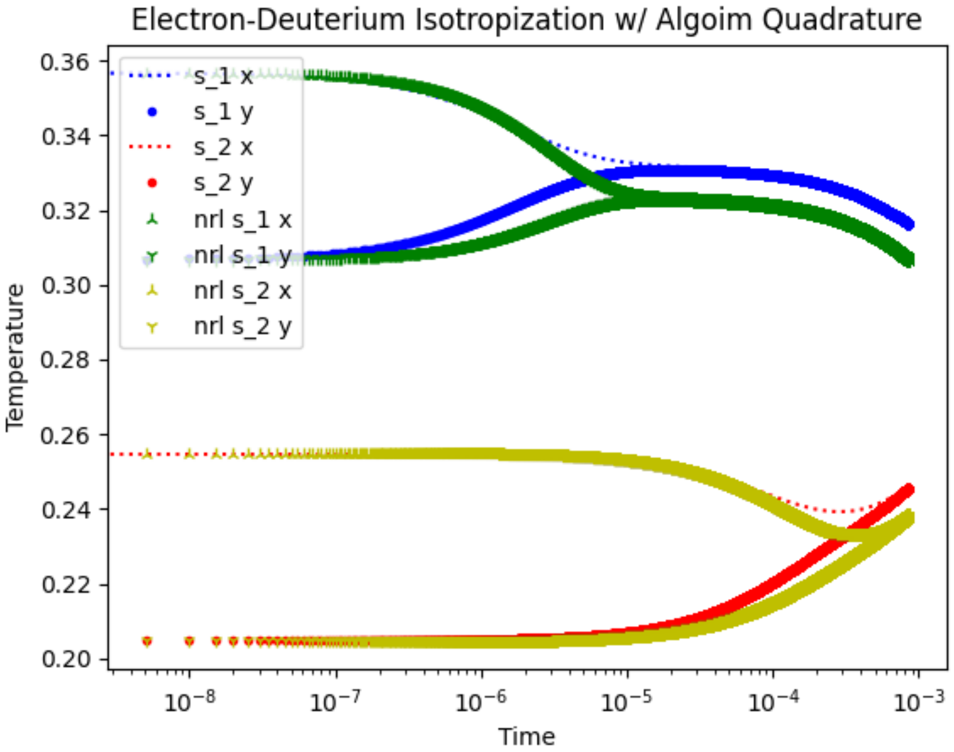




Pusztay, Zonta, Knepley, Adams, Paticle Basis Landau Collisions in PETSc PIC (in preparation)

Isotropization





Conclusion

- Conservative implementation from Adams et all in FE basis
  - Highly optimized
  - Multispecies support
- Conservative implementation in particle basis implementation underway
  - Undergoing optimization process
  - Multispecies support
- Monolithic system is a subject of future development
  - Relaxation RK, Monolithic Discrete Gradients

Regularized Entropy Form

- Cast as advective
- Particle basis entropy functional non smooth/continuous
- Mollify with smooth RBF

$$\frac{\partial f}{\partial t} = \frac{\partial}{\partial v} \cdot \int_{\Omega} Q(v - \bar{v})\{f(\bar{v})\frac{\partial f}{\partial v} - f(v)\frac{\partial f}{\partial \bar{v}}\}$$

$$\partial_v f = f\partial_v lnf = -f\partial_v \frac{\delta S}{\delta f}$$

$$S = -\int_{\Omega} flnf$$

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial v} \cdot (Ff) = 0$$

$$F(v_p) = \sum_{\bar{p}} w_{\bar{p}} Q(v_p - v_{\bar{p}})\{\frac{\partial}{\partial v_p}\frac{\delta S}{\delta f} - \frac{\partial}{\partial v_{\bar{p}}}\frac{\partial S}{\partial f}\}$$

$$\psi_\epsilon = \frac{1}{2\pi\epsilon} e^{\frac{-(v^2)}{2\epsilon}}$$

$$f * \psi = \int_{\Omega} \psi(v)f(v)dv$$

$$S[f * \psi_\epsilon] = -\int_{\Omega} f * \psi_\epsilon lnf * \psi_\epsilon$$

$$S_h = -\int_{\Omega} \psi_\epsilon ln \sum w\psi_\epsilon$$