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Conservative discretization of the Landau collision integral

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We describe a density, momentum, and energy conserving discretization of the nonlinear Landau collision integral. Our algorithm is suitable for both the finite-element and discontinuous Galerkin methods and does not require structured meshes. The conservation laws for the discretization are proven algebraically and demonstrated numerically for an axially symmetric nonlinear relaxation problem.

I. INTRODUCTION

Development of state-of-the-art numerical methods in plasma physics is set firmly on a course towards structure-preserving algorithms, and for an important reason. It is well known that integration of Hamiltonian systems with non-structure-preserving methods leads to numerical dissipation and, possibly, to false interpretation of the simulation results. For example, non-structure-preserving discretization of ideal MHD can lead to solutions that display reconnection, and tracing the full Larmor motion of charged particles with standard Runge-Kutta methods can lead to false changes in the orbit topologies. Naturally, one would prefer the discretizations to preserve the properties the continuous systems possess.

For many of the purely Hamiltonian or variational systems in plasma physics, recent research has indeed provided structure-preserving discretization methods¹⁻⁷. Yet dissipative effects reside on a largely uncharted territory: the *structure*, as it is understood for Hamiltonian or variational systems, is not that well understood for general dissipative systems. Exceptions do exist and, considering Coulomb collisions, the Landau collision integral⁸ can, in fact, be described in terms of a symmetric *metric* bracket⁹. Unfortunately, it is not clear yet how this specific bracket should be discretized to preserve the underlying structural properties.

Until an appropriate discretization of the metriplectic formulation is discovered, one could consider using a discrete version of the *Lagrange-d'Alembert principle* to embed a discrete Landau collision integral into structure preserving discretizations of the Vlasov-Maxwell system. Furthermore, as finite-element and discontinuous Galerkin methods are receiving increasing attention for addressing the Vlasov-Maxwell part of the kinetic system, we find it appealing to study how these two methods would adapt to the Landau collision integral.

The result we provide in this paper is a proof that discretization of the nonlinear Landau collision integral, either with the standard finite-element or discontinuous Galerkin method, indeed guarantees exact discrete conservation laws for density, momentum, and energy. As

we shall show, the only requirement is to retain the Landau's original integral formulation and not resort to the Rosenbluth-MacDonald-Judd potential formulation¹⁰: while the potential formulation is efficient in decreasing the numerical burden of evaluating the collision integral from $\mathcal{O}(N^2)$ down to $\mathcal{O}(N \log N)$, it simultaneously destroys numerical conservation laws so that artificial modification of the collision integral is necessary¹¹.

Although we focus purely on formulating an algorithm that delivers machine-precision conservation laws, we also note that the $\mathcal{O}(N^2)$ part of the algorithm belongs to the class of *embarrassingly parallel problems*. We thus expect our algorithm to scale well on highly vectorized platforms and, indeed, the feasibility of a (different) $\mathcal{O}(N^2)$ -algorithm has already been demonstrated^{12,13}.

The rest of the paper is following: The Landau collision integral and its properties are reviewed in Section II. The discretization, together with an algebraic proof of the related conservation laws, is detailed in Section III. In Section IV, the claimed properties are demonstrated numerically for an axially symmetric relaxation problem, and a summary of the results is given in Section V.

II. THE LANDAU COLLISION INTEGRAL

For clarity, we consider the like-species collisions, while the results generalize for multi-species collisions as well. Next, we review the explicit form of the collision integral, normalize it to dimensionless variables, and discuss the collisional invariants.

A. Single species collision operator

Under small-angle dominated Coulomb collisions, the evolution of the distribution function $f(t, \mathbf{u})$ in velocity space $\mathbf{u} \in \mathbb{R}^3$ is determined by the integro-differential equation⁸

$$\frac{\partial f}{\partial t} = \frac{\Gamma}{2m^2} \frac{\partial}{\partial \mathbf{u}} \cdot \int_{\mathbb{R}^3} d\bar{\mathbf{u}} \mathbf{U}(\mathbf{u}, \bar{\mathbf{u}}) \cdot \left(\bar{f} \frac{\partial f}{\partial \mathbf{u}} - f \frac{\partial \bar{f}}{\partial \bar{\mathbf{u}}} \right). \quad (1)$$

Here $\Gamma = e^4 \ln \Lambda / (4\pi \epsilon_0^2)$ can be considered a reference collision frequency, $\ln \Lambda$ is the Coulomb logarithm, e and m are the charge and mass, and $\mathbf{u} = \mathbf{p}/m$ is the

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momentum-per-rest-mass. The quantities with an overbar are evaluated at $\bar{\mathbf{u}}$.

The Landau tensor $\mathbf{U}(\mathbf{u}, \bar{\mathbf{u}})$, valid at non-relativistic energies, is a scaled projection matrix of the relative velocity $\mathbf{u} - \bar{\mathbf{u}}$ between the colliding particles:

$$\mathbf{U} = \frac{1}{|\mathbf{u} - \bar{\mathbf{u}}|^3} (|\mathbf{u} - \bar{\mathbf{u}}|^2 \mathbf{I} - (\mathbf{u} - \bar{\mathbf{u}})(\mathbf{u} - \bar{\mathbf{u}})). \quad (2)$$

In the relativistic case, the correct expression for the tensor $\mathbf{U}(\mathbf{u}, \bar{\mathbf{u}})$ was derived by Beliaev and Budker¹⁴

$$\mathbf{U}_{\text{BB}} = \frac{r^2}{\gamma \bar{\gamma} w^3} (w^2 \mathbf{I} - \mathbf{u}\mathbf{u} - \bar{\mathbf{u}}\bar{\mathbf{u}} + r(\mathbf{u}\bar{\mathbf{u}} + \bar{\mathbf{u}}\mathbf{u})), \quad (3)$$

where $r = \gamma \bar{\gamma} - \mathbf{u} \cdot \bar{\mathbf{u}}/c^2$, $w = c\sqrt{r^2 - 1}$, $\gamma = \sqrt{1 + u^2/c^2}$, $\bar{\gamma} = \sqrt{1 + \bar{u}^2/c^2}$, and c is the speed of light. In the limit $c \rightarrow \infty$, the Beliaev-Budker tensor \mathbf{U}_{BB} reduces to Landau tensor and the relativistic momenta, normalized to the rest mass, reduce to the non-relativistic expressions for velocities.

Although the focus of this paper is the nonrelativistic limit, we will show that standard finite-element or discontinuous Galerkin discretization of the relativistic collision integral will lead to exact density and momentum conservation while exact energy conservation would require development of a completely new set of basis functions.

B. Normalization

In numerical applications, one should always work in dimensionless variables to prevent accumulation of floating point errors. This is achieved by defining $\mathbf{x} = \mathbf{u}/c$ and $\bar{\mathbf{x}} = \bar{\mathbf{u}}/c$ with c some positive constant denoting a reference velocity. In the relativistic case c would naturally denote the speed of light but for the nonrelativistic case, it can be considered arbitrary, e.g., the thermal velocity. Obviously, \mathbf{x} , $\bar{\mathbf{x}}$ are not to be misunderstood as the configuration space variables.

The velocity-space gradients and differential volume elements transform according to

$$\partial/\partial\mathbf{u} = c^{-1}\nabla, \quad \partial/\partial\bar{\mathbf{u}} = c^{-1}\bar{\nabla}, \quad (4)$$

$$d\mathbf{u} = c^3 d\mathbf{x}, \quad d\bar{\mathbf{u}} = c^3 d\bar{\mathbf{x}}, \quad (5)$$

while the tensor \mathbf{U} transforms according to

$$\mathbf{U}(\mathbf{u}, \bar{\mathbf{u}}) = c^{-1}\mathbf{U}(\mathbf{x}, \bar{\mathbf{x}}). \quad (6)$$

Further, we normalize time according to

$$t = \frac{8\pi\epsilon_0^2 m^2}{e^4 \ln \Lambda} \tau, \quad (7)$$

so that the normalized Landau integral equation becomes

$$\frac{\partial f}{\partial \tau} = \nabla \cdot \int_{\mathbb{R}^3} d\bar{\mathbf{x}} \mathbf{U}(\mathbf{x}, \bar{\mathbf{x}}) \cdot (\bar{f}\nabla f - f\bar{\nabla}\bar{f}). \quad (8)$$

C. Conservation laws

Without loss of generality, we define a domain Ω and require that f vanishes at the boundary $\partial\Omega$. Additionally, the normal component of the velocity-space flux

$$\mathbf{J}(\mathbf{x}) \equiv \int_{\Omega} d\bar{\mathbf{x}} \mathbf{U}(\mathbf{x}, \bar{\mathbf{x}}) \cdot (\bar{f}\nabla f - f\bar{\nabla}\bar{f}), \quad (9)$$

is required to vanish at the boundary $\partial\Omega$, to satisfy density conservation. Obviously, both these conditions are true if Ω is chosen to be \mathbb{R}^3 . In numerical implementations the domain Ω must, however, be finite and, thus, we use Ω as an arbitrary domain for now.

If we now multiply Eq.(8) with a function ϕ , and integrate over the domain Ω and apply the boundary conditions, we find

$$\int d\mathbf{x} \phi \frac{\partial f}{\partial \tau} = \int_{\Omega} d\mathbf{x} \nabla \phi \cdot \int_{\Omega} d\bar{\mathbf{x}} \mathbf{U} \cdot (f\bar{\nabla}\bar{f} - \bar{f}\nabla f). \quad (10)$$

Upon rearranging the integration order, one obtains

$$\int d\mathbf{x} \phi \frac{\partial f}{\partial \tau} = \frac{1}{2} \int_{\Omega} d\mathbf{x} \int_{\Omega} d\bar{\mathbf{x}} (\nabla \phi - \bar{\nabla} \bar{\phi}) \cdot \mathbf{U} \cdot (f\bar{\nabla}\bar{f} - \bar{f}\nabla f). \quad (11)$$

For $\phi(\mathbf{x}) \in \{1, \mathbf{x}\}$, the above expression obviously vanishes. Further, $(\nabla \mathcal{E}(\mathbf{x}) - \bar{\nabla} \mathcal{E}(\bar{\mathbf{x}})) \cdot \mathbf{U}(\mathbf{x}, \bar{\mathbf{x}})$ vanishes for both the non-relativistic energy $\mathcal{E}(\mathbf{x}) = x^2$ (with \mathbf{U} the Landau tensor) and the relativistic energy $\mathcal{E}(\mathbf{x}) = \sqrt{1 + x^2}$ (with \mathbf{U} the Beliaev-Budker tensor \mathbf{U}_{BB}), due to the properties of the tensor \mathbf{U} . Thus, the quantities $\int_{\Omega} d\mathbf{x} \phi f$ for $\phi(\mathbf{x}) \in \{1, \mathbf{x}, \mathcal{E}(\mathbf{x})\}$ are referred to as *collisional invariants*.

III. DISCRETIZATION

One of the challenges in discretizing the Landau operator is to preserve the collisional invariants that exist for the continuous operator. Here we prove that discretization of the weak formulation

$$\begin{aligned} \int_{\Omega} d\mathbf{x} \phi \frac{\partial f}{\partial \tau} &= \int_{\Omega} d\mathbf{x} \nabla \phi \cdot \mathbf{J}, \\ \mathbf{J} &= \int_{\Omega} d\bar{\mathbf{x}} \mathbf{U} \cdot (f\bar{\nabla}\bar{f} - \bar{f}\nabla f) \\ f(\mathbf{x}) &= 0, \quad \forall \mathbf{x} \in \partial\Omega \end{aligned} \quad (12)$$

with either finite-element or discontinuous Galerkin methods succeeds in this feat. While we provide the explicit proof for the full three-dimensional velocity-space operator, the result holds true also for the axisymmetric or spherically symmetric cases. We also note that weak discretization of the multispecies collision operator similarly satisfies the related conservation laws.

A. Time-continuous equation for the degrees-of-freedom

Choose a *finite*-dimensional vector space V_h spanned by the set $\{\lambda_\ell(\mathbf{x})\}_\ell$ and approximate $(f, \phi) \approx (f_h, \phi_h)$ according to

$$f_h(\mathbf{x}, \tau) = \sum_\ell F_\ell(\tau) \lambda_\ell(\mathbf{x}), \quad (13)$$

$$\phi_h(\mathbf{x}) = \sum_\ell \phi_\ell \lambda_\ell(\mathbf{x}). \quad (14)$$

Denote also $F = \{F_\ell\}_\ell$ for convenience. Define the vector- and tensor-valued functionals

$$\mathbf{K}[F](\tau, \mathbf{x}) = \sum_\ell F_\ell(\tau) \mathbf{K}_\ell(\mathbf{x}), \quad (15)$$

$$\mathbf{D}[F](\tau, \mathbf{x}) = \sum_\ell F_\ell(\tau) \mathbf{D}_\ell(\mathbf{x}) \quad (16)$$

in terms of the vectors \mathbf{K}_ℓ and the tensors \mathbf{D}_ℓ

$$\mathbf{K}_\ell(\mathbf{x}) = \int_\Omega d\bar{\mathbf{x}} \mathbf{U}(\mathbf{x}, \bar{\mathbf{x}}) \cdot \bar{\nabla} \bar{\lambda}_\ell(\bar{\mathbf{x}}), \quad (17)$$

$$\mathbf{D}_\ell(\mathbf{x}) = \int_\Omega d\bar{\mathbf{x}} \mathbf{U}(\mathbf{x}, \bar{\mathbf{x}}) \bar{\lambda}_\ell(\bar{\mathbf{x}}) \quad (18)$$

Substitute f_h and ϕ_h into Eq. (12) to obtain the discretized time-continuous weak formulation

$$\sum_{ij} \phi_i \mathcal{M}_{ij} \frac{\partial F_j}{\partial \tau} = \sum_{ij} \phi_i \mathcal{C}_{ij}[F] F_j, \quad (19)$$

where the coefficients matrices are defined

$$\mathcal{M}_{ij} = \int_\Omega d\mathbf{x} \lambda_i \lambda_j, \quad (20)$$

$$\mathcal{C}_{ij}[F] = \int_\Omega d\mathbf{x} \nabla \lambda_i \cdot (\mathbf{K}[F] \lambda_j - \mathbf{D}[F] \cdot \nabla \lambda_j), \quad (21)$$

Since the discrete weak form (19) is to hold for arbitrary functions $\phi \in V_h$, we obtain the following nonlinear system of ordinary differential equations for the degrees-of-freedom F

$$\sum_j \mathcal{M}_{ij} \frac{\partial F_j}{\partial \tau} = \sum_j \mathcal{C}_{ij}[F] F_j, \quad \forall i. \quad (22)$$

B. Discrete conservation laws

If the vector space V_h is chosen so that the functions $\phi(\mathbf{x}) = \{1, \mathbf{x}, \mathcal{E}(\mathbf{x})\}$ are included in V_h exactly, i.e., $\phi(\mathbf{x}) \equiv \sum_i \phi_i \lambda_i(\mathbf{x})$, the weak discretization will automatically satisfy the conservation laws.

Consider the time rate of change of ϕ -moment of the numerical distribution function f_h . As long as ϕ belongs to V_h exactly, we can write

$$\int d\mathbf{x} \phi \frac{\partial f_h}{\partial \tau} = \sum_{ij} \phi_i \mathcal{M}_{ij} \frac{\partial F_j}{\partial t} = \sum_{ij} \phi_i \mathcal{C}_{ij}[F] F_j. \quad (23)$$

Let us then assume that a quadrature rule is used to approximate integrals over the domain Ω , with weights w_q and points $\boldsymbol{\xi}_q$. The vector $\sum_j \mathcal{C}_{ij}[F] F_j$ can then be evaluated as

$$\sum_j \mathcal{C}_{ij}[F] F_j = \sum_{j,q} w_q F_j \nabla \lambda_i(\boldsymbol{\xi}_q) \cdot \left(\mathbf{K}[F](\boldsymbol{\xi}_q) \lambda_j(\boldsymbol{\xi}_q) - \mathbf{D}[F](\boldsymbol{\xi}_q) \cdot \nabla \lambda_j(\boldsymbol{\xi}_q) \right). \quad (24)$$

The expressions for $\mathbf{K}[F]$ and $\mathbf{D}[F]$ at the points $\boldsymbol{\xi}_q$ are obtained using the same quadrature rule

$$\mathbf{K}[F](\boldsymbol{\xi}_q) = \sum_{\ell,p} w_p \mathbf{U}(\boldsymbol{\xi}_q, \boldsymbol{\xi}_p) \cdot \nabla \lambda_\ell(\boldsymbol{\xi}_p) F_\ell, \quad (25)$$

$$\mathbf{D}[F](\boldsymbol{\xi}_q) = \sum_{\ell,p} w_p \mathbf{U}(\boldsymbol{\xi}_q, \boldsymbol{\xi}_p) \lambda_\ell(\boldsymbol{\xi}_p) F_\ell, \quad (26)$$

and, when substituted to the expression for $\sum_j \mathcal{C}_{ij}[F] F_j$, we find

$$\begin{aligned} & \sum_j \mathcal{C}_{ij}[F^{(k)}] F_j^{(k)} \\ &= \sum_{j\ell,pq} w_p w_q F_\ell F_j \nabla \lambda_i(\boldsymbol{\xi}_q) \cdot \mathbf{U}(\boldsymbol{\xi}_q, \boldsymbol{\xi}_p) \\ & \quad \cdot \left(\nabla \lambda_\ell(\boldsymbol{\xi}_p) \lambda_j(\boldsymbol{\xi}_q) - \lambda_\ell(\boldsymbol{\xi}_p) \nabla \lambda_j(\boldsymbol{\xi}_q) \right). \end{aligned} \quad (27)$$

Since this expression is antisymmetric with respect to changing $j \leftrightarrow \ell$ and $p \leftrightarrow q$, we obtain

$$\begin{aligned} & \sum_{ij} \phi_i \mathcal{C}_{ij}[F^{(k)}] F_j^{(k)} \\ &= \frac{1}{2} \sum_{ij\ell,pq} w_p w_q F_\ell F_j \phi_i \left(\nabla \lambda_i(\boldsymbol{\xi}_q) - \nabla \lambda_i(\boldsymbol{\xi}_p) \right) \\ & \quad \cdot \mathbf{U}(\boldsymbol{\xi}_q, \boldsymbol{\xi}_p) \cdot \left(\nabla \lambda_\ell(\boldsymbol{\xi}_p) \lambda_j(\boldsymbol{\xi}_q) - \lambda_\ell(\boldsymbol{\xi}_p) \nabla \lambda_j(\boldsymbol{\xi}_q) \right). \end{aligned} \quad (28)$$

The exact conservation laws then follow trivially since

$$\sum_i \phi_i \left(\nabla \lambda_i(\boldsymbol{\xi}_q) - \nabla \lambda_i(\boldsymbol{\xi}_p) \right) \cdot \mathbf{U}(\boldsymbol{\xi}_q, \boldsymbol{\xi}_p), \quad (29)$$

vanishes identically for $\sum_i \phi_i \lambda_i(\mathbf{x}) \equiv \{1, \mathbf{x}, \mathcal{E}(\mathbf{x})\}$.

Here we wish to note that, in the nonrelativistic limit, the energy $\mathcal{E}(\mathbf{x}) = x^2$ is a polynomial, and can be exactly expressed with piecewise polynomials of order 2. Thus a standard finite-element or discontinuous Galerkin method will have no trouble satisfying the conservation laws. In the relativistic case, the energy $\mathcal{E}(\mathbf{x}) = \sqrt{1 + x^2}$ is, however, not a polynomial and cannot be exactly presented by piecewise polynomials of any order. Thus, standard finite-element or discontinuous Galerkin method will not achieve exact energy conservation in the relativistic case, although one could still expect the error to converge at the order of the basis functions.

C. A note on discretizing time

Although our purpose is not to focus on the time discretization – it should be chosen consistently with the discretization of the Vlasov-Maxwell part – the ordinary differential equation for the degrees-of-freedom will be nonlinear and stiff due to the presence of both advective and diffusive components, necessitating implicit time discretization and iterative methods. Here we comment on the importance of solving the nonlinear time-discrete equation exactly.

Consider Eq. (22) and assume we solve it using implicit Euler. Denote $F_\ell(\tau_k) = F_\ell^{(k)}$ so that

$$\frac{\partial F_\ell}{\partial \tau}(\tau_k) \approx \frac{F_\ell^{(k)} - F_\ell^{(k-1)}}{\delta \tau} \quad (30)$$

The time discrete equation for the degrees-of-freedom then becomes

$$\sum_j \mathcal{M}_{ij} \left(F_j^{(k)} - F_j^{(k-1)} \right) = \delta \tau \sum_j \mathcal{C}_{ij}[F^{(k)}] F_j^{(k)}, \quad \forall i. \quad (31)$$

Assume then that the iterative method provides us with a solution vector \tilde{F} that satisfies

$$\sum_j \mathcal{M}_{ij} \left(\tilde{F}_j - F_j^{(k-1)} \right) = \delta \tau \sum_j \mathcal{C}_{ij}[\tilde{F}] \tilde{F}_j + \epsilon_i, \quad \forall i \quad (32)$$

where $\epsilon = \{\epsilon_i\}_i$ is the residual from the iteration. For the collisional invariants $\phi(\mathbf{x}) \in \{1, \mathbf{x}, \mathcal{E}(\mathbf{x})\}$, we then have

$$\sum_{ij} \phi_i \mathcal{M}_{ij} \left(\tilde{F}_j - F_j^{(k-1)} \right) = \sum_i \phi_i \epsilon_i \leq |\epsilon|_\infty |\phi|_\infty. \quad (33)$$

The exactness of the conservation properties for the discretized collision operator thus depends only on the accuracy of the nonlinear solve.

IV. NUMERICAL EXAMPLE

For demonstration purposes we consider the relaxation of a nonrelativistic axially symmetric bi-Maxwellian distribution function

$$f(\mathbf{x}) = \frac{1}{2} (\pi \sigma^2)^{-3/2} \left[\exp\left(-\frac{r^2 + z^2}{\sigma^2}\right) + \exp\left(-\frac{r^2 + (z - 0.5)^2}{\sigma^2}\right) \right], \quad (34)$$

using cylindrical coordinates $\mathbf{x} = (r, \theta, z)$ that relate to cartesian coordinates according to $(x, y, z) = (r \cos \theta, r \sin \theta, z)$. For the computational domain we choose $\Omega = \{(r, z) \mid 0 \leq r \leq L, -L \leq z \leq L\}$ with $L = 2$. The parameter $\sigma = 1/\sqrt{20}$ is chosen so that the initial distribution f can be considered negligible at the Dirichlet boundary $\partial\Omega_D = \{(r, z) \mid z = \pm L \vee r = L\}$.

For the velocity-space discretization, we choose quadratic P2-Lagrange elements, while time is discretized with the Crank-Nicolson method. The resulting nonlinear system is solved with Newton iteration, using a numerical estimate for the system Jacobian matrix. Because we do not have an exact linearization of the Jacobian we only observe linear convergence in the Newton iteration, with a residual reduction rate of 0.16 for this specific problem. The mesh is generated with the open-source GMSH¹⁵ software, and the rest of the implementation is carried out within the PETSc^{16,17} framework, using PETSc PLEX for the finite-element operations and PETScs SNES for the nonlinear solver. The axially symmetric weak formulation is detailed in the Appendix and the source code for the test problem, written in C, will be made available online through `git`.

The time evolution of the distribution function is illustrated in Fig. 1, for six different time instances, while the evolution of momentum and energy are quantified in tables I and II for different nonlinear solver tolerances. The bi-Maxwellian distribution relaxes towards an equilibrium state in a qualitatively correct manner and, if the tolerance for the nonlinear solve is set to machine precision, energy and momentum are conserved to machine precision. Otherwise the errors in energy and momentum accumulate through time with a rate that correlates with the nonlinear solver tolerance.

V. SUMMARY

We have presented an algorithm for conservative discretization of the nonlinear Landau collision integral. We have provided both algebraic and numerical proof for achieving exact numerical conservation laws using either discontinuous Galerkin or standard finite-element method. Our method is not constrained by details of the discretization, admitting the use of structured as well as unstructured meshes. We have also argued that in the relativistic case, a polynomial basis of any order is not able to guarantee exact conservation of energy while density and momentum would be conserved even with linear basis functions. Future study will investigate the embedding of our discrete Landau operator to the Vlasov-Maxwell system using either the concept of Lagrange-d'Alembert principle or extended Lagrangians¹⁸. Another future study will focus on performance demonstrations.

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patience Prof. Matthew Knepley sustained while providing answers to all of our questions related to the use of PETS_c.

Appendix: Axially symmetric weak formulation

Using cylindrical coordinates $\mathbf{x} = (r, \theta, z)$, that relate to cartesian coordinates according to $(x, y, z) = (r \cos \theta, r \sin \theta, z)$, and assuming axially symmetric vector space V_h , i.e., $\partial f / \partial \theta = 0$ and $\partial \phi / \partial \theta = 0$, the weak formulation can be written

$$2\pi \int_{\Omega} dr dz r \phi \partial_{\tau} f = \int_{\Omega} dr dz r \partial_{\alpha} \phi (K^{\alpha} f - D^{\alpha\beta} \partial_{\beta} f) \quad (\text{A.1})$$

where the friction and diffusion coefficients are

$$K^{\alpha} = \int_{\Omega} d\bar{r} d\bar{z} \bar{r} U^{\alpha\bar{\beta}} \partial_{\bar{\beta}} \bar{f} \quad (\text{A.2})$$

$$D^{\alpha\beta} = \int_{\Omega} d\bar{r} d\bar{z} \bar{r} U^{\alpha\beta} \bar{f}, \quad (\text{A.3})$$

and the coefficients $U^{\alpha\beta}$ and $U^{\alpha\bar{\beta}}$ are defined

$$U^{\alpha\beta} = \int_0^{2\pi} \int_0^{2\pi} d\theta d\bar{\theta} \nabla x^{\alpha} \cdot \mathbf{U} \cdot \nabla x^{\beta} \quad (\text{A.4})$$

$$U^{\alpha\bar{\beta}} = \int_0^{2\pi} \int_0^{2\pi} d\theta d\bar{\theta} \nabla x^{\alpha} \cdot \mathbf{U} \cdot \bar{\nabla} \bar{x}^{\beta}. \quad (\text{A.5})$$

The expressions ∇x^{α} are the contravariant basis vectors for the curvilinear coordinate system.

For the nonrelativistic case, the angular integrals of $\nabla x^{\alpha} \cdot \mathbf{U} \cdot \nabla x^{\beta}$ are easily computed. Defining a parameter

$$s(r, z, \bar{r}, \bar{z}) = \frac{2r\bar{r}}{r^2 + \bar{r}^2 + (z - \bar{z})^2}, \quad (\text{A.6})$$

the exact expressions are

$$U^{rr} = 4\pi \left(\frac{s}{2r\bar{r}} \right)^{3/2} (\bar{r}^2 \mathcal{I}_1 + (z - \bar{z})^2 \mathcal{I}_2) \quad (\text{A.7})$$

$$U^{rz} = 4\pi \left(\frac{s}{2r\bar{r}} \right)^{3/2} (\bar{z} - z)(r\mathcal{I}_2 - \bar{r}\mathcal{I}_3) \quad (\text{A.8})$$

$$U^{zr} = U^{rz} \quad (\text{A.9})$$

$$U^{zz} = 4\pi \left(\frac{s}{2r\bar{r}} \right)^{3/2} ((r^2 + \bar{r}^2)\mathcal{I}_2 - 2r\bar{r}\mathcal{I}_3) \quad (\text{A.10})$$

$$U^{r\bar{r}} = 4\pi \left(\frac{s}{2r\bar{r}} \right)^{3/2} ((z - \bar{z})^2 \mathcal{I}_3 + r\bar{r}\mathcal{I}_1) \quad (\text{A.11})$$

$$U^{r\bar{z}} = U^{rz} \quad (\text{A.12})$$

$$U^{z\bar{r}} = 4\pi \left(\frac{s}{2r\bar{r}} \right)^{3/2} (\bar{z} - z)(r\mathcal{I}_3 - \bar{r}\mathcal{I}_2) \quad (\text{A.13})$$

$$U^{z\bar{z}} = U^{zz} \quad (\text{A.14})$$

where the integrals $\mathcal{I}(s)$ are defined

$$\mathcal{I}_1(s) = \int_{-1}^1 (1-x^2)^{1/2} (1-sx)^{-3/2} dx \quad (\text{A.15})$$

$$\mathcal{I}_2(s) = \int_{-1}^1 (1-x^2)^{-1/2} (1-sx)^{-3/2} dx \quad (\text{A.16})$$

$$\mathcal{I}_3(s) = \int_{-1}^1 x(1-x^2)^{-1/2} (1-sx)^{-3/2} dx \quad (\text{A.17})$$

and can be expressed in terms of the complete elliptic integrals $E[s]$ and $K[s]$ according to

$$\mathcal{I}_1(s) = \frac{4}{s^2 \sqrt{1+s}} \left(K \left[\frac{2s}{1+s} \right] - (1+s)E \left[\frac{2s}{1+s} \right] \right), \quad (\text{A.18})$$

$$\mathcal{I}_2(s) = \frac{2}{(1-s)\sqrt{1+s}} E \left[\frac{2s}{1+s} \right], \quad (\text{A.19})$$

$$\mathcal{I}_3(s) = \frac{2}{(1-s)s\sqrt{1+s}} \left(E \left[\frac{2s}{1+s} \right] - (1-s)K \left[\frac{2s}{1+s} \right] \right) \quad (\text{A.20})$$

¹Hong Qin and Xiaoyin Guan. Variational symplectic integrator for long-time simulations of the guiding-center motion of charged particles in general magnetic fields. *Phys. Rev. Lett.*, 100:035006, Jan 2008.

²J. Squire, H. Qin, and W. M. Tang. Geometric integration of the Vlasov-Maxwell system with a variational particle-in-cell scheme. *Physics of Plasmas*, 19(8):084501, 2012.

³Michael Kraus. *Variational Integrators in Plasma Physics*. PhD thesis, Technische Universität München, 2013.

⁴C Leland Ellison, J M Finn, H Qin, and W M Tang. Development of variational guiding center algorithms for parallel calculations in experimental magnetic equilibria. *Plasma Physics and Controlled Fusion*, 57(5):054007, 2015.

⁵Hong Qin, Jian Liu, Jianyuan Xiao, Ruili Zhang, Yang He, Yulei Wang, Yajuan Sun, Joshua W. Burby, Leland Ellison, and Yao Zhou. Canonical symplectic particle-in-cell method for long-term large-scale simulations of the vlasov-maxwell equations. *Nuclear Fusion*, 56(1):014001, 2016.

⁶Yang He, Yajuan Sun, Hong Qin, and Jian Liu. Hamiltonian particle-in-cell methods for Vlasov-Maxwell equations. *Physics of Plasmas*, 23(9):092108, 2016.

⁷Yao Zhou, Yi-Min Huang, Hong Qin, and A. Bhattacharjee. Formation of current singularity in a topologically constrained plasma. *Phys. Rev. E*, 93:023205, Feb 2016.

⁸L.D. Landau. The kinetic equation in the case of Coulomb interaction (translated from German). *Zh. Eksper. i Teoret. Fiz.*, 7:203–209, 1937.

⁹P. J. Morrison. A paradigm for joined Hamiltonian and dissipative systems. *Physica D Nonlinear Phenomena*, 18:410–419, January 1986.

¹⁰Marshall N. Rosenbluth, William M. MacDonald, and David L. Judd. Fokker-planck equation for an inverse-square force. *Phys. Rev.*, 107:1–6, Jul 1957.

¹¹W.T. Taitano, L. Chacón, A.N. Simakov, and K. Molvig. A mass, momentum, and energy conserving, fully implicit, scalable algorithm for the multi-dimensional, multi-species Rosenbluth–Fokker–Planck equation. *Journal of Computational Physics*, 297:357–380, 2015.

¹²E. S. Yoon and C. S. Chang. A Fokker-Planck-Landau collision equation solver on two-dimensional velocity grid and its application to particle-in-cell simulation. *Physics of Plasmas*, 21(3):032503, 2014.

- ¹³Robert Hager, E.S. Yoon, S. Ku, E.F. D’Azevedo, P.H. Worley, and C.S. Chang. A fully non-linear multi-species Fokker–Planck–Landau collision operator for simulation of fusion plasma. *Journal of Computational Physics*, 315:644–660, 2016.
- ¹⁴S. T. Beliaev and G. I. Budker. The Relativistic Kinetic Equation. *Soviet Physics Doklady*, 1:218, Oct 1956.
- ¹⁵C. Geuzaine and J.-F. Remacle. Gmsh: a three-dimensional finite element mesh generator with built-in pre- and post-processing facilities. *International Journal for Numerical Methods in Engineering*, 79:1309–1331, 2009.
- ¹⁶Satish Balay, Shirang Abhyankar, Mark F. Adams, Jed Brown, Peter Brune, Kris Buschelman, Lisandro Dalcin, Victor Eijkhout, William D. Gropp, Dinesh Kaushik, Matthew G. Knepley, Lois Curfman McInnes, Karl Rupp, Barry F. Smith, Stefano Zampini, Hong Zhang, and Hong Zhang. PETSc users manual. Technical Report ANL-95/11 - Revision 3.7, Argonne National Laboratory, 2016.
- ¹⁷Satish Balay, Shirang Abhyankar, Mark F. Adams, Jed Brown, Peter Brune, Kris Buschelman, Lisandro Dalcin, Victor Eijkhout, William D. Gropp, Dinesh Kaushik, Matthew G. Knepley, Lois Curfman McInnes, Karl Rupp, Barry F. Smith, Stefano Zampini, Hong Zhang, and Hong Zhang. PETSc Web page. <http://www.mcs.anl.gov/petsc>, 2016.
- ¹⁸Michael Kraus and Omar Maj. Variational integrators for non-variational partial differential equations. *Physica D: Nonlinear Phenomena*, 310:37–71, 2015.

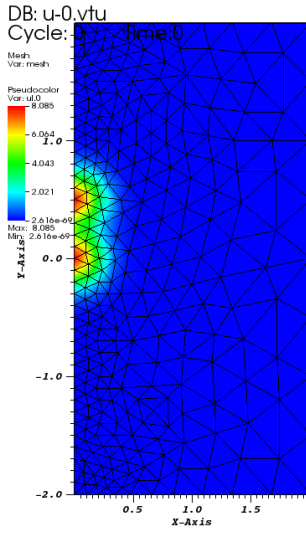
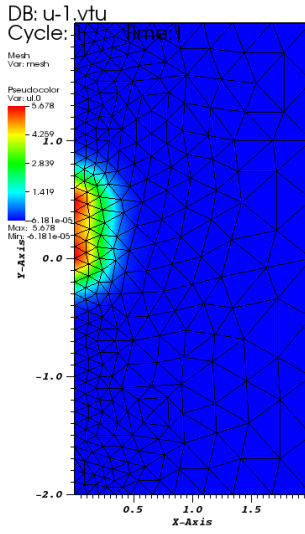
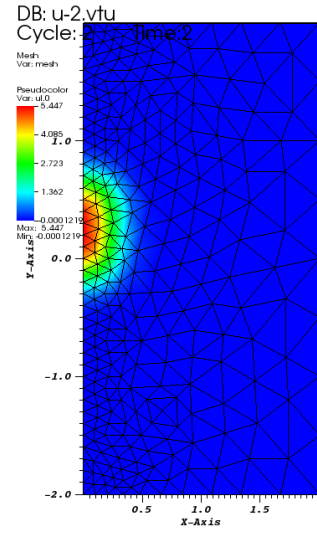
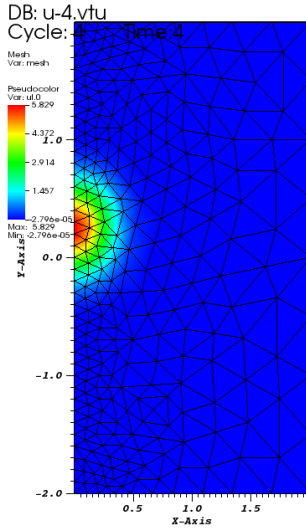
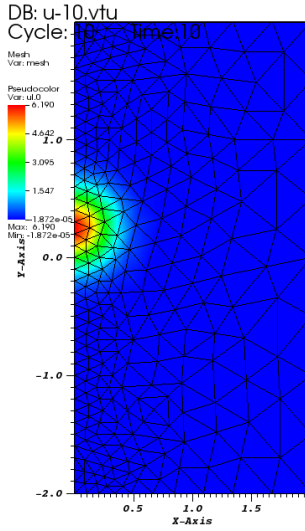
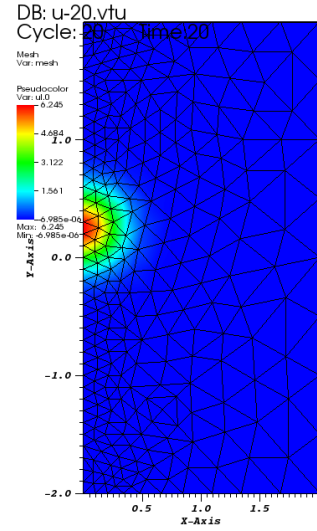
(a) $\tau = 0$ (b) $\tau = \delta\tau$ (c) $\tau = 2\delta\tau$ (d) $\tau = 4\delta\tau$ (e) $\tau = 10\delta\tau$ (f) $\tau = 20\delta\tau$

FIG. 1. Time slices of an initially bi-Maxwellian distribution function relaxing towards an equilibrium state.

TABLE I. Momentum conservation, measured with the innerproduct $\sum_{ij} \phi^i \mathcal{M}_{ij} F_j$ and $\phi = z$ for different nonlinear solver tolerances ϵ_{tol} . The incorrect digits are highlighted with red color.

| τ | $\epsilon_{\text{tol}} = 9.0\text{E-}01$ | $\epsilon_{\text{tol}} = 1.0\text{E-}06$ | $\epsilon_{\text{tol}} = 1.0\text{E-}14$ |
|--------|--|--|--|
| 0 | 3.97797664845241E-02 | 3.97797664845241E-02 | 3.97797664845248E-02 |
| 1 | 3.97791615978734E-02 | 3.97797664781777E-02 | 3.97797664845248E-02 |
| 2 | 3.97788912692161E-02 | 3.97797664743008E-02 | 3.97797664845247E-02 |
| 4 | 3.97786187222186E-02 | 3.97797664643968E-02 | 3.97797664845247E-02 |
| 10 | 3.97781761433900E-02 | 3.97797664423772E-02 | 3.97797664845247E-02 |
| 20 | 3.97775989653156E-02 | 3.97797663011934E-02 | 3.97797664845247E-02 |

TABLE II. Energy conservation, measured with the innerproduct $\sum_{ij} \phi^i \mathcal{M}_{ij} F_j$ and $\phi = r^2 + z^2$ for different nonlinear solver tolerances ϵ_{tol} . The incorrect digits are highlighted with red color.

| τ | $\epsilon_{\text{tol}} = 9.0\text{E-}01$ | $\epsilon_{\text{tol}} = 1.0\text{E-}06$ | $\epsilon_{\text{tol}} = 1.0\text{E-}14$ |
|--------|--|--|--|
| 0 | 3.17986788742740E-02 | 3.17986788742740E-02 | 3.17986788742740E-02 |
| 1 | 3.17606259814932E-02 | 3.17986790469298E-02 | 3.17986788742740E-02 |
| 2 | 3.17718385841557E-02 | 3.17986794847238E-02 | 3.17986788742741E-02 |
| 4 | 3.18140462853466E-02 | 3.17986808661484E-02 | 3.17986788742741E-02 |
| 10 | 3.18822521328414E-02 | 3.17986851426220E-02 | 3.17986788742741E-02 |
| 20 | 3.19077804661782E-02 | 3.17986927385047E-02 | 3.17986788742742E-02 |