Landau collision operator:

Stucture-preserving spatio-temporal methods

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Overview

- Energy, momentum, and density preservation can be achieved with a direct Galerkin discretization using a second order basis. This property translates also to temporal discretization as long as the nonlinear system of equations is solved to machine precision.
- Positivity preservation algebraically, without breaking the inherent conservation laws, has been a challenge.
- Exponential mapping of the distribution function together with so-called discrete gradient methods for temporal discretization, succeeds in providing the conservation laws, strict positivity, and a unique, physically exact equilibrium state.
- See arXiv:1804.08546 for the full story and a detailed list of relevant references.
1. Properties of the collision operator

2. Spatial discretization

3. Finite-dimensional metriplectic structure

4. Temporal discretization

5. Sparse system for iterative solution
Properties of the collision operator
A distribution function \( f(v, t) : \mathbb{R}^3 \times \mathbb{R}_{\geq 0} \mapsto \mathbb{R}_{\geq 0} \) is assumed to evolve according to the equation

\[
\frac{\partial f}{\partial t} = \frac{\partial}{\partial v} \cdot \int_{\mathbb{R}^3} Q(v - v') \cdot \left( f(v') \frac{\partial f}{\partial v} - f(v) \frac{\partial f}{\partial v'} \right) dv',
\]

(1)

corresponding to the dynamics driven by the nonlinear Landau collision operator. The dyad \( Q(\xi) = (I - \hat{\xi} \hat{\xi})/|\xi| \) in the above expression is an inversely scaled projection matrix with an eigenvector \( \xi \) corresponding to zero eigenvalue, and \( \hat{\xi} = \xi/|\xi| \).
A non-standard weak formulation of the problem

Given an arbitrary time-independent test function \( u(\mathbf{v}) \), the collisional relaxation problem can be formulated in a weak sense

\[
\frac{d}{dt} M(u, f) = C_f(u, \ln f). \tag{2}
\]

The symmetric, bilinear forms \( M \) and \( C_f \) are defined according to

\[
M(u, w) = \int_{\mathbb{R}^3} uw \, d\mathbf{v}, \tag{3}
\]

\[
C_f(u, w) = -\frac{1}{2} \int\int_{\mathbb{R}^3 \times \mathbb{R}^3} \left( \frac{\partial u}{\partial \mathbf{v}} - \frac{\partial u}{\partial \mathbf{v}'} \right) \cdot f(\mathbf{v}) Q(\mathbf{v} - \mathbf{v}') f(\mathbf{v}') \cdot \left( \frac{\partial w}{\partial \mathbf{v}} - \frac{\partial w}{\partial \mathbf{v}'} \right) \, d\mathbf{v} \, d\mathbf{v}'. \tag{4}
\]

The form \( C_f(u, w) \) is negative semidefinite, with a left-right null-space consisting of functions \( \phi = \{|\mathbf{v}|^2, \mathbf{v}, 1\} \).
Properties of the collision operator

The functions $\phi(v) = \{|v|^2, v, 1\}$ generate invariant forms $M(\phi, f)$ corresponding to conservation of energy, momentum and density.

The equilibrium condition $C_f(u, \ln f) = 0$, with respect to arbitrary $u$, requires that $\ln f$ is a linear combination of the functions $\phi = \{|v|^2, v, 1\}$, $f$ corresponding to a Maxwellian.

Since $M(1, f)$ is an invariant and $C_f(u, u) \leq 0$, one finds that $\partial_t M(−\ln f, f) \geq 0$, corresponding to entropy production.

Sign preservation: assuming $f$ to be at least twice differentiable and non-negative, then, at a point $v^*$ where $f(v^*) = 0$, $\partial_v f(v^*) = 0$, and $\partial_{vvv} f(v^*)$ is positive semi-definite, the evolution equation provides

$$\frac{\partial f(v^*)}{\partial t} = \int_{\mathbb{R}^3} Q(v^* - v') f(v') dv' : \frac{\partial^2 f(v^*)}{\partial v \partial v} \geq 0.$$  (5)
Spatial discretization
Introduce an exponentially-mapped Galerkin projection

Use the “$\ln f$ hint” in the weak formulation and choose an *ab initio* positive discretization

$$f_h = \exp(g_h), \quad g_h = \sum_{i \in I} g^i(t) \psi_i(v),$$

(6)

with $\{\psi_i\}_{i \in I}$ a second order Galerkin basis with compact support, and $\{g^i\}_{i \in I}$ the degrees of freedom for $g_h$.  

Finite-dimensional weak formulation using a test function $u = \psi_i$

$$\sum_{j \in I} M(\psi_i, f_h \psi_j) \frac{dg^j}{dt} = \sum_{j \in I} C_{f_h}(\psi_i, \psi_j) g^j, \quad \forall i \in I.$$  

(7)

Here, the integrals within the forms $M$ and $C_f$ are naturally limited to the domain of support for the basis. Also, note that the square matrices $M(\psi_i, f_h \psi_j)$ and $C_{f_h}(\psi_i, \psi_j)$ depend on the degrees of freedom via $f_h$, and that while $M(\psi_i, f_h \psi_j)$ is sparse, $C_{f_h}(\psi_i, \psi_j)$ is not.
Finite-dimensional collisional invariants

On the given mesh, the finite-dimensional versions of the energy, momentum, and density functionals can be written as

\[(E, P, N) = \sum_{i \in I} (e^i, v^i, 1^i) M(\psi_i, f_h).\]  \(\text{(8)}\)

The coefficients \(\{e^i\}_{i \in I}, \{v^i\}_{i \in I}, \text{ and } \{1^i\}_{i \in I}\) correspond to the expansion coefficients with respect to the chosen Galerkin basis for the functions \((|v|^2, v, 1), \text{ i.e.,}\)

\[|v|^2 = \sum_{i \in I} e^i \psi_i(v) \quad v = \sum_{i \in I} v^i \psi_i(v), \quad 1 = \sum_{i \in I} 1^i \psi_i(v).\]  \(\text{(9)}\)
The time derivatives of energy, momentum, and density vanish identically

\[
\frac{dE}{dt} = \sum_{i,j \in I} e^i M(\psi_i, f_h \psi_j) \frac{dg^j}{dt} = \sum_{j \in I} C_{f_h} \left( \sum_{i \in I} e^i \psi_i, \psi_j \right) g^j = 0, \quad (10)
\]

\[
\frac{dP}{dt} = \sum_{i,j \in I} v^i M(\psi_i, f_h \psi_j) \frac{dg^j}{dt} = \sum_{j \in I} C_{f_h} \left( \sum_{i \in I} v^i \psi_i, \psi_j \right) g^j = 0, \quad (11)
\]

\[
\frac{dN}{dt} = \sum_{i,j \in I} 1^i M(\psi_i, f_h \psi_j) \frac{dg^j}{dt} = \sum_{j \in I} C_{f_h} \left( \sum_{i \in I} 1^i \psi_i, \psi_j \right) g^j = 0. \quad (12)
\]

This follows from the equations of motion for the degrees of freedom (7), the bilinearity and the null-space of the form $C_f(u, w)$, and the requested property that the basis $\{\psi_i\}_{i \in I}$ reproduces quadratic functions exactly.
Note that $\{e^i\}_{i \in I}$, $\{v^i\}_{i \in I}$, and $\{1^i\}_{i \in I}$ are the only eigenvectors of the matrix $C_{f_h}(\psi_i, \psi_j)$, that correspond to zero eigenvalues.

Hence the equilibrium state $g^i_{eq}$ is a linear combination

$$g^i_{eq} = a e^i + b \cdot v^i + c 1^i,$$  \hspace{1cm} (13)

which, within the support of the Galerkin basis, corresponds to the numerical distribution function

$$f_{h,eq} = \exp \left( a |v|^2 + b \cdot v + c \right).$$  \hspace{1cm} (14)

Because the energy, momentum, and density are conserved, the coefficients $a$, $b$, and $c$ are uniquely determined in terms of the moments of a given initial state.
Note that the entropy $S = -\int f_h \ln f_h d\nu$ can be written as

$$S = -\sum_{i \in I} M(f_h, \psi_i) g^i.$$  \hspace{1cm} (15)

It's time derivative then becomes

$$\frac{dS}{dt} = -\sum_{i \in I} M(f_h, \psi_i) \frac{dg^i}{dt} - \sum_{i,j \in I} \frac{dg^j}{dt} M(\psi_j f_h, \psi_i) g^i$$

$$= -\frac{dN}{dt} - \sum_{i,j \in I} C_{f_h}(\psi_j, \psi_i) g^i g^j \geq 0.$$  \hspace{1cm} (16)

The last line follows from the density conservation and the fact that the form $C_f(u, w)$ is negative semidefinite, with the only nontrivial zero solution being a linear combination of the operator's null-space, corresponding to the equilibrium state.
Finite-dimensional metriplectic structure
Rearrange the finite-dimensional system of equations

Multiply (7) with the inverse of $M(\psi_i, f_h \psi_j)$

$$\frac{dg^k}{dt} = \sum_{i,j \in I} M^{-1}(\psi_i, f_h \psi_i) C_{f_h}(\psi_i, \psi_j) g^j, \quad \forall k \in I. \quad (17)$$

Use the finite-dimensional entropy (15), its derivative, and invert for

$$g^j + 1^j = - \sum_{\ell \in I} M^{-1}(\psi_j, f_h \psi_\ell) \frac{\partial S}{\partial g^\ell}, \quad \forall j \in I. \quad (18)$$

Use the fact that vector $1^j$ is an eigenvector of the matrix $C_{f_h}(\psi_i, \psi_j)$ with a zero eigenvalue, this gives

$$\frac{dg^k}{dt} = - \sum_{\ell \in I} G_{k\ell}(g) \frac{\partial S}{\partial g^\ell}, \quad \forall k \in I, \quad (19)$$

where we have collected the individual matrices together into

$$G_{k\ell}(g) = \sum_{i,j \in I} M^{-1}(\psi_k, f_h \psi_i) C_{f_h}(\psi_i, \psi_j) M^{-1}(\psi_j, f_h \psi_\ell). \quad (20)$$
Finite-dimensional metriplectic structure

Using the chain rule, time derivative of a generic function $U(g)$ becomes

$$\frac{dU}{dt} = - \sum_{k,\ell \in I} \frac{\partial U}{\partial g^k} G_{k\ell}(g) \frac{\partial S}{\partial g^\ell}, \quad \forall k \in I, \quad (21)$$

with the same matrix as previously

$$G_{k\ell}(g) = \sum_{i,j \in I} M^{-1}(\psi^k, f_h \psi^i) C_{f_h}(\psi^i, \psi^j) M^{-1}(\psi^j, f_h \psi^\ell). \quad (22)$$

The finite-dimensional metriplectic structure is then identified as

$$\frac{dU}{dt} = (U, -S) \quad (23)$$

where the bracket with respect to arbitrary functions $A(g)$ and $B(g)$ is

$$(A, B) = \sum_{k,\ell \in I} \frac{\partial A}{\partial g^k} G_{k\ell}(g) \frac{\partial B}{\partial g^\ell}, \quad \forall k \in I \quad (24)$$

The invariants are conserved and entropy produced as previously.
Temporal discretization
Discrete Gradient methods: generic recipe

Given $S(g)$, consider an ODE of the form

$$\frac{dg_k^k}{dt} = -\sum_{\ell \in I} G_{k\ell}(g) \frac{\partial S}{\partial g^\ell}, \quad \forall k \in I. \quad (25)$$

Denote time instances with $g(\delta t) = g_1$ and $g(0) = g_0$. Discrete gradient methods approximate the ODE according to

$$\frac{g_k^1 - g_k^0}{\delta t} = -\sum_{\ell \in I} \overline{G}_{k\ell}[g_0, g_1] \frac{\partial S}{\partial g^\ell}[g_0, g_1], \quad \forall k \in I. \quad (26)$$

The operator $\frac{\partial A}{\partial g^\ell}[g_0, g_1]$ is a discrete gradient and required to satisfy

$$\sum_{\ell \in I} \frac{\partial A}{\partial g^\ell}[g_0, g_1] (g_1^\ell - g_0^\ell) = A(g_1) - A(g_0), \quad \frac{\partial A}{\partial g^\ell}[g, g] = \frac{\partial A}{\partial g^\ell}(g). \quad (27)$$

Many such operators are known in the literature. Furthermore, requiring $\overline{G}_{k\ell}(g, g) = G_{k\ell}(g)$ guarantees that the limit $\delta t \to 0$ collapses (26) to the correct time-continuous ODE (25).
Using (27) and (26), the discrete evolution of a function $U(g)$ satisfies

$$U(g_1) - U(g_0) = -\delta t \sum_{k,\ell \in I} \frac{\partial U}{\partial g^k}[g_0, g_1] \overline{G}_{k\ell}[g_0, g_1] \frac{\partial S}{\partial g^\ell}[g_0, g_1].$$  

(28)

Hence, as long as the matrix operator $\overline{G}_{k\ell}[g_0, g_1]$ is negative semidefinite, entropy production will be guaranteed, according to

$$S(g_1) - S(g_0) = -\delta t \sum_{k,\ell \in I} \frac{\partial S}{\partial g^k}[g_0, g_1] \overline{G}_{k\ell}[g_0, g_1] \frac{\partial S}{\partial g^\ell}[g_0, g_1] \geq 0.$$

(29)

But what should the expression for $\overline{G}_{k\ell}[g_0, g_1]$ be? And how will it guarantee the energy, momentum, and density conservation?
For all invariants $C = (E, P, N)$, with $c^i = (e^i, v^i, 1^i)$, we have

$$\frac{\partial C}{\partial g^k} = \sum_{i \in I} c^i M(\psi_i, f_h \psi_k).$$  \hspace{1cm} (30)

A discrete gradient of the Casimirs is thus defined according to

$$\overline{\frac{\partial C}{\partial g^i}[g_0, g_1]} = \sum_{k \in I} c^k \overline{M}_{ki}[g_0, g_1],$$  \hspace{1cm} (31)

where $\overline{M}_{ki}[g_0, g_1]$ is required to satisfy $\overline{M}_{ki}[g, g] = M(\psi_i, f_h \psi_k)$. Hence the discrete evolution of the Casimirs satisfies

$$C(g_1) - C(g_0) = -\delta t \sum_{i \in I} \sum_{k, \ell \in I} c^i \overline{M}_{ik}[g_0, g_1] G_{k\ell}[g_0, g_1] \overline{\frac{\partial S}{\partial g^\ell}}[g_0, g_1].$$  \hspace{1cm} (32)
Discrete Gradient methods: Casimir invariance

To guarantee the invariance $C(g_1) - C(g_0) = 0$, we should choose

$$
\overline{G}_{k\ell}[g_0, g_1] = \sum_{i,j \in I} M^{-1}_{ki}[g_0, g_1] C_{fh}(\psi_i, \psi_j) \overline{M}^{-1}_{j\ell}[g_0, g_1], \quad (33)
$$

where $M^{-1}_{ij}[g_0, g_1]$ is the inverse of $M_{ij}[g_0, g_1]$. This satisfies also $\overline{G}_{k\ell}(g, g) = G_{k\ell}(g)$. The choice (33) then provides the desired result

$$
C(g_1) - C(g_0) = -\delta t \sum_{i \in I} \sum_{j, \ell \in I} c^i C_{fh}(\psi_i, \psi_j) \overline{M}^{-1}_{j\ell}[g_0, g_1] \frac{\partial S}{\partial g^\ell}[g_0, g_1] = 0,
$$

which follows from the property that the basis $\{\psi_i\}_{i \in I}$ can present the functions $\phi = \{|\psi|^2, \psi, 1\}$ exactly, and due to the null space of the form $C_f(u, w)$, which together lead to

$$
\sum_{i \in I} c^i C_{fh}(\psi_i, \psi_j) = 0, \quad \forall j \in I. \quad (35)
$$
For an equilibrium state to exist, one must have $g_1 = g_0 = g_{eq}$. This requirement, and the evolution equation (26), provides

$$\sum_{\ell \in I} G_{k\ell}[g_{eq}, g_{eq}] \frac{\partial S}{\partial g_{\ell}[g_{eq}, g_{eq}]} = 0, \quad \forall k \in I. \quad (36)$$

Next, using the defining properties $\frac{\partial S}{\partial g_{\ell}[g_{eq}, g_{eq}]} = \frac{\partial S}{\partial g_{\ell}(g_{eq})}$ and $G_{k\ell}[g_{eq}, g_{eq}] = G_{k\ell}(g_{eq})$, we obtain

$$\sum_{\ell \in I} G_{k\ell}(g_{eq}) \frac{\partial S}{\partial g_{\ell}(g_{eq})} = 0, \quad \forall k \in I. \quad (37)$$

From here the uniqueness of the equilibrium state follows trivially after using (18) and the null-space argument, leading to the observation that the numerical equilibrium state is given by

$$f_{h, eq}(v) = \exp(a|v|^2 + b \cdot v + c), \quad (38)$$
Sparse system for iterative solution
Use the second order $O(\delta t^2)$ average discrete gradient

$$\overline{\frac{\partial A}{\partial g^\ell}}[g_0, g_1] = \int_0^1 \frac{\partial A}{\partial g^\ell} ((1 - \xi)g_0 + \xi g_1) d\xi.$$  \hfill (39)

Define the short notations

$$g_{h0} = \sum_{k \in I} g_0^k \psi_k, \quad g_{h1} = \sum_{k \in I} g_1^k \psi_k.$$  \hfill (40)

Compute the matrix

$$\overline{M}_{ij}[g_0, g_1] = \int \psi_i \frac{\exp (g_{h0}) - \exp (g_{h1})}{g_{h0} - g_{h1}} \psi_j dv,$$  \hfill (41)

and the vector

$$\overline{\frac{\partial S - 1}{\partial g^\ell}}[g_0, g_1] = -\int \psi_\ell \frac{(g_{h0} - 1) \exp (g_{h0}) - (g_{h1} - 1) \exp (g_{h1})}{g_{h0} - g_{h1}} dv.$$  \hfill (42)
Put everything together and obtain a sparse iterable system

\[
\sum_{k \in I} \overline{M}_{ik}[g_0, g_1] \frac{g_1^k - g_0^k}{\delta t} = - \sum_{j \in I} C_{f_{h,1/2}}(\psi_i, \psi_j) F_j, \quad \forall i \in I,
\]

(43)

\[
\sum_{j \in I} \overline{M}_{ij}[g_0, g_1] F_j = \frac{\partial S - 1}{\partial g^i}[g_0, g_1], \quad \forall i \in I.
\]

(44)

Given \(g_0\), solving this system to machine precision for \(g_1\) provides the conservation laws the machine precision as well.