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.

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Time- and space-continuous collisional evolution

A distribution function $f(\boldsymbol{v}, t) : \mathbb{R}^3 \times \mathbb{R}_{\geq 0} \mapsto \mathbb{R}_{\geq 0}$ is assumed to evolve according to the equation

$$\frac{\partial f}{\partial t} = \frac{\partial}{\partial \boldsymbol{v}} \cdot \int_{\mathbb{R}^3} \mathbb{Q}(\boldsymbol{v} - \boldsymbol{v}') \cdot \left(f(\boldsymbol{v}') \frac{\partial f}{\partial \boldsymbol{v}} - f(\boldsymbol{v}) \frac{\partial f}{\partial \boldsymbol{v}'} \right) d\boldsymbol{v}', \qquad (1)$$

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

A non-standard weak formulation of the problem

Given an arbitrary time-independent test function $u(\boldsymbol{v})$, 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

$$M(u, w) = \int_{\mathbb{R}^3} uw \, d\boldsymbol{v}, \tag{3}$$

$$\begin{aligned} C_f(u, w) = -\frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} & \left(\frac{\partial u}{\partial \boldsymbol{v}} - \frac{\partial u}{\partial \boldsymbol{v}'} \right) \\ & \cdot f(\boldsymbol{v}) \mathbb{Q}(\boldsymbol{v} - \boldsymbol{v}') f(\boldsymbol{v}') \cdot \left(\frac{\partial w}{\partial \boldsymbol{v}} - \frac{\partial w}{\partial \boldsymbol{v}'} \right) d\boldsymbol{v} d\boldsymbol{v}'. \end{aligned} \tag{4}$$

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

Properties of the collision operator

The functions $\phi(\boldsymbol{v}) = \{|\boldsymbol{v}|^2, \boldsymbol{v}, 1\}$ 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 $\phi = \{|\boldsymbol{v}|^2, \boldsymbol{v}, 1\}$, 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 $\boldsymbol{v}^\star$ where $f(\boldsymbol{v}^\star) = 0$, $\partial_{\boldsymbol{v}} f(\boldsymbol{v}^\star) = 0$, and $\partial^2_{\boldsymbol{v}\boldsymbol{v}} f(\boldsymbol{v}^\star)$ is positive semi-definite, the evolution equation provides

$$\frac{\partial f(\boldsymbol{v}^\star)}{\partial t} = \int_{\mathbb{R}^3} \mathbb{Q}(\boldsymbol{v}^\star - \boldsymbol{v}') f(\boldsymbol{v}') d\boldsymbol{v}' : \frac{\partial^2 f(\boldsymbol{v}^\star)}{\partial \boldsymbol{v} \partial \boldsymbol{v}} \geq 0. \quad (5)$$

Spatial discretization

Introduce an exponentially-mapped Galerkin projection

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

$$f_h = \exp(g_h), \qquad g_h = \sum_{i\in I} g^i(t)\psi_i(\boldsymbol{v}), \tag{6}$$

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 $u = \psi_i$

$$\sum_{j\in I} M(\psi_i, f_h\psi_j)\frac{dg^j}{dt} = \sum_{j\in I} C_{f_h}(\psi_i,\psi_j)g^j, \quad \forall\, i \in I. \tag{7}$$

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

$$(E, \boldsymbol{P}, N) = \sum_{i \in I} (e^i, \boldsymbol{v}^i, 1^i) M(\psi_i, f_h). \tag{8}$$

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

$$|\boldsymbol{v}|^2 = \sum_{i \in I} e^i \psi_i(\boldsymbol{v}) \qquad \boldsymbol{v} = \sum_{i \in I} \boldsymbol{v}^i \psi_i(\boldsymbol{v}), \qquad 1 = \sum_{i \in I} 1^i \psi_i(\boldsymbol{v}). \tag{9}$$

Conservation of the finite-dimensional invariants

The time derivatives of energy, momentum, and density vanish identically

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

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

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

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.

H-theorem: equilibrium

Note that $\{e^i\}_{i\in I}$, $\{\boldsymbol{v}^i\}_{i\in I}$, 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

$$g^i_{\mathsf{eq}} = a\, e^i + \boldsymbol{b} \cdot \boldsymbol{v}^i + c\, 1^i, \tag{13}$$

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

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

Because the energy, momentum, and density are conserved, the coefficients a, $\boldsymbol{b}$, and c are uniquely determined in terms of the moments of a given initial state.

H-theorem: entropy production

Note that the entropy $S = -\int f_h \ln f_h d\boldsymbol{v}$ can be written as

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

It's time derivative then becomes

$$\begin{aligned} \frac{dS}{dt} &= -\sum_{i \in I} M(f_h, \psi_i) \frac{dg^i}{dt} - \sum_{i,j \in I} \frac{dg^j}{dt} M(\psi_j f_h, \psi_i) g^i \\ &= -\frac{dN}{dt} - \sum_{i,j \in I} C_{f_h}(\psi_j, \psi_i) g^i g^j \geq 0. \end{aligned} \tag{16}$$

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 $M(\psi_i, f_h \psi_j)$

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

Use the finite-dimensional entropy (15), it's derivative, and invert for

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

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

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

where we have collected the individual matrices together into

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

Finite-dimensional metriplectic structure

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

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

with the same matrix as previously

$$G_{k\ell}(g) = \sum_{i,j\in I} M^{-1}(\psi_k, f_h\psi_i)\, C_{f_h}(\psi_i, \psi_j)\, M^{-1}(\psi_j, f_h\psi_\ell). \tag{22}$$

The finite-dimensional metriplectic structure is then identifed as

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

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

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

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

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

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

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

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

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

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).

Discrete Gradient methods: entropy production

Using (27) and (26), the discrete evolution of a function $U(g)$ satisfies

$$U(g_1) - U(g_0) = -\delta t \sum_{k,\ell \in I} \overline{\frac{\partial U}{\partial g^k}}[g_0, g_1] \overline{G}_{k\ell}[g_0, g_1] \overline{\frac{\partial S}{\partial g^\ell}}[g_0, g_1]. \qquad (28)$$

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

$$S(g_1) - S(g_0) = -\delta t \sum_{k,\ell \in I} \overline{\frac{\partial S}{\partial g^k}}[g_0, g_1] \overline{G}_{k\ell}[g_0, g_1] \overline{\frac{\partial S}{\partial g^\ell}}[g_0, g_1] \geq 0. \qquad (29)$$

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?

Discrete Gradient methods: Casimir evolution

For all invariants $C = (E, \boldsymbol{P}, N)$, with $c^i = (e^i, \boldsymbol{v}^i, 1^i)$, we have

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

A discrete gradient of the Casimirs is thus defined according to

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

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

$$C(g_1) - C(g_0) = -\delta t \sum_{i \in I} \sum_{k, \ell \in I} c^i \overline{M}_{ik}[g_0, g_1] \overline{G}_{k\ell}[g_0, g_1] \overline{\frac{\partial S}{\partial g^\ell}}[g_0, g_1]. \tag{32}$$

Discrete Gradient methods: Casimir invariance

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

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

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

$$C(g_1) - C(g_0) = -\delta t \sum_{i\in I} \sum_{j,\ell\in I} c^i C_{f_h}(\psi_i, \psi_j)\, \overline{M}_{j\ell}^{-1}[g_0, g_1] \overline{\frac{\partial S}{\partial g^\ell}}[g_0, g_1] = 0, \tag{34}$$

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

$$\sum_{i\in I} c^i C_{f_h}(\psi_i, \psi_j) = 0, \quad \forall\, j \in I. \tag{35}$$

Discrete Gradient mehods: uniqueness of equilibrium

For an equilibrium state to exist, one must have $g_1 = g_0 = g_{\mathsf{eq}}$. This requirement, and the evolution equation (26), provides

$$\sum_{\ell \in I} \overline{G}_{k\ell}[g_{\mathsf{eq}}, g_{\mathsf{eq}}] \overline{\frac{\partial S}{\partial g^\ell}}[g_{\mathsf{eq}}, g_{\mathsf{eq}}] = 0, \quad \forall\, k \in I. \tag{36}$$

Next, using the defining properties $\overline{\partial S/\partial g^\ell}[g_{\mathsf{eq}}, g_{\mathsf{eq}}] = \partial S/\partial g^\ell(g_{\mathsf{eq}})$ and $\overline{G}_{k\ell}[g_{\mathsf{eq}}, g_{\mathsf{eq}}] = G_{k\ell}(g_{\mathsf{eq}})$, we obtain

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

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

$$f_{h,\mathsf{eq}}(\boldsymbol{v}) = \exp(a|\boldsymbol{v}|^2 + \boldsymbol{b} \cdot \boldsymbol{v} + c), \tag{38}$$

Sparse system for iterative solution

Average Discrete Gradient

Use the second order $\mathcal{O}(\delta t^2)$ average discrete gradient

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

Define the short notations

$$g_{h0} = \sum_{k\in I} g_0^k \psi_k, \qquad g_{h1} = \sum_{k\in I} g_1^k \psi_k. \tag{40}$$

Compute the matrix

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

and the vector

$$\overline{\frac{\partial S - 1}{\partial g^\ell}}[g_0, g_1] = -\int \psi_\ell \frac{(g_{h0} - 1)\exp(g_{h0}) - (g_{h1} - 1)\exp(g_{h1})}{g_{h0} - g_{h1}} \, d\boldsymbol{v}. \tag{42}$$

Sparse form suitable for iterative solution

Put everything together and obtain a sparse iterable system

$$\sum_{k\in I} \overline{M}_{ik}[g_0, g_1] \frac{g_1^k - g_0^k}{\delta t} = -\sum_{j\in I} C_{f_{h,1/2}}(\psi_i, \psi_j) F_j, \quad \forall\, i \in I, \tag{43}$$

$$\sum_{j\in I} \overline{M}_{ij}[g_0, g_1] F_j = \overline{\frac{\partial S - 1}{\partial g^i}}[g_0, g_1], \quad \forall\, i \in I. \tag{44}$$

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