Structure-preserving marker-particle discretization of the Landau collision operator

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Overview

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What is diffusive flow?

Hamiltonian systems describe incompressible flow driven by a Hamiltonian:

In a Hamiltonian system, a density f is transported according to the equation

$$\frac{\partial f}{\partial t} = \frac{\partial}{\partial z^i}(-V^i f). \tag{1}$$

The transporting velocity field and the Hamiltonian functional are connected by

$$V^i = \Pi^{ij} \frac{\partial}{\partial z^j} \frac{\delta \mathcal{H}}{\delta f}, \qquad \mathcal{H}[f] = \int f H. \tag{2}$$

The components V^i of the velocity field are the same thing as the equations of motion for a single particle with a Hamiltonian H and a Poisson matrix Π^{ij}.

Being Hamiltonian, the vector field V^i is incompressible. It also conserves the Hamiltonian along the flow due to the antisymmetry of the Poisson matrix:

$$V^i \frac{\partial}{\partial z^i} \frac{\delta \mathcal{H}}{\delta f} = \frac{\partial}{\partial z^i} \frac{\delta \mathcal{H}}{\delta f} \Pi^{ij} \frac{\partial}{\partial z^j} \frac{\delta \mathcal{H}}{\delta f} = 0 \tag{3}$$

Diffusive systems describe compressible flow driven by an entropy:

Consider a transport equation

$$\frac{\partial f}{\partial t} = \frac{\partial}{\partial z^i}\left(D^{ij}\frac{\partial f}{\partial z^j}\right). \tag{4}$$

Rewrite $D^{ij}\partial_j f = f D^{ij}\partial_j \ln f$ and define the entropy functional

$$\mathcal{S}[f] = -\int f \ln f. \tag{5}$$

The transport equation can now be written as

$$\frac{\partial f}{\partial t} = \frac{\partial}{\partial z^i}\left(-V^i f\right). \tag{6}$$

where the velocity field is given by the *entropic* flow

$$V^i = D^{ij}\frac{\partial}{\partial z^j}\frac{\delta \mathcal{S}}{\delta f}. \tag{7}$$

Along an entropic flow, the entropy is monotonically increased because the diffusion matrix D^{ij} has to be at least positive-semidefinite, if not positive-definite:

$$V^i \frac{\partial}{\partial z^i}\frac{\delta \mathcal{S}}{\delta f} = \frac{\partial}{\partial z^i}\frac{\delta \mathcal{S}}{\delta f} D^{ij}\frac{\partial}{\partial z^j}\frac{\delta \mathcal{S}}{\delta f} \geq 0 \tag{8}$$

Entropic flow can be discretized with particles, deterministically:

Consider particle coordinates, weights $(\boldsymbol{Z}; W) = \{(\boldsymbol{z}_p; w_p)\}_{p=1}^N$, and a distribution

$$f_h(\boldsymbol{z}, t) = \sum_{p=1}^{N} w_p \delta(\boldsymbol{z} - \boldsymbol{z}_p(t)). \tag{9}$$

A functional $\mathcal{A}[f]$ evaluated with respect to f_h becomes a function of the coordinates

$$\mathcal{A}[f_h] = A(\boldsymbol{Z}; W) \tag{10}$$

Varying this relation leads to the discrete form of the functional derivative

$$\frac{\partial}{\partial z^i} \frac{\delta \mathcal{A}[f_h]}{\delta f}\Big|_{\boldsymbol{z}=\boldsymbol{z}_p} = \frac{1}{w_p} \frac{\partial A(\boldsymbol{Z}; W)}{\partial z_p^i} \tag{11}$$

Evaluating the entropic flow at the particle position can be interpreted as an equation of motion for the particle $\boldsymbol{z}_p$, and results in the following *deterministic* expression

$$\frac{dz_p^i}{dt} = D^{ij}(\boldsymbol{z}_p) \frac{1}{w_p} \frac{\partial S(\boldsymbol{Z}; W)}{\partial z_p^j} \tag{12}$$

This guarantees that the discrete entropy never is decreased:

$$\frac{dS(\boldsymbol{Z}; W)}{dt} = \sum_p \frac{\partial S(\boldsymbol{Z}; W)}{\partial z_p^i} \frac{dz_p^i}{dt} = \sum_p \frac{1}{w_p} \frac{\partial S(\boldsymbol{Z}; W)}{\partial z_p^i} D^{ij}(\boldsymbol{z}_p) \frac{\partial S(\boldsymbol{Z}; W)}{\partial z_p^j} \geq 0 \tag{13}$$

But isn't the entropy badly behaving with respect to a delta distribution?

One can approximate and define a regularized entropy functional where the density function is convoluted with respect to a radial basis function ψ_ϵ according to

$$\mathcal{S}_\epsilon[f] \equiv \mathcal{S}[\psi_\epsilon * f]. \tag{14}$$

Utilizing the convolution strategy, a well behaving discrete entropy becomes

$$S_\epsilon(\boldsymbol{Z}; W) = -\int \Big(\sum_p w_p \psi_\epsilon(\boldsymbol{z} - \boldsymbol{z}_p(t)) \Big) \ln \Big(\sum_{\overline{p}} w_{\overline{p}} \psi_\epsilon(\boldsymbol{z} - \boldsymbol{z}_{\overline{p}}(t)) \Big) d\boldsymbol{z}. \tag{15}$$

Alternatively, one could consider the f_h to be a collection radial basis functions instead of δ-functions, effectively requiring no regularization. This would, however, open a can of worms and imply changes to the Hamiltonian parts of field theories. Let's just leave that part untouched for we know that variational geometric algorithms already work well for discretizing, e.g., the Vlasov–Maxwell action integral.

The regularization trick is not my invention

The trick has been used previously. See for example the papers

- Degond, Mustieles, (1989), doi:10.1137/0911018
- Russo, (1990), doi:10.1002/cpa.3160430602
- Carrillo, Graig, Patacchini, (2019) doi:10.1007/s00526-019-1486-3
- Carrillo, Hu, Wang, Wu, (2020), doi:10.1016/j.jcpx.2020.100066

The reference [Carrillo et al, (2020), doi:10.1016/j.jcpx.2020.100066] is also the first paper that uses the regularization trick to discretize the Landau operator deterministically with marker particles. The paper succeeds in reproducing continuous-time conservation laws and monotonic entropy production but falls short of these properties in discrete time. These issues can be fixed and, next, I show how.

Particle approximation of the Landau collision operator

Laundau operator as entropic flow:

The single-species Landau collision operator is given by

$$C[f] = \nu \frac{\partial}{\partial v^i} \int \mathbb{Q}^{ij}(\boldsymbol{v} - \overline{\boldsymbol{v}}) \left(f(\overline{\boldsymbol{v}}) \frac{\partial f}{\partial v^j} - f(\boldsymbol{v}) \frac{\partial f}{\partial \overline{v}^j} \right) d\overline{\boldsymbol{v}}. \tag{16}$$

The matrix $\mathbb{Q}$ in the collision operator is a scaled projection matrix

$$\mathbb{Q}^{ij}(\boldsymbol{\xi}) = |\boldsymbol{\xi}|^{-1}(\delta^{ij} - \xi^i \xi^j / |\boldsymbol{\xi}|^2). \tag{17}$$

Introducing the entropy functional $\mathcal{S}[f] = -\int f \ln f d\boldsymbol{v}$, the collision operator becomes

$$C[f] = \frac{\partial}{\partial v^i} \left(-U^i f \right), \tag{18}$$

where the velocity field is given by

$$U^i(\boldsymbol{v}) = \int f(\overline{\boldsymbol{v}}) \mathbb{Q}^{ij}(\boldsymbol{v} - \overline{\boldsymbol{v}}) \left(\frac{\partial}{\partial v^j} - \frac{\partial}{\partial \overline{v}^j} \right) \frac{\delta \mathcal{S}}{\delta f} d\overline{\boldsymbol{v}}. \tag{19}$$

This expression for the flow could be discretized directly. To reveal more structure, I discretize the bracket behind the operator instead.

Landau operator as a metric bracket:

The (single-species) Landau collision operator can be derived from the metric bracket

$$(\mathcal{A}, \mathcal{B}) = \frac{1}{2} \iint_{\boldsymbol{z}, \overline{\boldsymbol{z}}} \boldsymbol{\Gamma}(\mathcal{A}, \boldsymbol{z}, \overline{\boldsymbol{z}}) \cdot \mathbb{W}(\boldsymbol{z}, \overline{\boldsymbol{z}}) \cdot \boldsymbol{\Gamma}(\mathcal{B}, \boldsymbol{z}, \overline{\boldsymbol{z}}). \tag{20}$$

The vector $\boldsymbol{\Gamma}(\mathcal{A}, \boldsymbol{z}, \overline{\boldsymbol{z}})$ and the matrix $\mathbb{W}(\boldsymbol{z}, \overline{\boldsymbol{z}})$ are defined according to

$$\boldsymbol{\Gamma}(\mathcal{A}, \boldsymbol{z}, \overline{\boldsymbol{z}}) = \frac{\partial}{\partial \boldsymbol{v}} \frac{\delta \mathcal{A}}{\delta f}(\boldsymbol{z}) - \frac{\partial}{\partial \overline{\boldsymbol{v}}} \frac{\delta \mathcal{A}}{\delta f}(\overline{\boldsymbol{z}}), \tag{21}$$

$$\mathbb{W}(\boldsymbol{z}, \overline{\boldsymbol{z}}) = \nu \delta(\boldsymbol{x} - \overline{\boldsymbol{x}}) f(\boldsymbol{z}) f(\overline{\boldsymbol{z}}) \mathbb{Q}(\boldsymbol{v} - \overline{\boldsymbol{v}}). \tag{22}$$

Given an entropy functional $\mathcal{S}$, the collisional evolution of functionals becomes

$$\frac{d\mathcal{A}}{dt} = (\mathcal{A}, \mathcal{S}) \tag{23}$$

This result is one application of the so-called metriplectic dynamics. It has been known for some time now [Morrison, (1984), doi:10.1016/0375-9601(84)90635-2]

Discretizing the collisional bracket:

Take the following steps:

- Group together the degrees of freedom $(\boldsymbol{Z}; W) = \{(\boldsymbol{x}_p, \boldsymbol{v}_p; w_p)\}_{p=1}^{N}$
- Introduce the discrete distribution $f_h = \sum_p w_p \delta(\boldsymbol{x} - \boldsymbol{x}_p(t))\delta(\boldsymbol{v} - \boldsymbol{v}_p(t))$
- Discretize the functional derivative $\frac{\partial}{\partial \boldsymbol{v}} \frac{\delta \mathcal{A}[f_h]}{\delta f}\Big|_{\boldsymbol{z}_p} = \frac{1}{w_p} \frac{\partial A(\boldsymbol{Z}; W)}{\partial \boldsymbol{v}_p}$
- Approximate $\delta(\boldsymbol{x} - \overline{\boldsymbol{x}})$ in the bracket with an indicator function $\mathbf{1}(p, \overline{p})$

Substitute everything to the bracket and obtain a finite-dimensional bracket

$$(A, B)_h = \frac{1}{2} \sum_{p, \overline{p}} \boldsymbol{\Gamma}(A, p, \overline{p}) \cdot \mathbb{W}(p, \overline{p}) \cdot \boldsymbol{\Gamma}(B, p, \overline{p}). \tag{24}$$

The vector and the matrix in the discrete bracket are

$$\boldsymbol{\Gamma}(A, p, \overline{p}) = \frac{1}{w_p} \frac{\partial A(\boldsymbol{Z}; W)}{\partial \boldsymbol{v}_p} - \frac{1}{w_{\overline{p}}} \frac{\partial A(\boldsymbol{Z}; W)}{\partial \boldsymbol{v}_{\overline{p}}} \tag{25}$$

$$\mathbb{W}(p, \overline{p}) = \nu \, w_p w_{\overline{p}} \, \mathbf{1}(p, \overline{p}) \, \mathbb{Q}(\boldsymbol{v}_p - \boldsymbol{v}_{\overline{p}}) \tag{26}$$

Continuous-time dynamics:

Given a regularized entropy functional $S_\epsilon(\boldsymbol{Z}; W) = \mathcal{S}_\epsilon[f_h]$, assume the collisional dynamics of arbitrary functions $A(\boldsymbol{Z}; W)$ to obey

$$\frac{dA}{dt} = (A, S_\epsilon)_h. \tag{27}$$

Specifically, an equation of motion for a particle is obtained by choosing $A = \boldsymbol{v}_p$

$$\frac{d\boldsymbol{v}_p}{dt} = \sum_{\overline{p}} \nu\, w_{\overline{p}}\, \mathbf{1}(p, \overline{p})\, \mathbb{Q}(\boldsymbol{v}_p - \boldsymbol{v}_{\overline{p}}) \cdot \boldsymbol{\Gamma}(S_\epsilon, p, \overline{p}). \tag{28}$$

The indicator function decides if the particles p and $\overline{p}$ are within the same collision cell.

Continuous-time collisional invariants

Time evolution of momentum $\boldsymbol{P} = \sum w_p \boldsymbol{v}_p$ vanishes

$$\frac{d\boldsymbol{P}}{dt} = (\boldsymbol{P}, S_\epsilon)_h = 0 \tag{29}$$

Time evolution of kinetic energy $K = \sum_p w_p \frac{1}{2} |\boldsymbol{v}_p|^2$ vanishes

$$\frac{dK}{dt} = (K, S_\epsilon)_h = 0 \tag{30}$$

Time evolution of the regularized entropy functional is non-decreasing

$$\frac{dS_\epsilon}{dt} = (S_\epsilon, S_\epsilon)_h \geq 0 \tag{31}$$

The momentum conservation follows directly from $\boldsymbol{\Gamma}(\boldsymbol{P}, p, \overline{p}) = \boldsymbol{0}$, the energy conservation from $\boldsymbol{\Gamma}(K, p, \overline{p}) = \boldsymbol{v}_p - \boldsymbol{v}_{\overline{p}}$ being in the null space of $\mathbb{Q}(\boldsymbol{v}_p - \boldsymbol{v}_{\overline{p}})$, and the entropy behaviour from the positive-semidefinite nature of the matrix $\mathbb{Q}$.

Structure-preserving temporal discretization

Discrete-time dynamics:

Introduce the so-called discrete gradient operator which is required to satisfy

$$(\boldsymbol{x}-\boldsymbol{y})\cdot\overline{\nabla A}(\boldsymbol{x},\boldsymbol{y}) = A(\boldsymbol{x}) - A(\boldsymbol{y}) \tag{32}$$

$$\overline{\nabla A}(\boldsymbol{x},\boldsymbol{x}) = \nabla A(\boldsymbol{x}) \tag{33}$$

Modify the vector $\boldsymbol{\Gamma}(A,p,\overline{p})$ and the matrix $\mathbb{W}(p,\overline{p})$ to be evaluated with respect to two different time instances via the utilization of the discrete gradient operator

$$\overline{\boldsymbol{\Gamma}_n^{n+1}(A,p,\overline{p})} = \frac{1}{w_p}\overline{\frac{\partial A}{\partial \boldsymbol{v}_p}}(\boldsymbol{Z}^n,\boldsymbol{Z}^{n+1};W) - \frac{1}{w_{\overline{p}}}\overline{\frac{\partial A}{\partial \boldsymbol{v}_{\overline{p}}}}(\boldsymbol{Z}^n,\boldsymbol{Z}^{n+1};W) \tag{34}$$

$$\overline{\mathbb{W}_n^{n+1}(p,\overline{p})} = \nu\, w_p w_{\overline{p}}\,\mathbf{1}(p,\overline{p})\,\mathbb{Q}(\overline{\boldsymbol{\Gamma}_n^{n+1}(K,p,\overline{p})}) \tag{35}$$

Take the discrete-time evolution of functions to be given by

$$\frac{A^{n+1}-A^n}{\Delta t} = \frac{1}{2}\sum_{p,\overline{p}}\overline{\boldsymbol{\Gamma}_n^{n+1}(A,p,\overline{p})}\cdot\overline{\mathbb{W}_n^{n+1}(p,\overline{p})}\cdot\overline{\boldsymbol{\Gamma}_n^{n+1}(S_\epsilon,p,\overline{p})} \tag{36}$$

For a single particle this means

$$\frac{\boldsymbol{v}_p^{n+1}-\boldsymbol{v}_p^n}{\Delta t} = \sum_{\overline{p}}\nu\, w_{\overline{p}}\,\mathbf{1}(p,\overline{p})\,\mathbb{Q}(\overline{\boldsymbol{\Gamma}_n^{n+1}(K,p,\overline{p})})\cdot\overline{\boldsymbol{\Gamma}_n^{n+1}(S_\epsilon,p,\overline{p})} \tag{37}$$

Discrete-time collisional invariants

The evolution of momentum satisfies

$$\frac{\boldsymbol{P}^{n+1} - \boldsymbol{P}^{n}}{\Delta t} = \frac{1}{2} \sum_{p,\overline{p}} \overline{\boldsymbol{\Gamma}_n^{n+1}(P,p,\overline{p})} \cdot \overline{\mathbb{W}_n^{n+1}(p,\overline{p})} \cdot \overline{\boldsymbol{\Gamma}_n^{n+1}(S_\epsilon,p,\overline{p})} = 0 \tag{38}$$

The evolution of kinetic energy satisfies

$$\frac{K^{n+1} - K^{n}}{\Delta t} = \frac{1}{2} \sum_{p,\overline{p}} \overline{\boldsymbol{\Gamma}_n^{n+1}(K,p,\overline{p})} \cdot \overline{\mathbb{W}_n^{n+1}(p,\overline{p})} \cdot \overline{\boldsymbol{\Gamma}_n^{n+1}(S_\epsilon,p,\overline{p})} = 0 \tag{39}$$

The evolution of regularized entropy satisfies

$$\frac{S_\epsilon^{n+1} - S_\epsilon^{n}}{\Delta t} = \frac{1}{2} \sum_{p,\overline{p}} \overline{\boldsymbol{\Gamma}_n^{n+1}(S_\epsilon,p,\overline{p})} \cdot \overline{\mathbb{W}_n^{n+1}(p,\overline{p})} \cdot \overline{\boldsymbol{\Gamma}_n^{n+1}(S_\epsilon,p,\overline{p})} \geq 0 \tag{40}$$

These follow from the discrete gradient being exact for linear functions, meaning that $\overline{\boldsymbol{\Gamma}_n^{n+1}(\boldsymbol{P},p,\overline{p})} = \boldsymbol{0}$, the fact that $\overline{\boldsymbol{\Gamma}_n^{n+1}(K,p,\overline{p})}$ is in the null-space of the matrix $\mathbb{Q}(\overline{\boldsymbol{\Gamma}_n^{n+1}(K,p,\overline{p})})$, and that the matrix remains positive-semidefinite.

A numerical example

Collisional relaxation of a double Maxwellian in 2D:

Let's throw all the units out and choose an initial double-peaked distribution function

$$f(\boldsymbol{v}, t=0) = \frac{1}{4\pi}\left[\exp\left(-\frac{(\boldsymbol{v}-\boldsymbol{u}_1)^2}{2}\right) + \exp\left(-\frac{(\boldsymbol{v}-\boldsymbol{u}_2)^2}{2}\right)\right], \tag{41}$$

where the peaks of the Maxwellians are $\boldsymbol{u}_1 = (-2, 1)$ and $\boldsymbol{u}_2 = (0, -1)$. The energy and momentum of this distribution are $E = 2.5$ and $\boldsymbol{P} = (-1, 0)$ respectively.

Let's also choose the smoothing radial basis function ψ_ϵ to be a Gaussian

$$\psi_\epsilon(\boldsymbol{v}) = \frac{1}{2\pi\epsilon}\exp\left(-\frac{|\boldsymbol{v}|^2}{2\epsilon}\right), \tag{42}$$

with $\epsilon = 0.64h^{1.98}$, the parameter $h = 2L/\sqrt{N}$, $L = 10$, and the total particle number $N = 60^2 = 3600$. This setting now corresponds to the same test case as in [Carrillo et al. (2020), doi:10.1016/j.jcpx.2020.100066].

Then initialize all particles by placing them in a regular grid in the domain $[-L, L] \times [-L, L]$ and setting the weights to match the value of the initial distribution. For evaluating the discrete entropy functional, use a 2-D Gauss-Hermite quadrature, localizing a 6-by-6 mesh of quadrature points to the velocity position of each particle.

Finally, solve the non-linear system using fixed-point iteration and vectorize the summation over particles on a GPU.

Resulting temporal evolution:

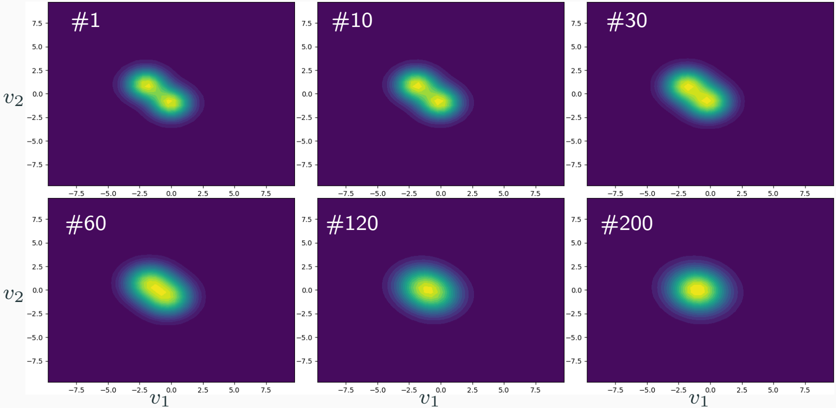

Figure 1: Illustrated evolution of $\psi_\epsilon * f_h$. The panels describe snapshots of the steps $\#(1, 10, 30, 60, 120, 200)$ from left to right and from top down. The axes in the panels refer to the velocity coordinates (v_1, v_2) in the domain $[-L, L] \times [-L, L]$ and the color indicates the level sets of the distribution function from zero (deep blue) to the instantaneous maximum values (bright yellow) for optimal visual contrast.

Conservation properties recorded during the simulation:

Step #	P_1	P_2	E
0	-1	0	2.5
1	-0.9999999999999982	-1.8617208789871285E-16	2.499999999999991
10	-0.9999999999999984	-4.263625043299246E-16	2.4999999999999907
30	-0.9999999999999981	-1.4125799054770516E-16	2.500000000000011
60	-0.9999999999999984	-1.2262462096082616E-15	2.5000000000000293
120	-0.9999999999999974	4.1795993749316196E-17	2.500000000000039
200	-0.9999999999999982	-4.68985202235761E-16	2.500000000000042

Table 1: Conservation of momentum and energy during the collisional relaxation of a double Maxwellian. The step numbers correspond to the panels in Fig.1.

I think this is quite good!

Summary

Thanks for listening!

A summary of the presentation:

- Diffusion processes can be interpreted as compressible flow driven by entropy.
- The Landau collision operator can be expressed as a metric bracket.
- The metric bracket representing collisions can be discretized with particles.
- Discrete-time thermodynamics and momentum conservation is achieved via utilization of the discrete gradient concept.

More details at Hirvijoki (2021), doi:10.1088/1361-6587/abe884, arXiv:2012.07187

Where to go next?

- Electrostatic gyrokinetics has a collisional bracket (Hirvijoki & Burby (2020)).
- Electromagnetic gyrokinetics has a collisional bracket (To Be Published (2022)).
- Discrete-time thermodynamics recovered but momentum conservation lacking.