Particle Method for the Landau Equation — A Gradient Flow Perspective

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Overview

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1. Introduction
   - Kinetic theory and the Landau equation
   - Existing numerical methods for the Landau equation
2. A deterministic particle method for the Landau equation
3. Extension to the spatially inhomogeneous case
4. Conclusion

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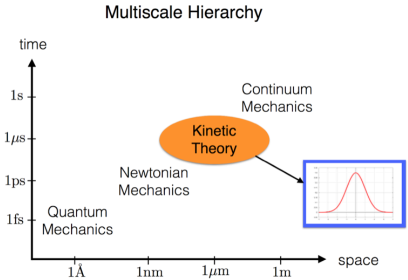
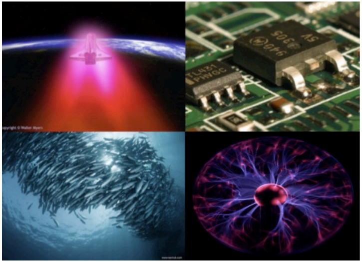
Kinetic theory

Kinetic theory models the non-equilibrium dynamics of a gas or any system comprised of a large number of particles using a **probability density function**

Applications: rarefied gas dynamics, electron/photon/neutron transport, plasma physics, collective behavior of biological and social systems, ...





Left: Role of kinetic theory in multiscale modeling hierarchy. **Right:** Some applications of kinetic theory. Clockwise: space shuttle reentry; semiconductor transport; plasmas; swarming fish.

Kinetic equations

$$\partial_t f + v \cdot \nabla_x f + F \cdot \nabla_v f = Q(f), \quad t > 0,\ x \in \Omega \subset \mathbb{R}^d,\ v \in \mathbb{R}^d$$

- $f = f(t, x, v)$: one-particle **probability density function (PDF)**
  — $f\mathrm{d}x\mathrm{d}v$ gives the probability of finding a fixed particle at time t, position x and velocity v in the phase space
- F: **acceleration** due to external or self-consistent forces
- $Q(f)$: **collision operator**
  — a linear or nonlinear operator modeling the interaction of particles with each other or with the surrounding environment

The Landau collision operator[1]

$$Q(f,f)(v) = \nabla_v \cdot \int_{\mathbb{R}^d} A(v-v_*)[f(v_*)\nabla_v f(v) - f(v)\nabla_{v_*} f(v_*)]\,\mathrm{d}v_*$$

where $d \geq 2$ and A is a (semi-positive-definite) matrix given by

$$A(z) = |z|^{\gamma+2}\left(I_d - \frac{z \otimes z}{|z|^2}\right), \quad -d-1 \leq \gamma \leq 1.$$

Note that $d=3$, $\gamma=-3$ corresponds to the Coulomb interaction.

- A nonlinear, nonlocal, diffusive type operator – also known as the Landau-Fokker-Planck operator
- Can be derived from the Boltzmann collision operator when all collisions become grazing (i.e., the scattering angle $\to 0$)
- Used to describe collisions between charged particles (e.g., in plasmas)

[1] Landau, '36.

A closer look at the Landau operator

$$Q(f,f)(v) = \nabla_v \cdot \int_{\mathbb{R}^d} A(v-v_*)[f(v_*)\nabla_v f(v) - f(v)\nabla_{v_*} f(v_*)]\,\mathrm{d}v_*$$

can be written equivalently in the **"log" form** (denote $f_* = f(v_*)$):

$$Q(f,f)(v) = \nabla_v \cdot \int_{\mathbb{R}^d} A(v-v_*)[\nabla_v \log f - \nabla_{v_*} \log f_*] f f_*\,\mathrm{d}v_*$$

from which one can derive the **weak form**:

$$\begin{aligned}
&\int_{\mathbb{R}^d} Q(f,f)(v)\phi(v)\,\mathrm{d}v \\
=& -\frac{1}{2}\iint_{\mathbb{R}^{2d}} [\nabla_v \phi - \nabla_{v_*}\phi_*]^T A(v-v_*)[\nabla_v \log f - \nabla_{v_*} \log f_*] f f_*\,\mathrm{d}v\mathrm{d}v_*
\end{aligned}$$

where ϕ is a test function.

Properties of the Landau operator

- **Conservation** of mass, momentum, and energy:

$$\int_{\mathbb{R}^d} Q(f,f)\,\mathrm{d}v = \int_{\mathbb{R}^d} Q(f,f)\,v\,\mathrm{d}v = \int_{\mathbb{R}^d} Q(f,f)\,|v|^2\,\mathrm{d}v = 0$$

- **Decay of entropy**:

$$\int_{\mathbb{R}^d} Q(f,f)\,\log f\,\mathrm{d}v \leq 0$$

- Equilibrium is a **Maxwellian**:

$$\text{``}=\text{''} \iff f = \mathcal{M}_{\rho,u,T} := \frac{\rho}{(2\pi T)^{d/2}} e^{-\frac{|v-u|^2}{2T}} \iff Q(f,f) = 0$$

with density $\rho = \int f\,\mathrm{d}v$; bulk velocity $u = \frac{1}{\rho}\int f\,v\,\mathrm{d}v$; temperature $T = \frac{1}{d\rho}\int f\,|v-u|^2\,\mathrm{d}v$

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Numerical challenges in solving the Landau equation

Here we focus on the spatially homogeneous Landau equation

$$\partial_t f = Q(f,f)(v), \quad f = f(t,v),\ v \in \mathbb{R}^d$$

- **collision operator**: a direct approximation of Q would require $O(N^{2d})$ numerical complexity (N is the number of discretization points used in each velocity dimension) — expensive in 2D/3D
- **maintain the physical properties at the discrete level**: conservation, positivity, entropy decay, etc. — needed for stable and robust numerical simulation

Existing numerical work

- **Finite difference method** (or **discrete velocity method**)
  - many works in the simplified setting (2D, radially symmetric solutions, etc.)
  - for the full 3D operator: conservative and entropic schemes[2], efficiency improved using sublattice method, multigrid method, or multipole method[3]

    (+) preserve physical properties
    (+, −) second order accuracy (rigid)
    (−) complexity $O(N^{2d})$

[2] Degond, Lucquin-Desreux, '94, Buet and Cordier, '99.
[3] Buet, Cordier, Degond, Lemou, '97; Lemou, '98.

Existing numerical work (cont'd)

- **Fourier-Galerkin spectral method**[4]: leverage the convolutional structure of the collision operator

  (+) complexity $O(N^d \log N)$
  (+) spectral accuracy
  (−) no positivity, no conservation (except mass), no entropy decay

[4] Pareschi, Russo, Toscani, '00; H., Jin, Yan, '12; Zhang and Gamba, '17.

Existing numerical work (cont'd)

- **Rosenbluth form** is often used by plasma physicists[5]

$$Q(f,f) = \nabla \cdot (A_f \nabla f - f \nabla a_f),$$

where A_f and a_f can be obtained from

$$\Delta a_f = -8\pi f, \quad \Delta G_f = a_f, \quad A_f = D^2 G_f.$$

(+) complexity $O(N^d)$ provided a fast Poisson solver
(+) can be made conservative and positive using limiters
(−) no entropy decay

[5] Taitano, Chacon, Simakov, Molvig, '15.

Existing numerical work (cont'd)

- **Monte Carlo** methods:
  - based on approximation of Coulomb collisions (analog of DSMC for the Boltzmann equation)[6]
  - based on solving the SDE[7]: $dv_i = F_i dt + D_{ij} dW_j$

$(+,-)$ converges as $O(N^{-1/2})$ (N: number of particles), dimension independent
$(-)$ solution contains noise, typically require averaging for a large number of runs
$(-)$ no entropy decay

[6] Takizuka and Abe, '77. Bobylev and Nanbu, '00.
[7] Rosin, Ricketson, Dimits, Caflisch, and Cohen, '14.

Overview

Classical particle method

Consider the **linear transport** equation

$$\partial_t u + \nabla \cdot (a(t,x)u) = 0.$$

The classical particle method[a] seeks a (weak) solution of the form

$$u^N(t,x) = \sum_{p=1}^{N} w_p \delta(x - x_p(t)),$$

where x_p: particle locations, w_p: particle weights, N: number of particles. Then x_p satisfies

$$\frac{\mathrm{d}x_p(t)}{\mathrm{d}t} = a(t, x_p(t)), \quad p = 1, \ldots, N.$$

[a] Raviart, '85.

A motivating example

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Q: Can this method be applied to the **heat** equation $\partial_t u = \Delta u$ (since Landau is a diffusive type operator)?

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Q: Can this method be applied to the **heat** equation $\partial_t u = \Delta u$ (since Landau is a diffusive type operator)?

A: Need to interpret it in a "transport" form.

A motivating example (cont'd)

Approach 1 (Degond and Mustieles, '90):

$$\partial_t u = \Delta u = \nabla \cdot [(\nabla \log u) u]$$

View the heat equation as a "transport" equation with velocity field $U = \nabla \log u$. However, $\log u$ is not well-defined for a sum of δ-functions. One can regularize u to obtain

$$U \approx \nabla \log u_\varepsilon, \quad u_\varepsilon := \varphi_\varepsilon * u, \quad \varphi_\varepsilon \text{ is a mollifier.}$$

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Approach 2 (Carrillo, Craig, and Patacchini, '19):

$$\partial_t u = \Delta u = \nabla \cdot [(\nabla \log u) u] = \nabla \cdot \left[\left(\nabla \frac{\delta E}{\delta u} \right) u \right] = -\nabla_{W_2} E(u)$$

where $E(u) := \int u \log u \, dx$, ∇_{W_2} is the gradient under the quadratic Wasserstein metric. Instead of regularizing u, one can regularize the energy E to obtain

$$U \approx \nabla \frac{\delta E_\varepsilon}{\delta u}, \quad E_\varepsilon := \int (\varphi_\varepsilon * u) \log(\varphi_\varepsilon * u) \, dx, \quad \varphi_\varepsilon \text{ is a mollifier.}$$

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Approach 2 seems better as it respects the variational or gradient flow structure of the equation. Let's convince ourself!

The Landau equation – main idea[8]

Now let's consider the Landau equation

$$\partial_t f = Q(f, f)$$

where the operator Q can be written as

$$\begin{aligned} Q(f,f) &= \nabla_v \cdot \left\{ \left(\int_{\mathbb{R}^d} A(v - v_*) \left(\nabla_v \log f - \nabla_{v_*} \log f_* \right) f_* \, \mathrm{d}v_* \right) f \right\} \\ &= \nabla_v \cdot \left\{ \left(\int_{\mathbb{R}^d} A(v - v_*) \left(\nabla_v \frac{\delta E}{\delta f} - \nabla_{v_*} \frac{\delta E_*}{\delta f_*} \right) f_* \, \mathrm{d}v_* \right) f \right\} \end{aligned}$$

where

$$E(f) := \int_{\mathbb{R}^d} f \log f \, \mathrm{d}v$$

[8]Carrillo-H-Wang-Wu, JCP-X 2020.

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where

$$E(f) := \int_{\mathbb{R}^d} f \log f \, \mathrm{d}v$$

Similarly as in the heat equation, we propose to regularize E as

$$E_\varepsilon(f) := \int (\varphi_\varepsilon * f) \log(\varphi_\varepsilon * f) \, \mathrm{d}v, \quad \varphi_\varepsilon(v) = \frac{1}{(2\pi\varepsilon)^{d/2}} \exp\left(-\frac{|v|^2}{2\varepsilon} \right)$$

[8] Carrillo-H-Wang-Wu, JCP-X 2020.

The Landau equation – main idea (cont'd)

Accordingly, the equation is modified to

Regularized Landau equation

$$\partial_t f = Q_\varepsilon(f,f) := \nabla_v \cdot (U_\varepsilon(f) f)$$

with the velocity field given by

$$U_\varepsilon(f) = \int_{\mathbb{R}^d} A(v - v_*) \left(\nabla_v \frac{\delta E_\varepsilon}{\delta f} - \nabla_{v_*} \frac{\delta E_{\varepsilon,*}}{\delta f_*} \right) f_* \, \mathrm{d}v_*$$

where

$$\frac{\delta E_\varepsilon}{\delta f} = \varphi_\varepsilon * \log(\varphi_\varepsilon * f), \quad \nabla_v \frac{\delta E_\varepsilon}{\delta f} = (\nabla \varphi_\varepsilon) * \log(\varphi_\varepsilon * f)$$

Why the proposed regularization is good?

For the regularized Landau operator Q_ε, one still has a **weak** form:

$$\int Q_\varepsilon(f,f)\phi\,\mathrm{d}v = -\frac{1}{2}\iint [\nabla_v\phi - \nabla_{v_*}\phi_*]^T A(v-v_*)\left(\nabla_v \frac{\delta E_\varepsilon}{\delta f} - \nabla_{v_*}\frac{\delta E_{\varepsilon,*}}{\delta f_*}\right) ff_*\,\mathrm{d}v\mathrm{d}v_*$$

hence

- **conservation** of mass, momentum, and energy:

$$\int Q_\varepsilon(f,f)\,\mathrm{d}v = \int Q_\varepsilon(f,f)\,v\,\mathrm{d}v = \int Q_\varepsilon(f,f)\,|v|^2\,\mathrm{d}v = 0$$

- **decay of entropy**:

$$\int Q_\varepsilon(f,f)\frac{\delta E_\varepsilon}{\delta f}\,\mathrm{d}v \le 0$$

Why the regularization is good (cont'd)?

- the equilibrium of Q_ε is still a **Maxwellian**:

$$\int Q_\varepsilon(f,f)\frac{\delta E_\varepsilon}{\delta f}\,\mathrm{d}v = 0 \Longleftrightarrow \frac{\delta E_\varepsilon}{\delta f} = \lambda^{(0)} + \lambda^{(1)}\cdot v + \frac{\lambda^{(2)}}{2}|v|^2 \Longleftrightarrow Q_\varepsilon(f,f) = 0$$

Since $\frac{\delta E_\varepsilon}{\delta f} = \varphi_\varepsilon * \log(\varphi_\varepsilon * f)$, one can further deduce that

$$f = \mathcal{M}_{\rho,u,T}$$

with

$$\begin{cases} \rho & = \left(\frac{2\pi}{|\lambda^{(2)}|}\right)^{\frac{d}{2}} \exp\left\{\lambda^{(0)} + \frac{\varepsilon|\lambda^{(2)}|d}{2} - \frac{\varepsilon|\lambda^{(1)}|^2}{2(1-\varepsilon|\lambda^{(2)}|)} + \frac{|\lambda^{(1)}|^2}{2|\lambda^{(2)}|(1-\varepsilon|\lambda^{(2)}|)}\right\} \\ u & = \frac{\lambda^{(1)}}{|\lambda^{(2)}|} \\ T & = \frac{1}{|\lambda^{(2)}|} - \varepsilon \end{cases}$$

The deterministic particle method

For the initial value problem

$$\partial_t f = \nabla_v \cdot (U_\varepsilon(f) f), \quad f(0, v) = f^0(v)$$

we look for a particle solution as

$$f^N(t, v) = \sum_{p=1}^{N} w_p \delta(v - v_p(t))$$

where N is the number of particles, $v_p(t)$ is the velocity of particle p. The initial velocity and the weight w_p are set as

$$v_p(0) = v_i^c, \quad w_p = h^d f^0(v_i^c),$$

where the computational domain is $[-L, L]^d$, $h = 2L/n$, $N = n^d$, and v_i^c is the center of the square Q_i.

The deterministic particle method (cont'd)

Then the particle velocity $v_p(t)$ satisfies

$$\frac{dv_p(t)}{dt} = -U_\varepsilon(f^N)(v_p(t))$$
$$= -\sum_q w_q A(v_p - v_q)\left[\nabla \frac{\delta E_\varepsilon^N}{\delta f}(v_p) - \nabla \frac{\delta E_\varepsilon^N}{\delta f}(v_q)\right]$$

where

$$\frac{\delta E_\varepsilon^N}{\delta f} := \varphi_\varepsilon * \log(\varphi_\varepsilon * f^N) = \int_{\mathbb{R}^d} \varphi_\varepsilon(v-u) \log\left(\sum_p w_p \varphi_\varepsilon(u - v_p)\right) \mathrm{d}u$$
$$\approx \sum_i h^d \varphi_\varepsilon(v - v_i^c) \log\left(\sum_p w_p \varphi_\varepsilon(v_i^c - v_p)\right)$$

Properties of the particle solution

Theorem

The particle solution $v_p(t)$, $p = 1, \ldots, N$ satisfies

1) *conservation of mass, momentum, and energy:*

$$\frac{d}{dt}\sum_{p=1}^{N} w_i \phi(v_p) = 0, \quad \phi(v_p) = 1, v_p, |v_p|^2$$

2) *decay of entropy: let*

$$E_\varepsilon^N = E_\varepsilon(f^N) = \int_{\mathbb{R}^d} (\varphi_\varepsilon * f^N) \log(\varphi_\varepsilon * f^N)\, dv$$

be the discrete entropy, then

$$\frac{d}{dt} E_\varepsilon^N = -D_\varepsilon^N \leq 0$$

$$D_\varepsilon^N = \frac{1}{2}\sum_{p,q} w_p w_q \left(\nabla \frac{\delta E_\varepsilon^N}{\delta f}(v_p) - \nabla \frac{\delta E_\varepsilon^N}{\delta f}(v_q)\right)^T A(v_p - v_q) \left(\nabla \frac{\delta E_\varepsilon^N}{\delta f}(v_p) - \nabla \frac{\delta E_\varepsilon^N}{\delta f}(v_q)\right)$$

2D BKW solution with Maxwell kernel

Consider the collision kernel

$$A(z) = \frac{1}{16}(|z|^2 I_d - z \otimes z),$$

and an exact solution is given by

$$f^{\text{ext}}(t, v) = \frac{1}{2\pi K} \exp\left(-\frac{|v|^2}{2K}\right)\left(\frac{2K-1}{K} + \frac{1-K}{2K^2}|v|^2\right),$$

with $K = 1 - \exp(-t/8)/2$.

We choose $t_0 = 0$ and compute the solution until $t = 5$. The forward Euler with $\Delta t = 0.01$ is used for time discretization. Given $v_p(t)$, the numerical solution on the mesh is constructed as

$$f_\varepsilon^N(t, v_i^c) = f^N * \varphi_\varepsilon = \sum_{p=1}^{N} w_p \varphi_\varepsilon(v_i^c - v_p(t)).$$

The mesh size h is related to ε and is chosen as $\varepsilon = 0.64h^{1.98}$.

2D BKW solution with Maxwell kernel

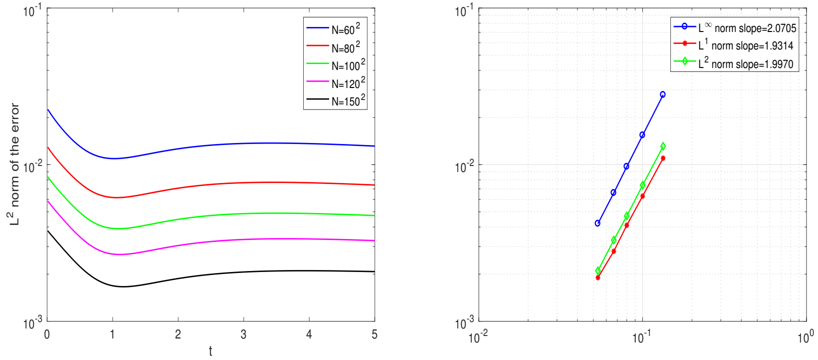

Figure: Left: Time evolution of $\|f^{\text{num}} - f^{\text{ext}}\|_{L^2}/\|f^{\text{ext}}\|_{L^2}$ with respect to different number of particles. Right: Relative L^∞, L^1, and L^2 norms of the error at time $t = 5$ with respect to different h.

Overview

The Vlasov-Landau-Maxwell system[9]

Consider

$$\partial_t f + v \cdot \nabla_x f + \frac{q}{m}(E + v \times B) \cdot \nabla_v f = Q(f, f),$$

coupled with the Maxwell's equations. We consider a particle solution as

$$f^N(t, x, v) = \sum_{p=1}^{N} w_p \delta(x - x_p(t))\delta(v - v_p(t)),$$

where N is the number of particles, w_p, x_p, v_p are the particle weight, position, and velocity, respectively. Following the characteristics, we require $x_p(t)$ and $v_p(t)$ to solve

Collisional Particle In Cell (CPIC) method

$$\begin{cases} \dfrac{\mathrm{d}x_p}{\mathrm{d}t} = v_p, \\ \dfrac{\mathrm{d}v_p}{\mathrm{d}t} = \dfrac{q}{m}(E(t, x_p) + v_p \times B(t, x_p)) - \mathcal{U}(f^N)(x_p, v_p), \end{cases}$$

where $E(t, x_p)$ and $B(t, x_p)$ are the electromagnetic fields at particle locations, $\mathcal{U}(f^N)(x_p, v_p)$ is the contribution from the collision term mimicking what happened in the homogeneous case (need proper regularization in both x and v).

[9] Bailo-Carrillo-H, work in progress.

Overview

Conclusion

A new particle method was introduced for the homogeneous Landau equation

- The method is based on the variational form of the Landau operator and regularization of the "free energy" (view the Landau equation as a modified 2-Wasserstein gradient flow)
- The main physical properties of the original equation: conservation of mass, momentum, energy, and decay of entropy can be maintained
- Easy extension to the spatially inhomogeneous case

Thank you!