



Mathematical
Institute

The Landau equation: Particle Methods & Gradient Flow Structure

J.A. CARRILLO

*Mathematical Institute
University of Oxford*

Jean-Morlet Chair - Conference - Kinetic Equations: from
Modeling Computation to Analysis, March 2021

Oxford
Mathematics

This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No 883363)



Outline

- 1 The Landau Equation
 - Basic Properties
 - Existing numerical methods for solving the Landau equation

- 2 A deterministic particle method
 - The Particle Method: Theory
 - The Particle Method: Practice

- 3 Metric Gradient Flows and the Landau equation
 - The Landau Equation as a Gradient Flow
 - Main Results

- 4 Global Conclusions

Outline

- 1 The Landau Equation
 - Basic Properties
 - Existing numerical methods for solving the Landau equation
- 2 A deterministic particle method
 - The Particle Method: Theory
 - The Particle Method: Practice
- 3 Metric Gradient Flows and the Landau equation
 - The Landau Equation as a Gradient Flow
 - Main Results
- 4 Global Conclusions

The Landau equation

Written by Landau in the second half of the 20th century^a.

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

^aE.M. Lifschitz. Perspectives in theoretical physics. Pergamon Press, Oxford, 1992.

- $f(t, x, v)$ is the **probability density function (PDF)** of time t , position x , and particle velocity v
- F is the acceleration due to external or self-consistent forces
- $Q(f, f)$ is the **(Fokker-Planck-)Landau collision operator**, a diffusive type integral operator modeling the grazing collisions between particles (can be derived from the Boltzmann collision operator)
- The equation is widely used to describe collisional plasmas

The Landau collision operator

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

where A is a (semi-positive-definite) matrix given by

$$A(z) = |z|^{\gamma+2} \Pi[z] \quad \text{with} \quad \Pi[z] = \left(\text{Id} - \frac{z \otimes z}{|z|^2} \right), \quad -d - 1 \leq \gamma \leq 1,$$

$d = 3, \gamma = -3$ is the **Coulomb** potential.

The log form is useful to identify its properties

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

from which we can derive the weak form

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

The Landau collision operator

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

where A is a (semi-positive-definite) matrix given by

$$A(z) = |z|^{\gamma+2} \Pi[z] \quad \text{with} \quad \Pi[z] = \left(\text{Id} - \frac{z \otimes z}{|z|^2} \right), \quad -d - 1 \leq \gamma \leq 1,$$

$d = 3, \gamma = -3$ is the **Coulomb** potential.

The log form is useful to identify its properties

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

from which we can derive the weak form

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

The Landau collision operator

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

where A is a (semi-positive-definite) matrix given by

$$A(z) = |z|^{\gamma+2} \Pi[z] \quad \text{with} \quad \Pi[z] = \left(\text{Id} - \frac{z \otimes z}{|z|^2} \right), \quad -d - 1 \leq \gamma \leq 1,$$

$d = 3, \gamma = -3$ is the **Coulomb** potential.

The log form is useful to identify its properties

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

from which we can derive the weak form

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

Properties of Q

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

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

- **entropy decay**:

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

- **equilibrium** function:

$$“ = ” \iff f = \mathcal{M}_{\rho, u, T} := \frac{\rho}{(2\pi T)^{d/2}} e^{-\frac{|v-u|^2}{2T}} \iff Q(f, f) = 0$$

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

More on entropy dissipation

Formally, the H-theorem for Landau reads

$$\begin{aligned} \frac{d}{dt} \int_{\mathbb{R}^d} f \log f dv &= -D(f) := \\ &- \frac{1}{2} \iint_{\mathbb{R}^{2d}} ff_* \left| |v - v_*|^{1+\frac{\gamma}{2}} \Pi[v - v_*] (\nabla \log f - \nabla_* \log f_*) \right|^2 dv dv_* \leq 0. \end{aligned}$$

- Crucial for bypassing unavailable L^p_v estimates to make sense of weak solution for sufficiently negative γ (c.f. H-solutions of Villani¹).
- Furthermore, this gives a variational formulation of Landau with entropy decrease.
- Landau entropy dissipation $D(f)$ is reminiscent of weighted Fisher information regularity estimate/heat flow entropy dissipation (c.f. entropy dissipation estimates of Desvillettes²).

¹On a New Class of Weak Solutions to the Spatially Homogeneous Boltzmann and Landau Equations, ARMA 1998.

²Entropy dissipation estimates for the Landau equation in the Coulomb case and applications, JFA 2015.

More on entropy dissipation

Formally, the H-theorem for Landau reads

$$\begin{aligned} \frac{d}{dt} \int_{\mathbb{R}^d} f \log f dv &= -D(f) := \\ &- \frac{1}{2} \iint_{\mathbb{R}^{2d}} ff_* \left| |v - v_*|^{1+\frac{\gamma}{2}} \Pi[v - v_*] (\nabla \log f - \nabla_* \log f_*) \right|^2 dv dv_* \leq 0. \end{aligned}$$

- Crucial for bypassing unavailable L^p_v estimates to make sense of weak solution for sufficiently negative γ (c.f. H-solutions of Villani¹).
- Furthermore, this gives a variational formulation of Landau with entropy decrease.
- Landau entropy dissipation $D(f)$ is reminiscent of weighted Fisher information regularity estimate/heat flow entropy dissipation (c.f. entropy dissipation estimates of Desvillettes²).

¹On a New Class of Weak Solutions to the Spatially Homogeneous Boltzmann and Landau Equations, ARMA 1998.

²Entropy dissipation estimates for the Landau equation in the Coulomb case and applications, JFA 2015.

More on entropy dissipation

Formally, the H-theorem for Landau reads

$$\begin{aligned} \frac{d}{dt} \int_{\mathbb{R}^d} f \log f dv &= -D(f) := \\ &- \frac{1}{2} \iint_{\mathbb{R}^{2d}} ff_* \left| |v - v_*|^{1+\frac{\gamma}{2}} \Pi[v - v_*] (\nabla \log f - \nabla_* \log f_*) \right|^2 dv dv_* \leq 0. \end{aligned}$$

- Crucial for bypassing unavailable L^p_v estimates to make sense of weak solution for sufficiently negative γ (c.f. H-solutions of Villani¹).
- Furthermore, this gives a variational formulation of Landau with entropy decrease.
- Landau entropy dissipation $D(f)$ is reminiscent of weighted Fisher information regularity estimate/heat flow entropy dissipation (c.f. entropy dissipation estimates of Desvillettes²).

¹On a New Class of Weak Solutions to the Spatially Homogeneous Boltzmann and Landau Equations, ARMA 1998.

²Entropy dissipation estimates for the Landau equation in the Coulomb case and applications, JFA 2015.

Outline

- 1 The Landau Equation
 - Basic Properties
 - Existing numerical methods for solving the Landau equation
- 2 A deterministic particle method
 - The Particle Method: Theory
 - The Particle Method: Practice
- 3 Metric Gradient Flows and the Landau equation
 - The Landau Equation as a Gradient Flow
 - Main Results
- 4 Global Conclusions

Numerical challenges in solving the Landau equation

Here we focus on the spatially homogeneous Landau equation

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

- **collision operator:** a direct approximation of Q would require $O(N^{2d})$ numerical complexity — expensive in 2D/3D
- **maintain the physical properties at the discrete level:** conservation, positivity, entropy decay, etc.
- **time discretization:** explicit time discretization would suffer from the parabolic CFL condition $\Delta t = O(\Delta v^2)$; even worse in the high collision regime $\Delta t = O(\varepsilon \Delta v^2)$ (ε is the Knudsen number)

Approximation of the collision operator

- **Finite difference method** (aka **discrete velocity method**)

- many works in the simplified setting (2D, radially symmetric solutions, etc.)
- for the full 3D operator: conservative and entropic schemes³, efficiency further improved using sublattice method, multigrid method, multipole method, etc.⁴
 - (+) preserve physical properties
 - (+, -) second order accuracy (rigid)
 - (-) expensive $O(N^{2d})$

³Degond, Lucquin-Desreux, '94, Buet and Cordier, '99.

⁴Buet, Cordier, Degond, Lemou, '97; Lemou, '98.

Approximation of the collision operator (cont'd)

- **Fourier-Galerkin spectral method**⁵: 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

⁵Pareschi, Russo, Toscani, '00; H., Jin, Yan, '12; Zhang and Gamba, '17.

Approximation of the collision operator (cont'd)

- **Rosenbluth form** is often used by plasma physicists⁶

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

$$A_f = \int A(v - v_*) f(v_*) dv_*, \quad a_f = \text{tr}(A_f)$$

A_f and a_f can be computed from the Rosenbluth potentials G and H

$$A_f = D^2 G, \quad a_f = H,$$

and G and H can be solved from

$$\Delta H = -f, \quad \Delta G = H.$$

(+) complexity $O(N^d)$ provided a fast Poisson solver

(+) can be made conservative and positive by using some limiters

(-) no entropy decay

⁶Taitano, Chacon, Simakov, Molvig, '15.

Approximation of the collision operator (cont'd)

- **Monte Carlo** method: based on particle collision⁷ or based on solving the SDE⁸:

$$dv_i = F_i dt + D_{ij} dW_j$$

(+) highly efficient, dimension independent

(-) converges slowly $O(N^{-1/2})$ (N : number of particles)

(-) solution contains noise

⁷Takizuka, '77. Lemons, Winske, Daughton, and Albright, '09.

⁸Rosin, Ricketson, Dimits, Caflisch, and Cohen, '14.

Outline

- 1 The Landau Equation
 - Basic Properties
 - Existing numerical methods for solving the Landau equation
- 2 A deterministic particle method
 - **The Particle Method: Theory**
 - The Particle Method: Practice
- 3 Metric Gradient Flows and the Landau equation
 - The Landau Equation as a Gradient Flow
 - Main Results
- 4 Global Conclusions

Main idea

Recall the Landau operator can be written as

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

where

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

We propose to modify it to

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

with

$$E_\varepsilon(f) = \int_{\mathbb{R}^d} (f * \psi_\varepsilon) \log(f * \psi_\varepsilon) \, dv, \quad \psi_\varepsilon(v) = \frac{1}{(2\pi\varepsilon)^{d/2}} \exp\left(-\frac{|v|^2}{2\varepsilon}\right)$$

Main idea

Recall the Landau operator can be written as

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

where

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

We propose to modify it to

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

with

$$E_\varepsilon(f) = \int_{\mathbb{R}^d} (f * \psi_\varepsilon) \log(f * \psi_\varepsilon) \, dv, \quad \psi_\varepsilon(v) = \frac{1}{(2\pi\varepsilon)^{d/2}} \exp\left(-\frac{|v|^2}{2\varepsilon}\right)$$

Main idea (cont'd)

Accordingly, the equation is modified to

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

with

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

Note also

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

That is, we rewrite the Landau equation into a convection equation with regularized velocity $U_\varepsilon(f)$, hence giving access to particle solutions.⁹

⁹Carrillo, Craig, and Patacchini, '19.

Why the regularization is good?

For the regularized Landau operator, one has

$$\int_{\mathbb{R}^d} Q_\varepsilon(f, f) \phi \, dv = -\frac{1}{2} \iint_{\mathbb{R}^{2d}} ff_* [\nabla_v \phi - \nabla_{v_*} \phi_*]^T A(v - v_*) \left(\nabla_v \frac{\delta E_\varepsilon}{\delta f} - \nabla_{v_*} \frac{\delta E_{\varepsilon,*}}{\delta f_*} \right) dv_* \, dv$$

hence

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

$$\int_{\mathbb{R}^d} Q_\varepsilon(f, f) \, dv = \int_{\mathbb{R}^d} Q_\varepsilon(f, f) v \, dv = \int_{\mathbb{R}^d} Q_\varepsilon(f, f) |v|^2 \, dv = 0$$

- **entropy decay:**

$$\int_{\mathbb{R}^d} Q_\varepsilon(f, f) \frac{\delta E_\varepsilon}{\delta f} \, dv \leq 0$$

Why the regularization is good (cont'd)?

- **equilibrium** function:

$$“ = ” \iff \frac{\delta E_\varepsilon}{\delta f} = \lambda^{(0)} + \lambda^{(1)} \cdot v + \frac{\lambda^{(2)}}{2} |v|^2 \iff \mathcal{Q}_\varepsilon(f, f) = 0$$

Furthermore, since $\frac{\delta E_\varepsilon}{\delta f} = \psi_\varepsilon * \log(f * \psi_\varepsilon)$, one can deduce that

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

where

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

The particle method

For the equation

$$\partial_t f + \nabla_v \cdot (U_\varepsilon(f)f) = 0$$

we look for a particle solution as

$$f^N(t, v) = \sum_{i=1}^N w_i \delta(v - v_i(t))$$

where N is the number of particles, $v_i(t)$ is the velocity of particle i . The the initial velocity and the weight w_i are set as

$$v_i(0) = v_i^c, \quad w_i = f_0(v_i^c) h^d,$$

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 particle method (cont'd)

For the equation

$$\partial_t f + \nabla_v \cdot (U_\varepsilon(f)f) = 0$$

we look for a particle solution as

$$f^N(t, v) = \sum_{i=1}^N w_i \delta(v - v_i(t))$$

where N is the number of particles, then the particle velocity $v_i(t)$ satisfies

$$\frac{dv_i(t)}{dt} = U_\varepsilon(f^N)(t, v_i(t)) = - \sum_j w_j A(v_i - v_j) \left[\nabla \frac{\delta E_\varepsilon^N}{\delta f}(v_i) - \nabla \frac{\delta E_\varepsilon^N}{\delta f}(v_j) \right]$$

where

$$\frac{\delta E_\varepsilon^N}{\delta f} := \psi_\varepsilon * \log(f^N * \psi_\varepsilon) = \int_{\mathbb{R}^d} \psi_\varepsilon(v - u) \log \left(\sum_k w_k \psi_\varepsilon(u - v_k) \right) du$$

Properties of the particle solution

Theorem

The particle solution $v_i(t)$, $i = 1, \dots, N$ satisfies

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

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

- 2) dissipation of entropy: let

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

be the discrete entropy, then

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

$$D_\varepsilon^N = \frac{1}{2} \sum_{i,j} w_i w_j \left(\nabla \frac{\delta E_\varepsilon^N}{\delta f}(v_i) - \nabla \frac{\delta E_\varepsilon^N}{\delta f}(v_j) \right)^T A(v_i - v_j) \left(\nabla \frac{\delta E_\varepsilon^N}{\delta f}(v_i) - \nabla \frac{\delta E_\varepsilon^N}{\delta f}(v_j) \right)$$

A further approximation

$$\frac{dv_i(t)}{dt} = U_\varepsilon(f^N)(t, v_i(t)) = - \sum_j w_j A(v_i - v_j) \left[\nabla \frac{\delta E_\varepsilon^N}{\delta f}(v_i) - \nabla \frac{\delta E_\varepsilon^N}{\delta f}(v_j) \right]$$

$$\begin{aligned} \nabla \frac{\delta E_\varepsilon^N}{\delta f}(v_i) &= \int_{\mathbb{R}^d} \nabla \psi_\varepsilon(v_i - v) \log \left(\sum_k w_k \psi_\varepsilon(v - v_k) \right) dv \\ &\approx \sum_l h^d \nabla \psi_\varepsilon(v_i - v_l^c) \log \left(\sum_k w_k \psi_\varepsilon(v_l^c - v_k) \right) \end{aligned}$$

where v_l^c is the mesh for initialization.

Properties of the particle solution

With this further quadrature approximation, one can still show the conservation of mass, momentum, and energy. The fully discrete entropy

$$E_\varepsilon^N = \sum_l h^d \left(\sum_i w_i \psi_\varepsilon(v_l^c - v_i) \right) \log \left(\sum_k w_k \psi_\varepsilon(v_l^c - v_k) \right)$$

satisfies

$$\frac{d}{dt} E_\varepsilon^N = -D_\varepsilon^N + O(h^2)$$

with

$$D_\varepsilon^N = \frac{1}{2} \sum_{i,j} w_i w_j \left(\nabla \frac{\delta E_\varepsilon^N}{\delta f}(v_i) - \nabla \frac{\delta E_\varepsilon^N}{\delta f}(v_j) \right)^T A(v_i - v_j) \left(\nabla \frac{\delta E_\varepsilon^N}{\delta f}(v_i) - \nabla \frac{\delta E_\varepsilon^N}{\delta f}(v_j) \right)$$

Outline

- 1 The Landau Equation
 - Basic Properties
 - Existing numerical methods for solving the Landau equation
- 2 A deterministic particle method
 - The Particle Method: Theory
 - **The Particle Method: Practice**
- 3 Metric Gradient Flows and the Landau equation
 - The Landau Equation as a Gradient Flow
 - Main Results
- 4 Global Conclusions

Some implementation details

Given $v_i(t)$, the numerical solution is constructed as

$$f_\varepsilon^N(t, v) = f^N * \psi_\varepsilon = \sum_{i=1}^N w_i \psi_\varepsilon(v - v_i)$$

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

2D BKW solution for Maxwell molecules

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.

2D BKW solution for Maxwell molecules

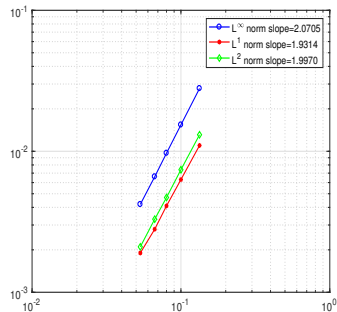
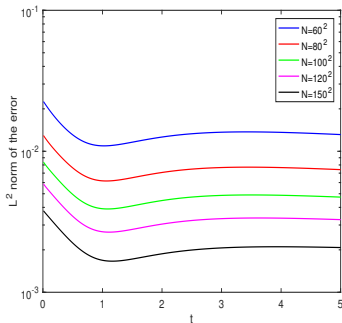


Figure: Left: Time evolution of $\|f^{\text{num}} - f^{\text{ext}}\|_{L^2} / \|f^{\text{ext}}\|_{L^2}$ with respect to different number of particles. Right: Relative L^∞ , L^1 , and L^2 norms of the error at time $t = 5$ with respect to different h .

3D BKW solution for Maxwell molecules

Consider the collision kernel

$$A(z) = \frac{1}{24} (|z|^2 I_d - z \otimes z),$$

and an exact solution is given by

$$f^{\text{ext}}(t, v) = \frac{1}{(2\pi K)^{3/2}} \exp\left(-\frac{|v|^2}{2K}\right) \left(\frac{5K-3}{2K} + \frac{1-K}{2K^2} |v|^2\right),$$

with $K = 1 - \exp(-t/6)$.

We choose $t_0 = 5.5$ and compute the solution until $t = 6$. The forward Euler with $\Delta t = 0.01$ is used for time discretization.

3D BKW solution for Maxwell molecules

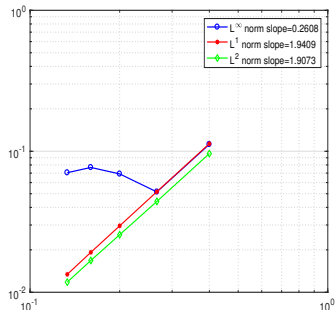
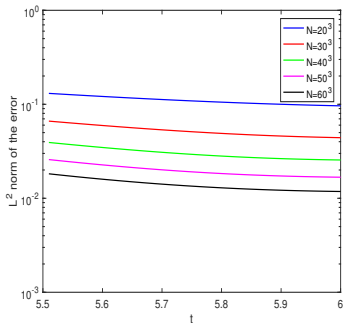


Figure: Left: Time evolution of $\|f^{\text{num}} - f^{\text{ext}}\|_{L^2} / \|f^{\text{ext}}\|_{L^2}$ with respect to different number of particles. Right: Relative L^∞ , L^1 , and L^2 norms of the error at time $t = 6.5$ with respect to different h .

2D anisotropic solution with Coulomb potential

Consider the collision kernel

$$A(z) = \frac{1}{16} \frac{1}{|z|^3} (|z|^2 I_d - z \otimes z),$$

and the initial condition

$$f(0, v) = \frac{1}{4\pi} \left\{ \exp\left(-\frac{(v - u_1)^2}{2}\right) + \exp\left(-\frac{(v - u_2)^2}{2}\right) \right\},$$

with $u_1 = (-2, 1)$, $u_2 = (0, -1)$.

We compare with the **Fourier spectral method**¹⁰ since there is no analytical solution. The same computational domain is used by both methods. For the particle method, the forward Euler with $\Delta t = 0.1$ is used for time discretization. For the spectral method, the second order Heun's method with $\Delta t = 0.1$ is used for time discretization.

¹⁰Pareschi, Russo, and Toscani, '00.

2D anisotropic solution with Coulomb potential

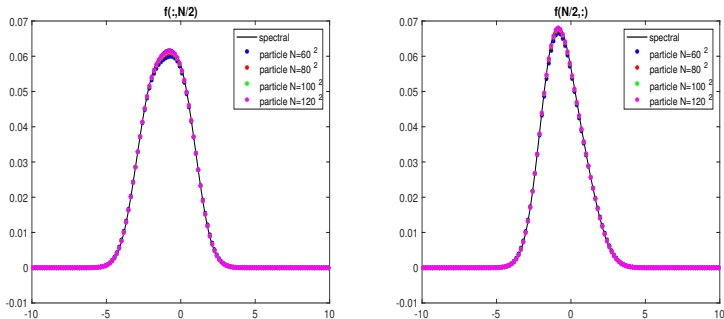


Figure: Comparison of the particle method (using different particle numbers) with the spectral method ($N_v = 128^2$). Slices of the solutions at time $t = 20$.

2D anisotropic solution with Coulomb potential

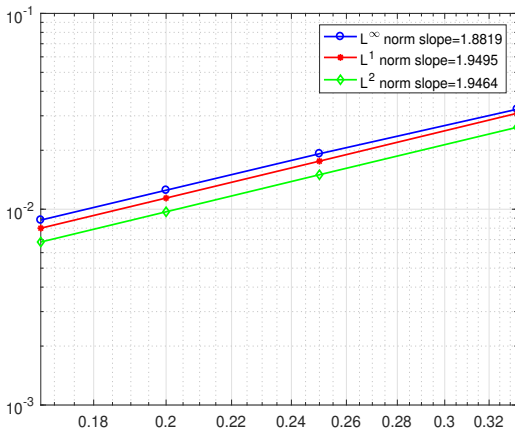


Figure: Relative L^∞ , L^1 , and L^2 norms of the error at time $t = 20$ with respect to different h .

3D Rosenbluth problem with Coulomb potential

Consider the collision kernel

$$A(z) = \frac{1}{4\pi} \frac{1}{|z|^3} (|z|^2 I_d - z \otimes z),$$

and the initial condition

$$f(0, v) = \frac{1}{S^2} \exp\left(-S \frac{(|v| - \sigma)^2}{\sigma^2}\right), \quad \sigma = 0.3, \quad S = 10.$$

The cost of the (direct) particle method in 3D is $O(N^2)$, $N = n^3$ (n the initial mesh in each dimension). Hence we speed it up using the **treecode**¹¹, whose complexity is $O(N \log N)$.

¹¹Li, Johnston, and Krasny, '09.

3D Rosenbluth problem with Coulomb potential

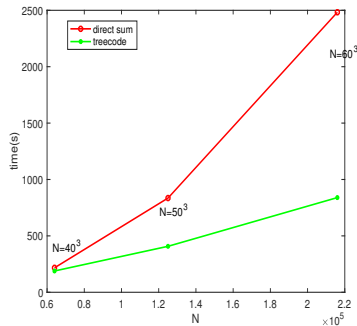
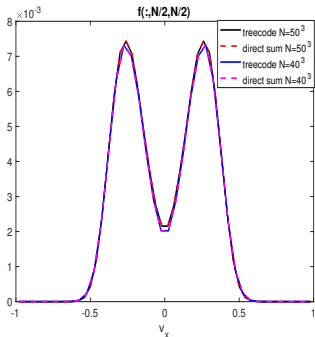


Figure: Left: comparison a slice of solution with direct sum and treecode at $t = 20$, $N = 50^3$ or $N = 40^3$. Right: comparison of computational sum time (in seconds) for one step with the treecode solver and with the direct sum solver.

Conclusions on the numerical side

A new particle method was introduced for the homogeneous Landau equation

- Based on regularization of the entropy term in the collision operator
- The main physical properties: conservation of mass, momentum, energy, and decay of entropy can be maintained
- The second order accuracy can be observed

Future work

- Couple with the PIC to solve the full Vlasov-Poisson-Landau equation
- Investigate fast techniques to accelerate the method while maintaining the physical properties
- Study the convergence/accuracy of the method

Outline

- 1 The Landau Equation
 - Basic Properties
 - Existing numerical methods for solving the Landau equation
- 2 A deterministic particle method
 - The Particle Method: Theory
 - The Particle Method: Practice
- 3 Metric Gradient Flows and the Landau equation
 - The Landau Equation as a Gradient Flow
 - Main Results
- 4 Global Conclusions

Rewriting the Landau Equation

Consider a test function $\phi \in C_c^\infty(\mathbb{R}^d)$, the weak formulation is given by

$$\frac{d}{dt} \int_{\mathbb{R}^d} \phi f dv = -\frac{1}{2} \iint_{\mathbb{R}^{2d}} ff_* (\nabla \phi - \nabla_* \phi_*)^T A[v - v_*] (\nabla \log f - \nabla_* \log f_*) dv_* dv, \quad (1)$$

where the change of variables $v \leftrightarrow v_*$ has been exploited. Building an analogy with the heat equation and the 2-Wasserstein distance, we define an appropriate gradient

$$\tilde{\nabla} \phi := |v - v_*|^{1+\frac{\gamma}{2}} \Pi[v - v_*] (\nabla \phi - \nabla_* \phi_*),$$

so that equation (1) now looks like

$$\frac{d}{dt} \int_{\mathbb{R}^d} \phi f dv = -\frac{1}{2} \iint_{\mathbb{R}^{2d}} ff_* \tilde{\nabla} \phi \cdot \tilde{\nabla} \log f dv_* dv,$$

noting that $\Pi^2 = \Pi$.

Rewriting the Landau Equation

Consider a test function $\phi \in C_c^\infty(\mathbb{R}^d)$, the weak formulation is given by

$$\frac{d}{dt} \int_{\mathbb{R}^d} \phi f dv = -\frac{1}{2} \iint_{\mathbb{R}^{2d}} ff_* (\nabla \phi - \nabla_* \phi_*)^T A[v - v_*] (\nabla \log f - \nabla_* \log f_*) dv_* dv, \quad (1)$$

where the change of variables $v \leftrightarrow v_*$ has been exploited. Building an analogy with the heat equation and the 2-Wasserstein distance, we define an appropriate gradient

$$\tilde{\nabla} \phi := |v - v_*|^{1+\frac{\gamma}{2}} \Pi[v - v_*] (\nabla \phi - \nabla_* \phi_*),$$

so that equation (1) now looks like

$$\frac{d}{dt} \int_{\mathbb{R}^d} \phi f dv = -\frac{1}{2} \iint_{\mathbb{R}^{2d}} ff_* \tilde{\nabla} \phi \cdot \tilde{\nabla} \log f dv_* dv,$$

noting that $\Pi^2 = \Pi$.

Rewriting the Landau Equation 2

The Landau metric is built by considering a minimizing action principle over curves that are solutions to the appropriate continuity equation, that is

$$d_L(f, g) := \min_{\substack{\partial_t \mu + \frac{1}{2} \tilde{\nabla} \cdot (V \mu \mu_*) = 0 \\ \mu_0 = f, \mu_1 = g}} \left\{ \frac{1}{2} \int_0^1 \iint_{\mathbb{R}^{2d}} |V|^2 d\mu(v) d\mu(v_*) dt \right\},$$

where the $\tilde{\nabla} \cdot$ is the appropriate divergence; the formal adjoint to the gradient operator $\tilde{\nabla} \phi$.

The Landau equation can be formally re-written as

$$\partial_t f = \frac{1}{2} \tilde{\nabla} \cdot (ff_* \tilde{\nabla} \log f),$$

equivalent to the continuity equation with non-local velocity field given by

$$\begin{cases} \partial_t f + \nabla \cdot (U(f)f) = 0 \\ U(f) := - \int_{\mathbb{R}^d} |v - v_*|^{2+\gamma} \Pi[v - v_*] (\nabla \log f - \nabla_* \log f_*) f_* dv_* . \end{cases}$$

Rewriting the Landau Equation 2

The Landau metric is built by considering a minimizing action principle over curves that are solutions to the appropriate continuity equation, that is

$$d_L(f, g) := \min_{\substack{\partial_t \mu + \frac{1}{2} \tilde{\nabla} \cdot (V \mu \mu_*) = 0 \\ \mu_0 = f, \mu_1 = g}} \left\{ \frac{1}{2} \int_0^1 \iint_{\mathbb{R}^{2d}} |V|^2 d\mu(v) d\mu(v_*) dt \right\},$$

where the $\tilde{\nabla} \cdot$ is the appropriate divergence; the formal adjoint to the gradient operator $\tilde{\nabla} \phi$.

The Landau equation can be formally re-written as

$$\partial_t f = \frac{1}{2} \tilde{\nabla} \cdot (ff_* \tilde{\nabla} \log f),$$

equivalent to the continuity equation with non-local velocity field given by

$$\begin{cases} \partial_t f + \nabla \cdot (U(f)f) = 0 \\ U(f) := - \int_{\mathbb{R}^d} |v - v_*|^{2+\gamma} \Pi[v - v_*] (\nabla \log f - \nabla_* \log f_*) f_* dv_* . \end{cases}$$

Comparison to classical Wasserstein gradient flows

Gradient Flows with respect to the Wasserstein distance:

$$\begin{cases} \partial_t f + \nabla \cdot (Uf) = 0 \\ U := -\nabla \frac{\delta \mathcal{H}}{\delta f} . \end{cases}$$

Gradient Flows with respect to the Landau distance:

$$\begin{cases} \partial_t f + \frac{1}{2} \tilde{\nabla} \cdot (Uff_*) = 0 \\ U := -\tilde{\nabla} \frac{\delta \mathcal{H}}{\delta f} . \end{cases}$$

Comparison to classical Wasserstein gradient flows

Gradient Flows with respect to the Wasserstein distance:

$$\begin{cases} \partial_t f + \nabla \cdot (Uf) = 0 \\ U := -\nabla \frac{\delta \mathcal{H}}{\delta f} . \end{cases}$$

Gradient Flows with respect to the Landau distance:

$$\begin{cases} \partial_t f + \frac{1}{2} \tilde{\nabla} \cdot (Uff_*) = 0 \\ U := -\tilde{\nabla} \frac{\delta \mathcal{H}}{\delta f} . \end{cases}$$

Outline

- 1 The Landau Equation
 - Basic Properties
 - Existing numerical methods for solving the Landau equation
- 2 A deterministic particle method
 - The Particle Method: Theory
 - The Particle Method: Practice
- 3 Metric Gradient Flows and the Landau equation
 - The Landau Equation as a Gradient Flow
 - **Main Results**
- 4 Global Conclusions

The Landau distance

The Landau distance¹² is defined by

$$d_L^2(\lambda, \nu) := \inf \left\{ T \int_0^T \mathcal{A}(\mu_t, M_t) dt \mid (\mu, M) \in \mathcal{GC}\mathcal{E}_T^{2,E}(\lambda, \nu) \right\}.$$

Theorem

The (pseudo)-metric d_L on $\mathcal{P}_{2,E}(\mathbb{R}^d)$, satisfies:

- d_L -convergent sequences are weakly convergent.
- d_L -bounded sets are weakly compact.
- The map $(\mu_0, \mu_1) \mapsto d_L(\mu_0, \mu_1)$ is weakly lower semicontinuous.
- For any $\tau \in \mathcal{P}_2(\mathbb{R}^d)$ the subset $\mathcal{P}_\tau(\mathbb{R}^d) := \{ \mu \in \mathcal{P}_{2,m_2(\tau)}(\mathbb{R}^d) \mid d_L(\mu, \tau) < \infty \}$ is a complete geodesic space.

¹²M. Erbar, preprint 2016.

ϵ -Landau equation

A regularized version of the Landau equation can be written as

$$\partial_t f = \nabla \cdot \left\{ f \int_{\mathbb{R}^d} f_* |v - v_*|^{2+\gamma} \Pi[v - v_*] \left(\nabla \frac{\delta \mathcal{H}_\epsilon}{\delta f} - \nabla_* \frac{\delta \mathcal{H}_\epsilon}{\delta f_*} \right) dv_* \right\}.$$

where the regularised entropy and its first variation are

$$\mathcal{H}_\epsilon[f] = \int_{\mathbb{R}^d} (f * G_\epsilon) \log(f * G_\epsilon) dv, \quad \frac{\delta \mathcal{H}_\epsilon}{\delta f} = G_\epsilon * \log(f * G_\epsilon)$$

and G_ϵ is a mollifier.

- This idea was used earlier for nonlinear diffusions to approximate them by nonlocal equations¹³.
- This approximation can be used to write a deterministic particle method for the regularized Landau equation¹⁴ by choosing an empirical measure ansatz.

¹³C.-Craig-Patacchini, A Blob Method For Diffusion, CVPDE 2019

¹⁴C.-Hu-Wang-Wu, A particle method for the homogeneous Landau equation, JCP-X 2020.

ϵ -Landau equation

A regularized version of the Landau equation can be written as

$$\partial_t f = \nabla \cdot \left\{ f \int_{\mathbb{R}^d} f_* |v - v_*|^{2+\gamma} \Pi[v - v_*] \left(\nabla \frac{\delta \mathcal{H}_\epsilon}{\delta f} - \nabla_* \frac{\delta \mathcal{H}_\epsilon}{\delta f_*} \right) dv_* \right\}.$$

where the regularised entropy and its first variation are

$$\mathcal{H}_\epsilon[f] = \int_{\mathbb{R}^d} (f * G_\epsilon) \log(f * G_\epsilon) dv, \quad \frac{\delta \mathcal{H}_\epsilon}{\delta f} = G_\epsilon * \log(f * G_\epsilon)$$

and G_ϵ is a mollifier.

- This idea was used earlier for nonlinear diffusions to approximate them by nonlocal equations¹³.
- This approximation can be used to write a deterministic particle method for the regularized Landau equation¹⁴ by choosing an empirical measure ansatz.

¹³C.-Craig-Patacchini, A Blob Method For Diffusion, CVPDE 2019

¹⁴C.-Hu-Wang-Wu, A particle method for the homogeneous Landau equation, JCP-X 2020.

ϵ -Landau equation

A regularized version of the Landau equation can be written as

$$\partial_t f = \nabla \cdot \left\{ f \int_{\mathbb{R}^d} f_* |v - v_*|^{2+\gamma} \Pi[v - v_*] \left(\nabla \frac{\delta \mathcal{H}_\epsilon}{\delta f} - \nabla_* \frac{\delta \mathcal{H}_\epsilon}{\delta f_*} \right) dv_* \right\}.$$

where the regularised entropy and its first variation are

$$\mathcal{H}_\epsilon[f] = \int_{\mathbb{R}^d} (f * G_\epsilon) \log(f * G_\epsilon) dv, \quad \frac{\delta \mathcal{H}_\epsilon}{\delta f} = G_\epsilon * \log(f * G_\epsilon)$$

and G_ϵ is a mollifier.

- This idea was used earlier for nonlinear diffusions to approximate them by nonlocal equations¹³.
- This approximation can be used to write a deterministic particle method for the regularized Landau equation¹⁴ by choosing an empirical measure ansatz.

¹³C.-Craig-Patacchini, A Blob Method For Diffusion, CVPDE 2019

¹⁴C.-Hu-Wang-Wu, A particle method for the homogeneous Landau equation, JCP-X 2020.

Equivalence and Existence for the regularised Landau

Theorem

For $\epsilon > 0$, the notion of gradient flow solution with respect to the Landau distance on the regularised entropy functional

$$\mathcal{H}_\epsilon[f] = \int_{\mathbb{R}^d} f * G_\epsilon \log(f * G_\epsilon), \quad G_\epsilon(v) = \frac{1}{\epsilon^d} G\left(\frac{v}{\epsilon}\right),$$

is equivalent to the notion of weak solution of the ϵ -regularisation of the Landau equation. Here, $G(v)$ is the smooth convolution kernel

$$G(v) = C_d \exp\left\{-\sqrt{1 + |v|^2}\right\}.$$

Theorem

There exists a curve of maximal slope to the ϵ -regularised entropy with respect to the Landau distance.

Equivalence and Existence for the regularised Landau

Theorem

For $\epsilon > 0$, the notion of gradient flow solution with respect to the Landau distance on the regularised entropy functional

$$\mathcal{H}_\epsilon[f] = \int_{\mathbb{R}^d} f * G_\epsilon \log(f * G_\epsilon), \quad G_\epsilon(v) = \frac{1}{\epsilon^d} G\left(\frac{v}{\epsilon}\right),$$

is equivalent to the notion of weak solution of the ϵ -regularisation of the Landau equation. Here, $G(v)$ is the smooth convolution kernel

$$G(v) = C_d \exp\left\{-\sqrt{1 + |v|^2}\right\}.$$

Theorem

There exists a curve of maximal slope to the ϵ -regularised entropy with respect to the Landau distance.

Gradient Flow solutions = Weak solutions for Landau

Theorem

The notion of gradient flow solution with respect to the Landau distance of the Boltzmann entropy functional is equivalent to the notion of weak solutions of the Landau equation.

- The control using the Landau entropy dissipation of Fisher information like functionals due to Desvillettes¹⁵ is crucial for this result.
- The strategy of the proof is to pass to the limit in the chain rule of the Boltzmann entropy from the regularized Landau equations for a given fixed curve defined by the grazing continuity equation.
- We are not able yet to show the existence of a curve of maximal slope to the entropy with respect to the Landau distance. This needs stability estimates for a sequence of solutions of the regularized Landau problems leading to good compactness properties from the control of the Landau dissipation functional.

¹⁵Entropy dissipation estimates for the Landau equation in the Coulomb case and applications, JFA 2015.

Gradient Flow solutions = Weak solutions for Landau

Theorem

The notion of gradient flow solution with respect to the Landau distance of the Boltzmann entropy functional is equivalent to the notion of weak solutions of the Landau equation.

- The control using the Landau entropy dissipation of Fisher information like functionals due to Desvillettes¹⁵ is crucial for this result.
- The strategy of the proof is to pass to the limit in the chain rule of the Boltzmann entropy from the regularized Landau equations for a given fixed curve defined by the grazing continuity equation.
- We are not able yet to show the existence of a curve of maximal slope to the entropy with respect to the Landau distance. This needs stability estimates for a sequence of solutions of the regularized Landau problems leading to good compactness properties from the control of the Landau dissipation functional.

¹⁵Entropy dissipation estimates for the Landau equation in the Coulomb case and applications, JFA 2015.

Conclusions

- The Landau equation is written as a gradient flow introducing a bespoke distance.
- Efficient deterministic Particle Methods can be derived for the Landau equation.
- Gradient flow solutions are equivalent to weak distributional solutions of Landau with finite entropy and entropy dissipation and certain propagation of moment condition.
- Existence of solutions for a regularized Landau equation via this approach using the DiGiorgi minimizing movement scheme approach.
- **Perspectives:** Use of Γ -convergence techniques to show the convergence of the gradient flow solutions constructed by Erbar for the Boltzmann equation towards the gradient flow solutions of the Landau equation.
- References:
 - ① C.-Hu-Wang-Wu (JCP-X 2020).
 - ② C.-Delgadino-Desvillettes-Wu (Preprint ArXiv).

Conclusions

- The Landau equation is written as a gradient flow introducing a bespoke distance.
- Efficient deterministic Particle Methods can be derived for the Landau equation.
- Gradient flow solutions are equivalent to weak distributional solutions of Landau with finite entropy and entropy dissipation and certain propagation of moment condition.
- Existence of solutions for a regularized Landau equation via this approach using the DiGiorgi minimizing movement scheme approach.
- **Perspectives:** Use of Γ -convergence techniques to show the convergence of the gradient flow solutions constructed by Erbar for the Boltzmann equation towards the gradient flow solutions of the Landau equation.
- References:
 - ① C.-Hu-Wang-Wu (JCP-X 2020).
 - ② C.-Delgado-Desvilletes-Wu (Preprint ArXiv).

Conclusions

- The Landau equation is written as a gradient flow introducing a bespoke distance.
- Efficient deterministic Particle Methods can be derived for the Landau equation.
- Gradient flow solutions are equivalent to weak distributional solutions of Landau with finite entropy and entropy dissipation and certain propagation of moment condition.
- Existence of solutions for a regularized Landau equation via this approach using the DiGiorgi minimizing movement scheme approach.
- **Perspectives:** Use of Γ -convergence techniques to show the convergence of the gradient flow solutions constructed by Erbar for the Boltzmann equation towards the gradient flow solutions of the Landau equation.
- References:
 - ① C.-Hu-Wang-Wu (JCP-X 2020).
 - ② C.-Delgadino-Desvillettes-Wu (Preprint ArXiv).

Conclusions

- The Landau equation is written as a gradient flow introducing a bespoke distance.
- Efficient deterministic Particle Methods can be derived for the Landau equation.
- Gradient flow solutions are equivalent to weak distributional solutions of Landau with finite entropy and entropy dissipation and certain propagation of moment condition.
- Existence of solutions for a regularized Landau equation via this approach using the DiGiorgi minimizing movement scheme approach.
- **Perspectives:** Use of Γ -convergence techniques to show the convergence of the gradient flow solutions constructed by Erbar for the Boltzmann equation towards the gradient flow solutions of the Landau equation.
- References:
 - ① C.-Hu-Wang-Wu (JCP-X 2020).
 - ② C.-Delgadino-Desvilletes-Wu (Preprint ArXiv).

Conclusions

- The Landau equation is written as a gradient flow introducing a bespoke distance.
- Efficient deterministic Particle Methods can be derived for the Landau equation.
- Gradient flow solutions are equivalent to weak distributional solutions of Landau with finite entropy and entropy dissipation and certain propagation of moment condition.
- Existence of solutions for a regularized Landau equation via this approach using the DiGiorgi minimizing movement scheme approach.
- **Perspectives:** Use of Γ -convergence techniques to show the convergence of the gradient flow solutions constructed by Erbar for the Boltzmann equation towards the gradient flow solutions of the Landau equation.
- References:
 - ① C.-Hu-Wang-Wu (JCP-X 2020).
 - ② C.-Delgadino-Desvillettes-Wu (Preprint ArXiv).

Conclusions

- The Landau equation is written as a gradient flow introducing a bespoke distance.
- Efficient deterministic Particle Methods can be derived for the Landau equation.
- Gradient flow solutions are equivalent to weak distributional solutions of Landau with finite entropy and entropy dissipation and certain propagation of moment condition.
- Existence of solutions for a regularized Landau equation via this approach using the DiGiorgi minimizing movement scheme approach.
- **Perspectives:** Use of Γ -convergence techniques to show the convergence of the gradient flow solutions constructed by Erbar for the Boltzmann equation towards the gradient flow solutions of the Landau equation.
- References:
 - ① C.-Hu-Wang-Wu (JCP-X 2020).
 - ② C.-Delgadino-Desvillettes-Wu (Preprint ArXiv).