A deterministic particle method for the homogeneous Landau equation

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Overview

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The Landau equation

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

- $f(t, x, v)$ 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

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

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

$$A(z) = |z|^{\gamma+2}\left(\mathrm{Id} - \frac{z\otimes z}{|z|^2}\right), \quad -d \le \gamma \le 1,$$

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

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

Sometimes, we use the log form

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

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

from which we can derive the weak form

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

Properties of Q

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

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

- **entropy decay**:

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

- **equilibrium** function:

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

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

Overview

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 schemes[1], efficiency further improved using sublattice method, multigrid method, multipole method, etc.[2]
    (+) preserve physical properties
    (+, −) second order accuracy (rigid)
    (−) expensive $O(N^{2d})$

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

Approximation of the collision operator (cont'd)

- **Fourier-Galerkin spectral method**[3]: 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

[3] Pareschi, 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 physicists[4]

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

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

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

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

Approximation of the collision operator (cont'd)

- **Monte Carlo** method: based on particle collision[5] or based on solving the SDE[6]:

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

(+) highly efficient, dimension independent
(−) converges slowly $O(N^{-1/2})$ (N: number of particles)
(−) solution contains noise

[5] Takizuka, '77. Lemons, Winske, Daughton, and Albright, '09.
[6] Rosin, Ricketson, Dimits, Caflisch, and Cohen, '14.

Overview

Main idea

Recall the Landau operator can be written as

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

where

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

Main idea

Recall the Landau operator can be written as

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

where

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

We propose to modify it to

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

with

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

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

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

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.[7]

[7] Carrillo, Craig, and Patacchini, '19.

Why the regularization is good?

For the regularized Landau operator, one has

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

hence

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

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

- **entropy decay**:

$$\int_{\mathbb{R}^d} Q_\varepsilon(f,f)\frac{\delta E_\varepsilon}{\delta f}\,\mathrm{d}v \le 0$$

Why the regularization is good (cont'd)?

- **equilibrium** function:

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

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

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

The 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

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

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

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

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

A further approximation

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

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

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

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

Overview

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

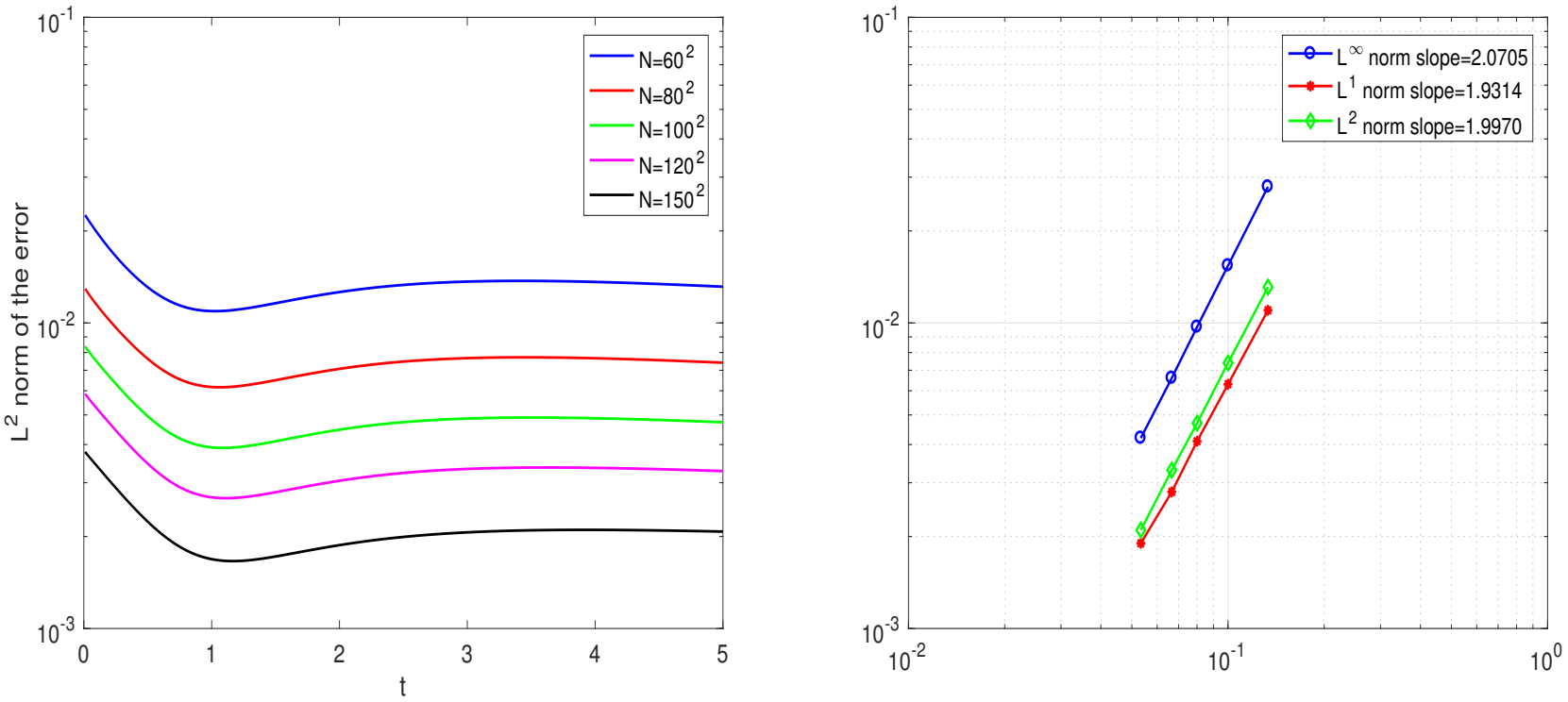


Figure: Left: Time evolution of $\|f^{\text{num}} - f^{\text{ext}}\|_{L^2} / \|f^{\text{ext}}\|_{L^2}$ with respect to different number of particles. Right: Relative L^∞, L^1, and L^2 norms of the error at time $t = 5$ with respect to different h.

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

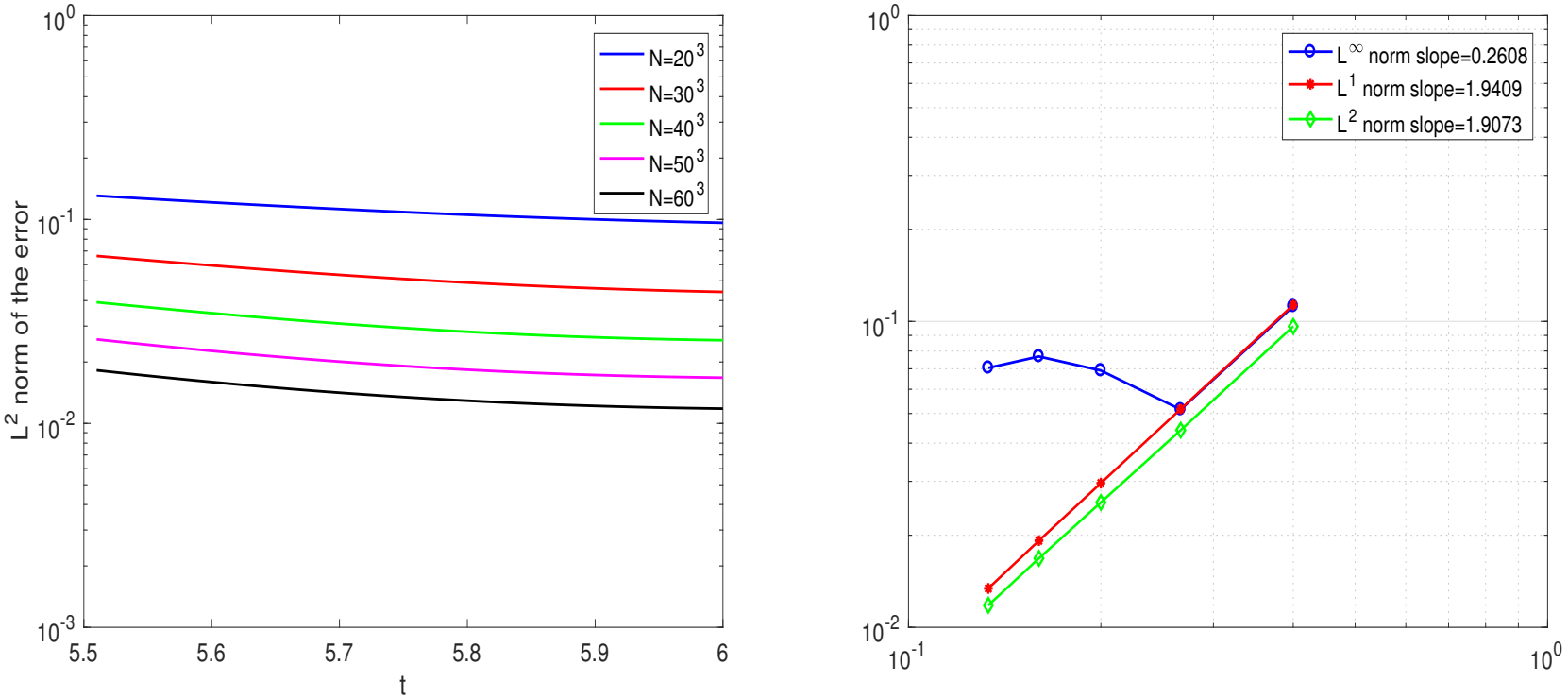


Figure: Left: Time evolution of $\|f^{\text{num}} - f^{\text{ext}}\|_{L^2} / \|f^{\text{ext}}\|_{L^2}$ with respect to different number of particles. Right: Relative L^∞, L^1, and L^2 norms of the error at time $t = 6.5$ with respect to different h.

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**[8] 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.

[8] Pareschi, Russo, and Toscani, '00.

2D anisotropic solution with Coulomb potential

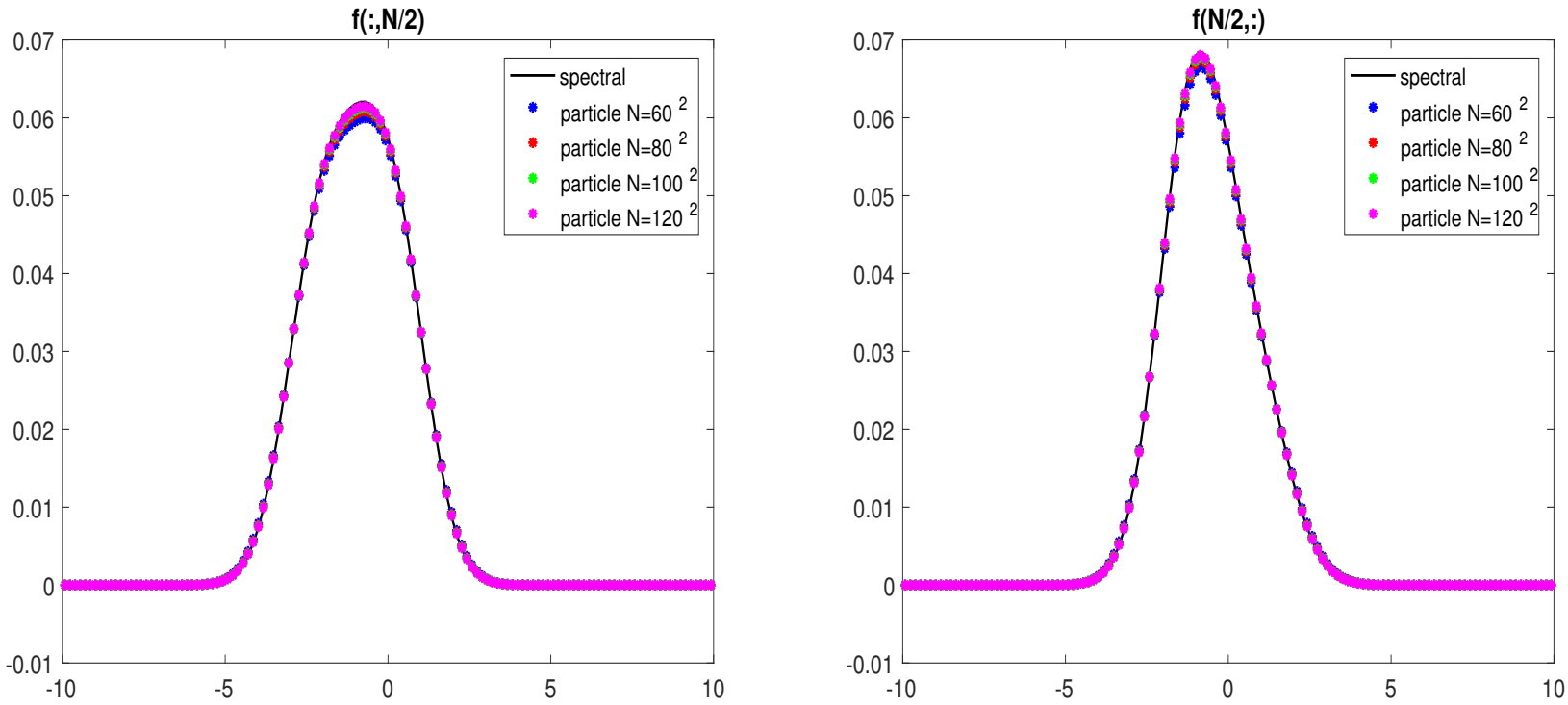


Figure: Comparison of the particle method (using different particle numbers) with the spectral method ($N_v = 128^2$). Slices of the solutions at time $t = 20$.

2D anisotropic solution with Coulomb potential

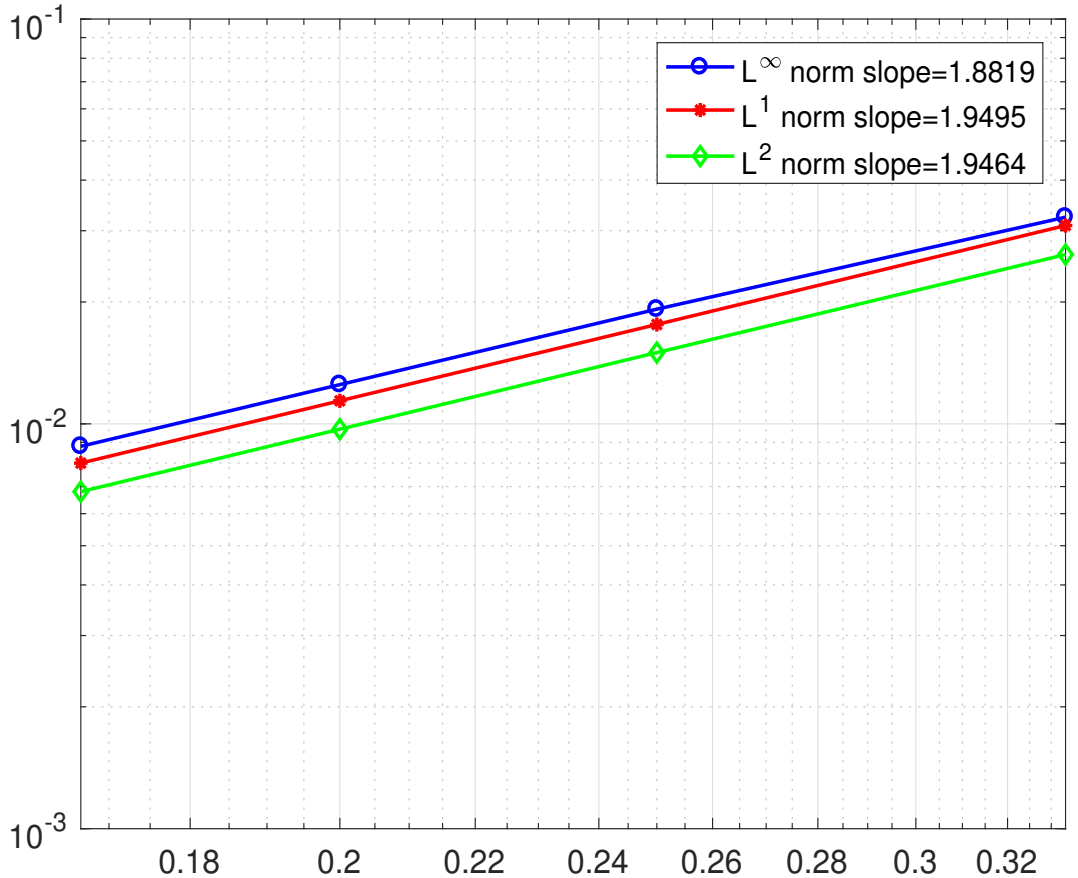


Figure: Relative L^∞, L^1, and L^2 norms of the error at time $t = 20$ with respect to different h.

3D Rosenbluth problem with Coulomb potential

Consider the collision kernel

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

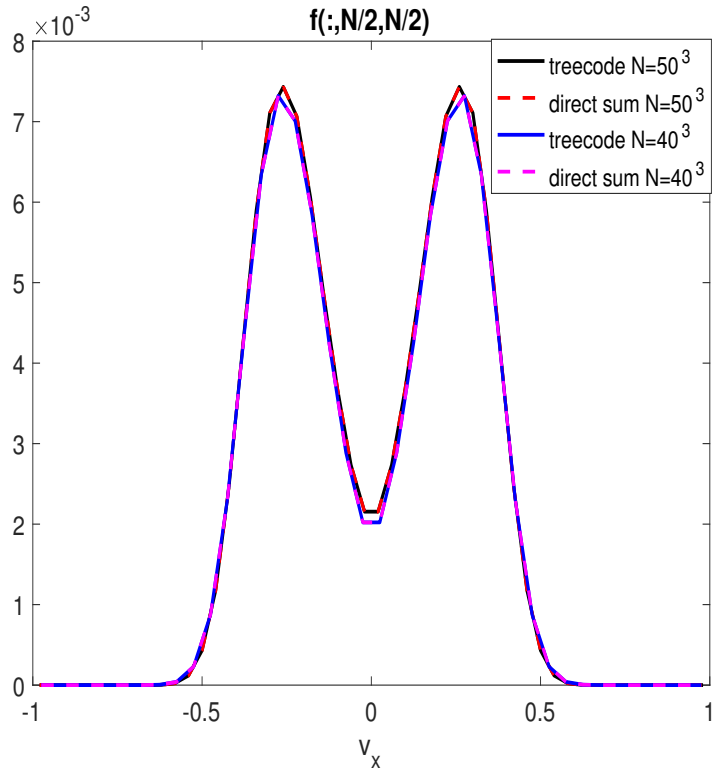
and the initial condition

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

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**[9], whose complexity is $O(N \log N)$.

[9] Li, Johnston, and Krasny, '09.

3D Rosenbluth problem with Coulomb potential



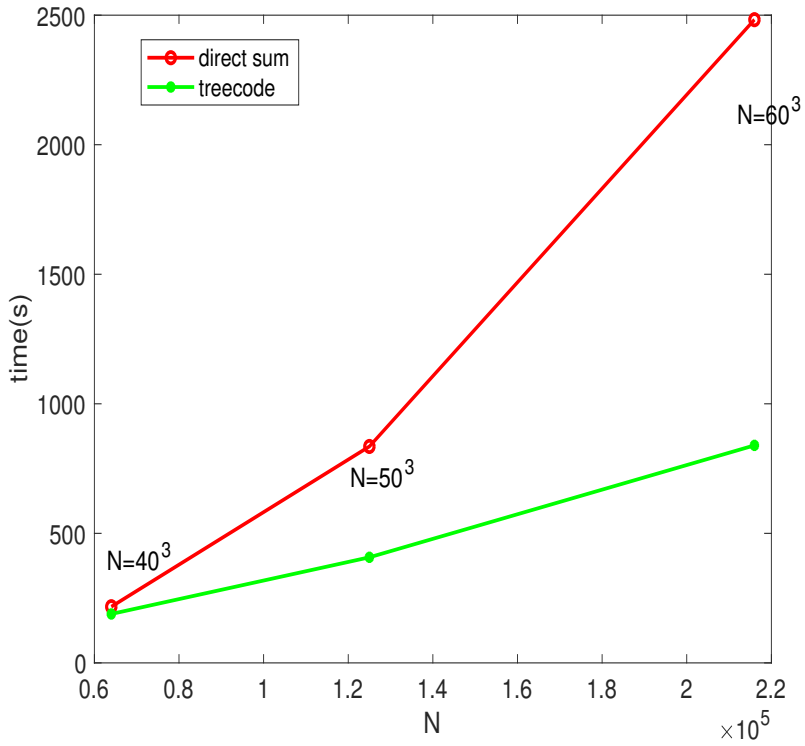


Figure: Left: comparison a slice of solution with direct sum and treecode at $t = 20$, $N = 50^3$ or $N = 40^3$. Right: comparison of computational time (in seconds) for one step with the treecode solver and with the direct sum solver.

Overview

Conclusion

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