Novel approaches for the reliable and efficient numerical integration of the Landau equation

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Objectives

Future objective. Study operator splitting methods for multi-species Vlasov–Maxwell–Landau equations. A favourable solver for the Landau equation represents a fundamental component of the entire algorithm.

Current objective. Focus on the study of the collision integral, that is, design reliable and efficient methods for

- the numerical evaluation of the Landau operator and
- the time integration of the spatially homogeneous Landau equation.

In preparation. J. A. CARRILLO, M. TH. *Novel approaches for the reliable and efficient numerical evaluation of the Landau operator.*

Scope of applications

In the lines of CARRILLO ET AL. (2020).

The Landau equation represents a fundamental kinetic equation. It describes the evolution of the distribution of charged particles in a collisional plasma where grazing collisions are predominant.

Together with the Boltzmann equation, the Landau equation is considered to be one of the most important equations in kinetic theory. Relevant applications related to fusion reactors and the International Thermonuclear Experimental Reactor (ITER) project gave rise to a renewed interest, amongst others in the field of computational plasma physics.

In the special *Maxwellian molecules case*, the equation is reduced to a sort of degenerate linear Fokker–Planck equation which preserves the same moments as the Landau equation.

The physically relevant Coulomb case can be derived from the Boltzmann equation in the grazing collision limit when particles interact via Coulomb forces.

Starting point

Landau equation. Consider the spatially homogeneous Landau equation

$$\partial_t f(v,t) = (Q(f,f))(v,t), \quad (v,t) \in \Omega \times [t_0,T] \subset \mathbb{R}^3 \times \mathbb{R}$$

By means of convenient abbreviations for the integral kernel and the term involving the outer product

$$\varphi(u) = C |u|^{-3}, \quad P(u) = |u|^2 I - u \otimes u,$$

the Landau operator takes the compact form

$$(Q(f,f))(v,t) = \partial_v \cdot \int_{\Omega} \varphi(v-w) P(v-w) \left(\partial_v f(v,t) f(w,t) - f(v,t) \partial_w f(w,t) \right) \mathrm{d}w.$$

Challenges

Computational issues. The numerical simulation of the physically most relevant case with Coulomb interaction requires

- computations in three dimensions (integrand involves $(v, w) \in \mathbb{R}^6$),
- a careful treatment of the singular integral kernel $\varphi(u) = C |u|^{-3}$.



Guide line

Stepwise generalisation of the approach and validation of the implementation for test problems with known solutions.

- Constant integral kernel. Maxwellian molecules case with BKW solution on unbounded domain.
- Regular integral kernel. First test problem on bounded domain and second test problem with localised solution.
- Singular integral kernel.

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Sorry, certain technicalities will arise ...

Focus

- Accuracy of results. Verification of approach on basis of several test problems.
- Efficiency of approach. Exploitation of savings by precomputations.
- Reliability in integration. Study of stability and conserved quantities.



Maxwellian molecules case (BKW solution)

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Alternative approaches

Approach CST2

Based on the conservative formulation of the Landau operator.

Uses numerical differentiation of the integral operator.

Adapted to kernels with an isolated singularity at the origin.

The integral transform is applied to the singular kernel and its regularisation.

Approach CST1

Based on the conservative formulation of the Landau operator.

Uses numerical differentiation of the integral operator.

Adapted to kernels with an isolated singularity at the origin.

The integral transform is applied to the singular kernel.

Approach NST1

Based on the non-conservative formulation of the Landau operator.

Avoids numerical differentiation of the integral operator.

Adapted to kernels with an isolated singularity at the origin.

The integral transform is applied to the singular kernel and its derivatives.

Different approaches for the numerical evaluation of the Landau collision operator (Coulomb case, kernel with isolated singularity).

Maxwellian molecules and Coulomb case Summary and open questions Main references and additional material First representation Fundamental means

General approach

First representation of Landau operator. Fundamental means regarding implementation.

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First representation Fundamental means

First representation

Approach. Specify the Landau operator in components

$$\begin{split} & \left(Q(f,f)\right)(v) \\ & = \begin{pmatrix} \partial v_1 \\ \partial v_2 \\ \partial v_3 \end{pmatrix} \cdot \int_{\Omega} \varphi(v-w) \\ & \times \begin{pmatrix} (v_2 - w_2)^2 + (v_3 - w_3)^2 & -(v_1 - w_1)(v_2 - w_2) & -(v_1 - w_1)(v_3 - w_3) \\ -(v_1 - w_1)(v_2 - w_2) & (v_1 - w_1)^2 + (v_3 - w_3)^2 & -(v_2 - w_2)(v_3 - w_3) \\ -(v_1 - w_1)(v_3 - w_3) & -(v_2 - w_2)(v_3 - w_3) & (v_1 - w_1)^2 + (v_2 - w_2)^2 \end{pmatrix} \\ & \times \begin{pmatrix} \partial_{v_1} f(v) f(w) - f(v) \partial_{w_1} f(w) \\ \partial_{v_2} f(v) f(w) - f(v) \partial_{w_2} f(w) \\ \partial_{v_3} f(v) f(w) - f(v) \partial_{w_3} f(w) \end{pmatrix} dw, \quad v = (v_1, v_2, v_3) \in \Omega, \end{split}$$

and perform straightforward calculations (expand integrand, determine divergence).

Notation. For notational simplicity, omit the dependence of the density function and the Landau operator on time.

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First representation Fundamental means

First representation

Approach. Obtain a first representation of the Landau operator involving derivatives of the density function and linear operators that comprise (quite a few) integrals

 $\begin{aligned} & (Q(f,f))(v) \\ &= (Q_{000}(f))(v) f(v) \\ &+ (Q_{100}(f))(v) \partial_{v_1} f(v) + (Q_{010}(f))(v) \partial_{v_2} f(v) \\ &+ (Q_{001}(f))(v) \partial_{v_3} f(v) \\ &+ (Q_{200}(f))(v) \partial_{v_1}^2 f(v) + (Q_{110}(f))(v) \partial_{v_1 v_2} f(v) \\ &+ (Q_{101}(f))(v) \partial_{v_1 v_3} f(v) + (Q_{020}(f))(v) \partial_{v_2}^2 f(v) \\ &+ (Q_{011}(f))(v) \partial_{v_2 v_3} f(v) + (Q_{002}(f))(v) \partial_{v_2}^2 f(v), \quad v \in \Omega. \end{aligned}$

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First representation Fundamental means

Decisive integrals

Notation. Employ a convenient symbolic notation for the arising decisive integrals (indicate the degrees of the monomials as well as the orders of the derivatives of the integral kernel and the density function)

$$\begin{split} I_{wi_1i_2i_3\varphi j_1j_2j_3fk_1k_2k_3}(v) \\ &= \int_{\Omega} w_1^{i_1} w_2^{i_2} w_2^{i_3} \partial_{v_1}^{j_1} \partial_{v_2}^{j_2} \partial_{v_3}^{j_3} \varphi(v-w) \partial_{w_1}^{k_1} \partial_{w_2}^{k_2} \partial_{w_3}^{k_3} f(w) \,\mathrm{d}w, \quad v \in \Omega \end{split}$$

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Arising operators

A glance at the arising operators is enough ... ;-)

$$\begin{split} & (Q_{200}(f))(v) \\ &= v_2^2 \, I_{w\,000\,\varphi\,000\,f\,000\,(v)} + v_3^2 \, I_{w\,000\,\varphi\,000\,f\,000\,(v)} - 2 \, v_2 \, I_{w\,010\,\varphi\,000\,f\,000\,(v)} \\ &\quad - 2 \, v_3 \, I_{w\,001\,\varphi\,000\,f\,000\,(v)} + I_{w\,020\,\varphi\,000\,f\,000\,(v)} + I_{w\,002\,\varphi\,000\,f\,000\,(v)}, \\ & (Q_{110}(f))(v) \\ &= -2 \, v_1 \, v_2 \, I_{w\,000\,\varphi\,000\,f\,000\,(v)} + 2 \, v_1 \, I_{w\,010\,\varphi\,000\,f\,000\,(v)} + 2 \, v_2 \, I_{w\,100\,\varphi\,000\,f\,000\,(v)} \\ &\quad - 2 \, I_{w\,110\,\varphi\,000\,f\,000\,(v)}. \end{split}$$

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Arising operators

 $(Q_{100}(f))(v)$ $= v_1 v_2 \left(-I_{w \, 000 \, \varphi \, 010 \, f \, 000}(v) + I_{w \, 000 \, \varphi \, 000 \, f \, 010}(v) \right)$ $+ v_1 v_3 (-I_{w 000 \varphi 001 f 000}(v) + I_{w 000 \varphi 000 f 001}(v))$ $+v_2^2 (I_{w000\varphi 100f000}(v) - I_{w000\varphi 000f100}(v))$ $+ v_3^2 (I_{w \, 000 \, \varphi \, 100 \, f \, 000}(v) - I_{w \, 000 \, \varphi \, 000 \, f \, 100}(v))$ $+v_1(-2I_{w000}\omega_{000}f_{000}(v)+I_{w010}\omega_{010}f_{000}(v)+I_{w001}\omega_{001}f_{000}(v)$ $-I_{w010}\varphi_{000}f_{010}(v) - I_{w001}\varphi_{000}f_{001}(v)$ $+ v_2 (-2I_w 010 \omega 100 f 000(v) + I_w 100 \omega 010 f 000(v) + 2I_w 010 \omega 000 f 100(v)$ $-I_{w \, 100 \, \varphi \, 000 \, f \, 010}(v)$ $+ v_3 (-2I_{w001}\omega_{100}f_{000}(v) + I_{w100}\omega_{001}f_{000}(v) + 2I_{w001}\omega_{000}f_{100}(v)$ $-I_{w 100 \varphi 000 f 001}(v)$ $+2I_{w100}\varphi_{000}f_{000}(v)+I_{w020}\varphi_{100}f_{000}(v)+I_{w002}\varphi_{100}f_{000}(v)$ $-I_{w 110 \varphi 010 f 000}(v) - I_{w 101 \varphi 001 f 000}(v) - I_{w 020 \varphi 000 f 100}(v)$ $-I_{w002}\omega_{000}f_{100}(v) + I_{w110}\omega_{000}f_{010}(v) + I_{w101}\omega_{000}f_{001}(v).$

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First representation Fundamental means

Arising operators

 $\big(Q_{000}(f)\big)(v)$

- $$\begin{split} &= -v_1^2 \Big(I_{w\,000\,\varphi\,010\,f\,010\,(v)} + I_{w\,000\,\varphi\,001\,f\,001\,(v)} \Big) + v_1\,v_2 \big(I_{w\,000\,\varphi\,010\,f\,100\,(v)} + I_{w\,000\,\varphi\,100\,f\,010\,(v)} \Big) \\ &+ v_1\,v_3 \, \big(I_{w\,000\,\varphi\,001\,f\,100\,(v)} + I_{w\,000\,\varphi\,100\,f\,001\,(v)} \Big) v_2^2 \, \big(I_{w\,000\,\varphi\,100\,f\,100\,(v)} + I_{w\,000\,\varphi\,001\,f\,001\,(v)} \Big) \\ &+ v_2\,v_3 \, \big(I_{w\,000\,\varphi\,001\,f\,010\,(v)} + I_{w\,000\,\varphi\,010\,f\,001\,(v)} \Big) v_3^2 \, \big(I_{w\,000\,\varphi\,100\,f\,100\,(v)} + I_{w\,000\,\varphi\,010\,f\,010\,(v)} \Big) \\ &+ v_1\,(2\,I_{w\,000\,\varphi\,000\,f\,100\,(v)} I_{w\,010\,\varphi\,010\,f\,100\,(v)} I_{w\,010\,\varphi\,010\,f\,100\,(v)} I_{w\,010\,\varphi\,010\,f\,010\,(v)} + 2\,I_{w\,100\,\varphi\,010\,f\,010\,(v)} \Big) \end{split}$$
 - $-I_{w\,001\,\varphi\,100\,f\,001\,(v)\,+\,2\,I_{w\,100\,\varphi\,001\,f\,001\,(v)})$
 - $+ v_2 (2I_{w010\varphi100f100}f_{100}^{(v)} I_{w100\varphi010f100}^{(v)} + 2I_{w000\varphi000f010}^{(v)} I_{w100\varphi100f010}^{(v)} I_{w001\varphi001f010}^{(v)} I_{w001\varphi001f010}^{(v)} + 2I_{w000\varphi001f010}^{(v)})$
 - $+v_3 \left(2 I_{w001} \varphi_{100} f_{100} (v) I_{w100} \varphi_{001} f_{100} (v) + 2 I_{w001} \varphi_{010} f_{010} (v) I_{w010} \varphi_{001} f_{010} (v) + 2 I_{w000} \varphi_{000} f_{001} (v) I_{w100} \varphi_{100} f_{010} (v) I_{w010} \varphi_{010} f_{010} (v) I_{w010} \varphi_{010} f_{010} (v) \right)$
 - $-2\,I_{w}_{100\varphi_{000}f_{100}(v)}-I_{w}_{020\varphi_{100}f_{100}(v)}-I_{w}_{002\varphi_{100}f_{100}(v)}+I_{w}_{110\varphi_{010}f_{100}(v)}+I_{w}_{101\varphi_{001}f_{100}(v)}$
 - $^{-2I}w_{010}\varphi_{000}f_{010}{}^{(v)+I}w_{110}\varphi_{100}f_{010}{}^{(v)-I}w_{200}\varphi_{010}f_{010}{}^{(v)-I}w_{002}\varphi_{010}f_{010}{}^{(v)+I}w_{011}\varphi_{001}f_{010}{}^{(v)}$
 - $-2\,I_{w\,001}\varphi_{000}f_{001}(v)+I_{w\,101}\varphi_{100}f_{001}(v)+I_{w\,011}\varphi_{010}f_{001}(v)-I_{w\,200}\varphi_{001}f_{001}(v)-I_{w\,020}\varphi_{001}f_{001}(v).$

The numerical verification of the correctness of all terms on test problems with known solutions seemed to be a good idea ... ;-)

First representation Fundamental means

Fundamental means

Main task. Compute suitable approximations to the arising derivatives and the decisive integrals, e.g.

$$\partial_{v_1}^2 f(v)\,,\quad I_{w\,000\,\varphi\,000\,f\,000}(v)=\int_\Omega \varphi(v-w)\,f(w)\,\mathrm{d} w\,,\quad v\in\Omega\,.$$

Approach.

- Application of Fourier spectral method
- Quadrature approximation nearby singularity of kernel
- Identification of basic integrals involving Fourier functions

Implementation.

- Use of fast Fourier techniques (FFT / IFFT)
- Summation along certain directions (einsum)
- Observation of reduced computational complexity

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First representation Fundamental means

Fourier spectral method

Fourier functions. Consider well-known Fourier functions

$$\begin{aligned} \mathscr{F}_{\kappa}^{(\alpha)}(\xi) &= \frac{1}{\sqrt{\alpha_{2} - \alpha_{1}}} e^{\mu_{\kappa}^{(\alpha)}(\xi - \alpha_{1})}, \quad \mu_{\kappa}^{(\alpha)} &= \frac{2\pi i \kappa}{\alpha_{2} - \alpha_{1}}, \\ \mathscr{F}_{\kappa}^{(\alpha)}(\alpha_{1}) &= \frac{1}{\sqrt{\alpha_{2} - \alpha_{1}}} = \mathscr{F}_{\kappa}^{(\alpha)}(\alpha_{2}), \quad \partial_{\xi} \mathscr{F}_{\kappa}^{(\alpha)}(\xi) = \mu_{\kappa}^{(\alpha)} \mathscr{F}_{\kappa}^{(\alpha)}(\xi), \\ \xi \in \mathbb{R}, \quad \kappa \in \mathbb{Z}, \quad \alpha = (\alpha_{1}, \alpha_{2}) \in \mathbb{R}^{2}, \quad \alpha_{1} < \alpha_{2}. \end{aligned}$$

In particular, in three dimensions, denote

$$\begin{split} F_m(v) &= \mathcal{F}_{m_1}^{(b_{11}, b_{12})}(v_1) \mathcal{F}_{m_2}^{(b_{21}, b_{22})}(v_2) \mathcal{F}_{m_3}^{(b_{31}, b_{32})}(v_3), \\ v &= (v_1, v_2, v_3) \in \Omega_{\mathcal{F}}, \quad m = (m_1, m_2, m_3) \in \mathcal{M}, \\ \Omega_{\mathcal{F}} &= [b_{11}, b_{12}] \times [b_{21}, b_{22}] \times [b_{31}, b_{32}], \\ \mathcal{M} &= \{-\frac{1}{2}M_1, \dots, \frac{1}{2}M_1 - 1\} \times \dots \times \{-\frac{1}{2}M_3, \dots, \frac{1}{2}M_3 - 1\} \subset \mathbb{Z}^3. \end{split}$$

First representation Fundamental means

Fourier spectral method

General benefits.

- High accuracy for localised regular functions
- High efficiency (implementation based on FFT / IFFT)



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First representation Fundamental means

Fourier spectral method

Within our setting. Recall the typical form of the decisive integrals

$$I_{w\,000\,\varphi\,000\,f\,000}(v) = \int_{\Omega} \varphi(v-w)\,f(w)\,\mathrm{d}w\,,\quad v\in\Omega\,.$$

Specific advantage. The particular identity

$$F_{\ell}(v-w)F_{m}(w) = \Gamma_{\ell}^{(b)}F_{\ell}(v)F_{m-\ell}(w),$$

$$\Gamma_{\ell}^{(b)} = e^{-\mu_{\ell_{1}}^{(b_{11},b_{12})}b_{11}}e^{-\mu_{\ell_{2}}^{(b_{21},b_{22})}b_{21}}e^{-\mu_{\ell_{3}}^{(b_{31},b_{32})}b_{31}},$$

suggests to study Fourier series expansions for both, the density function and the integral kernel.

First representation Fundamental means

Fourier spectral method

Fourier series expansions. Use approximations based on Fourier series expansions for the integral kernel and its (known) derivatives

$$\begin{split} \varphi(v) &\approx \sum_{\ell \in \mathcal{L}} \varphi_{\ell} F_{\ell}(v), \\ \partial_{v_1}^{j_1} \partial_{v_2}^{j_2} \partial_{v_3}^{j_3} \varphi(v) &\approx \sum_{\ell \in \mathcal{L}} \varphi_{j_1 j_2 j_3 \ell} F_{\ell}(v). \end{split}$$

Employ a Fourier series expansion for the density function and the resulting representations for its derivatives

$$f(v) \approx \sum_{m \in \mathcal{M}} f_m F_m(v),$$

$$\partial_{v_1}^{k_1} \partial_{v_2}^{k_2} \partial_{v_3}^{k_3} f(v) \approx \sum_{m \in \mathcal{M}} f_m \left(\mu_{m_1}^{(b_{11}, b_{12})}\right)^{k_1} \left(\mu_{m_2}^{(b_{21}, b_{22})}\right)^{k_2} \left(\mu_{m_3}^{(b_{31}, b_{32})}\right)^{k_3} F_m(v).$$

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First representation Fundamental means

Basic integrals

Calculations. Straightforward calculations yield explicit representations for basic integrals involving monomials and Fourier functions

$$I_{j}(k,m_{j}) = \int_{b_{j1}}^{b_{j2}} w_{j}^{k} \mathscr{F}_{m_{j}}^{(b_{j1},b_{j2})}(w_{j}) dw_{j} = \begin{cases} \sqrt{\frac{b_{j2} - b_{j1}}{2\sqrt{b_{j2} - b_{j1}}}}, & m_{j} = 0, \ k = 0, \\ \frac{b_{j2}^{2} - b_{j1}^{2}}{2\sqrt{b_{j2} - b_{j1}}}, & m_{j} = 0, \ k = 1, \\ \frac{b_{j2}^{2} - b_{j1}^{2}}{3\sqrt{b_{j2} - b_{j1}}}, & m_{j} = 0, \ k = 2, \\ 3\sqrt{b_{j2} - b_{j1}}, & m_{j} \neq 0, \ k = 0, \\ \frac{\sqrt{b_{j2} - b_{j1}}}{(b_{j1}^{2} - b_{j2}^{2})}, & m_{j} \neq 0, \ k = 1, \\ \frac{(b_{j2}^{2} - b_{j1}^{2})(m_{j1}^{2} - b_{j2}^{2})}{\sqrt{b_{j2} - b_{j1}}(m_{j1}^{2} - b_{j2}^{2})}, & m_{j} \neq 0, \ k = 2, \end{cases}$$

Reductions. The observed simplification leads to significant reductions in computational complexity for three dimensions.

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First representation Fundamental means

A few more (surprising) details ...

Implementation and observation. Essential ingredients for the efficient implementation are

- matrix multiplications,
- summations along certain directions (einsum),
- inverse fast Fourier transforms.

First representation Fundamental means

A few more (surprising) details ...

Reduced computational complexity (Arising inner sums). A crucial observation is that the costs for the computation of inner sums amount to the evaluation of single and double sums, but no triple sums.

Type of decisive integral	# Summations along directions (einsum)
w 000	0
w 100, w 010, w 001	1
w 200, w 020, w 002	1
w 110, w 101, w 011	2

First representation Fundamental means

A few more (surprising) details ...

Reduced computational complexity (quadrature approximation on small domain). Test problem (regular integral kernel, unbounded domain, known solution) in two dimensions. Numerical evaluation of the Landau operator based on 256×256 uniform grid points covering the truncated velocity domain $[-10, 10] \times [-10, 10]$. Precomputation times observed for a quadrature approximation based on 5×5 grid points versus a quadrature approximation on the whole domain based on 256×256 grid points. In both cases, an overall relative accuracy of about $4 \cdot 10^{-11}$ is obtained.

Quadrature on a small neighbourhood	Precomputation time CT
Quadrature on the whole domain	88×CT

Numerical simulations (Maxwellian molecules case) Numerical simulations (Coulomb case)

Constant and singular integral kernels

Detailed study of Maxwellian molecules case. BKW solution on unbounded domain. Conclusions for Coulomb case.

Maxwellian molecules case (BWK solution)

Landau equation. The BKW solution to the Landau equation involving a constant kernel is given by

$$\begin{split} \varphi(v) &= C = \frac{1}{24}, \quad (\alpha_1, \alpha_2, \alpha_3) = \left(\frac{5}{2}, \frac{3}{2}, \frac{1}{6}\right), \quad K(t) = 1 - \frac{1}{2} e^{-\alpha_3 t}, \\ f(v, t) &= \frac{1}{(2\pi K(t))^{3/2}} e^{-\frac{1}{2} \frac{1}{K(t)} |v|^2} \left(\alpha_1 - \alpha_2 \frac{1}{K(t)} + \frac{1}{2} \frac{1 - K(t)}{(K(t))^2} |v|^2\right), \\ \partial_t f(v, t) &= \left(Q(f, f)\right)(v, t), \quad (v, t) \in \Omega \times [t_0, T]. \end{split}$$

Landau operator. For a particular choice of the density function, the associated Landau operator reads as

$$\begin{split} f(v) &= \frac{1}{2\pi^{3/2}} \, \mathrm{e}^{-|v|^2} \left(2 \, |v|^2 - 1 \right), \\ \left(Q(f,f) \right)(v) &= \frac{1}{6\pi^{3/2}} \, \mathrm{e}^{-|v|^2} \left(|v|^4 - 5 \, |v|^2 + \frac{15}{4} \right), \quad v \in \Omega. \end{split}$$

An ideal situation to verify our approach and perform first numerical tests. :-)

Numerical simulations (Maxwellian molecules case) Numerical simulations (Coulomb case)

Illustration (BWK)



Profiles of the BKW solution at two times (right) and corresponding cross sections (left).

 $https://techmath.uibk.ac.at/mecht/MyHomepage/Research/Movie_Maxwellian_Solution3d.m4v https://techmath.uibk.ac.at/mecht/MyHomepage/Research/Movie_Maxwellian_Solution3dSection.m4v https://techmatk.uibk.ac.at/mecht/MyHomepage/Research/Movie_Maxwellian_Solution3dSection.m4v https://techmatk.uibk.ac.at/mecht/MyHomepage/Research/Movie_Maxwellian_Solution3dSection.m4v https://techmatk.uibk.ac.at/mecht/MyHomepage/Research/Movie_Maxwellian_Solution3dSection.m4v https://techmatk.uibk.ac.at/mecht/MyHomepage/Research/Movie_Maxwellian_Solution3dSection.m4v https://techmatk.uibk.ac.at/mecht/MyHomepage/Research/Movie_Maxwellian_Solution3dSection.m4v https://techmatk.uibk.ac.at/mecht/MyHomepage/Research/Movie_Maxwellian_Solution3dSection.m4v https://techmatk.uibk.ac.at/mecht/MyHomepage/Research/MyHomepage/Resea$

Numerical simulations (Maxwellian molecules case) Numerical simulations (Coulomb case)

Numerical tests (BWK)

Verification, computation time, accuracy. Study the numerical evaluation of the Landau operator based on slightly differing implementations for a non-symmetric domain versus a symmetric domain

$$\begin{split} \Omega_{\mathscr{F}} &= [-9,10] \times [-10,11] \times [-11,12], \quad |\mathcal{M}| = M_1 \cdot M_2 \cdot M_3 = 100 \cdot 110 \cdot 120, \\ \Omega_{\mathscr{F}} &= [-10,10]^3, \quad |\mathcal{M}| = M^3 = 100^3. \end{split}$$

Verify the correctness of the approach. Observe a reasonable magnitude of the overall computation times and highly accurate results (confirmed by a comparison with the two-dimensional case).



Mechthild Thalhammer Numerical integration of the Landau equation

Numerical simulations (Maxwellian molecules case) Numerical simulations (Coulomb case)

Numerical tests (BWK)

Stability, accuracy, conserved quantities. Study the time integration of the Landau equation based on a fourth-order explicit Runge–Kutta method.

- At each time step, compute the discrete L^2 -error of the solution.
- Determine approximations to mass and energy (conserved quantities)

$$\int_\Omega f(v,t)\,\mathrm{d}v = \int_\Omega f(v,t_0)\,\mathrm{d}v\,,\quad \int_\Omega |v|^2\,f(v,t)\,\mathrm{d}v = \int_\Omega |v|^2\,f(v,t_0)\,\mathrm{d}v\,,$$

and observe the decay of the entropy

$$\int_{\Omega} f(v,t) \ln \left(f(v,t) \right) \mathrm{d} v \leq \int_{\Omega} f(v,t_0) \ln \left(f(v,t_0) \right) \mathrm{d} v \,, \quad t \in [t_0,T] \,.$$

Numerical simulations (Maxwellian molecules case) Numerical simulations (Coulomb case)

Numerical tests (BWK, d = 3)

Short-time integration (d = 3).



Time integration by explicit Runge–Kutta methods. Approximation of the solution and corresponding errors.

Numerical simulations (Maxwellian molecules case) Numerical simulations (Coulomb case)

Numerical tests (BWK, d = 3)

Long-term integration (d = 3).



Approximation of mass, momentum, energy, entropy.

Numerical simulations (Maxwellian molecules case) Numerical simulations (Coulomb case)

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Numerical tests (BWK, d = 2)

Long-term integration (d = 2).



Exact solution and convergence towards equilibrium (time T = 100).

Numerical simulations (Maxwellian molecules case) Numerical simulations (Coulomb case)

Numerical tests (BWK, d = 2)

Long-term integration (d = 2).



Numerical solution obtained by an adaptive explicit Runge–Kutta methods (ode45) and convergence towards equilibrium (time T = 100).

Numerical simulations (Maxwellian molecules case) Numerical simulations (Coulomb case)

Illustration (Coulomb, d = 3)



Choice of the initial state accordingly to CARRILLO ET AL. (2020). Profiles of the solution to the Landau equation with Coulomb interaction at the initial time and a later time ($M^3 = 100^3$ Fourier functions). https://techmath.uibk.ac.at/mecht/MyHomepage/Research/Movie_CoulombPotential_Solution3d.m4v

Summary and open questions

Summary.

• Study of flexible novel approaches for the reliable and efficient evaluation of the Landau collision operator.

Open tasks and questions.

- Specification of the spatial and temporal discretisation errors.
- Generalisation of the employed approach (e.g. Hermite functions).
- Enhancement of the stability behaviour for large time stepsizes. Extension of splitting-type methods to regular and singular kernels.
- Extensions to Vlasov–Poisson–Landau and Vlasov–Maxwell–Landau equations by Hamiltonian operator splitting methods.

Thank you!

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Inspiration

J. A. CARRILLO, J. HU, L. WANG, J. WU. *A particle method for the homogeneous Landau equation.* Journal of Computational Physics X 7 (2020) 100066. www.sciencedirect.com/science/article/pii/S2590055220300184

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Vlasov-Poisson-Landau equation

Classical mean-field model for collisional plasmas. For a single species, the time evolution of the distribution function

$$f:\Omega^{(x)}\times\Omega^{(v)}\times[t_0,T]\longrightarrow\mathbb{R}$$

is described by the inhomogeneous Fokker–Planck–Landau equation coupled with the Poisson equation (charge *q*, electrostatic field *E*, binary collision operator *Q* involving Coulomb potential)

$$\begin{cases} \partial_t f(x,v,t) + v \cdot \nabla_x f(x,v,t) + q \left(E(f) \right)(x,t) \cdot \nabla_v f(x,v,t) = \left(Q(f,f) \right)(x,v,t), \\ \left(E(f) \right)(x,t) = -\nabla_x \left(\Phi(f) \right)(x,t), \quad -\Delta_x \left(\Phi(f) \right)(x,t) = \int_{\Omega^{(v)}} f(x,v,t) \, \mathrm{d}v, \\ (x,v,t) \in \Omega^{(x)} \times \Omega^{(v)} \times [t_0,T] \subset \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}. \end{cases}$$

Generalisation. Models for multiple species rely on coupled Vlasov–Poisson–Landau systems.

Associated subproblems

Operator splitting. Decompose the original problem into the Vlasov–Poisson equation (collisionless)

$$\begin{cases} \partial_t f(x, v, t) + v \cdot \nabla_x f(x, v, t) + q \left(E(f) \right)(x, t) \cdot \nabla_v f(x, v, t) = 0, \\ (x, v, t) \in \Omega^{(x)} \times \Omega^{(v)} \times [t_0, T] \subset \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}. \end{cases}$$

and the Fokker-Planck-Landau equation (homogeneous)

$$\begin{cases} \partial_t f(x, v, t) = (Q(f, f))(x, v, t), \\ (x, v, t) \in \Omega^{(x)} \times \Omega^{(v)} \times [t_0, T] \subset \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}. \end{cases}$$

Reference. See CH. ZHANG, I. GAMBA (*A conservative scheme for Vlasov Poisson Landau modeling collisional plasmas*, 2017).

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Approaches for higher-order time-splitting methods

Real coefficients. Design of schemes based on real coefficients

- provides favourable approximations for Schrödinger equations,
- but presence of negative coefficients for order *p* ≥ 4 leads to instabilities for parabolic equations.

Complex coefficients. Design of schemes based on complex coefficients with positive real parts

- provides favourable approximations for parabolic equations,
- but implies loss of invariance properties for Schrödinger equations.

Modified methods. Incorporation of iterated commutators permits design of favourable schemes with positive coefficients, but neccessary considerations in nonlinear case are involved.

Reference. Recent and current works in collaboration with S. BLANES F. CASAS, C. GONZÁLEZ (2022, 2023).