On the numerical evaluation of the Landau operator

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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.*

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

Y. Li, Y. He, Y. Sun, J. Niesen, H. Qin, J. Liu.
Solving the Vlasov–Maxwell equations using Hamiltonian splitting.
Journal of Computational Physics 396 (2019) 381–399.
www.sciencedirect.com/science/article/pii/S0021999119304784

L. Pareschi, G. Russo, G. Toscani.
Fast spectral methods for the Fokker–Planck–Landau collision operator.
Journal of Computational Physics 165 (2000) 216–236.
www.sciencedirect.com/science/article/pii/S0021999100966129

Y. Wang.
The two-species Vlasov–Maxwell–Landau system in $\mathbb{R}^3$.
Annales de l'Institut Henri Poincaré C, Analyse non linéaire 32 (2015) 1099–1123.
www.sciencedirect.com/science/article/pii/S0294144914000523

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

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

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

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

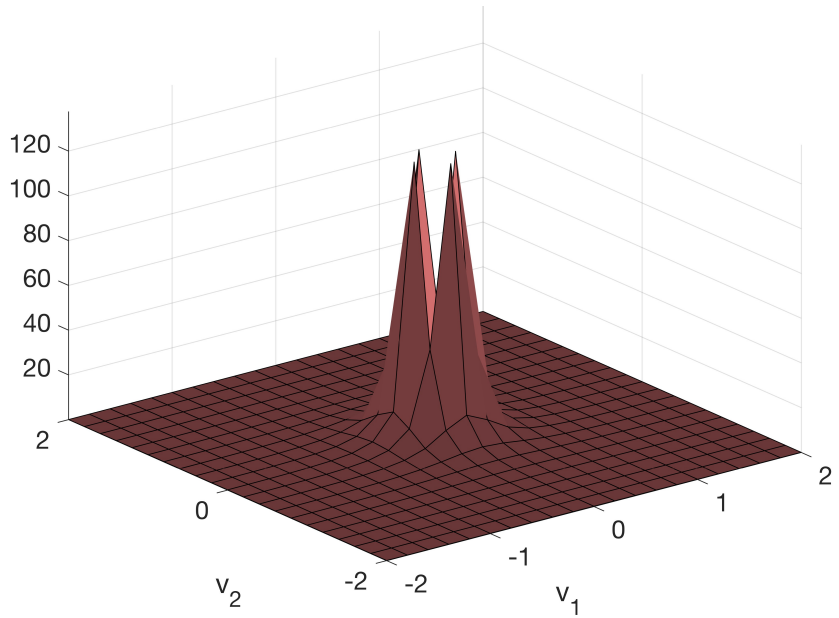
the Landau operator takes the compact form

$$\begin{aligned}&\big(Q(f,f)\big)(v,t)\\ &\quad = \partial_v \cdot \int_\Omega \varphi(v-w)\, P(v-w) \big(\partial_v f(v,t)\, f(w,t) - f(v,t)\, \partial_w f(w,t)\big)\, \mathrm{d}w.\end{aligned}$$

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 $\varphi(u) = C|u|^{-3}$.

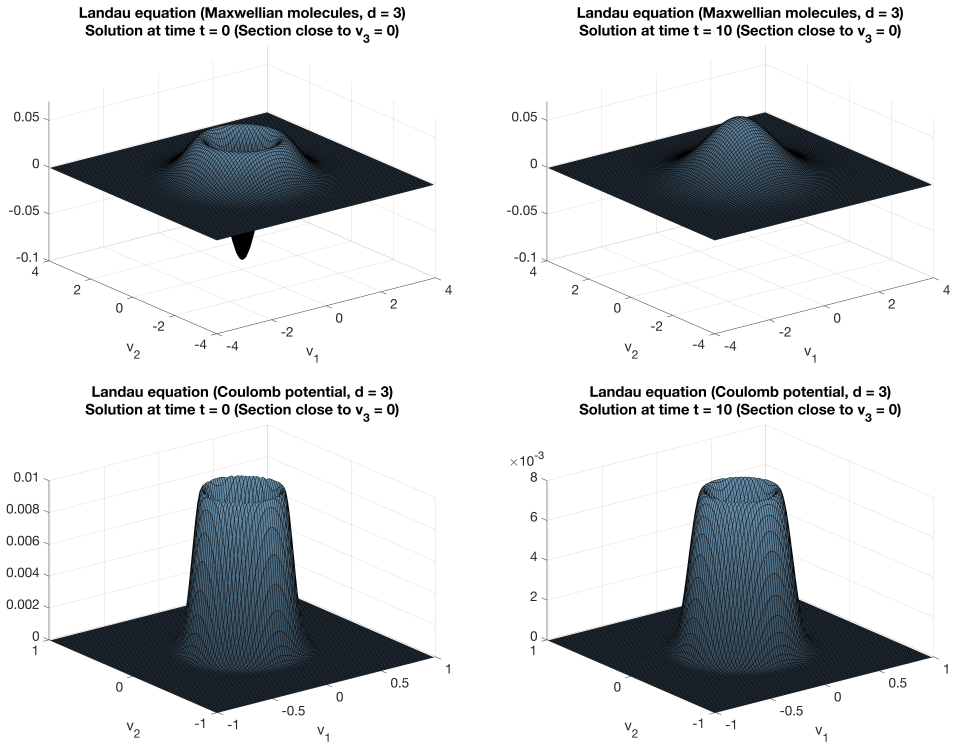


Integral kernel (intersection along $v_3 = 0$)

Guide line

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

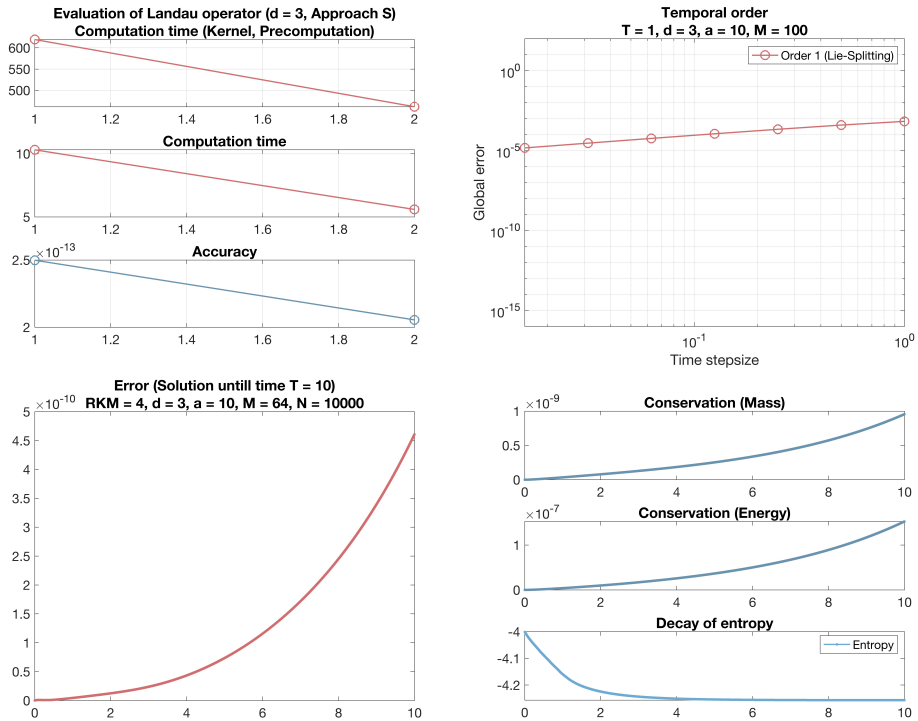
- Constant integral kernel.
  Maxwellian molecules case with BKW solution on unbounded domain.
- Regular integral kernel.
  First test problem on bounded domain and second test problem with localised solution.
- Singular integral kernel.



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)

General approach

First representation of Landau operator. Fundamental means regarding implementation.

First representation

Approach. Specify the Landau operator in components

$$
\begin{aligned}
&\big(Q(f,f)\big)(v) \\
&\quad = \begin{pmatrix} \partial_{v_1} \\ \partial_{v_2} \\ \partial_{v_3} \end{pmatrix} \cdot \int_\Omega \varphi(v-w) \\
&\qquad \times \begin{pmatrix} (v_2-w_2)^2 + (v_3-w_3)^2 & -(v_1-w_1)(v_2-w_2) & -(v_1-w_1)(v_3-w_3) \\ -(v_1-w_1)(v_2-w_2) & (v_1-w_1)^2 + (v_3-w_3)^2 & -(v_2-w_2)(v_3-w_3) \\ -(v_1-w_1)(v_3-w_3) & -(v_2-w_2)(v_3-w_3) & (v_1-w_1)^2 + (v_2-w_2)^2 \end{pmatrix} \\
&\qquad \times \begin{pmatrix} \partial_{v_1} f(v) f(w) - f(v) \partial_{w_1} f(w) \\ \partial_{v_2} f(v) f(w) - f(v) \partial_{w_2} f(w) \\ \partial_{v_3} f(v) f(w) - f(v) \partial_{w_3} f(w) \end{pmatrix} \mathrm{d}w, \quad v = (v_1, v_2, v_3) \in \Omega,
\end{aligned}
$$

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.

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

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

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)

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

Arising operators

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

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

Arising operators

$$
\begin{aligned}
&\big(Q_{100}(f)\big)(v) \\
&\quad = v_1\, v_2 \big(- I_{w000\varphi 010} f_{000}(v) + I_{w000}\varphi_{000} f_{010}(v)\big) \\
&\qquad + v_1\, v_3 \big(- I_{w000\varphi 001} f_{000}(v) + I_{w000}\varphi_{000} f_{001}(v)\big) \\
&\qquad + v_2^2 \big(I_{w000\varphi 100} f_{000}(v) - I_{w000}\varphi_{000} f_{100}(v)\big) \\
&\qquad + v_3^2 \big(I_{w000\varphi 100} f_{000}(v) - I_{w000}\varphi_{000} f_{100}(v)\big) \\
&\qquad + v_1 \big(- 2\, I_{w000}\varphi_{000} f_{000}(v) + I_{w010\varphi 010} f_{000}(v) + I_{w001\varphi 001} f_{000}(v) \\
&\qquad - I_{w010}\varphi_{000} f_{010}(v) - I_{w001}\varphi_{000} f_{001}(v)\big) \\
&\qquad + v_2 \big(- 2\, I_{w010\varphi 100} f_{000}(v) + I_{w100\varphi 010} f_{000}(v) + 2\, I_{w010}\varphi_{000} f_{100}(v) \\
&\qquad - I_{w100}\varphi_{000} f_{010}(v)\big) \\
&\qquad + v_3 \big(- 2\, I_{w001\varphi 100} f_{000}(v) + I_{w100\varphi 001} f_{000}(v) + 2\, I_{w001}\varphi_{000} f_{100}(v) \\
&\qquad - I_{w100}\varphi_{000} f_{001}(v)\big) \\
&\qquad + 2\, I_{w100}\varphi_{000} f_{000}(v) + I_{w020\varphi 100} f_{000}(v) + I_{w002\varphi 100} f_{000}(v) \\
&\qquad - I_{w110\varphi 010} f_{000}(v) - I_{w101\varphi 001} f_{000}(v) - I_{w020}\varphi_{000} f_{100}(v) \\
&\qquad - I_{w002}\varphi_{000} f_{100}(v) + I_{w110}\varphi_{000} f_{010}(v) + I_{w101}\varphi_{000} f_{001}(v)\,.
\end{aligned}
$$

Arising operators

$$
\begin{aligned}
&\left(Q_{000}(f)\right)(v) \\
&\quad = -v_1^2\left(I_{w000\varphi010 f010}(v) + I_{w000\varphi001 f001}(v)\right) + v_1\, v_2\left(I_{w000\varphi010 f100}(v) + I_{w000\varphi100 f010}(v)\right) \\
&\qquad + v_1\, v_3\left(I_{w000\varphi001 f100}(v) + I_{w000\varphi100 f001}(v)\right) - v_2^2\left(I_{w000\varphi100 f100}(v) + I_{w000\varphi001 f001}(v)\right) \\
&\qquad + v_2\, v_3\left(I_{w000\varphi001 f010}(v) + I_{w000\varphi010 f001}(v)\right) - v_3^2\left(I_{w000\varphi100 f100}(v) + I_{w000\varphi010 f010}(v)\right) \\
&\qquad + v_1\left(2\, I_{w000\varphi000 f100}(v) - I_{w010\varphi010 f100}(v) - I_{w001\varphi001 f100}(v) - I_{w010\varphi100 f010}(v) + 2\, I_{w100\varphi010 f010}(v)\right. \\
&\qquad \left. - I_{w001\varphi100 f001}(v) + 2\, I_{w100\varphi001 f001}(v)\right) \\
&\qquad + v_2\left(2\, I_{w010\varphi100 f100}(v) - I_{w100\varphi010 f100}(v) + 2\, I_{w000\varphi000 f010}(v) - I_{w100\varphi100 f010}(v) - I_{w001\varphi001 f010}(v)\right. \\
&\qquad \left. - I_{w001\varphi010 f001}(v) + 2\, I_{w010\varphi001 f001}(v)\right) \\
&\qquad + v_3\left(2\, I_{w001\varphi100 f100}(v) - I_{w100\varphi001 f100}(v) + 2\, I_{w001\varphi010 f010}(v) - I_{w010\varphi001 f010}(v) + 2\, I_{w000\varphi000 f001}(v)\right. \\
&\qquad \left. - I_{w100\varphi100 f001}(v) - I_{w010\varphi010 f001}(v)\right) \\
&\qquad - 2\, I_{w100\varphi000 f100}(v) - I_{w020\varphi100 f100}(v) - I_{w002\varphi100 f100}(v) + I_{w110\varphi010 f100}(v) + I_{w101\varphi001 f100}(v) \\
&\qquad - 2\, I_{w010\varphi000 f010}(v) + I_{w110\varphi100 f010}(v) - I_{w200\varphi010 f010}(v) - I_{w002\varphi010 f010}(v) + I_{w011\varphi001 f010}(v) \\
&\qquad - 2\, I_{w001\varphi000 f001}(v) + I_{w101\varphi100 f001}(v) + I_{w011\varphi010 f001}(v) - I_{w200\varphi001 f001}(v) - I_{w020\varphi001 f001}(v).
\end{aligned}
$$

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

Fundamental means

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

$$\partial_{v_1}^2 f(v), \quad I_{w000\varphi000 f000}(v) = \int_\Omega \varphi(v-w) f(w) \, \mathrm{d}w, \quad v \in \Omega.$$

Approach.

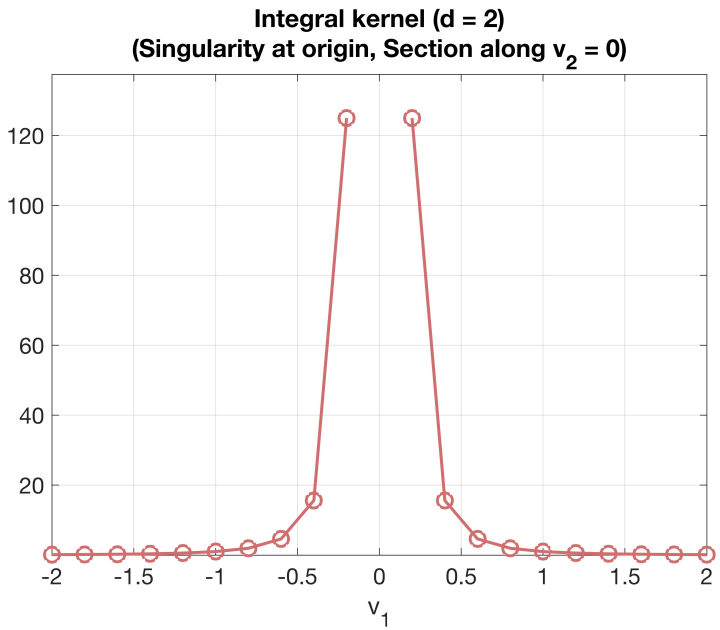
- Application of Fourier spectral method
- Quadrature approximation nearby singularity of kernel
- Identification of basic integrals involving Fourier functions

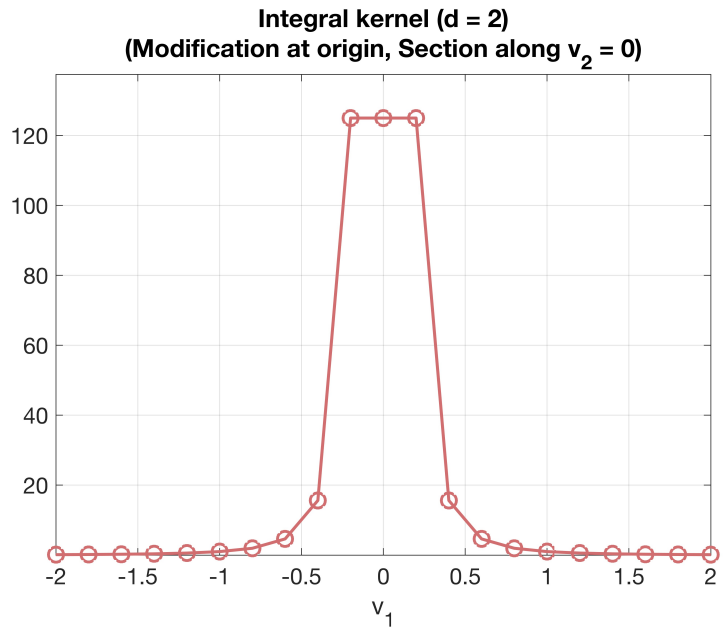
Implementation.

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

For the moment ...

Remark. The following considerations are valid for a regular integral kernel. The modified approach for a kernel with a singularity at the origin is detailed below.





Just for the moment, to have a picture in mind ...

Fourier spectral method

Fourier functions. Consider well-known Fourier functions

$$\mathscr{F}_\kappa^{(\alpha)}(\xi) = \frac{1}{\sqrt{\alpha_2-\alpha_1}}\, \mathrm{e}^{\mu_\kappa^{(\alpha)}(\xi-\alpha_1)}, \quad \mu_\kappa^{(\alpha)} = \frac{2\pi \mathrm{i}\kappa}{\alpha_2-\alpha_1},$$

$$\mathscr{F}_\kappa^{(\alpha)}(\alpha_1) = \frac{1}{\sqrt{\alpha_2-\alpha_1}} = \mathscr{F}_\kappa^{(\alpha)}(\alpha_2), \quad \partial_\xi \mathscr{F}_\kappa^{(\alpha)}(\xi) = \mu_\kappa^{(\alpha)}\, \mathscr{F}_\kappa^{(\alpha)}(\xi),$$

$$\xi \in \mathbb{R}, \quad \kappa \in \mathbb{Z}, \quad \alpha = (\alpha_1, \alpha_2) \in \mathbb{R}^2, \quad \alpha_1 < \alpha_2.$$

In particular, in three dimensions, denote

$$F_m(v) = \mathscr{F}_{m_1}^{(b_{11}, b_{12})}(v_1)\, \mathscr{F}_{m_2}^{(b_{21}, b_{22})}(v_2)\, \mathscr{F}_{m_3}^{(b_{31}, b_{32})}(v_3),$$

$$v = (v_1, v_2, v_3) \in \Omega_{\mathscr{F}}, \quad m = (m_1, m_2, m_3) \in \mathscr{M},$$

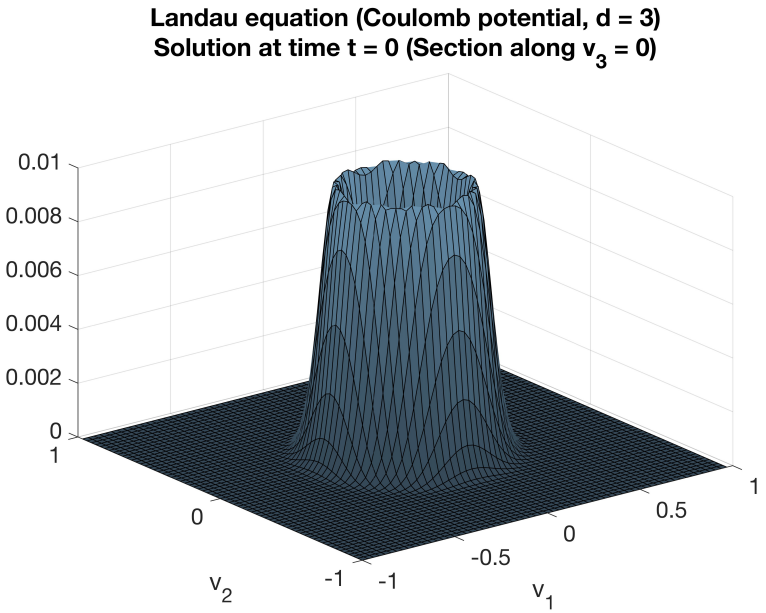
$$\Omega_{\mathscr{F}} = [b_{11}, b_{12}] \times [b_{21}, b_{22}] \times [b_{31}, b_{32}],$$

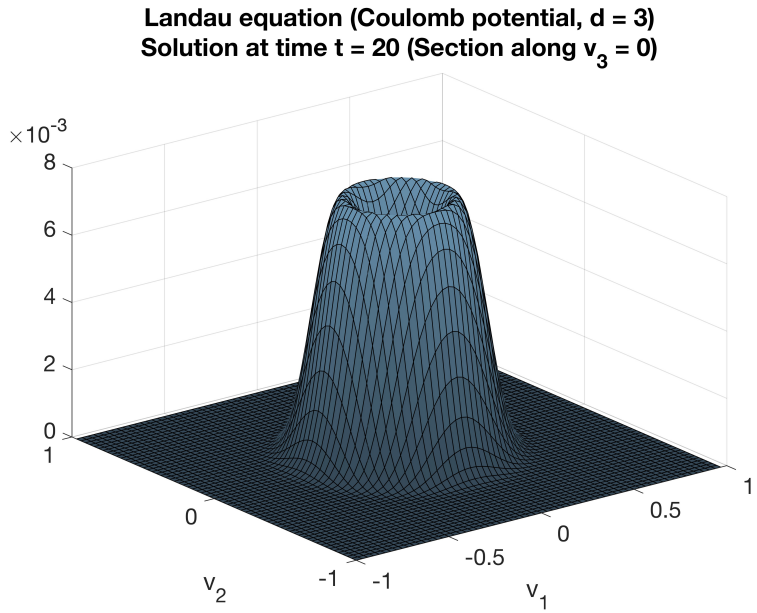
$$\mathscr{M} = \{-\tfrac{1}{2} M_1, \dots, \tfrac{1}{2} M_1 - 1\} \times \cdots \times \{-\tfrac{1}{2} M_3, \dots, \tfrac{1}{2} M_3 - 1\} \subset \mathbb{Z}^3.$$

Fourier spectral method

General benefits.

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





Fourier spectral method

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

$$I_{w000\varphi000f000}(v) = \int_\Omega \varphi(v-w)\, f(w)\, \mathrm{d}w\,, \quad v \in \Omega\,.$$

Specific advantage. The particular identity

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

$$\Gamma_\ell^{(b)} = \mathrm{e}^{-\mu_{\ell_1}^{(b_{11},b_{12})}\, b_{11}}\, \mathrm{e}^{-\mu_{\ell_2}^{(b_{21},b_{22})}\, b_{21}}\, \mathrm{e}^{-\mu_{\ell_3}^{(b_{31},b_{32})}\, b_{31}}\,,$$

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

Fourier spectral method

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

$$\varphi(v) \approx \sum_{\ell \in \mathscr{L}} \varphi_\ell \, F_\ell(v),$$

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

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

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

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

Basic integrals

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

$$I_j(k,m_j) = \int_{b_{j1}}^{b_{j2}} w_j^k \, \mathcal{F}_{m_j}^{(b_{j1},b_{j2})}(w_j)\,\mathrm{d}w_j = \begin{cases} \sqrt{b_{j2}-b_{j1}}, & m_j = 0, \quad k = 0, \\ \frac{b_{j2}^2-b_{j1}^2}{2\sqrt{b_{j2}-b_{j1}}}, & m_j = 0, \quad k = 1, \\ \frac{b_{j2}^3-b_{j1}^3}{3\sqrt{b_{j2}-b_{j1}}}, & m_j = 0, \quad k = 2, \\ 0, & m_j \neq 0, \quad k = 0, \\ \frac{\sqrt{b_{j2}-b_{j1}}}{\mu_{m_j}^{(b_{j1},b_{j2})}}, & m_j \neq 0, \quad k = 1, \\ \frac{(b_{j2}^2-b_{j1}^2)\,\mu_{m_j}^{(b_{j1},b_{j2})} - 2(b_{j2}-b_{j1})}{\sqrt{b_{j2}-b_{j1}}\,(\mu_{m_j}^{(b_{j1},b_{j2})})^2}, & m_j \neq 0, \quad k = 2, \end{cases} \qquad j \in \{1,\ldots,d\}.$$

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

Constant integral kernel

Maxwellian molecules case.
BKW solution on unbounded domain.

Maxwellian molecules case

Setting. Study the particular situation, where the underlying domain for the velocity coincides with the Euclidian space and the Landau operator involves a constant integral kernel

$$\varphi(v) = C,$$

$$\big(Q(f,f)\big)(v) = C\,\partial_v \cdot \int_\Omega P(v-w)\big(\partial_v f(v)\, f(w) - f(v)\,\partial_w f(w)\big)\,\mathrm{d}w,$$

$$v \in \Omega = \mathbb{R}^d.$$

BWK solution

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

$$\varphi(v) = C = \tfrac{1}{24}, \quad (\alpha_1, \alpha_2, \alpha_3) = \left(\tfrac{5}{2}, \tfrac{3}{2}, \tfrac{1}{6}\right), \quad K(t) = 1 - \tfrac{1}{2}\,\mathrm{e}^{-\alpha_3 t},$$

$$f(v,t) = \frac{1}{(2\pi K(t))^{3/2}}\,\mathrm{e}^{-\frac{1}{2}\frac{1}{K(t)}|v|^2}\left(\alpha_1 - \alpha_2\,\frac{1}{K(t)} + \frac{1}{2}\,\frac{1-K(t)}{(K(t))^2}\,|v|^2\right),$$

$$\partial_t f(v,t) = \big(Q(f,f)\big)(v,t), \quad (v,t) \in \Omega \times [t_0, T].$$

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

$$f(v) = \frac{1}{2\pi^{3/2}}\,\mathrm{e}^{-|v|^2}\left(2|v|^2 - 1\right),$$

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

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

A few more details ...

Recall the representation for the Landau operator

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

Based on the Fourier spectral coefficients $(f_m)_{m\in\mathcal{M}}$ of the density function, approximations to its derivatives are computed through

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

A few more details ...

Due to the fact that the integral kernel is constant and its derivatives vanish, approximations to the decisive integrals are obtained through

$$
\begin{aligned}
&C\,\widetilde{I}_{w\,i_1 i_2 i_3\,f\,k_1 k_2 k_3} \\
&\quad = C \sum_{m \in \mathcal{M}} f_m^{(F)} \left(\mu_{m_1}^{(b_{11}, b_{12})}\right)^{k_1} \left(\mu_{m_2}^{(b_{21}, b_{22})}\right)^{k_2} \left(\mu_{m_3}^{(b_{31}, b_{32})}\right)^{k_3} \\
&\qquad\qquad \times I_1(i_1, m_1)\, I_2(i_2, m_2)\, I_3(i_3, m_3)\,, \\
&\quad \approx I_{w\,i_1 i_2 i_3\,\varphi 000\,f\,k_1 k_2 k_3} = C \int_\Omega w_1^{i_1} w_2^{i_2} w_3^{i_3}\, \partial_{w_1}^{k_1} \partial_{w_2}^{k_2} \partial_{w_3}^{k_3} f(w)\, \mathrm{d}w\,.
\end{aligned}
$$

A few more details ...

Overall, the implementation is simpler ...

$$(Q_{000}(f))(v) \approx 2C(-\tilde{I}_{w100}f_{100} - \tilde{I}_{w010}f_{010} - \tilde{I}_{w001}f_{001}),$$

$$(Q_{100}(f))(v) \approx C\Big(v_1(-2\tilde{I}_{w000}f_{000} - \tilde{I}_{w010}f_{010} - \tilde{I}_{w001}f_{001}) + 2\tilde{I}_{w100}f_{000} + \tilde{I}_{w110}f_{010} + \tilde{I}_{w101}f_{001}\Big),$$

$$(Q_{010}(f))(v) \approx C\Big(v_2(-2\tilde{I}_{w000}f_{000} - \tilde{I}_{w100}f_{100} - \tilde{I}_{w001}f_{001}) + 2\tilde{I}_{w010}f_{000} + \tilde{I}_{w110}f_{100} + \tilde{I}_{w011}f_{001}\Big),$$

$$(Q_{001}(f))(v) \approx C\Big(v_3(-2\tilde{I}_{w000}f_{000} - \tilde{I}_{w100}f_{100} - \tilde{I}_{w010}f_{010}) + 2\tilde{I}_{w001}f_{000} + \tilde{I}_{w101}f_{100} + \tilde{I}_{w011}f_{010}\Big),$$

$$(Q_{200}(f))(v) \approx C(v_2^2\tilde{I}_{w000}f_{000} + v_3^2\tilde{I}_{w000}f_{000} - 2v_2\tilde{I}_{w010}f_{000} - 2v_3\tilde{I}_{w001}f_{000} + \tilde{I}_{w020}f_{000} + \tilde{I}_{w002}f_{000}),$$

$$(Q_{110}(f))(v) \approx 2C(-v_1v_2\tilde{I}_{w000}f_{000} + v_1\tilde{I}_{w010}f_{000} + v_2\tilde{I}_{w100}f_{000} - \tilde{I}_{w110}f_{000}),$$

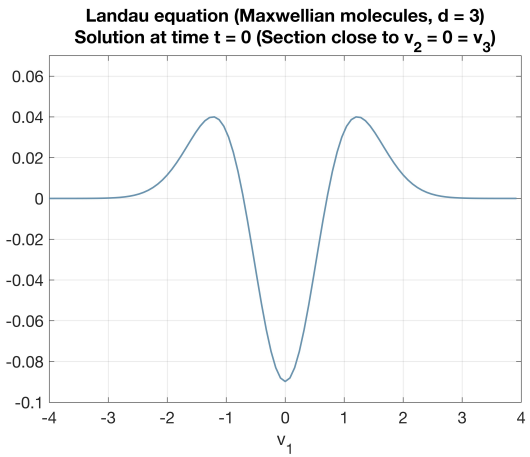
$$(Q_{101}(f))(v) \approx 2C(-v_1v_3\tilde{I}_{w000}f_{000} + v_1\tilde{I}_{w001}f_{000} + v_3\tilde{I}_{w100}f_{000} - \tilde{I}_{w101}f_{000}),$$

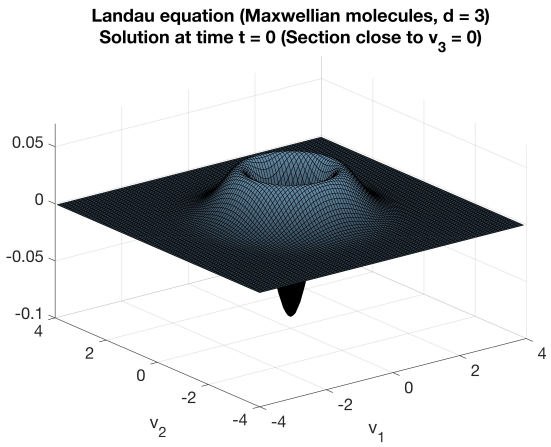
$$(Q_{020}(f))(v) \approx C(v_1^2\tilde{I}_{w000}f_{000} + v_3^2\tilde{I}_{w000}f_{000} - 2v_1\tilde{I}_{w100}f_{000} - 2v_3\tilde{I}_{w001}f_{000} + \tilde{I}_{w200}f_{000} + \tilde{I}_{w002}f_{000}),$$

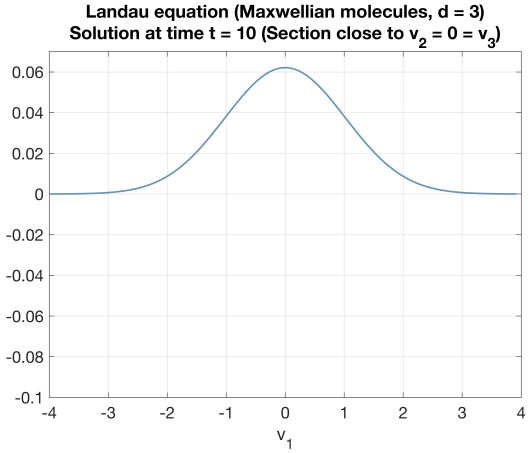
$$(Q_{011}(f))(v) \approx 2C(-v_2v_3\tilde{I}_{w000}f_{000} + v_2\tilde{I}_{w001}f_{000} + v_3\tilde{I}_{w010}f_{000} - \tilde{I}_{w011}f_{000}),$$

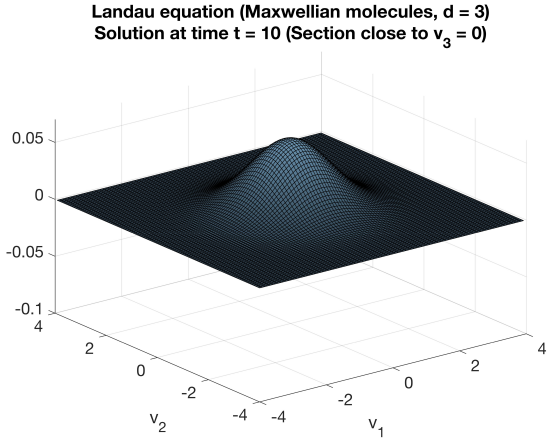
$$(Q_{002}(f))(v) \approx C(v_1^2\tilde{I}_{w000}f_{000} + v_2^2\tilde{I}_{w000}f_{000} - 2v_1\tilde{I}_{w100}f_{000} - 2v_2\tilde{I}_{w010}f_{000} + \tilde{I}_{w200}f_{000} + \tilde{I}_{w020}f_{000}).$$

Illustration









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

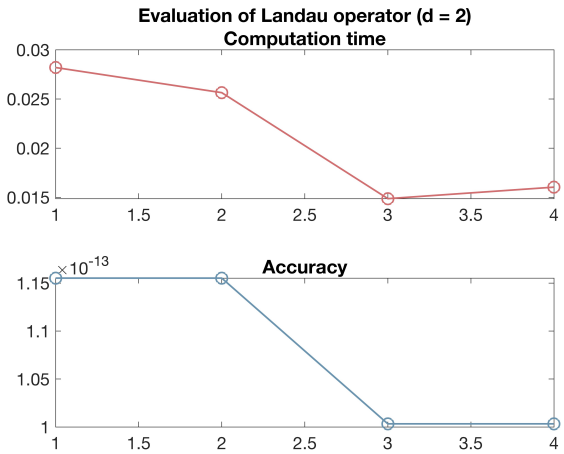
https://techmath.uibk.ac.at/mecht/MyHomepage/Research/Movie_Maxwellian_Solution3d.m4v
https://techmath.uibk.ac.at/mecht/MyHomepage/Research/Movie_Maxwellian_Solution3dSection.m4v

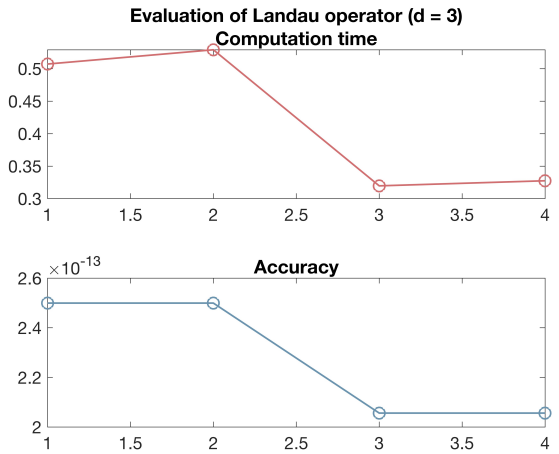
Numerical tests

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

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

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).





Numerical tests

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 (not illustrated here)

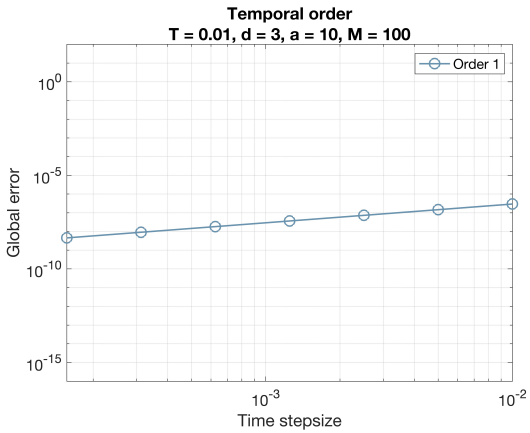
$$\int_\Omega f(v,t)\ln\big(f(v,t)\big)\,\mathrm{d}v \le \int_\Omega f(v,t_0)\ln\big(f(v,t_0)\big)\,\mathrm{d}v, \quad t\in[t_0,T].$$

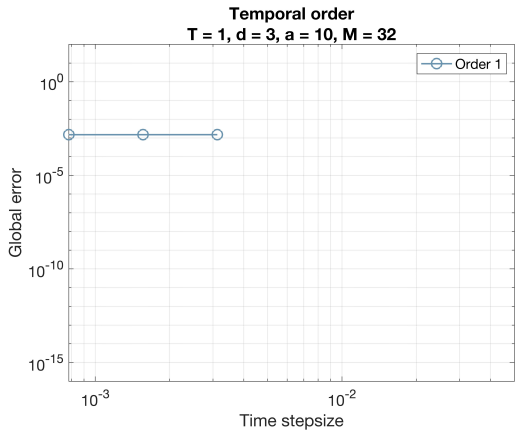
Splitting approach. Contrast the results with those obtained by a Lie-splitting-type method, which provides a reliable first-order alternative, since in particular the terms related to the second-order derivatives $\partial_{v_1}^2 f, \partial_{v_2}^2 f, \partial_{v_3}^2 f$ are treated separately in a semi-implicit manner.

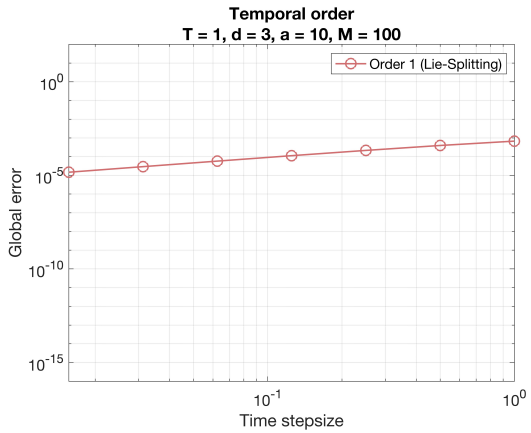
Numerical tests

Stability. Verify the temporal orders of time integration methods.

- The observations hold for the explicit Euler method and higher-order explicit Runge–Kutta methods.
- For relatively small time stepsizes, obtain the expected results. For larger time stepsizes, the procedure failes due to severe stability issues!
- A first-order Lie–Splitting-type method provides a robust alternative. Even for a significantly higher number of Fourier functions ($M^3 = 100^3$), it yields a reliable result for any choice of the time stepsize.

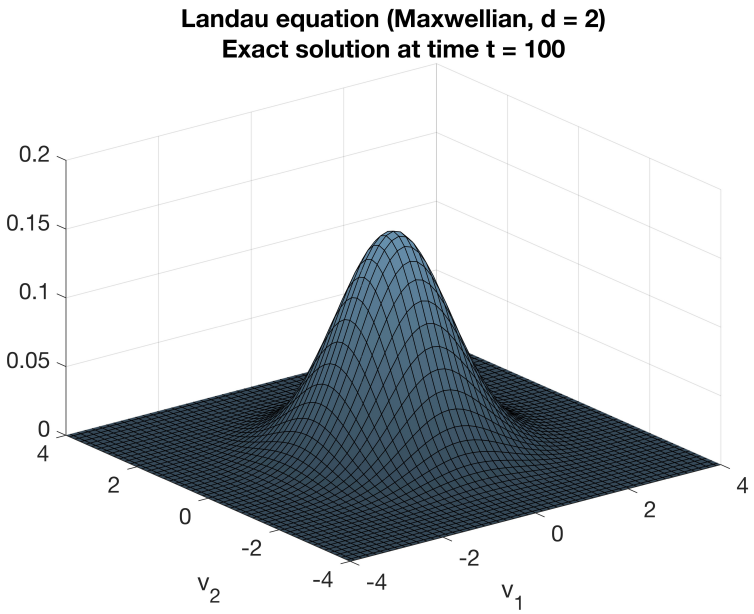


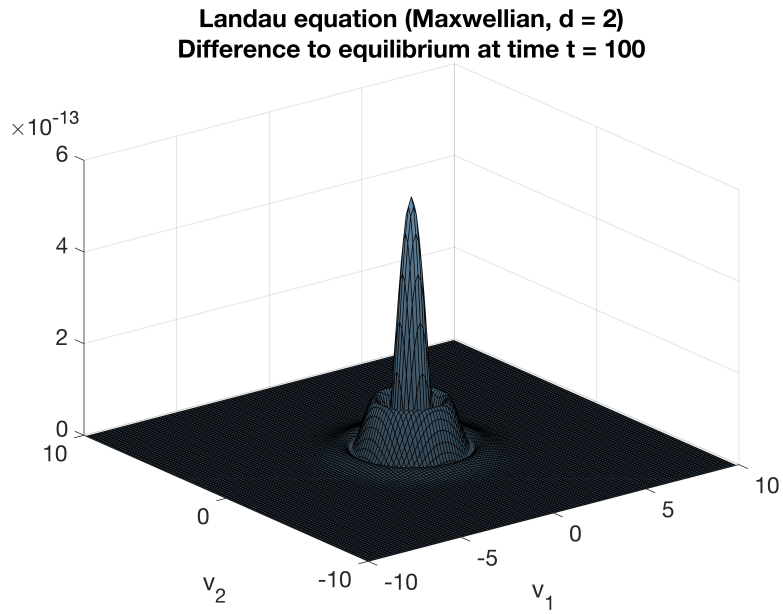




Numerical tests ($d = 2$)

Long-term integration ($d = 2$).

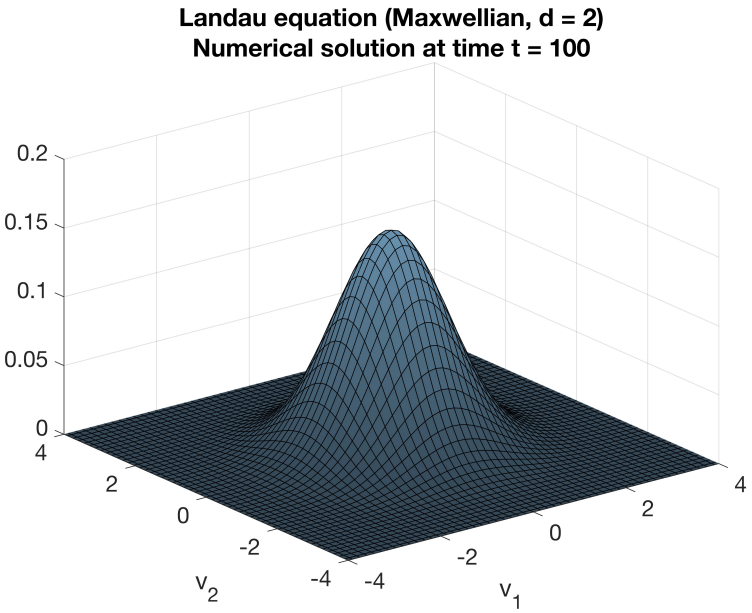


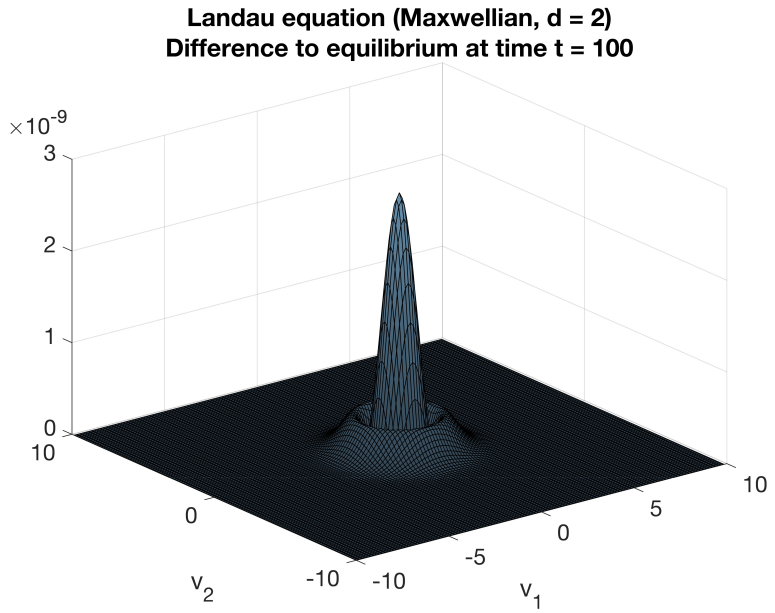


Exact solution and convergence towards equilibrium (time $T = 100$).

Numerical tests ($d = 2$)

Long-term integration ($d = 2$).

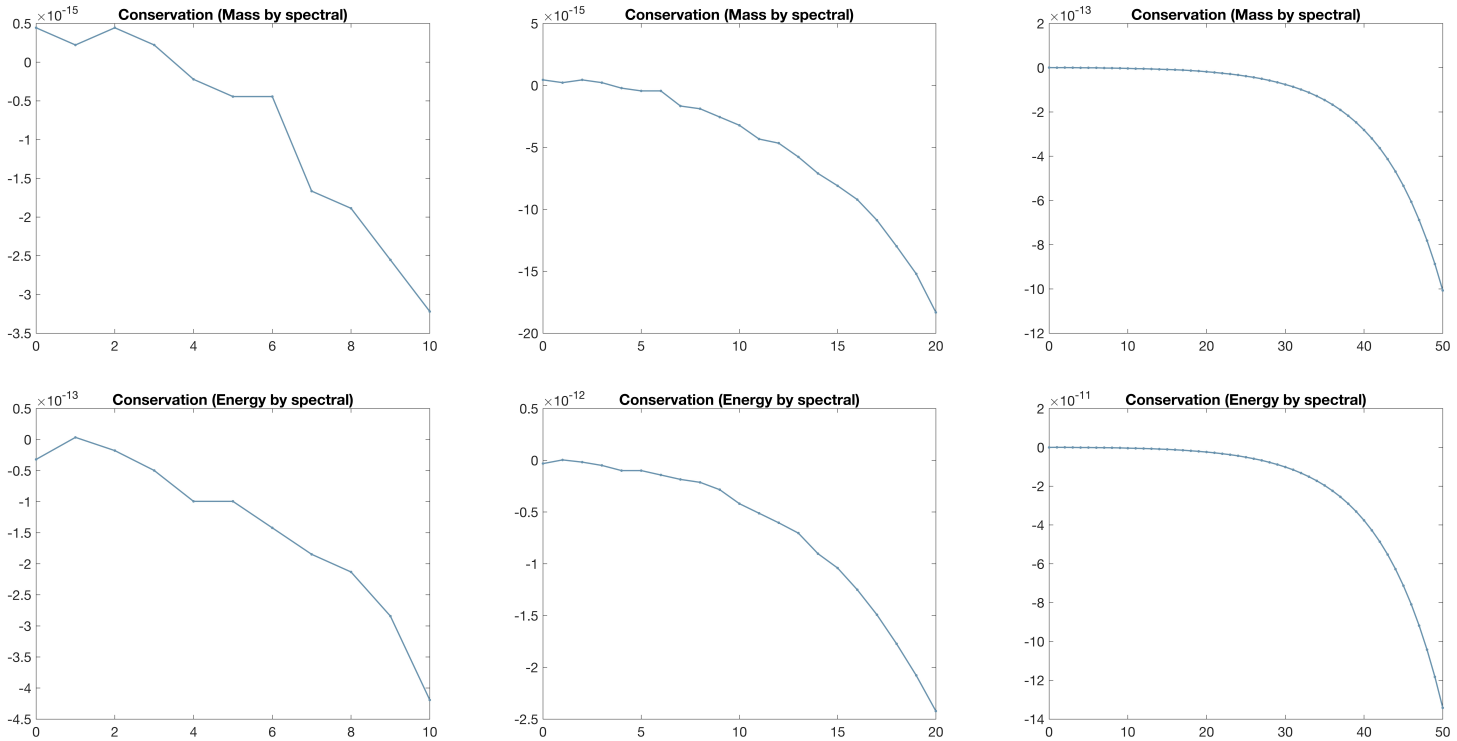




Numerical solution obtained by an adaptive explicit Runge–Kutta methods (ode45) and convergence towards equilibrium (time $T = 100$).

Numerical tests ($d = 2$)

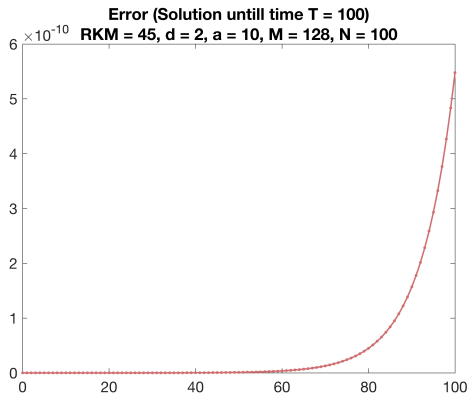
Long-term integration ($d = 2$).

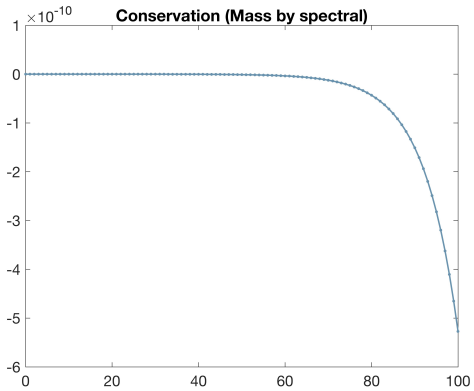


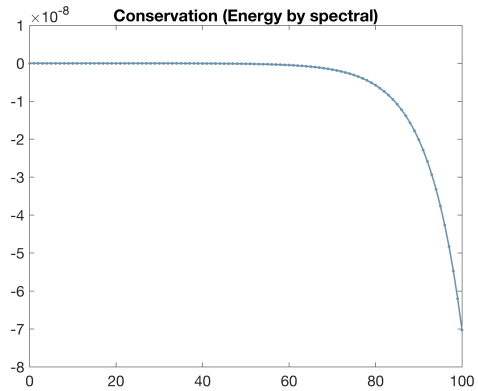
Time integration by an adaptive explicit Runge–Kutta methods (ode45).
Approximation of mass and energy at times $t = 10, 20, 50$ (left to right).

Numerical tests ($d = 2$)

Long-term integration ($d = 2$).







Time integration by an adaptive explicit Runge–Kutta methods (ode45).
Approximation of the solution and associated quantities untill time $T = 100$.

Regular integral kernel

First test problem on bounded domain.
Second test problem with localised solution.

Approach

Setting. Extend the former approach for the Maxwellian molecules case and study the more general situation, where the Landau operator involves a regular integral kernel

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

$$v \in \Omega.$$

Use that favourable approximations to the kernel and its derivatives are provided by Fourier series expansions.

A few more details ...

Fundamental means. Recall the relations for the decisive integrals, the approximations by Fourier series for the kernel and the density functions as well as their derivatives, and the particular identity for Fourier functions

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

$$\partial_{v_1}^{j_1} \partial_{v_2}^{j_2} \partial_{v_3}^{j_3} \varphi(v-w) \approx \sum_{\ell \in \mathcal{L}} \varphi_{j_1 j_2 j_3 \ell}\, F_\ell(v-w)\,,$$

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

$$F_\ell(v-w)\, F_m(w) = \Gamma_\ell^{(b)}\, F_\ell(v)\, F_{m-\ell}(w)\,, \quad \Gamma_\ell^{(b)} = \mathrm{e}^{-\mu_{\ell_1}^{(b_{11},b_{12})} b_{11}}\, \mathrm{e}^{-\mu_{\ell_2}^{(b_{21},b_{22})} b_{21}}\, \mathrm{e}^{-\mu_{\ell_3}^{(b_{31},b_{32})} b_{31}}\,.$$

A few more details ...

Resulting approximations. Based on these relations, approximations to the decisive integrals are obtained

$$
\begin{aligned}
&\widetilde{I}_{w\,i_1 i_2 i_3\,\varphi\,j_1 j_2 j_3\,f\,k_1 k_2 k_3}(v) \\
&\quad = \sum_{\ell \in \mathscr{L}} \varphi_\ell \, \Gamma_\ell^{(b)} \left(\mu_{\ell_1}^{(b_{11},b_{12})}\right)^{j_1} \left(\mu_{\ell_2}^{(b_{21},b_{22})}\right)^{j_2} \left(\mu_{\ell_3}^{(b_{31},b_{32})}\right)^{j_3} F_\ell(v) \\
&\qquad \times \sum_{m \in \mathscr{M}} f_m \, I_1(i_1, m_1 - \ell_1) \, I_2(i_2, m_2 - \ell_2) \, I_3(i_3, m_3 - \ell_3) \\
&\qquad \times \left(\mu_{m_1}^{(b_{11},b_{12})}\right)^{k_1} \left(\mu_{m_2}^{(b_{21},b_{22})}\right)^{k_2} \left(\mu_{m_3}^{(b_{31},b_{32})}\right)^{k_3} \\
&\quad \approx I_{w\,i_1 i_2 i_3\,\varphi\,j_1 j_2 j_3\,f\,k_1 k_2 k_3}(v), \qquad v \in \Omega_{\mathscr{F}}\,.
\end{aligned}
$$

A few more details ...

Implementation and observation. Essential ingredients for the efficient implementation are

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

A crucial observation is that the costs for the computation of the inner sums amount to the evaluation of single and double 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

Basic test problem

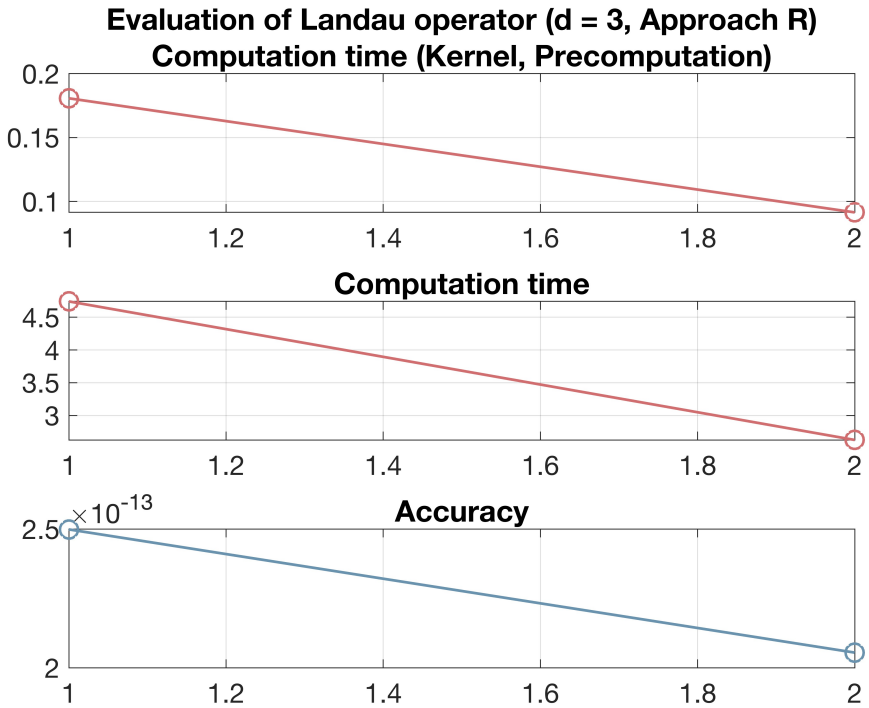
Maxwellian molecules case. For a constant kernel and a prescribed density function, the associated Landau operator is given by

$$f(v) = \frac{1}{2\pi^{3/2}} \mathrm{e}^{-|v|^2} \left(2|v|^2 - 1\right),$$

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

Numerical tests

Main purpose. Consider the Maxwellian molecules case as a preliminary test problem to verify the extended approach and implementation for regular integral kernels.



Maxwellian molecules case

Artificial test problem

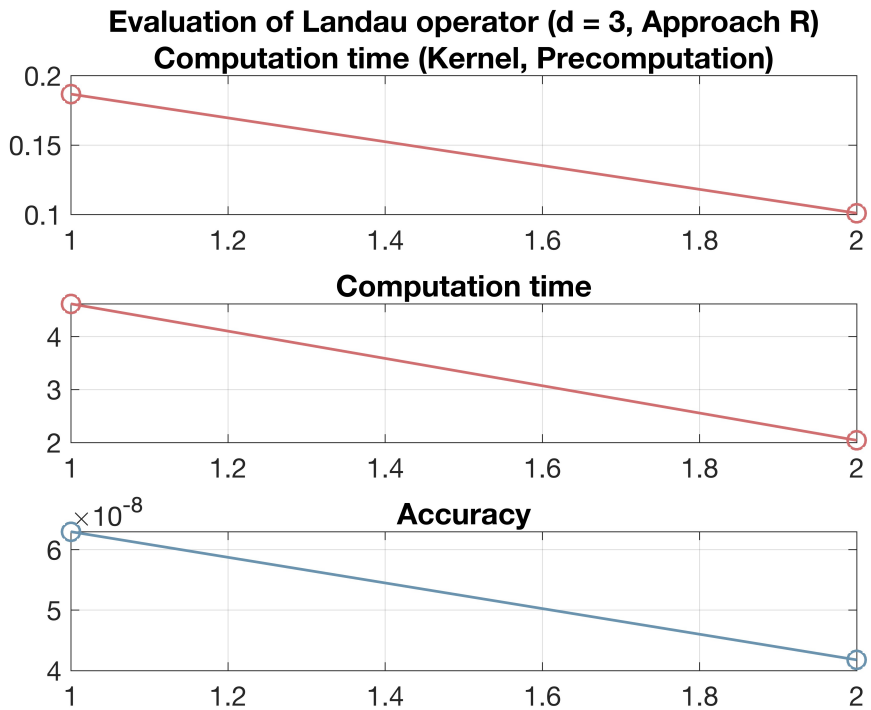
Bounded domain. For a prescribed kernel and a prescribed density function, the associated Landau operator is given by

$$\varphi(v) = \cos(v_1)\cos(v_2)\cos(v_3)\,,$$
$$f(v) = \sin(v_1)\sin(v_2)\sin(v_3)\,,$$
$$q_{11}(v) = v_2\sin(2\,v_2)\cos(2\,v_3) + v_3\cos(2\,v_2)\sin(2\,v_3) - \tfrac{1}{2}\,v_2\sin(2\,v_2) - \tfrac{1}{2}\,v_3\sin(2\,v_3)\,,$$
$$q_{12} = \tfrac{1}{2}\cos(2\,v_2) + \tfrac{1}{2}\cos(2\,v_3) - \tfrac{1}{2}\,,$$
$$q_1(v) = q_{11}(v) + q_{12}(v)\,,$$
$$q_2(v) = v_1\sin(2\,v_1)\cos(2\,v_3) + \tfrac{1}{2}\cos(2\,v_3) - \tfrac{1}{2}\,v_1\sin(2\,v_1) - \tfrac{1}{2}\,v_3\sin(2\,v_3) - \tfrac{1}{2}\,,$$
$$q_3(v) = -\tfrac{1}{2}\,v_1\sin(2\,v_1) - \tfrac{1}{2}\,v_2\sin(2\,v_2)\,,$$
$$\big(Q(f,f)\big)(v) = \tfrac{\pi^3}{2}\left(q_1(v)\cos(2\,v_1) + q_2(v)\cos(2\,v_2) + q_3(v)\cos(2\,v_3) - \cos^2(v_3) + \tfrac{1}{2}\right),$$
$$v = (v_1, v_2, v_3) \in \Omega = [-\pi,\pi]^3\,.$$

Remark. The above test problem is not suitable for the verification of the general approach (considerations in the context of quadrature approximations apply to unbounded domains).

Numerical tests

Main purpose. Consider the above test problem on a bounded domain. Verify the extended approach and implementation for regular kernels. Observe reasonable computation times and high accuracy.



Test problem on bounded domain

Artificial test problem

Unbounded domain. For a prescribed kernel and a prescribed density function, the associated Landau operator is given by

$$\varphi(v) = C\,\mathrm{e}^{-v_1^2-2\,v_2^2-3\,v_3^2}\,,$$

$$f(v) = \mathrm{e}^{-\frac{1}{2}\,v_1^2-\frac{1}{4}\,v_2^2-\frac{1}{8}\,v_3^2}\,,$$

$$q_1(v) = -\,C\,\frac{\pi^{3/2}\,\sqrt{3}}{41006250}\,\mathrm{e}^{-\frac{5}{6}\,v_1^2-\frac{17}{36}\,v_2^2-\frac{49}{200}\,v_3^2}\,,$$

$$q_2(v) = 17500\,v_1^2\,v_2^2 + 7047\,v_1^2\,v_3^2 + 135\,v_2^2\,v_3^2 - 1005300\,v_1^2 + 111000\,v_2^2 + 46899\,v_3^2 + 369900\,,$$

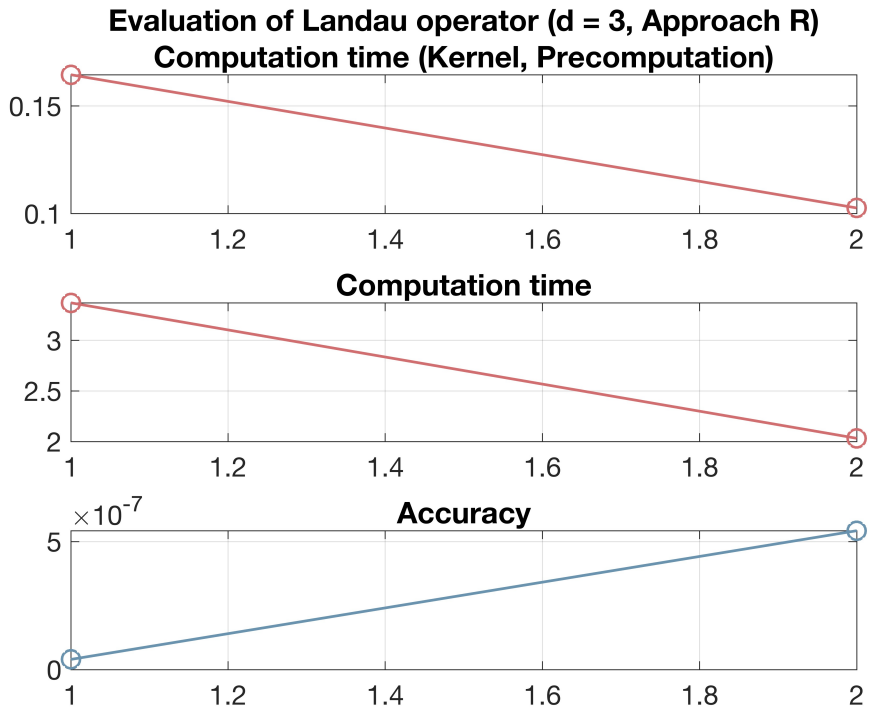
$$\big(Q(f,f)\big)(v) = q_1(v)\,q_2(v)\,,$$

$$v = (v_1, v_2, v_3) \in \Omega = \mathbb{R}^3\,.$$

Remark. The above test problem is suitable for the verification of the general approach (considerations in the context of quadrature approximations apply).

Numerical tests

Main purpose. Consider the above test problem on a bounded domain. Verify the extended approach and implementation for regular kernels. Observe reasonable computation times and high accuracy.



Test problem on unbounded domain

Singular integral kernel

Approach

Setting. Extend the former approach for regular integral kernels and study the relevant situation, where the Landau operator involves an integral kernel with a singularity at the origin

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

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

Approach

Starting point. Use the evident identity

$$\varphi = \underbrace{\psi}_{\substack{\text{regular function} \\ \text{above approach applies}}} + \underbrace{\varphi - \psi}_{\substack{\text{singular function} \\ \text{non-zero on small domain}}}$$

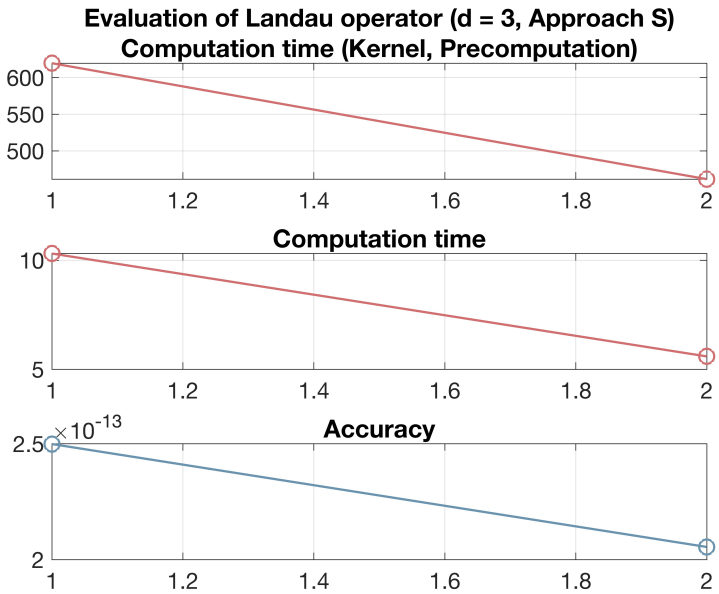
and analogous relations for the (known) derivatives of the kernel.

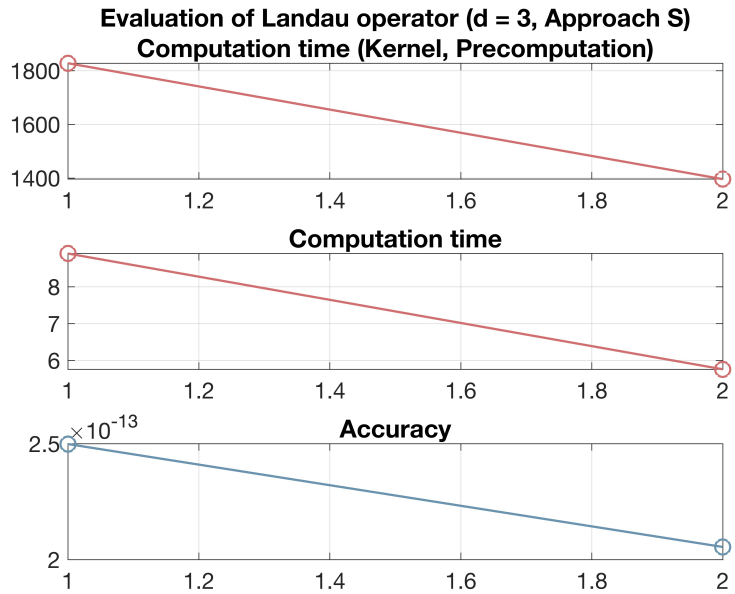
Realisation and implementation.

- Define a small neighbourhood of the origin, and determine the linear interpolants of the kernel and its derivatives.
- For the remaining differences, employ quadrature approximations.
- Transfer the main part of the additional effort to precomputations.

Preliminary numerical tests

Main purpose. Consider the Maxwellian molecules case as a preliminary test problem to verify the extended implementation for (possibly) singular integral kernels. Base quadrature approximations on width two (left) and four (right), respectively, and observe increasing precomputation times.





Maxwellian molecules case

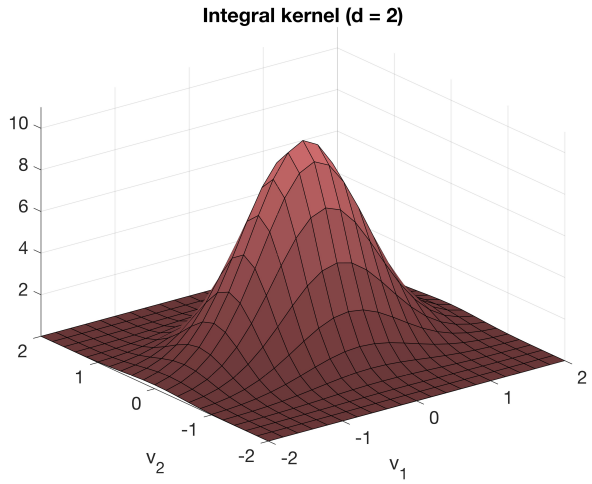
Approach and artificial test problem

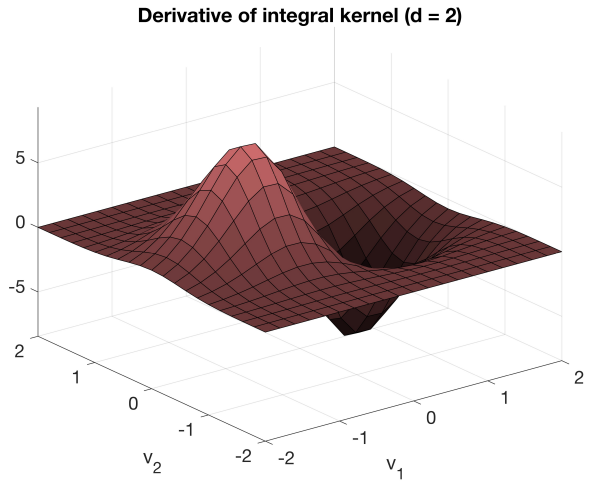
Test problem. Consider the above stated, more meaningful artificial test problem involving the regular integral kernel

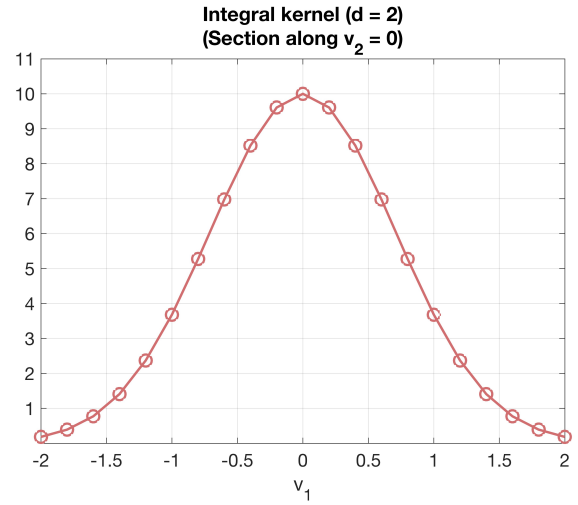
$$\varphi(v) = C\,\mathrm{e}^{-v_1^2 - 2\,v_2^2 - 3\,v_3^2}\,, \qquad v = (v_1, v_2, v_3) \in \Omega = \mathbb{R}^3\,.$$

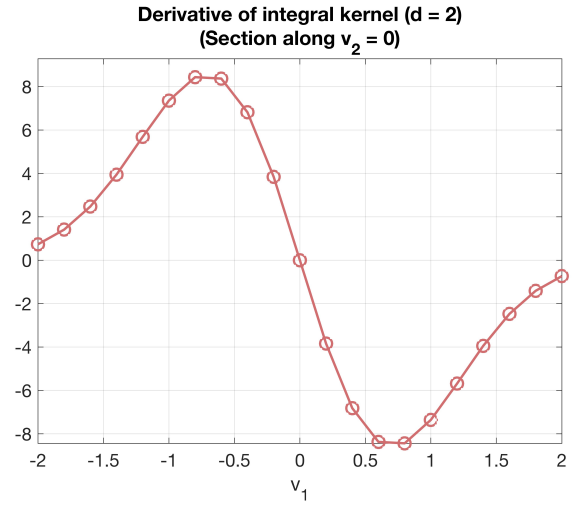
How to proceed when including quadrature approximations?
Pictures say more than a thousand words ...

Approach and artificial test problem



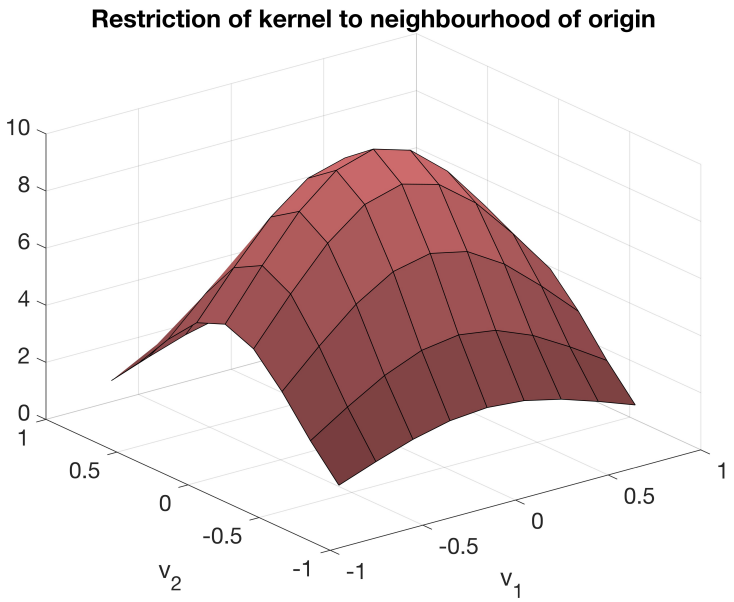


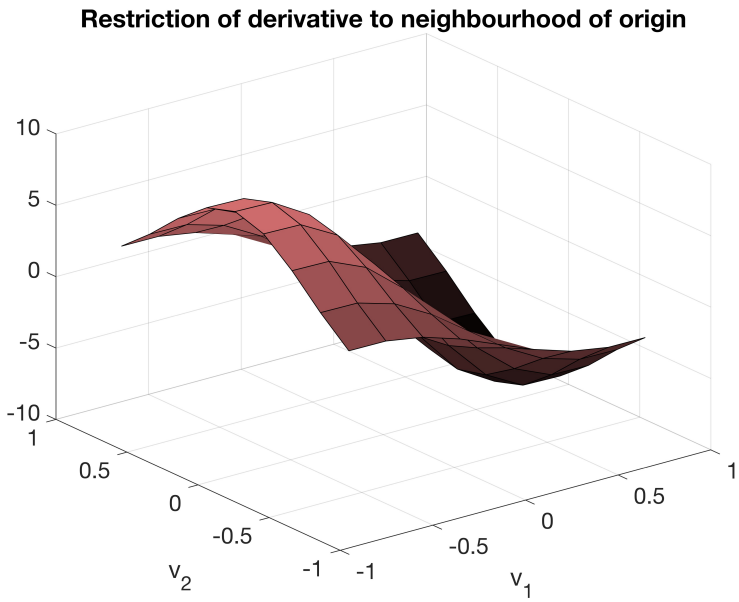




Regular integral kernel and its first derivative.

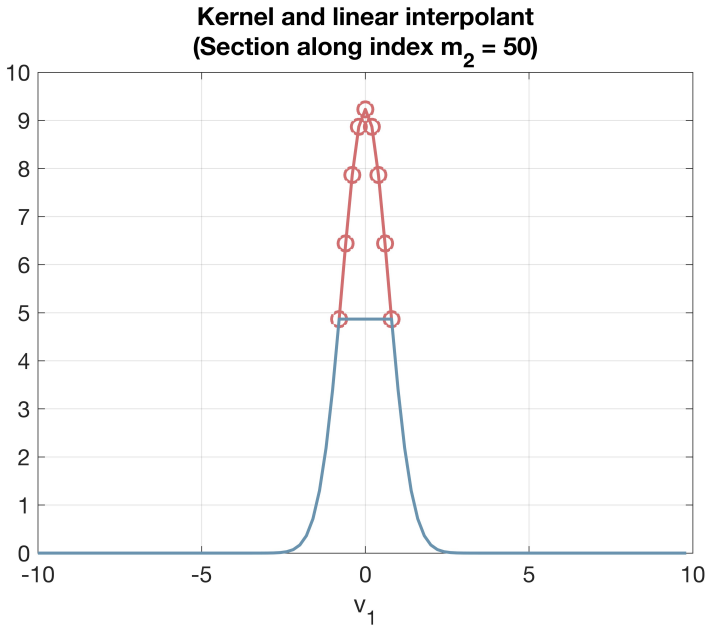
Approach and artificial test problem

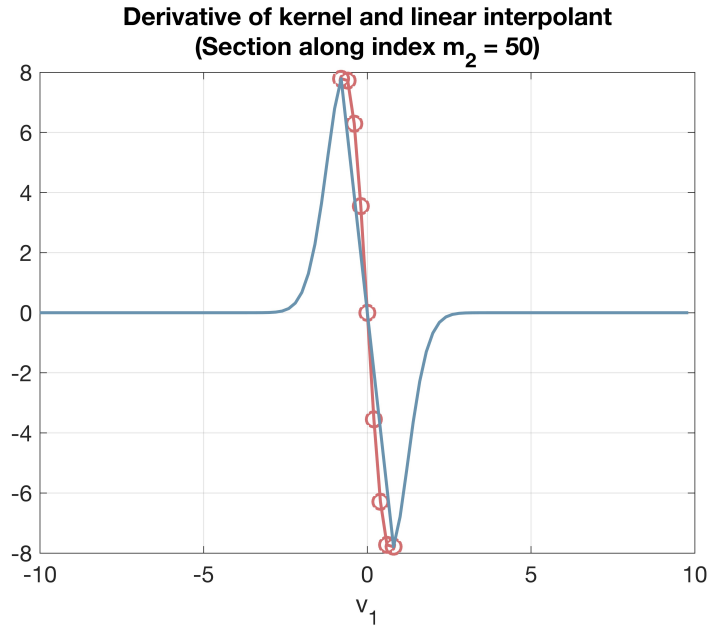




Restriction of the regular integral kernel and its derivative to a (small) neighbourhood of the origin, where linear interpolation is applied.

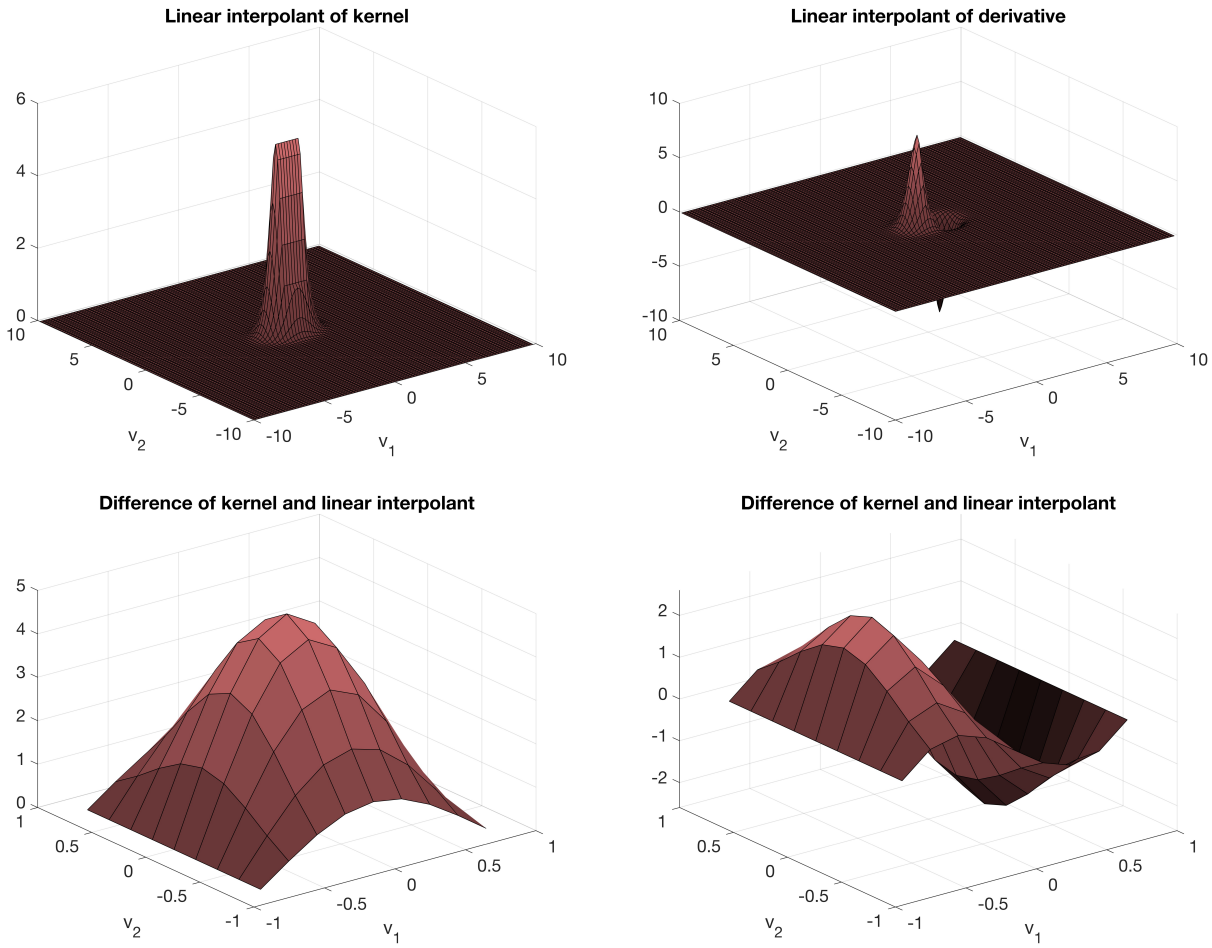
Approach and artificial test problem





Regular kernel and its derivative. Linear interpolants. Sections along indices.

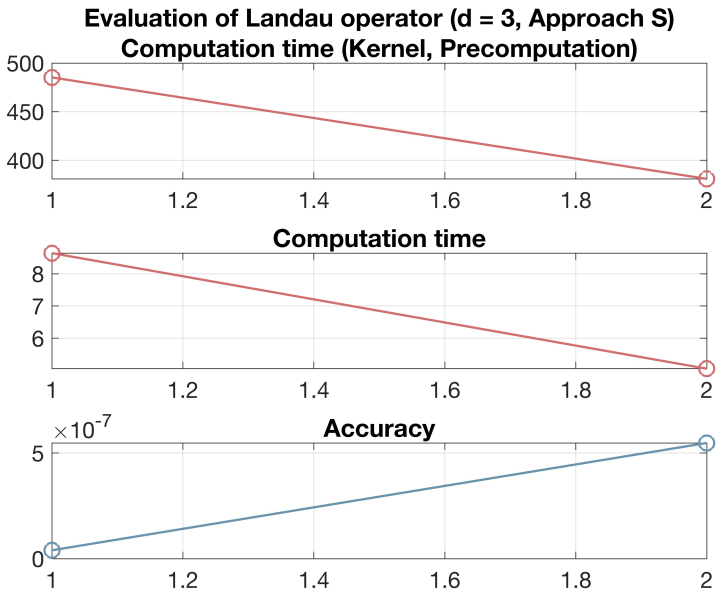
Approach and artificial test problem

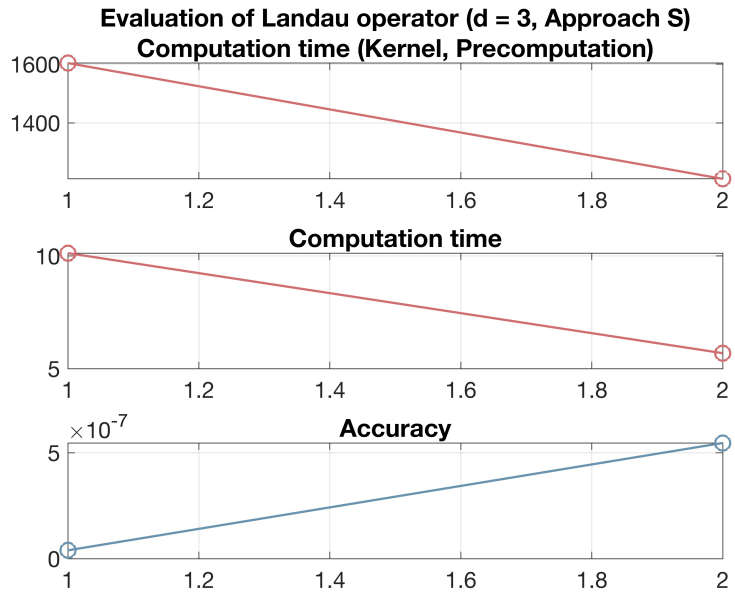


Linear interpolants of the regular kernel and its derivative (used in Fourier series approximation). Corresponding differences (used in quadrature approximation).

Approach and artificial test problem

Main purpose. Consider the artificial test problem involving a regular integral kernel. Verify the extended approach and implementation for a possibly singular kernel. Base the quadrature approximations on width two (left) and four (right), respectively. Observe high accuracy.

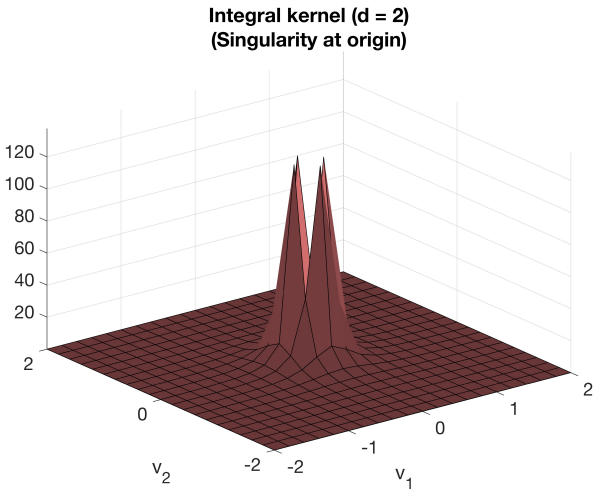


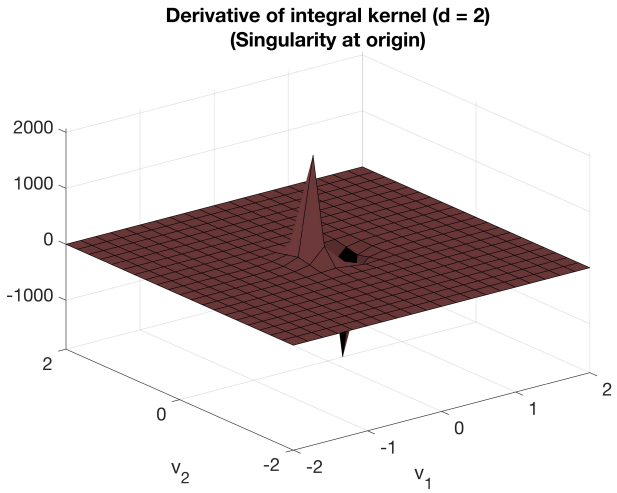


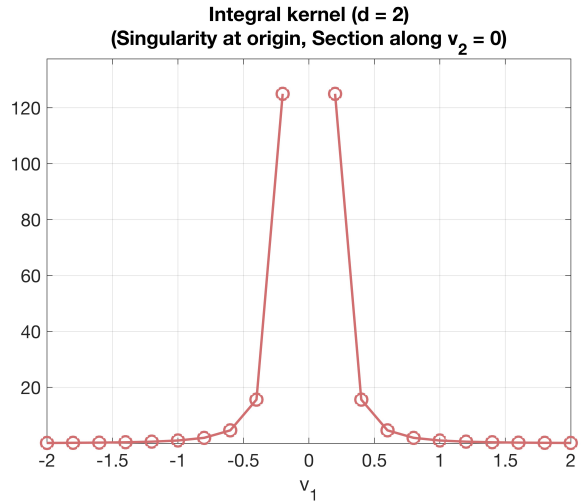
Finally ...

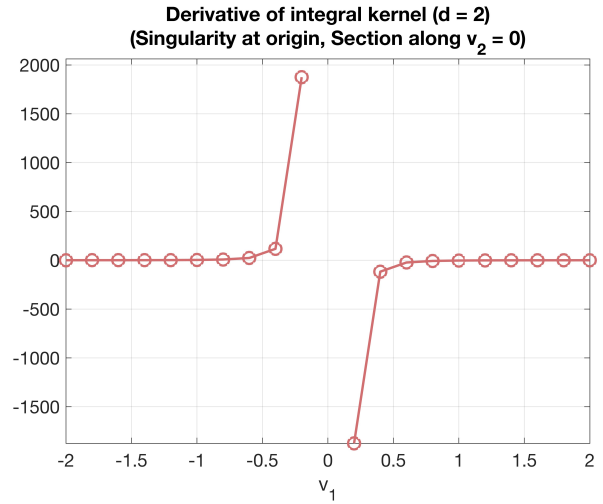
... we are ready for numerical evaluation of the Landau operator in three dimensions with Coulomb interaction.

Approach and numerical tests



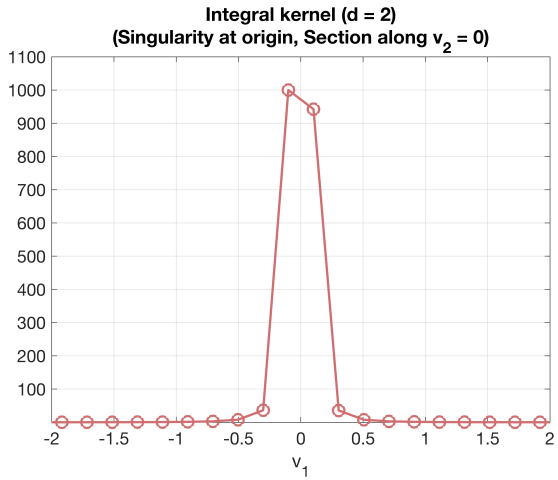


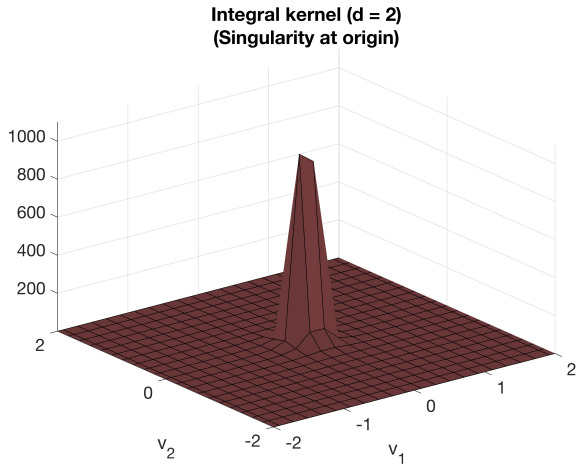


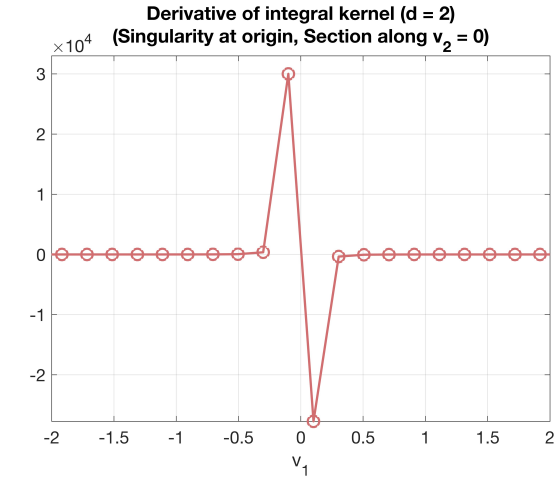


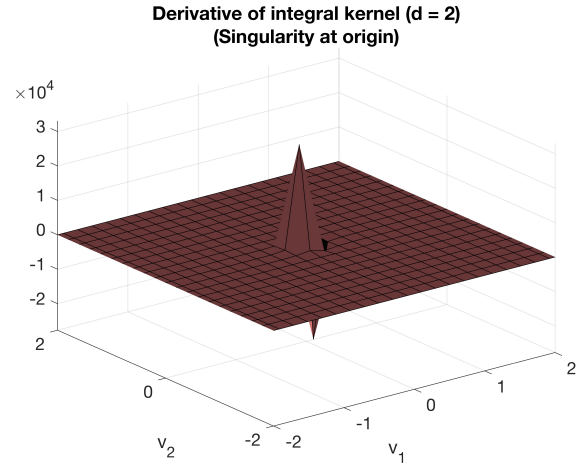
Integral kernel with a singularity at the origin and its first derivative.

Approach and numerical tests



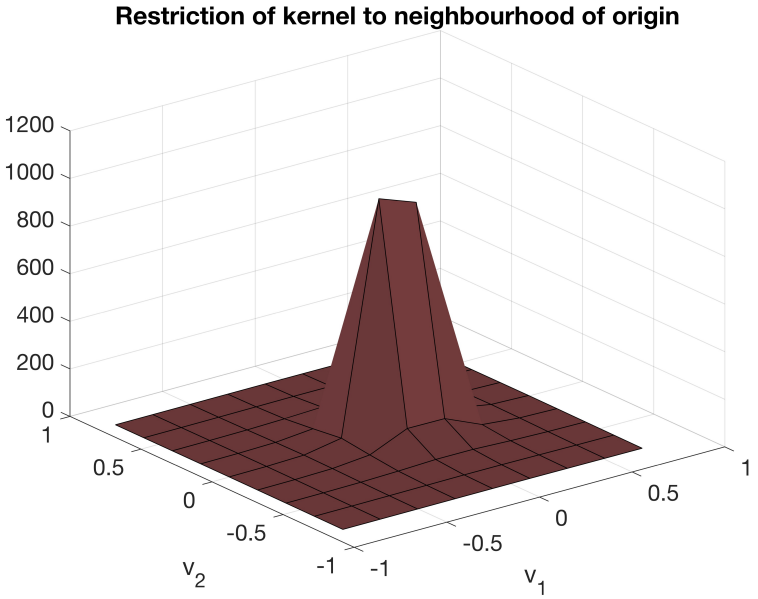


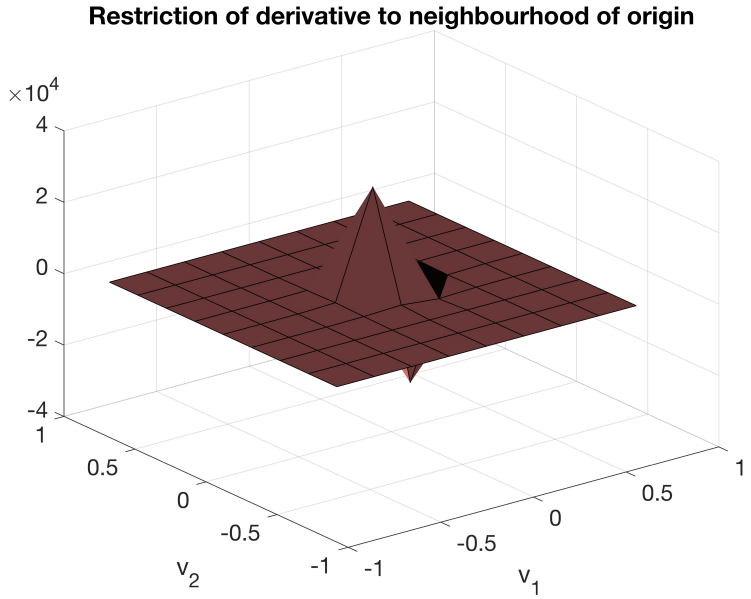




Slight modification of the domain. By the choice of a non-symmetric domain the coincidence of a grid point with the singularity at the origin is avoided.

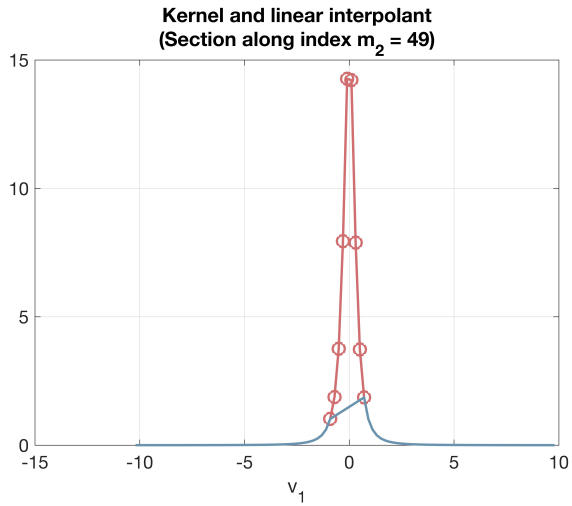
Approach and numerical tests

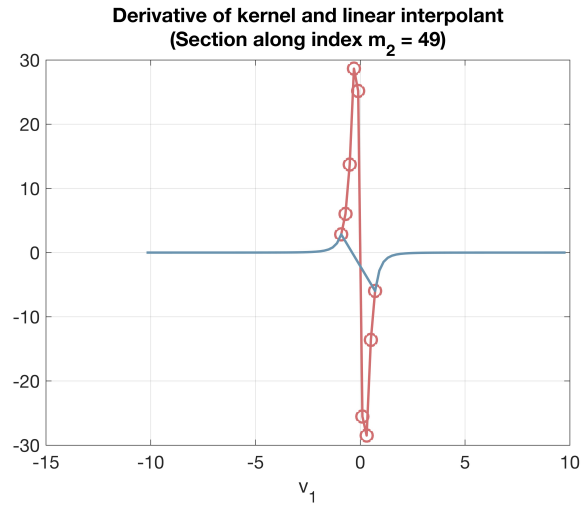


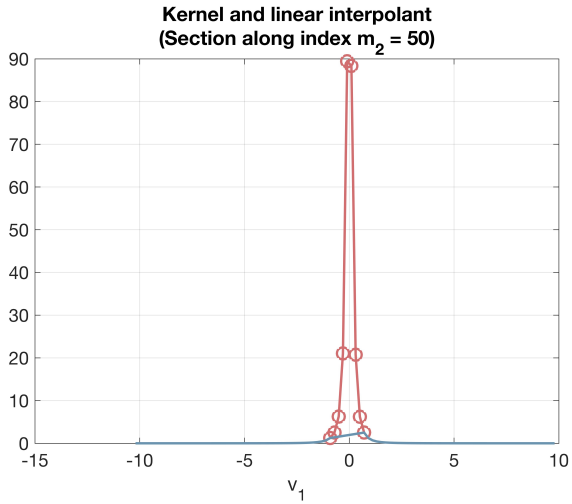


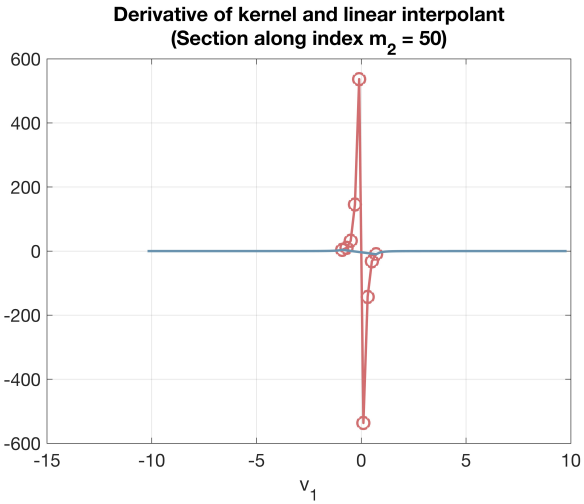
Restriction of the singular integral kernel and its derivative to a (small) neighbourhood of the origin, where linear interpolation is applied.

Approach and numerical tests



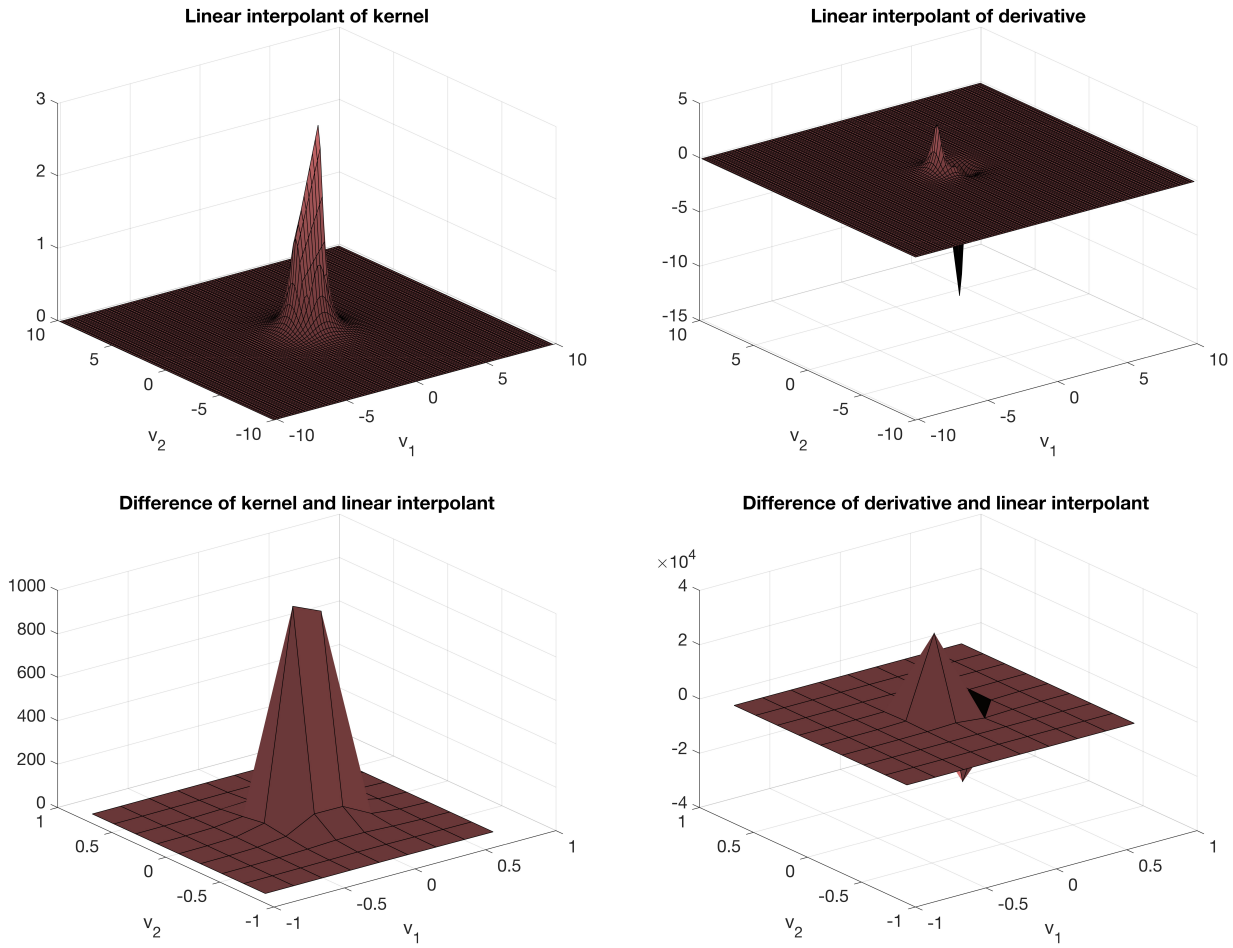






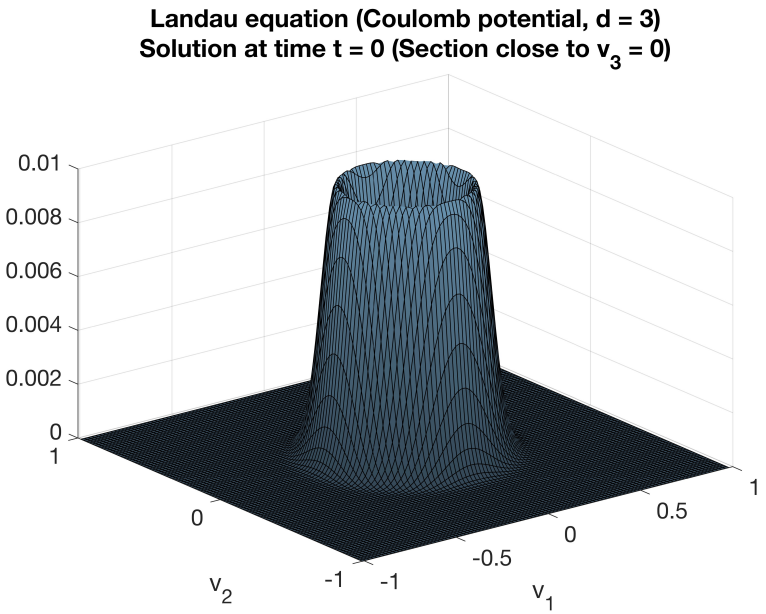
Singular kernel and its derivative. Linear interpolants. Sections along indices.

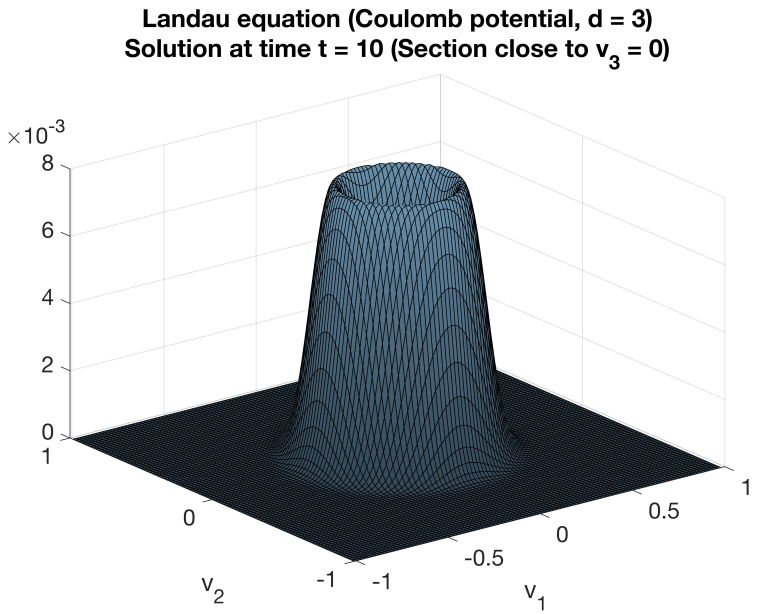
Approach and numerical tests



Linear interpolants of the singular kernel and its derivative (used in Fourier series approximation). Corresponding differences (used in quadrature approximation).

Illustration

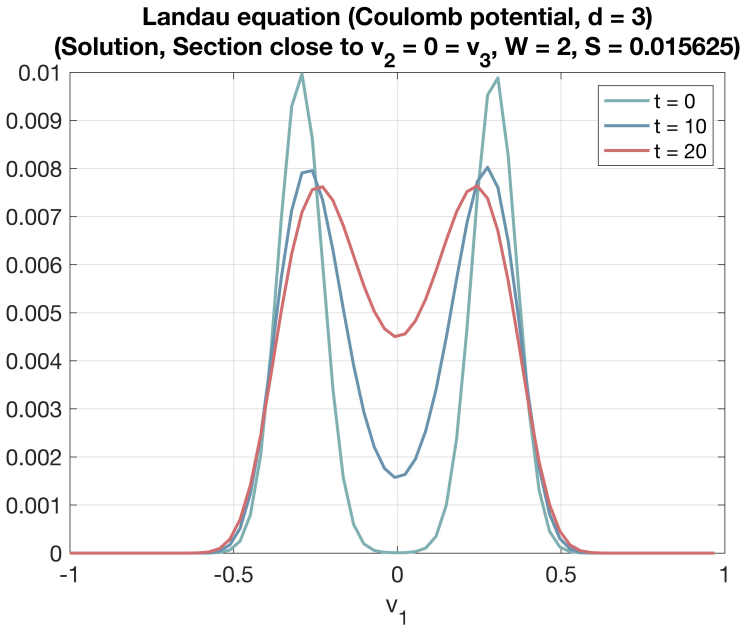


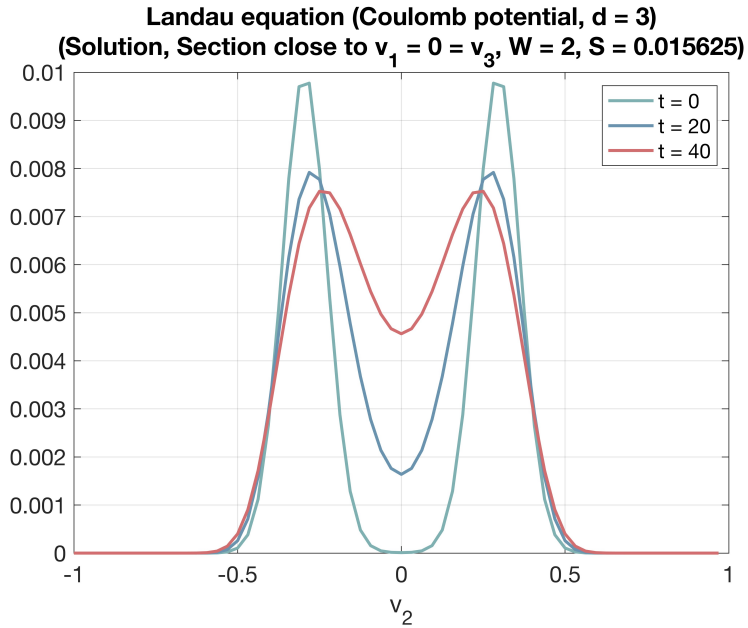


Choice of the initial state accordingly to CARRILLO ET AL. (2020).
Profiles of the solution to the Landau equation with Coulomb interaction
at the initial time and a later time ($M^3 = 100^3$ Fourier functions).

https://techmath.uibk.ac.at/mecht/MyHomepage/Research/Movie_CoulombPotential_Solution3d.m4v

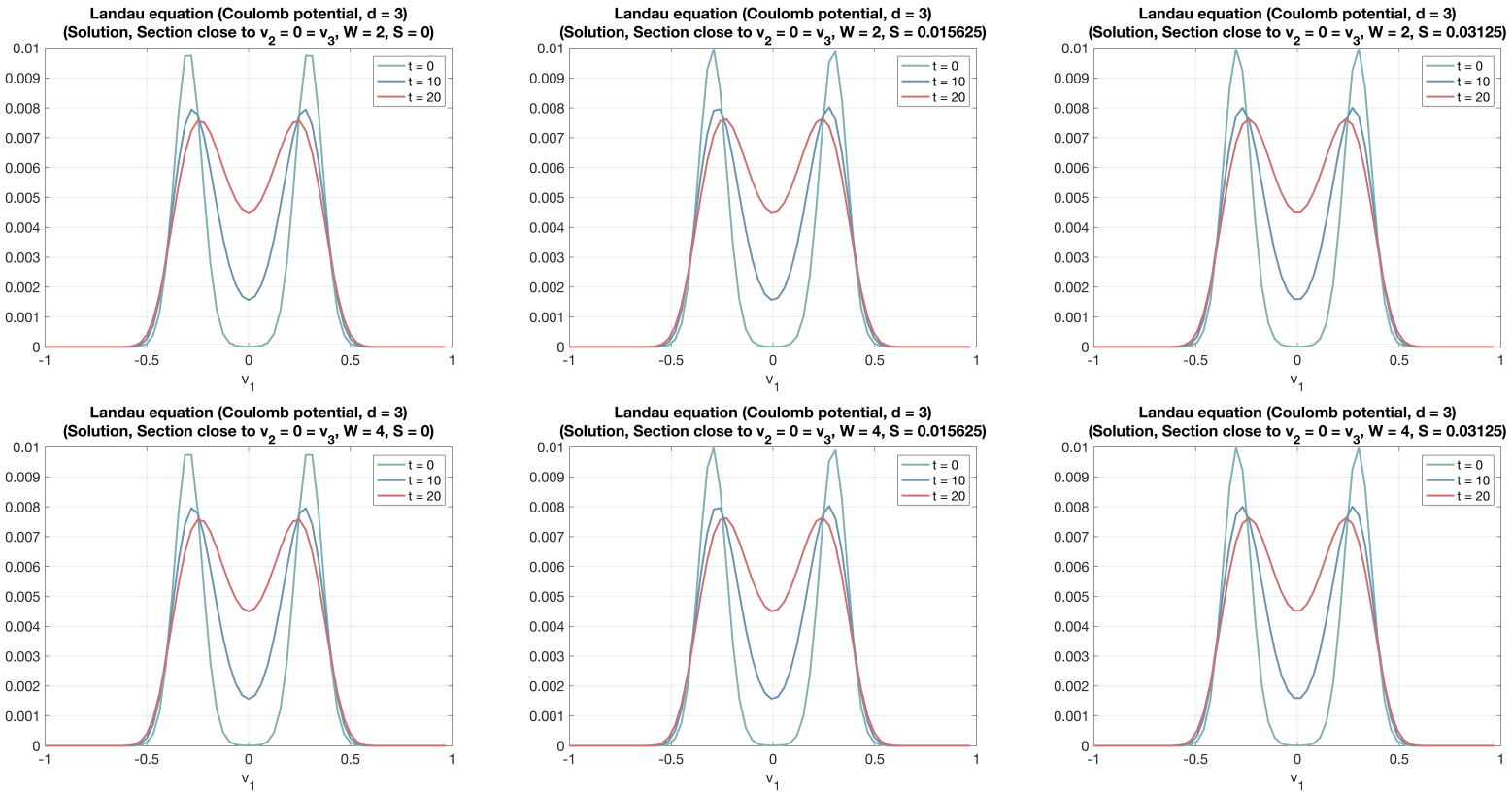
Numerical tests





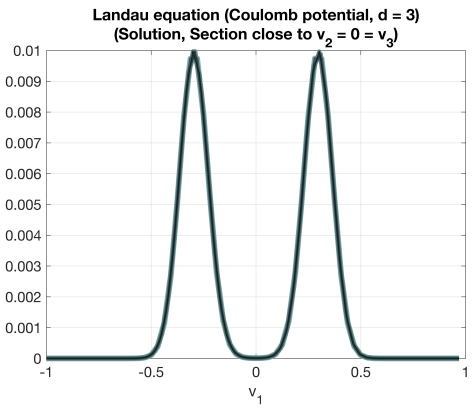
Choice of the initial state and $M^3 = 64^3$ accordingly to CARRILLO ET AL. (2020).
Observation of consistent results with CARRILLO ET AL. (2020) for a certain width and a certain shift of the domain to avoid coincidence of the singularity with a grid point.

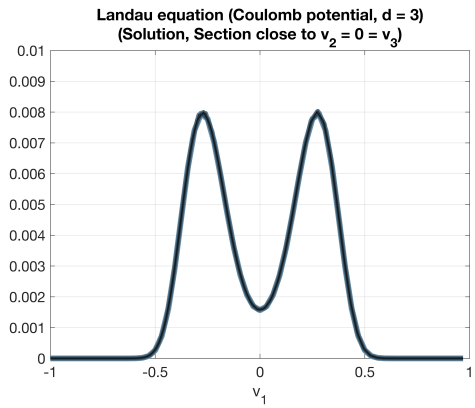
Numerical tests

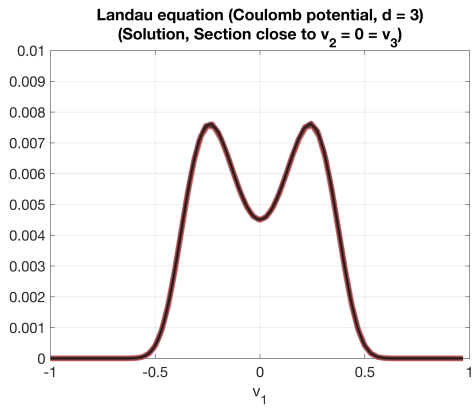


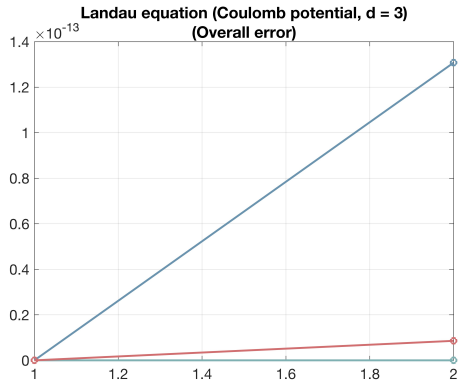
Comparison of the solution profiles for different widths and shifts of domains.

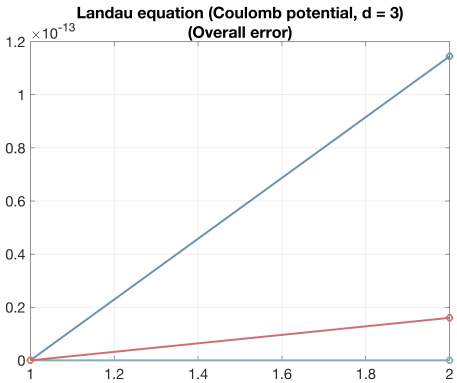
Numerical tests

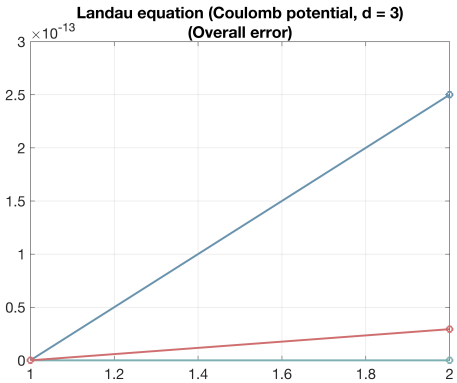












Comparison of the solution profiles for different widths and shifts of domains.
For the same shift, consistent results are observed (second row).

Summary and open questions

Summary.

- Study of a flexible novel approach for the reliable and efficient evaluation of the Landau collision operator.

Open tasks and questions.

- Improvement of the implementation (e.g. parallelisation).
- Thorough numerical comparisons with existing approaches.
- 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.

Thank you!