A new stability and convergence proof of the Fourier-Galerkin spectral method for the spatially homogeneous Boltzmann equation

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Overview

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The Boltzmann equation

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

- $f = f(t,x,v)$: one-particle **probability density function**
  — $f\mathrm{d}x\mathrm{d}v$ gives the probability of finding a fixed particle at time t, position x and velocity v in the phase space
- $Q(f,f)$: **Boltzmann collision operator**
  — a nonlinear integral operator modeling the binary collisions among particles

The Boltzmann collision operator

$$Q(f,f)(v) = \int_{\mathbb{R}^d} \int_{S^{d-1}} \mathcal{B}(v - v_*, \sigma)[f(v')f(v'_*) - f(v)f(v_*)]\, d\sigma\, dv_*$$

(v, v_*) and (v', v'_*) are the velocity pairs before and after a collision:

$$\begin{cases} v' = \dfrac{v + v_*}{2} + \dfrac{|v - v_*|}{2}\sigma \\ v'_* = \dfrac{v + v_*}{2} - \dfrac{|v - v_*|}{2}\sigma \end{cases}$$

$\mathcal{B}(v - v_*, \sigma) = B(|v - v_*|, \cos\theta)$
$\cos\theta = \sigma \cdot (v - v_*)/|v - v_*|$

e.g. variable hard sphere (VHS) model[1]
$B = |v - v_*|^\lambda, \; 0 \le \lambda \le 1$

$\lambda = 1$: hard sphere; $\lambda = 0$: Maxwell molecule

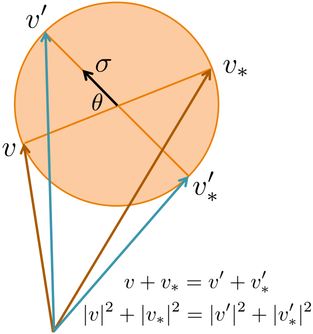

Figure: Illustration of a 2D elastic collision.

[1] Bird, 1994.

Properties of Q

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

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

- **Boltzmann's H-theorem**:

$$-\int_{\mathbb{R}^d} Q(f,f)\,\ln f\,\mathrm{d}v \geq 0$$

- **equilibrium** function:

$$-\int_{\mathbb{R}^d} Q(f,f)\,\ln f\,\mathrm{d}v = 0 \Longleftrightarrow Q(f,f) = 0 \Longleftrightarrow f = \frac{\rho}{(2\pi T)^{d/2}} e^{-\frac{(v-u)^2}{2T}}$$

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

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Numerical challenge

The **major difficulty** of numerically solving the Boltzmann equation comes from the collision operator

$$Q(f,f)(v) = \int_{\mathbb{R}^d} \int_{S^{d-1}} B(|v - v_*|, \cos\theta)[f(v')f(v'_*) - f(v)f(v_*)]\, d\sigma\, dv_*$$

- a five-fold ($d = 3$) integral that needs to be evaluated at every v, x and t
- a nonlinear (quadratic) operator
- better to preserve the physical structure: conservation, positivity, entropy decay, etc.

General strategy

Probabilistic approach

- direct simulation Monte Carlo (DSMC) method[2]
  — easy implementation, efficient, low accuracy, random fluctuations

Deterministic approach

- discrete velocity method (DVM)[3]
  — expensive, low accuracy, maintain physical properties (positivity, conservation, and entropy decay)
- (Fourier) spectral method[4]
  — relatively expensive, high accuracy, does not maintain most physical properties

[2]Bird, Nanbu, ...

[3]Bobylev, Buet, Goldstein, Heintz, Palczewski, Panferov, Rogier, Schneider, ...

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Fourier-Galerkin spectral method[5]

Consider the spatially homogeneous Boltzmann equation:

$$\begin{cases} \partial_t f(t,v) = Q(f,f), & v \in \mathbb{R}^d \ (d \geq 2), \\ f(0,v) = f^0(v). \end{cases}$$

- Truncate the domain $\mathbb{R}^d$ to a torus $\mathcal{D}_L = [-L, L]^d$.
- Change of variable $v_* \to q = v - v_*$ in $Q(f,f)$, and truncate q to a ball $\mathcal{B}_R$:

$$Q^R(f,f)(v) = \int_{\mathcal{B}_R} \int_{S^{d-1}} B(|q|, \sigma \cdot \hat{q}) [f(v')f(v'_*) - f(v)f(v-q)] \, \mathrm{d}\sigma \, \mathrm{d}q,$$

  where $|q|$ and $\hat{q}$ are the magnitude and direction of q.
- Approximate f by a truncated Fourier series:

$$f(t,v) \approx f_N(t,v) = \sum_{k=-N/2}^{N/2} f_k(t) e^{i \frac{\pi}{L} k \cdot v} \in \mathbb{P}_N,$$

  where $k = (k_1, \dots, k_d)$, and $-N/2 \leq k \leq N/2$ means $-N/2 \leq k_j \leq N/2$ for each $j = 1, \dots, d$.

[5] Pareschi and Russo, *SIAM J. Numer. Anal.*, 2000.

Fourier-Galerkin spectral method (cont'd)

- Substitute f_N into the equation and conduct the Galerkin projection onto the space $\mathbb{P}_N$:

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t} f_k = Q_k^R \\ f_k(0) = f_k^0 \end{cases} \quad \text{for } -N/2 \leq k \leq N/2,$$

where f_k^0 is the k-th Fourier mode of the initial condition f^0, and

$$Q_k^R = \sum_{\substack{l,m=-N/2 \\ l+m=k}}^{N/2} \mathcal{G}(l,m) f_l f_m,$$

with the weight given by

$$\begin{aligned} \mathcal{G}(l,m) &= \int_{\mathcal{B}_R} \int_{S^{d-1}} B(|q|, \sigma \cdot \hat{q}) \left[e^{-i\frac{\pi}{2L}(l+m)\cdot q + i\frac{\pi}{2L}|q|(l-m)\cdot\sigma} - e^{-i\frac{\pi}{L} m\cdot q} \right] \mathrm{d}\sigma \, \mathrm{d}q \\ &:= G(l,m) - G(m,m). \end{aligned}$$

The direct Fourier spectral method

The algorithm then proceeds as follows:

0. precompute the weight $\mathcal{G}(l, m)$ — storage requirement $O(N^{2d})$;
1. prepare the initial data f_k^0 — computational cost $O(N^d)$;
2. at each time step, evaluate Q_k^R — computational cost $O(N^{2d})$;
3. time stepping to obtain f_k at new time step — computational cost $O(N^d)$; repeat steps 2 and 3 until the final time.

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We have introduced a fast algorithm[a] to accelerate the direct Fourier spectral method as well as to alleviate its memory constraint in the precomputation stage

- move some offline computation to online using quadratures
- weighted convolution is rendered to a few pure convolutions which can be evaluated by FFT.

The idea has been generalized to multi-species Boltzmann equation[b], inelastic Boltzmann equation[c], and non-cutoff Boltzmann equation[d].

[a] Gamba, Haack, Hauck, and H., *SIAM J. Sci. Comput.*, 2017.
[b] Jaiswal, Alexeenko and H., *Comput. Methods Appl. Mech. Engrg., 2019.*
[c] H. and Ma, *J. Comput. Phys., 2019.*
[d] H. and Qi, *J. Comput. Phys., 2020.*

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- ☹ The equation is nonlinear.
- ☹ The method does not necessarily preserve the positivity of the solution.

  Positivity is the key to many stability estimates of the Boltzmann equation

$$\|f\|_{L^1} \overset{\text{if } f \geq 0}{=\!=\!=} \int f \, \mathrm{d}v \overset{\text{if mass conservation}}{=\!=\!=\!=\!=\!=} \int f^0 \, \mathrm{d}v$$

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- ☺ The method does preserve the mass (1 lies in the expansion basis).
- ☺ The domain is bounded.

Existing work and our contribution

- Pareschi and Russo, *Transport Theory Statist. Phys.*, 2000.
  — A positivity-preserving filter is applied to the equation to enforce the positivity of the solution (then the proof for the continuous equation follows). Filtering introduces too much smearing hence destroying the spectral accuracy.
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In our recent work[6], we give a new proof

- estimate the L^2 norm of the negative part of the solution and show that it can be controlled (the solution is allowed to be negative for the method to remain stable)
- does not rely on sophisticated property of the collision operator

[6] H., Qi, and Yang, *SIAM J. Numer. Anal.*, 2021.

Main stability result

The Fourier spectral method can be written as[7]:

$$\begin{cases} \partial_t f = Q^R(f,f), \ v \in \mathcal{D}_L \\ f(0,v) = f^0 \end{cases} \Longrightarrow \quad (*) \begin{cases} \partial_t f_N = \mathcal{P}_N Q^R(f_N, f_N), \ v \in \mathcal{D}_L \\ f_N(0,v) = \mathcal{P}_N f^0 := f_N^0 \end{cases}$$

Basic assumptions:

- $B = |v - v_*|^\lambda b(\cos\theta)$, $0 \le \lambda \le 1$, $\int_{S^{d-1}} b(\cos\theta)\, \mathrm{d}\sigma < \infty$ (cut-off assumption).
- $f^0 \in L^1 \cap H^1(\mathcal{D}_L)$, periodic and non-negative.
- For any ε, $\exists N_0$, s.t. $N > N_0$, $\|f_N^0\|_{L^1} \le 2\|f^0\|_{L^1}$ and $\|f_N^{0,-}\|_{L^2} < \varepsilon$.

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Theorem (H., Qi, and Yang, 2020)

Under the above assumptions, there exists an integer N_0 depending only on the (arbitrary) final time T and initial condition f^0, such that for all $N > N_0$, the numerical system $(*)$ admits a unique solution $f_N(t,\cdot) \in L^1 \cap H^1(\mathcal{D}_L)$ on $[0, T]$. Furthermore, f_N satisfies the stability estimate

$$\forall t \in [0,T], \quad \|f_N(t)\|_{L^1} \le 2\|f^0\|_{L^1}.$$

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Main strategy of the proof

Step (i): Initially choose N such that $\|f_N^0\|_{L^1} \leq 2\|f^0\|_{L^1}$, then determine a small time τ such that there exists a unique solution f_N on $[0,\tau]$ and satisfies

$$\forall t \in [0,\tau], \quad \|f_N(t)\|_{L^1} \leq 4\|f^0\|_{L^1}.$$

Using this L^1 bound, one can show that

$$\forall t \in [0,\tau], \quad \|f_N^-(t)\|_{L^2} \leq K_0(f^0,T)\left(\|f_N^{0,-}\|_{L^2} + \frac{K_1(f^0,T)}{N}\right).$$

On the other hand,

$$\begin{aligned}\|f_N(t)\|_{L^1} &= \int |f_N(t,v)|\,\mathrm{d}v = 2\int f_N^-(t,v)\,\mathrm{d}v + \int f_N(t,v)\,\mathrm{d}v \\ &= 2\|f_N^-(t)\|_{L^1} + \int f^0(v)\,\mathrm{d}v \leq 2(2L)^{d/2}\|f_N^-(t)\|_{L^2} + \|f^0\|_{L^1}.\end{aligned}$$

Therefore, we can choose N large enough (depending only on T and f^0) to obtain

$$\forall t \in [0,\tau], \quad \|f_N(t)\|_{L^1} \leq 2\|f^0\|_{L^1}. \Longleftarrow \text{back to the initial condition}$$

Step (ii): Iterate the above process to build the solution to $[\tau,2\tau]$, $[2\tau,3\tau]$, ... until T.

Elaboration of the key estimate of $\left\|f_N^-(t)\right\|_{L^2}$

We first rewrite the method as

$$\partial_t f_N = Q^{R,+}(f_N, f_N) - Q^{R,-}(f_N, f_N) + E_N(f_N),$$

with $E_N(f_N) := \mathcal{P}_N Q^R(f_N, f_N) - Q^R(f_N, f_N)$. We then estimate[8]:

$$\int Q^{R,+}(f_N, f_N) f_N \mathbf{1}_{\{f_N \le 0\}} \, \mathrm{d}v \le C_0 \left\|f_N\right\|_{L^1} \left\|f_N^-\right\|_{L^2}^2 + C_0' \left\|f_N\right\|_{L^2} \left\|f_N^-\right\|_{L^2}^2$$

$$-\int Q^{R,-}(f_N, f_N) f_N \mathbf{1}_{\{f_N \le 0\}} \mathrm{d}v \le C_1 \left\|f_N\right\|_{L^1} \left\|f_N^-\right\|_{L^2}^2$$

$$\int E_N(f_N) f_N \mathbf{1}_{\{f_N \le 0\}} \, \mathrm{d}v \le \left\|E_N(f_N)\right\|_{L^2} \left\|f_N^-\right\|_{L^2} \le \frac{C_2}{N} \left\|f_N\right\|_{H^1}^2 \left\|f_N^-\right\|_{L^2}.$$

Note also

$$f_N \mathbf{1}_{\{f_N \le 0\}} \partial_t f_N = f_N^- \partial_t f_N^-.$$

The Gronwall's inequality finally yields the desired estimate of $\left\|f_N^-(t)\right\|_{L^2}$.

[8] Use $f_N = f_N^+ - f_N^-$, $|f_N| = f_N^+ + f_N^-$, and $\|Q^{R,\pm}(g, f)\|_{L^p} \le C\|g\|_{L^1}\|f\|_{L^p}$.

Convergence and spectral accuracy

Basic assumptions:

- $B = |v - v_*|^\lambda b(\cos\theta)$, $0 \le \lambda \le 1$, $\int_{S^{d-1}} b(\cos\theta)\,d\sigma < \infty$ (cut-off assumption).
- $f^0 \in L^1 \cap H^k(\mathcal{D}_L)$, periodic and non-negative.
- For any ε, $\exists N_0$, s.t. $N > N_0$, $\|f_N^0\|_{L^1} \le 2\|f^0\|_{L^1}$ and $\|f_N^{0,-}\|_{L^2} < \varepsilon$.

Define the error function $e_N(t,v) = \mathcal{P}_N f(t,v) - f_N(t,v)$, where f is the exact solution and f_N is the numerical solution. Then

Corollary

Under the above assumptions, there exists N_0 such that the Fourier spectral method is convergent for all $N > N_0$ and exhibits spectral accuracy, that is,

$$\forall t \in [0,T], \quad \|e_N(t)\|_{L^2} \le \frac{C(f^0,T)}{N^k}, \quad \text{for all } N > N_0.$$

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Conclusion

A new stability and convergence proof of the Fourier-Galerkin spectral method is established for the spatially homogeneous (cutoff) Boltzmann equation.

Ongoing/Future work: 1) Obtain stability/convergence for the fast algorithms where quadratures are added. 2) Stability/convergence in the non-cutoff case.

Thank you!

Papers and preprints can be found at
`https://jingweihu-math.github.io/webpage/`