Fast Fourier Spectral Methods for Nonlinear Boltzmann Kinetic Equations — Algorithm and Analysis

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Overview

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The Boltzmann equation

$$\partial_t f + v \cdot \nabla_x f = \frac{1}{\mathrm{Kn}} Q(f,f), \quad t > 0,\ x \in \Omega \subset \mathbb{R}^3,\ v \in \mathbb{R}^3$$

- $f = f(t,x,v)$: one-particle **probability density function**
  — $f\,dx\,dv$ gives the probability of finding a fixed particle at time t, position x and velocity v in the phase space
- Kn: **Knudsen number** (ratio of the mean free path and typical length scale)
  — Kn $= O(1)$ kinetic/rarefied regime; Kn $\ll 1$ fluid/continuum regime
- $Q(f,f)$: **Boltzmann collision operator**
  — a nonlinear integral operator modeling the binary collisions among particles

The Boltzmann collision operator

$$Q(f,f)(v) = \int_{\mathbb{R}^3}\int_{S^2} \mathcal{B}(v-v_*,\sigma)[f(v')f(v'_*) - f(v)f(v_*)]\,\mathrm{d}\sigma\,\mathrm{d}v_*$$

(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

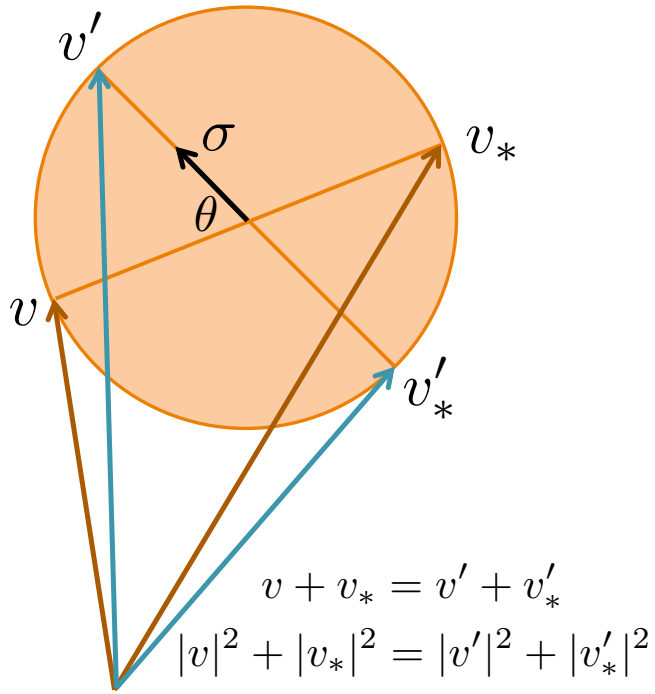

Figure: Illustration of a 2D elastic collision.

[1] Bird, 1994.

Overview

Numerical challenge and general strategy

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

- a five-fold integral that needs to be evaluated at every v, x and t
- a nonlinear (quadratic) operator

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, ...

[4] Bobylev, Filbet, Gamba, Mouhot, Pareschi, Perthame, Rjasanow, Russo, Tharkabhushanam, ...

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The direct Fourier spectral method[5]

Consider the spatially homogeneous Boltzmann equation:

$$\begin{cases} \partial_t f(t,v) = Q(f,f), \quad v \in \mathbb{R}^3, \\ f(0,v) = f^0(v). \end{cases}$$

- Truncate the domain $\mathbb{R}^3$ to a torus $\mathcal{D}_L = [-L, L]^3$.
- Change of variable $v_* \to q = v - v_*$ in $Q(f,f)$, and truncate q to a ball $\mathcal{B}_R$:

$$Q^R(f,f)(v) = \int_{\mathcal{B}_R} \int_{S^2} B(|q|, \sigma \cdot \hat{q}) [f(v')f(v'_*) - f(v)f(v-q)] \, \mathrm{d}\sigma \, \mathrm{d}q,$$

  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 $k = (k_1, k_2, k_3)$, and $-N/2 \le k \le N/2$ means $-N/2 \le k_j \le N/2$ for each j.

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

The direct Fourier spectral method (cont'd)

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

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

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

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

The direct Fourier spectral method (cont'd)

The algorithm then proceeds as follows:

0. precompute the weight $\mathcal{G}(l, m)$ — storage requirement $O(N^6)$;
1. prepare the initial data f_k^0 — computational cost $O(N^3)$;
2. at each time step, evaluate Q_k^R — computational cost $O(N^6)$;
3. time stepping to obtain f_k at new time step — computational cost $O(N^3)$;

   repeat steps 2 and 3 until the final time.

The direct Fourier spectral method (cont'd)

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 $O(N^3)$;
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 $O(N^3)$;

   repeat steps 2 and 3 until the final time.

Step 2 is certainly the most expensive part in this procedure. Step 0 can be completed in advance, but it requires a huge memory[6] to store the precomputed weight, which quickly becomes a bottleneck for large-scale problems.

[6] For example, when $N = 40$, it takes over 30 GB of data to store the weights. This becomes over 500 GB when $N = 64$.

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Q: Can we have a fast algorithm to accelerate the computation as well as alleviate the memory constraint?

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Fast Fourier spectral method – a quick summary

- Mouhot and Pareschi, *Math. Comp.*, 2006.
  - $O(MN^3 \log N)$, $M \ll N$, using Carleman representation
  - Fastest method available to date but only works for single species, hard sphere kernel
  - Extension to other cases (general collision kernel, multi-species, inelastic) can be done but requires additional approximation and computational cost
- Gamba, Haack, Hauck, and H., *SIAM J. Sci. Comput.*, 2017.
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The fast Fourier spectral method

Recall

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

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- **What is nice about** Q_k^R? Its loss term is a convolution

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

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  hence can be computed using FFT in $O(N^3 \log N)$ complexity.

- **What is not nice about** Q_k^R? Its gain term of Q_k^R is a weighted convolution

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

  hence has to be computed directly in $O(N^6)$ complexity.

The fast Fourier spectral method

If we can find a lowrank separated expansion for $G(l, m)$:

$$G(l, m) \approx \sum_{t=1}^{T} \alpha_t(l)\beta_t(m), \quad T \text{ is small},$$

then we can render the gain term $Q_k^{R,+}$ into a sum of convolutions.

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If we can find a lowrank separated expansion for $G(l, m)$:

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Indeed,

$$Q_k^{R,+} = \sum_{\substack{l,m=-N/2 \\ l+m=k}}^{N/2} G(l,m) f_l f_m \approx \sum_{t=1}^{T} \gamma_t(k) \sum_{\substack{l,m=-N/2 \\ l+m=k}}^{N/2} [\alpha_t(l) f_l][\beta_t(m) f_m].$$

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How?

$$G(l,m) = \int_{\mathcal{B}_R} \int_{S^2} B(|q|, \sigma\cdot\hat{q}) e^{-i\frac{\pi}{2L}(l+m)\cdot q + i\frac{\pi}{2L}|q|(l-m)\cdot\sigma} \mathrm{d}\sigma\, \mathrm{d}q$$

$$= \int_0^R \int_{S^2} \left(\int_{S^2} B(|q|, \sigma\cdot\hat{q}) e^{-i\frac{\pi}{2L}|q|(l+m)\cdot\hat{q}}\, \mathrm{d}\hat{q} \right) e^{i\frac{\pi}{2L}|q|(l-m)\cdot\sigma} \mathrm{d}\sigma\, |q|^2 \mathrm{d}|q|.$$

The fast Fourier spectral method[7]

If we precompute

$$F(l+m,|q|,\sigma) := \int_{S^2} B(|q|,\sigma\cdot\hat{q}) e^{-i\frac{\pi}{2L}|q|(l+m)\cdot\hat{q}}\,\mathrm{d}\hat{q},$$

and carry out the integration in σ and $|q|$ using a quadrature, we obtain

$$G(l,m) \approx \sum_{|q|,\sigma} |q|^2 w_{|q|} w_\sigma F(l+m,|q|,\sigma) e^{i\frac{\pi}{2L}|q|(l-m)\cdot\sigma}.$$

Then

$$Q_k^{R,+} \approx \sum_{|q|,\sigma} |q|^2 w_{|q|} w_\sigma F(k,|q|,\sigma) \sum_{\substack{l,m=-N/2 \\ l+m=k}}^{N/2} \left[e^{i\frac{\pi}{2L}|q|l\cdot\sigma} f_l\right]\left[e^{-i\frac{\pi}{2L}|q|m\cdot\sigma} f_m\right].$$

[7] Gamba, Haack, Hauck, and H., *SIAM J. Sci. Comput.*, 2017.

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- We use the Gauss-Legendre quadrature in the radial direction; the Lebedev quadrature or spherical design on the sphere.
- It is found that $N_{|q|} = O(N)$, $N_\sigma = M \ll N^2$. The total complexity is $O(MN^4 \log N)$ and the storage requirement is $O(MN^4)$ (compare with $O(N^6)$ of the direct spectral method).

[7] Gamba, Haack, Hauck, and H., *SIAM J. Sci. Comput.*, 2017.

Bobylev-Krook-Wu (BKW) analytical solution

If the collision kernel $B = 1/(4\pi)$ is a constant, one can construct an exact solution to the homogeneous Boltzmann equation:

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

where $K = 1 - \exp(-t/6)$. One thus has the exact $Q(f,f)$ by calculating $\partial_t f$.

N	direct	fast
8	6.91e-04	7.33e-04
16	7.83e-05	7.63e-05
32	3.90e-08	3.90e-08
64	—	3.81e-08

N	direct	fast
8	0.09s	0.14s
16	6.31s	0.26s
32	542.34s	1.78s
64	—	33.15s

Table: Left: $\|Q^{\text{num}} - Q^{\text{ext}}\|_{L^\infty}$ evaluated at $t = 6.5$. Right: Average running time for one time evaluation of the collision operator. N is the number of points in each velocity dimension. 14-point Lebedev rule ($M = 14$) is used on the sphere.

Overview

Generalization to other collision operators

- **Multi-species Boltzmann collision operator** for gas mixtures[8]

$$m_i v + m_j v_* = m_i v' + m_j v'_*, \quad m_i |v|^2 + m_j |v_*|^2 = m_i |v'|^2 + m_j |v'_*|^2$$

$$\partial_t f^{(i)} + v \cdot \nabla_x f^{(i)} = \sum_{j=1}^{s} \frac{1}{\mathrm{Kn}_{ij}} Q^{(ij)}(f^{(i)}, f^{(j)})$$

$$Q_k^{(ij),+} \approx \sum_{|q|,\sigma} |q|^2 w_{|q|} w_\sigma F^{(ij)}(k, |q|, \sigma) \sum_{\substack{l,m=-N/2 \\ l+m=k}}^{N/2} \left(e^{i \frac{\pi}{L} |q| \frac{m_j}{m_i+m_j} l \cdot \sigma} f_l^{(i)} \right) \left(e^{-i \frac{\pi}{L} |q| \frac{m_i}{m_i+m_j} m \cdot \sigma} f_m^{(j)} \right)$$

$$F^{(ij)}(k, |q|, \sigma) = \int_{S^2} B_{ij}(|q|, \sigma \cdot \hat{q}) e^{-i \frac{\pi}{L} |q| \frac{m_j}{m_i+m_j} k \cdot \hat{q}} \, \mathrm{d}\hat{q}$$

[8] Jaiswal, Alexeenko, and H., *Comput. Methods Appl. Mech. Engrg.*, 2019.

Generalization to other collision operators (cont'd)

- **Inelastic Boltzmann collision operator** for granular gases[9]

$$v + v_* = v' + v'_*, \quad |v|^2 + |v_*|^2 \geq |v'|^2 + |v'_*|^2$$

- **Non-cutoff Boltzmann collision operator** (collision kernel is non-integrable in the angular direction)[10]

$$B = |v - v_*|^\lambda b(\cos\theta), \quad \sin\theta b(\cos\theta)\Big|_{\theta\to 0} \sim \theta^{-1-\nu}, \quad 0 < \nu < 2,$$

with $\nu = 2$ being the Coulomb interaction.

$$\int_{\mathbb{R}^3} Q(f,f)(v)\,\varphi(v)\,\mathrm{d}v = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{S^2} B(|q|,\sigma\cdot\hat{q}) f(v) f(v_*)\left(\varphi(v') - \varphi(v)\right)\mathrm{d}\sigma\,\mathrm{d}v\,\mathrm{d}v_*$$

$$\varphi(v) = e^{-i\frac{\pi}{L}k\cdot v} \Longrightarrow Q_k \approx \sum_{|q|,\hat{q}} |q|^2 w_{|q|} w_{\hat{q}} F(k,|q|,\hat{q}) \sum_{\substack{l,m=-N/2\\ l+m=k}}^{N/2} f_l\left(e^{-i\frac{\pi}{L}|q|m\cdot\hat{q}} f_m\right)$$

$$F(k,|q|,\hat{q}) = \int_{S^2} B(|q|,\sigma\cdot\hat{q})\left(e^{i\frac{\pi}{L}|q|\frac{1+e}{4}k\cdot(\hat{q}-\sigma)} - 1\right)\mathrm{d}\sigma, \quad e < 1 \text{ inelastic; } e = 1 \text{ elastic}$$

[9] H. and Ma, *J. Comput. Phys.*, 2019.
[10] H. and Qi, *J. Comput. Phys.*, 2020.

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Now we have a Fourier spectral method for the Boltzmann equation

- achieves a good accuracy-efficiency tradeoff
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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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  — Use the "spreading" or "mixing" property of the gain term of the collision operator to show that the solution will become everywhere positive after a certain time if it is initially negative.

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In our recent work[11], 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

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

Main stability result

The Fourier spectral method can be written as[12]:

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

Basic assumptions:

- $B = |v - v_*|^\lambda b(\cos\theta)$, $0 \le \lambda \le 1$, $\int_{S^2} b(\cos\theta)\,\mathrm{d}\sigma < \infty$ (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, 2021)

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): Determine a small time τ such that there exists a unique solution f_N on $[0,\tau]$ and satisfies

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

Using this L^1 bound, one can show that

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

On the other hand,

$$\begin{aligned}\|f_N(t)\|_{L^1} &= \int |f_N(t,v)|\,\mathrm{d}v = 2\int f_N^-(t,v)\,\mathrm{d}v + \int f_N(t,v)\,\mathrm{d}v \\ &= 2\|f_N^-(t)\|_{L^1} + \int f^0(v)\,\mathrm{d}v \le 2(2L)^{3/2}\|f_N^-(t)\|_{L^2} + \|f^0\|_{L^1}.\end{aligned}$$

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

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

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

Convergence and spectral accuracy

Basic assumptions:

- $B = |v - v_*|^\lambda b(\cos\theta)$, $0 \le \lambda \le 1$, $\int_{S^2} b(\cos\theta)\,\mathrm{d}\sigma < \infty$ (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,

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

Overview

Numerical method for the full Boltzmann equation

Going back to the full Boltzmann equation:

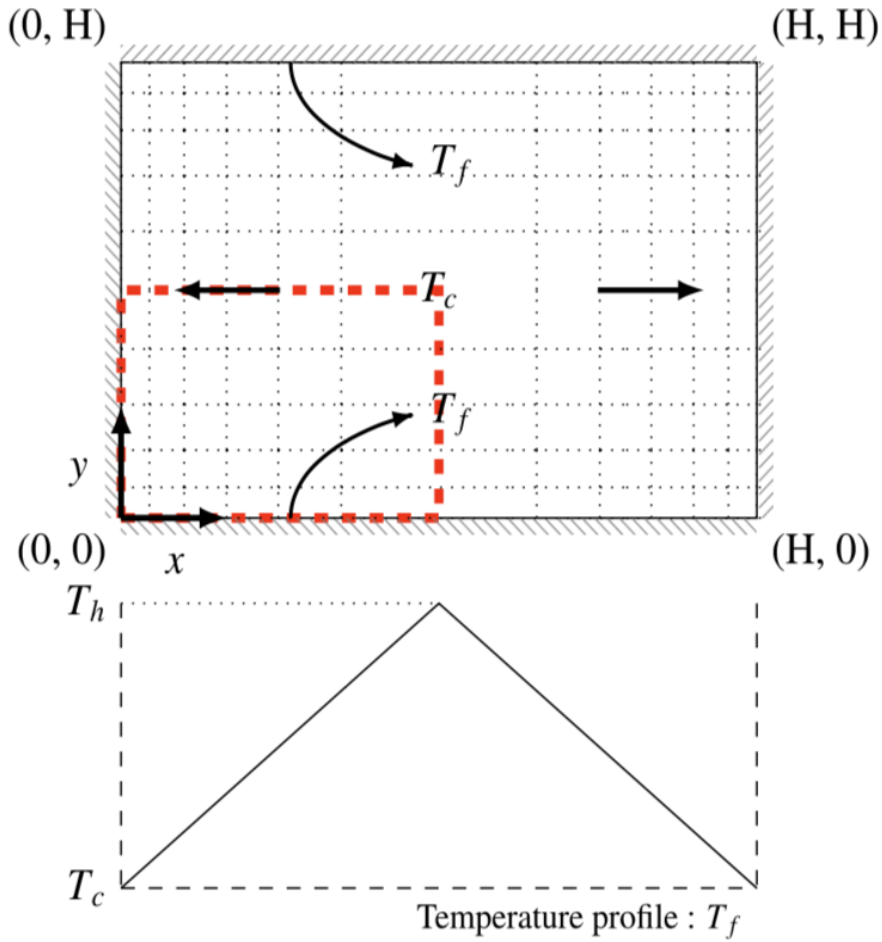
$$\partial_t f + v \cdot \nabla_x f = \frac{1}{\mathrm{Kn}} Q(f, f)$$

One also needs an accurate discretization in the physical space to handle the convection term.

We couple the discontinuous Galerkin (DG) method in the physical space and the fast spectral (FS) method in the velocity space to obtain a highly accurate deterministic method, **DGFS**, for the full Boltzmann equation[13] [14] [15].

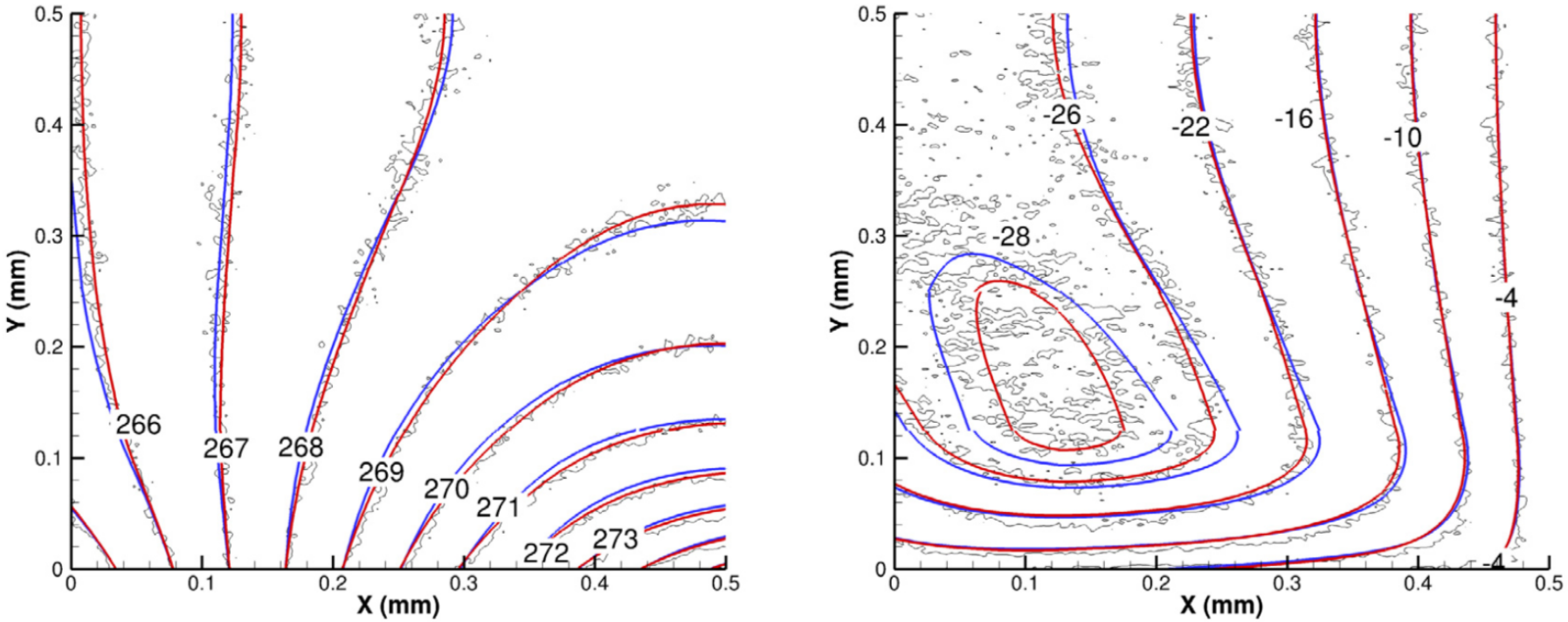
[13] Jaiswal, Alexeenko, and H., *J. Comput. Phys.*, 2019.
[14] Jaiswal, Alexeenko, and H., *Comput. Methods Appl. Mech. Engrg.*, 2019.
[15] Jaiswal, Pikus, Strongrich, Sebastiao, H., and Alexeenko, *Phys. Fluids*, 2019.

2D thermally driven cavity flow



The walls are at rest and with the temperature shown above ($T_c = 263K$, $T_h = 283K$). The simulation is carried out at Kn = 1. Argon gas with VHS collision kernel is taken as the working gas.

2D thermally driven cavity flow (cont'd)

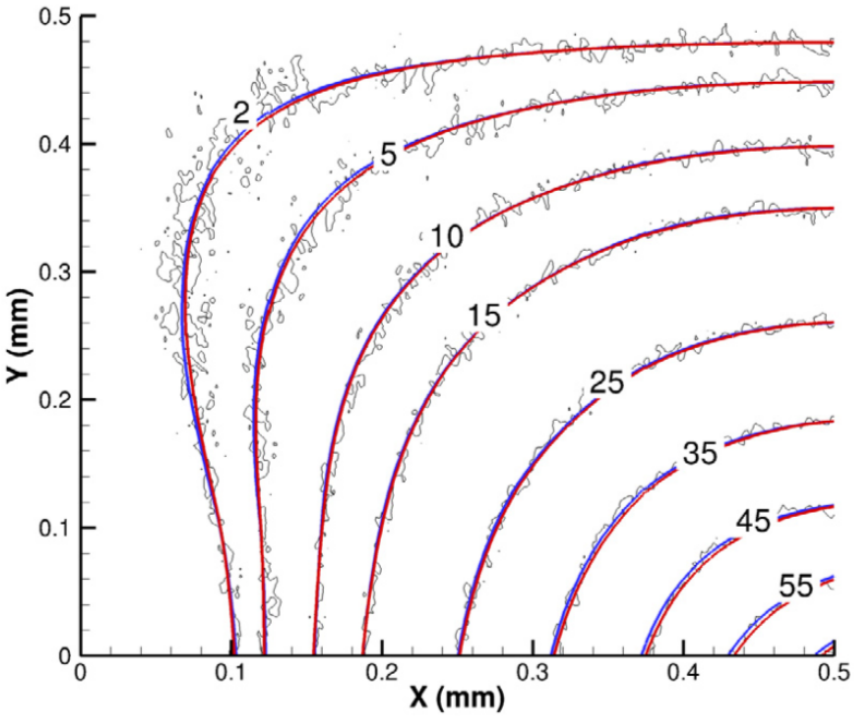


(a) temperature

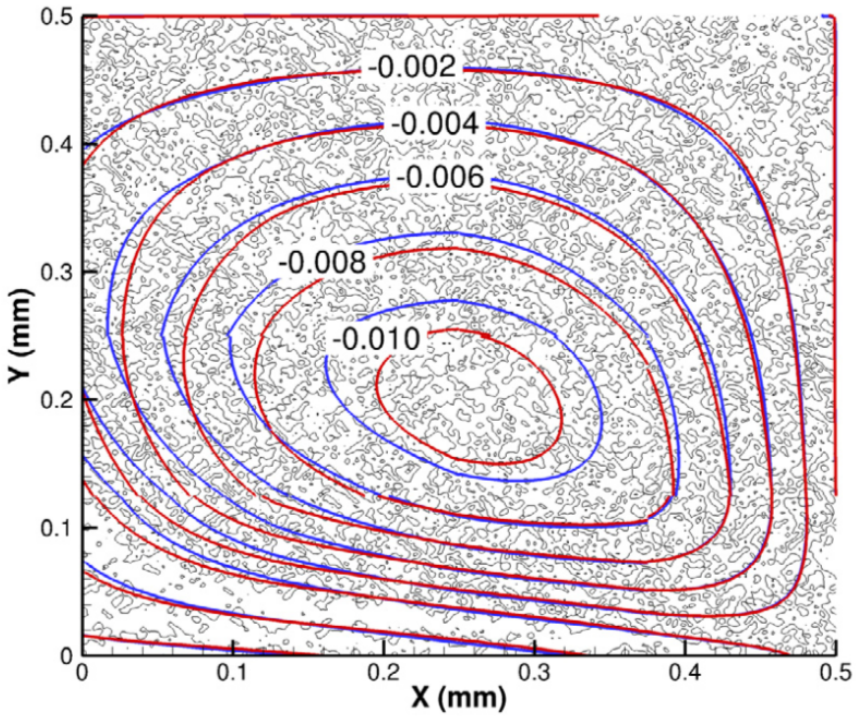
(b) x-component of heat-flux

Figure: Contours of the temperature and heat flux (x-component). DSMC results (thin black lines). For DGFS, 8^2 cells and 3rd order polynomial are used in the physical space; 24^3 points (solid blue lines) and 48^3 points (solid red lines) are used in the velocity space.

2D thermally driven cavity flow (cont'd)



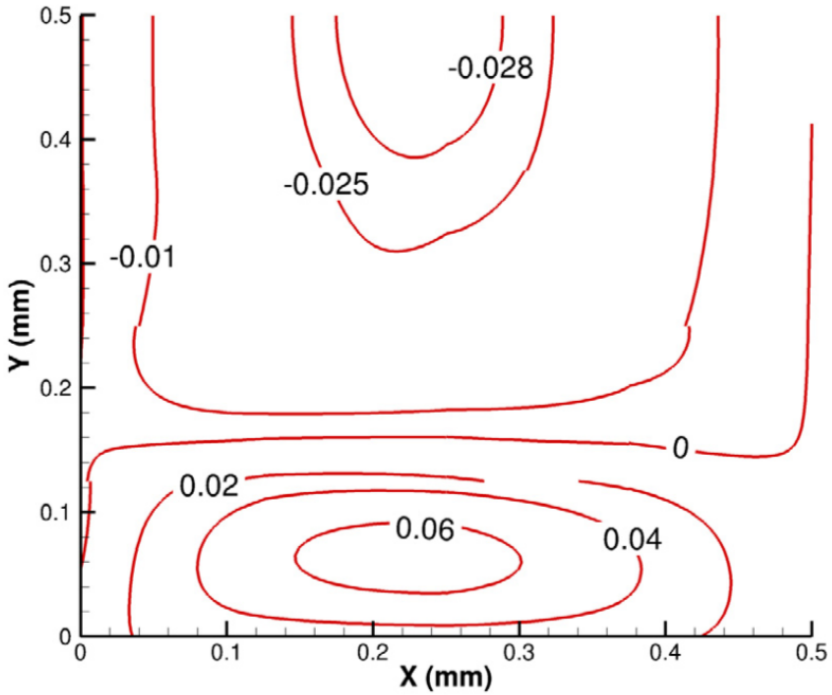
(c) y-component of heat-flux



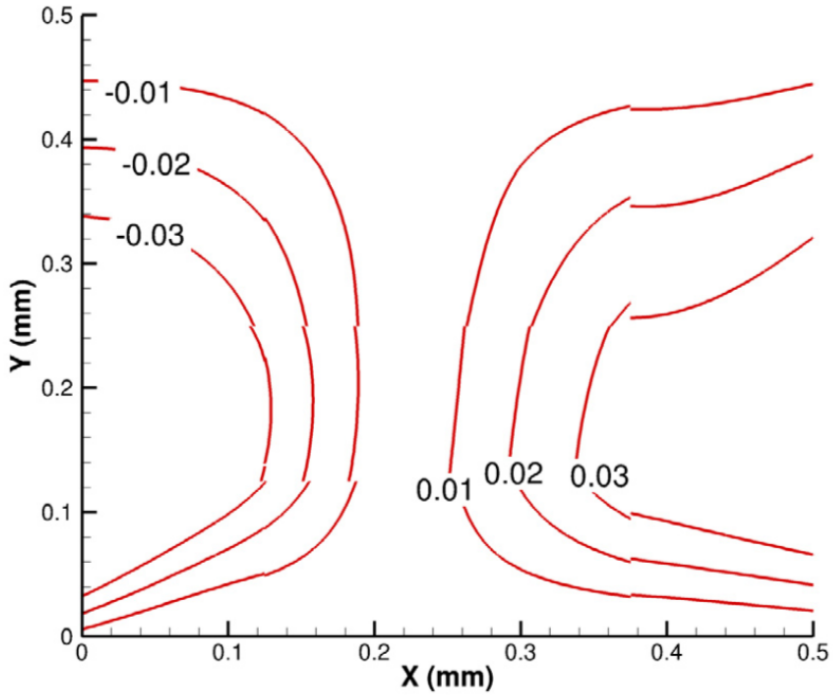
(d) xy-component of stress

Figure: Contours of the heat flux (y-component) and stress (xy-component). DSMC results (thin black lines). For DGFS, 8^2 cells and 3rd order polynomial are used in the physical space; 24^3 points (solid blue lines) and 48^3 points (solid red lines) are used in the velocity space.

2D(3V) thermally driven cavity flow (cont'd)



(e) x-component of velocity



(f) y-component of velocity

Figure: Contours of the velocity. For DGFS, 8^2 cells and 3rd order polynomial are used in the physical space; 48^3 points (solid red lines) are used in the velocity space. Note that DSMC results are not shown due to the huge statistical noise.

Overview

Conclusion

A simple yet effective strategy is introduced to accelerate the direct Fourier spectral method for the Boltzmann collision operator

- can handle the general collision kernels (with and without angular cutoff), the multi-species and inelastic Boltzmann collision operators;
- can be coupled with the proper spatial discretization to yield a highly accurate deterministic solver for the full Boltzmann equation
- applicable to a series of engineering applications

A new stability and convergence proof of the Fourier spectral method is provided for the (cutoff) Boltzmann equation.

Ongoing and future work: 1) Stability/convergence in the non-cutoff case. 2) Some low-rank method to further reduce the cost.

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Thank you!

Papers and preprints can be found at

`https://jingweihu-math.github.io/webpage/`