A fast spectral method for the Boltzmann collision operator with general collision kernels

Jingwei Hu

Purdue University

Math Colloquium
City University of Hong Kong
June 15, 2017

Joint work with Irene Gamba (UT-Austin), Jeff Haack (LANL), and Cory Hauck (ORNL)

Overview

Overview

Overview

Kinetic theory

Kinetic theory models the non-equilibrium dynamics of a gas (or any system comprised of a large number of particles)

Applications

- aerospace engineering
- nuclear, plasma, and radiological engineering
- condensed matter physics
- biological and social sciences
- ...

The Boltzmann equation

A nonlinear phase space equation modeling

- **particle transport**
- **binary collisions**

— the most fundamental equation in kinetic theory

Figure: Ludwig Boltzmann (1844-1906)

The Boltzmann equation

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = \mathcal{Q}(f, f)(v), \quad x \in \Omega \subset \mathbb{R}^3, \ v \in \mathbb{R}^3$$

- $f(t, x, v)$ is the **phase space distribution function** of time t, position x, and particle velocity v
- $\mathcal{Q}(f, f)$ is the **collision operator**, a nonlinear integral operator modeling the binary interaction among particles

The Boltzmann collision operator

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

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

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

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

Variable hard sphere (VHS) model

$B = b_\lambda |v-v_*|^\lambda,\ -3 < \lambda \le 1$

$\lambda = 1$: hard sphere

$\lambda = 0$: Maxwell molecule

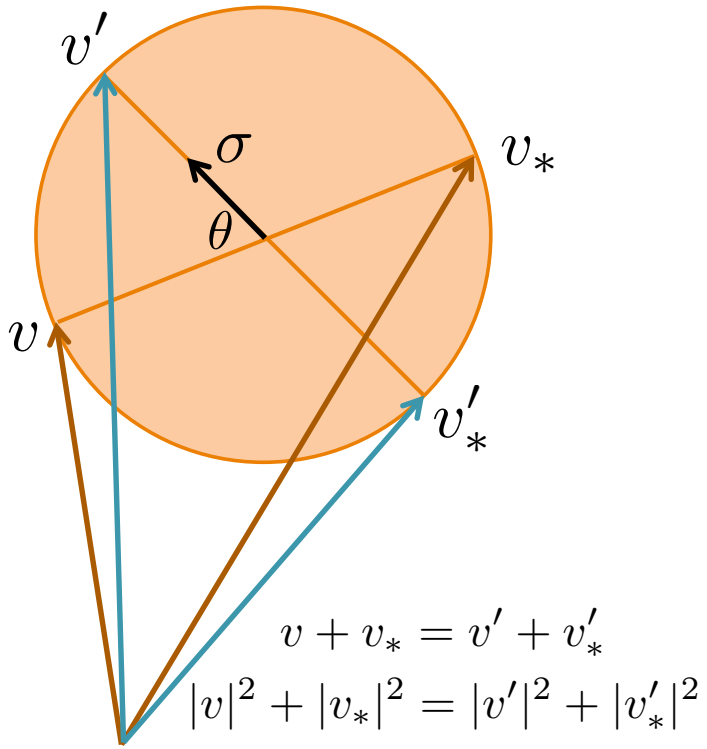

Figure: Illustration of 2D elastic collision.

Properties of $\mathcal{Q}$

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

$$\int_{\mathbb{R}^3} \mathcal{Q}(f,f)\,\mathrm{d}v = \int_{\mathbb{R}^3} \mathcal{Q}(f,f)\,v\,\mathrm{d}v = \int_{\mathbb{R}^3} \mathcal{Q}(f,f)\,|v|^2\,\mathrm{d}v = 0$$

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

$$-\int_{\mathbb{R}^3} \mathcal{Q}(f,f)\,\ln f\,\mathrm{d}v \geq 0$$

- **equilibrium** function:

$$\text{“}=\text{”} \Longleftrightarrow \mathcal{Q}(f,f)=0 \Longleftrightarrow f=\mathcal{M}:=\frac{\rho}{(2\pi T)^{3/2}}e^{-\frac{(v-u)^2}{2T}}$$

with density $\rho := \int f\,\mathrm{d}v$; bulk velocity $u := \frac{1}{\rho}\int f\,v\,\mathrm{d}v$; temperature $T := \frac{1}{3\rho}\int f\,|v-u|^2\,\mathrm{d}v$

Overview

Numerical challenge

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

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

- five-fold integral that needs to be evaluated at every v, x, and t
- quadratic operator
- need to maintain conservation at discrete level, capture high-order moments with good accuracy

General strategy

Probabilistic approach

- direct simulation Monte Carlo (DSMC) methods[1]
  — easy implementation, efficient, half-order accuracy, random fluctuations

Deterministic approach

- discrete velocity models (DVM)[2]
  — expensive, first or second order accuracy, maintain conservation
- (Fourier) spectral methods[3]
  — relatively expensive, spectral accuracy, do not maintain conservation

[1] Bird, Nanbu, ...

[2] Bobylev, Buet, Palczewski, Rogier, Schneider, ...

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

General strategy

Probabilistic approach

- direct simulation Monte Carlo (DSMC) methods[1]
  — easy implementation, efficient, half-order accuracy, random fluctuations

Deterministic approach

- discrete velocity models (DVM)[2]
  — expensive, first or second order accuracy, maintain conservation
- (Fourier) spectral methods[3]
  — relatively expensive, spectral accuracy, do not maintain conservation

[1] Bird, Nanbu, ...

[2] Bobylev, Buet, Palczewski, Rogier, Schneider, ...

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

Overview

Overview

The classical spectral method[4]

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

where $g := v - v_*$.

[4] Pareschi and Perthame 1996; Pareschi and Russo 2000.

The classical spectral method[4]

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

where $g := v - v_*$.

- Truncate the integral in g to a ball $\mathcal{B}_R$ with $R \geq 2S$, $\mathcal{B}_S \approx \mathrm{supp}_v(f)$.

[4] Pareschi and Perthame 1996; Pareschi and Russo 2000.

The classical spectral method[4]

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

where $g := v - v_*$.

- Truncate the integral in g to a ball $\mathcal{B}_R$ with $R \geq 2S$, $\mathcal{B}_S \approx \mathrm{supp}_v(f)$.
- Periodize f on the domain $\mathcal{D}_L = [-L, L]^d$. Choose $L \geq \frac{3\sqrt{2}+1}{2}S$ for antialiasing.

[4] Pareschi and Perthame 1996; Pareschi and Russo 2000.

The classical spectral method[4]

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

where $g := v - v_*$.

- Truncate the integral in g to a ball $\mathcal{B}_R$ with $R \geq 2S$, $\mathcal{B}_S \approx \mathrm{supp}_v(f)$.
- Periodize f on the domain $\mathcal{D}_L = [-L, L]^d$. Choose $L \geq \frac{3\sqrt{2}+1}{2}S$ for antialiasing.
- Approximate f by a truncated Fourier series (k is a 3D index):

$$f(v) \approx \sum_{k=-\frac{N}{2}}^{\frac{N}{2}-1} \hat{f}_k e^{i\frac{\pi}{L}k\cdot v}, \quad \hat{f}_k = \frac{1}{(2L)^3}\int_{\mathcal{D}_L} f(v)e^{-i\frac{\pi}{L}k\cdot v}\,\mathrm{d}v.$$

[4] Pareschi and Perthame 1996; Pareschi and Russo 2000.

The classical spectral method[4]

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

where $g := v - v_*$.

- Truncate the integral in g to a ball $\mathcal{B}_R$ with $R \geq 2S$, $\mathcal{B}_S \approx \mathrm{supp}_v(f)$.
- Periodize f on the domain $\mathcal{D}_L = [-L, L]^d$. Choose $L \geq \frac{3\sqrt{2}+1}{2}S$ for antialiasing.
- Approximate f by a truncated Fourier series (k is a 3D index):

$$f(v) \approx \sum_{k=-\frac{N}{2}}^{\frac{N}{2}-1} \hat{f}_k e^{i\frac{\pi}{L}k\cdot v}, \quad \hat{f}_k = \frac{1}{(2L)^3}\int_{\mathcal{D}_L} f(v)e^{-i\frac{\pi}{L}k\cdot v}\,\mathrm{d}v.$$

- Substitute the Fourier expansion of f into $\mathcal{Q}$, and project to the space $\mathbb{P}^N = \{e^{i\frac{\pi}{L}k\cdot v} | -N/2 \leq k < N/2 - 1\}$.

[4] Pareschi and Perthame 1996; Pareschi and Russo 2000.

The classical spectral method (cont'd)

Then one has

$$\hat{\mathcal{Q}}_k = \sum_{\substack{l,m=-\frac{N}{2} \\ l+m=k}}^{\frac{N}{2}-1} \mathcal{G}(l,m)\hat{f}_l\hat{f}_m, \quad k = -\frac{N}{2}, \ldots, \frac{N}{2}-1,$$

where

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

The classical spectral method (cont'd)

Then one has

$$\hat{\mathcal{Q}}_k = \sum_{\substack{l,m=-\frac{N}{2} \\ l+m=k}}^{\frac{N}{2}-1} \mathcal{G}(l,m)\hat{f}_l\hat{f}_m, \quad k = -\frac{N}{2}, \ldots, \frac{N}{2}-1,$$

where

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

This is a weighted convolution. One has to evaluate the sum directly if there is no special treatment.

The classical spectral method (cont'd)

The algorithm then proceeds as follows:

0. precompute the weights $\mathcal{G}(l, m)$ — storage requirement $O(N^6)$;
1. compute $\hat{f}_k$ using the Fast Fourier Transform (FFT) — cost $O(N^3 \log N)$;
2. compute the weighted convolution — cost $O(N^6)$;
3. take the inverse Fourier transform of $\hat{\mathcal{Q}}_k$ to obtain $\mathcal{Q}$ — cost $O(N^3 \log N)$.

[5] For example, when $N = 40$, it takes over 30 gigabytes of data to store the weights — an amount that almost reaches the maximum memory capacity on a typical compute node of ORNL's Titan supercomputer.

The classical spectral method (cont'd)

The algorithm then proceeds as follows:

0. precompute the weights $\mathcal{G}(l, m)$ — storage requirement $O(N^6)$;
1. compute $\hat{f}_k$ using the Fast Fourier Transform (FFT) — cost $O(N^3 \log N)$;
2. compute the weighted convolution — cost $O(N^6)$;
3. take the inverse Fourier transform of $\hat{\mathcal{Q}}_k$ to obtain $\mathcal{Q}$ — cost $O(N^3 \log N)$.

Step 2 is certainly the most expensive part in this procedure. Step 0 can be completed in advance, but it requires a huge memory[5] to store the precomputed weights, which quickly become a bottleneck for large-scale problems.

[5] For example, when $N = 40$, it takes over 30 gigabytes of data to store the weights — an amount that almost reaches the maximum memory capacity on a typical compute node of ORNL's Titan supercomputer.

A fast spectral method based on Carleman representation[6]

This method is based on an equivalent representation of the collision operator:

$$\mathcal{Q}(f,f)(v)=\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\tilde{B}(|x|,|y|)\delta(x\cdot y)[f(v+x)f(v+y)-f(v)f(v+x+y)]\mathrm{d}x\mathrm{d}y$$

where $v_*=v+x+y$, $v'=v+x$, $v'_*=v+y$,

$$\tilde{B}(|x|,|y|)=\frac{4}{\sqrt{|x|^2+|y|^2}}B(\sqrt{|x|^2+|y|^2},\cos\theta).$$

As will be shown, this method requires $\tilde{B}$ to be separated in x and y:

$$B(|x|,|y|)=\sum_t a_t(|x|)b_t(|y|),$$

generally not hold (hard sphere is an exception).

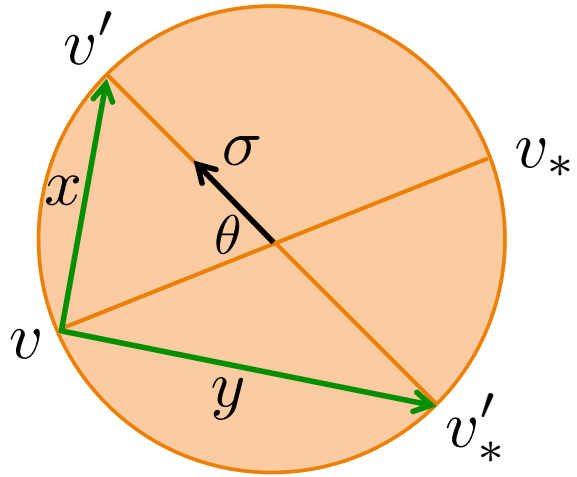

Figure: Carleman representation.

[6] Mouhot and Pareschi, 2006.

Hard sphere case of the Carleman spectral method

Now $\tilde{B}$ is a constant. Under a similar Fourier-Galerkin projection as before, one has

$$\hat{\mathcal{Q}}_k = \sum_{\substack{l,m=-\frac{N}{2} \\ l+m=k}}^{\frac{N}{2}-1} \mathcal{G}(l,m)\hat{f}_l\hat{f}_m, \quad k = -\frac{N}{2}, \ldots, \frac{N}{2}-1,$$

where

$$\begin{aligned}\mathcal{G}(l,m) &= \int_{\mathcal{B}_R}\int_{\mathcal{B}_R} \delta(x\cdot y)\left[e^{i\frac{\pi}{L}l\cdot x}e^{i\frac{\pi}{L}m\cdot y} - e^{i\frac{\pi}{L}m\cdot x}e^{i\frac{\pi}{L}m\cdot y}\right]\mathrm{d}x\,\mathrm{d}y \\ &= G(l,m) - G(m,m).\end{aligned}$$

Hard sphere case of the Carleman spectral method

Now $\tilde{B}$ is a constant. Under a similar Fourier-Galerkin projection as before, one has

$$\hat{\mathcal{Q}}_k = \sum_{\substack{l,m=-\frac{N}{2} \\ l+m=k}}^{\frac{N}{2}-1} \mathcal{G}(l,m)\hat{f}_l\hat{f}_m, \quad k = -\frac{N}{2}, \ldots, \frac{N}{2}-1,$$

where

$$\begin{aligned}\mathcal{G}(l,m) &= \int_{\mathcal{B}_R}\int_{\mathcal{B}_R} \delta(x\cdot y)\left[e^{i\frac{\pi}{L}l\cdot x}e^{i\frac{\pi}{L}m\cdot y} - e^{i\frac{\pi}{L}m\cdot x}e^{i\frac{\pi}{L}m\cdot y}\right]\mathrm{d}x\,\mathrm{d}y \\ &= G(l,m) - G(m,m).\end{aligned}$$

This form allows us to represent $\mathcal{G}(l,m)$ in a separated form in l and m, then the weighted convolution turns into a pure convolution, hence can be evaluated by the FFT.

Hard sphere case of the Carleman spectral method (cont'd)

$$G(l,m) = \int_{S^2}\int_{S^2} \delta(\sigma_1\cdot\sigma_2)\left(\int_0^R \rho e^{i\frac{\pi}{L}\rho(l\cdot\sigma_1)}\,\mathrm{d}\rho\right)\left(\int_0^R \rho e^{i\frac{\pi}{L}\rho(m\cdot\sigma_2)}\,\mathrm{d}\rho\right)\mathrm{d}\sigma_1\mathrm{d}\sigma_2$$
$$= \int_{S^2} \alpha_t(l\cdot\sigma)\beta_t(\sqrt{|m|^2-(m\cdot\sigma)^2})\,\mathrm{d}\sigma$$

where α and β are some functions that can be precomputed (or have analytical forms).

Hard sphere case of the Carleman spectral method (cont'd)

$$G(l,m) = \int_{S^2}\int_{S^2} \delta(\sigma_1\cdot\sigma_2)\left(\int_0^R \rho e^{i\frac{\pi}{L}\rho(l\cdot\sigma_1)}\,\mathrm{d}\rho\right)\left(\int_0^R \rho e^{i\frac{\pi}{L}\rho(m\cdot\sigma_2)}\,\mathrm{d}\rho\right)\mathrm{d}\sigma_1\mathrm{d}\sigma_2$$
$$= \int_{S^2} \alpha_t(l\cdot\sigma)\beta_t(\sqrt{|m|^2-(m\cdot\sigma)^2})\,\mathrm{d}\sigma$$

where α and β are some functions that can be precomputed (or have analytical forms).

Now if one discretizes σ on the sphere S^2 in $G(l,m)$, one has

$$\hat{\mathcal{Q}}_k^+ \approx \sum_\sigma w_\sigma \sum_{\substack{l,m=-\frac{N}{2}\\ l+m=k}}^{\frac{N}{2}-1} (\alpha_t(l\cdot\sigma)\hat{f}_l)(\beta_t(\sqrt{|m|^2-(m\cdot\sigma)^2})\hat{f}_m).$$

The total numerical complexity is thus $O(MN^3\log N)$, where M is the number of points on the sphere (usually $M \ll N$).

Overview

Motivation

- The Carleman spectral method is very efficient $O(MN^3 \log N)$, but limited to certain collision kernels (cannot handle even the VHS case: $B = b_\lambda |v - v_*|^\lambda$).
- The classical spectral method is more generic (can handle any collision kernels, not limited to VHS), but requires huge memory to store the precomputed weight and $O(N^6)$ numerical complexity.

Motivation

- The Carleman spectral method is very efficient $O(MN^3 \log N)$, but limited to certain collision kernels (cannot handle even the VHS case: $B = b_\lambda |v - v_*|^\lambda$).
- The classical spectral method is more generic (can handle any collision kernels, not limited to VHS), but requires huge memory to store the precomputed weight and $O(N^6)$ numerical complexity.

Q: Can we design a fast algorithm that is able to treat general collision kernels?

The new method

We will start with the classical spectral formulation:

$$\hat{\mathcal{Q}}_k = \sum_{\substack{l,m=-\frac{N}{2} \\ l+m=k}}^{\frac{N}{2}-1} \mathcal{G}(l,m)\hat{f}_l\hat{f}_m,$$

where $\mathcal{G}(l,m) = G(l,m) - G(m,m)$, and

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

The goal is similar as in the Carleman spectral method: we would like to find a lowrank separated expansion for $G(l,m)$

$$G(l,m) = \sum_t \alpha_t(l)\beta_t(m)$$

The new method

We will start with the classical spectral formulation:

$$\hat{\mathcal{Q}}_k = \sum_{\substack{l,m=-\frac{N}{2} \\ l+m=k}}^{\frac{N}{2}-1} \mathcal{G}(l,m)\hat{f}_l\hat{f}_m,$$

where $\mathcal{G}(l,m) = G(l,m) - G(m,m)$, and

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

The goal is similar as in the Carleman spectral method: we would like to find a lowrank separated expansion for $G(l,m)$

$$G(l,m) = \sum_t \alpha_t(l)\beta_t(m)\gamma_t(l+m)$$

The new method (cont'd)

The weight $G(l,m)$ can be written as

$$G(l,m)=\int_0^R\int_{S^2}F(l+m,\rho,\sigma)e^{i\frac{\pi}{L}\rho\frac{(l-m)}{2}\cdot\sigma}\mathrm{d}\sigma\,\mathrm{d}\rho,$$

where

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

Now if we precompute F and carry out the integration in σ and ρ using a fixed numerical quadrature, then

$$\hat{\mathcal{Q}}_k^+=\sum_{\rho,\sigma}w_\rho w_\sigma F(k,\rho,\sigma)\sum_{\substack{l,m=-\frac{N}{2}\\ l+m=k}}^{\frac{N}{2}-1}\left[e^{i\frac{\pi}{L}\rho\frac{l}{2}\cdot\sigma}\hat{f}_l\right]\left[e^{-i\frac{\pi}{L}\rho\frac{m}{2}\cdot\sigma}\hat{f}_m\right]$$

Usually $N_\rho=O(N)$, $N_\sigma=M\ll N$. Therefore, the total numerical complexity is $O(MN^4\log N)$ and the storage requirement is $O(MN^4)$.

The new method (cont'd)

- We use the Gauss-Legendre quadrature in the radial direction
- We use the Lebedev quadrature[7] for the integration on the sphere, which is the near optimal quadrature on the sphere and requires fewer quadrature points than tensor product based Gauss quadratures for a large class of functions. The Lebedev quadrature is designed to enforce the exact integration of spherical harmonics up to a given order and only a certain number of quadrature points are available.

[7] Lebedev and Laikov, 1999.

A comparison of the three methods

	classical	new	Carleman
storage requirement	$O(N^6)$	$O(MN^4)$	$O(MN^3)$
numerical complexity	$O(N^6)$	$O(MN^4 \log N)$	$O(MN^3 \log N)$

Table: N is the number of points in each velocity dimension. M is the total points on a sphere.

Note that the Carleman spectral method only works for the hard sphere case, while both the classical and the new spectral methods can treat general collision kernels.

Overview

3D Maxwell molecule — BKW solution

If $B = 1/(4\pi)$ is a constant, we know the exact solution

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

where $K = 1 - \exp(-t/6)$. The initial time has to be greater than $6\ln(5/2) \approx 5.498$ for f to be positive.

The above f satisfies exactly the space homogeneous Boltzmann equation, so we know the exact value of $\mathcal{Q}(f)$ is $\frac{\partial f}{\partial t}$.

3D Maxwell molecule — BKW solution

N	classical spectral	new spectral $M = 14$
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

Table: $\|\mathcal{Q}^{\text{num}}(f) - \mathcal{Q}^{\text{ext}}(f)\|_{L^\infty}$ evaluated at $t = 6.5$. M-points Lebedev rule is used on the sphere.

N	classical spectral	new spectral $M = 14$
8	0.09s	0.14s
16	6.31s	0.26s
32	542.34s	1.78s
64	—	33.15s

Table: Average running time for one time evaluation of the collision operator.

3D Maxwell molecule — evolution of higher order moments

Consider $B = 1/(4\pi)$ and the initial condition

$$f_0(v) = \frac{1}{2(2\pi)^{3/2}} \left\{ \exp\left(-\frac{(v-u_1)^2}{2}\right) + \exp\left(-\frac{(v-u_2)^2}{2}\right) \right\},$$

with $u_1 = (-2, 2, 0)$, $u_2 = (2, 0, 0)$.

Define the momentum flow and the energy flow as

$$P_{ij} = \int_{\mathbb{R}^3} f v_i v_j \, \mathrm{d}v, \quad q_i = \frac{1}{2} \int_{\mathbb{R}^3} f v_i v^2 \, \mathrm{d}v, \quad i, j = 1, 2, 3,$$

then we have the exact formula

$$P_{11} = \frac{7}{3} \exp\left(-\frac{t}{2}\right) + \frac{8}{3}, \quad P_{22} = -\frac{2}{3} \exp\left(-\frac{t}{2}\right) + \frac{11}{3},$$
$$P_{33} = -\frac{5}{3} \exp\left(-\frac{t}{2}\right) + \frac{8}{3}, \quad P_{12} = -2 \exp\left(-\frac{t}{2}\right),$$

and

$$q_1 = -2 \exp\left(-\frac{t}{2}\right), \quad q_2 = -\frac{2}{3} \exp\left(-\frac{t}{2}\right) + \frac{43}{6}.$$

3D Maxwell molecule — evolution of higher order moments

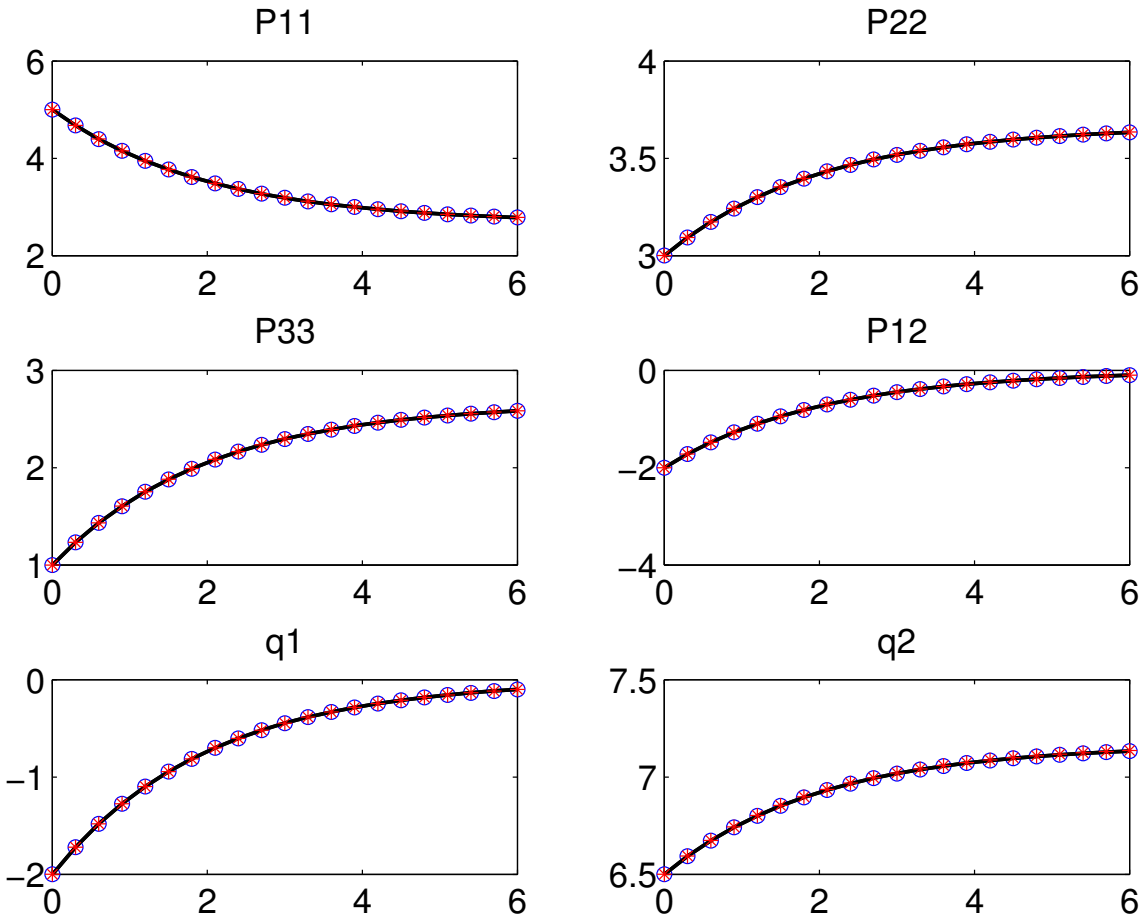

Figure: Time evolution for higher order moments. Solid line: exact solution. Blue circle: classical spectral method. Red star: new fast spectral method. $N = 32$, $M = 74$. $\Delta t = 0.3$, RK4 for time discretization.

Variable soft sphere (VSS) model

We finally consider a more realistic collision kernel — variable soft sphere (VSS) model[8]:

$$B = |g|^{\gamma} \left(1 + \frac{\sigma \cdot g}{|g|}\right)^{\eta}.$$

The VSS molecular model depends on both relative velocity and deviation angle, and can reproduce the measured values of the coefficient of diffusion as well as the coefficient of viscosity.

For Argon gas in normal temperature range: $\gamma = 0.38$, $\eta = 0.4$.

[8] Bird, 1994.

Argon gas — evolution of higher order moments

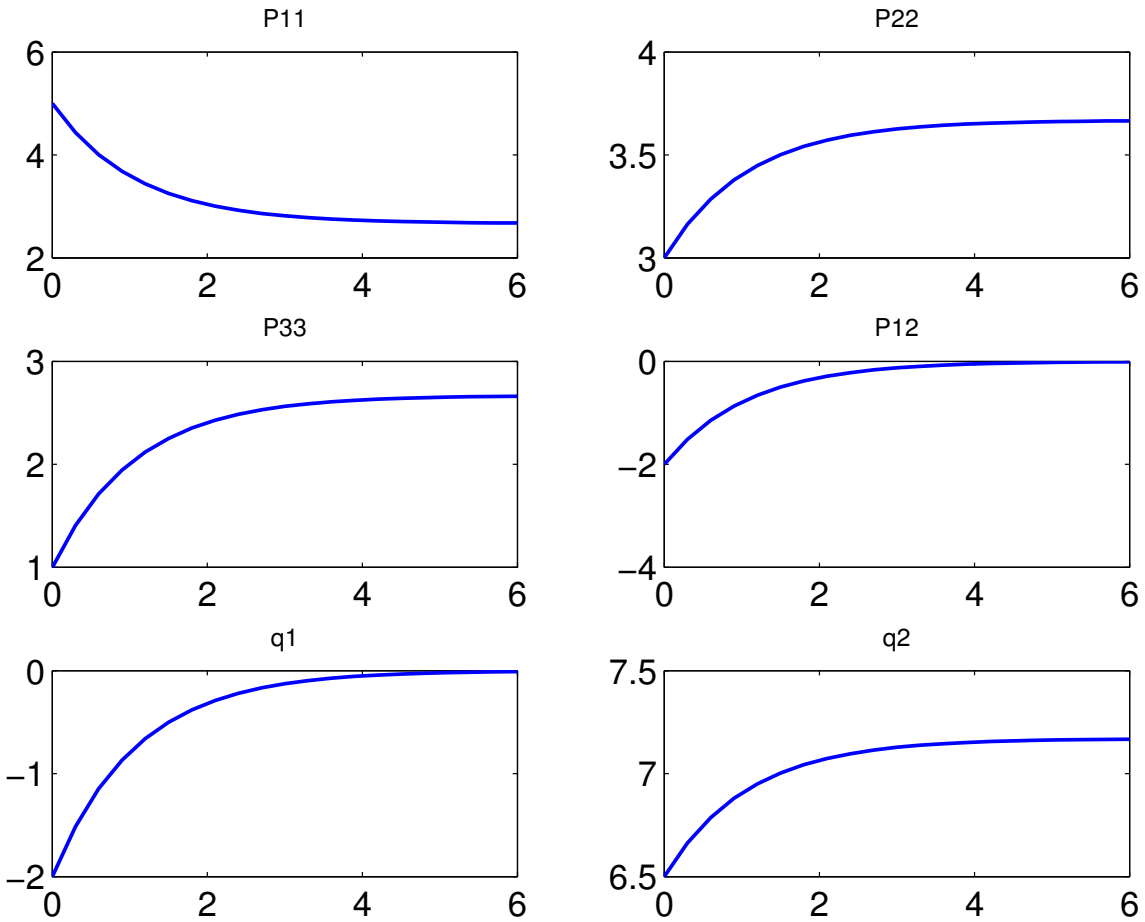

Figure: Time evolution for higher order moments. Blue line: new fast spectral method. $N = 32$, $M = 74$. $\Delta t = 0.3$, RK4 for time discretization.

Overview

Conclusion and future work

We introduced a new strategy to accelerate the classical spectral method as well as relieve its memory bottleneck in the precomputation:

- easy to implement
- can handle general collision kernels including both velocity and angular dependence

Future work

- investigate the property of sphere integration with respect to anisotropic function
- develop adaptive quadrature to further reduce the cost
- couple with spatial discretization to simulate benchmark examples

References

L. Pareschi and G. Russo

Numerical solution of the Boltzmann equation I: spectrally accurate approximation of the collision operator. *SIAM J. Numer. Anal.*, 37 (2000), pp. 1217–1245.

I. Gamba and S. Tharkabhushanam

Spectral-Lagrangian methods for collisional models of non-equilibrium statistical states. *J. Comput. Phys.*, 228 (2009), pp. 2012–2036.

C. Mouhot and L. Pareschi

Fast algorithms for computing the Boltzmann collision operator. *Math. Comp.*, 75 (2006), pp. 1833–1852.

I. Gamba, J. Haack, C. Hauck, and J. Hu (This talk)

A fast spectral method for the Boltzmann collision operator with general collision kernels. *SIAM J. Sci. Comput.*, to appear.

References

L. Pareschi and G. Russo

Numerical solution of the Boltzmann equation I: spectrally accurate approximation of the collision operator. *SIAM J. Numer. Anal.*, 37 (2000), pp. 1217–1245.

I. Gamba and S. Tharkabhushanam

Spectral-Lagrangian methods for collisional models of non-equilibrium statistical states. *J. Comput. Phys.*, 228 (2009), pp. 2012–2036.

C. Mouhot and L. Pareschi

Fast algorithms for computing the Boltzmann collision operator. *Math. Comp.*, 75 (2006), pp. 1833–1852.

I. Gamba, J. Haack, C. Hauck, and J. Hu (This talk)

A fast spectral method for the Boltzmann collision operator with general collision kernels. *SIAM J. Sci. Comput.*, to appear.

Thank you!