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

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We propose a simple fast spectral method for the Boltzmann collision operator with general collision kernels. Compared with the direct spectral method [8] which requires $O(N^6)$ memory to store precomputed weights and has $O(N^6)$ numerical complexity, the new method has complexity $O(MN^4 \log N)$, where N is the number of discretization points in each velocity dimension, M is the total number discretization points on a sphere and $M \ll N^2$. Furthermore, it requires only $O(MN^4)$ memory to store precomputed functions for more general collision kernels. Unlike previous methods, our new method can apply to arbitrary collision kernels including angularly dependent models. A series of numerical tests is performed to illustrate the efficiency and accuracy of the proposed method.

Background and Motivation

Proposed by Ludwig Boltzmann in 1872, the Boltzmann equation is one of the fundamental equations of kinetic theory. Yet its numerical approximation still presents a huge computational challenge, even on today's supercomputers, due to the high-dimensional, nonlinear, nonlocal structure of the collision integral. Two approaches have been primarily employed for solving the Boltzmann equation numerically: one stochastic and one deterministic. Direct simulation Monte Carlo (DSMC) methods [1, 6, 3] have been historically popular because they avoid the curse of dimensionality for this problem, however they can suffer from slow convergence for certain types of problems such as transient and low-speed flows and give noisy results due to their stochastic nature. The other approach is to use deterministic solvers, which have undergone considerable development over the past twenty years. These methods include discrete velocity models (DVM) and Fourier spectral methods [7, 2, 8, 4]. Spectral methods are invariably hindered in most real-world applications since they require $O(N^6)$ operations per evaluation of the collision operator, with N being the number of discretization points in each velocity dimension, as well as $O(N^6)$ bytes of memory to store precomputed weight functions which quickly becomes a bottleneck when solving large-scale problems [8, 4]. While fast spectral methods were earlier proposed in [2, 5] based on the Carleman representation of the collision integral (complexity $O(MN^3 \log N)$, where M is the total discrete points on a sphere and $M \ll N^2$), this steps required to obtain this formulation will only give the needed decoupling for fast evaluation in the case of the hard sphere model. Therefore, the goal of this paper is to introduce a fast spectral method for the Boltzmann collision operator that can handle general collision kernels as well as mitigate the memory requirement in the direct spectral method. Specifically, the numerical complexity of our new method will be $O(MN^4 \log N)$, and only $O(MN^4)$ memory is needed to store precomputed functions for more general collision kernels. The proposed method can serve as a "black-box" solver in the velocity domain to be used in conjunction with existing time and spatial discretization methods to treat more practical problems with complex geometries, multiple temporal/spatial scales, etc.

Description/Impact

To try to obtain a form for the weights in the spectral formulation that can be expressed as a convolution, we seek an approximation of the weight $G(l,m)$ in the following decoupled form

$$G(l,m) \approx \sum_{p=1}^{N_p} \alpha_p(l+m)\beta_p(l)\gamma_p(m),$$

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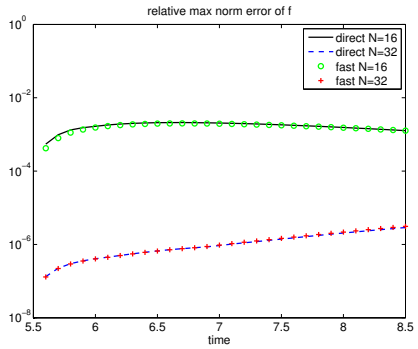
where α_p, β_p, γ_p represent appropriate functions of $l+m$, l, and m respectively, and the total number of terms N_p in the expansion is relatively small. Using a fixed numerical quadrature in the definition of $G(l.m)$ allows us to make this decomposition

$$G(l,m) \approx \sum_{\rho,\phi_1,\phi_2} w_\rho w_{\phi_1} w_{\phi_2} \sin\phi_2 F(l+m,\rho,\omega) e^{i\frac{\pi}{L}\rho\frac{l}{2}\cdot\omega} e^{-i\frac{\pi}{L}\rho\frac{m}{2}\cdot\omega}.$$

This form allows us a large increase in computational efficiency without sacrificing much accuracy.

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

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



Time evolution of error between the direct spectral (lines) and fast spectral (symbols) for the BKW solution to the Boltzmann equation.

Anticipated Impact

The new method was designed to accelerate the direct spectral method as well as relieve its memory bottleneck in the precomputation. Through a series of examples, we were able to demonstrate that the proposed method can be orders of magnitude faster than the direct method to achieve the same level of accuracy. Furthermore, it can be applied not only for the VHS model but also for more general collision kernels that have both velocity and angular dependence, unlike existing fast spectral methods which can only treat hard sphere molecules.

Path Forward

Ongoing work includes careful investigation of the dependence of spherical discretization on the property of the solution and development of adaptive quadrature to further improve the method. The reduction in computational complexity allows for implementation for much higher dimensional problems than could previously be obtained.

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