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Note on Divergence of the Chapman–Enskog Expansion for Solving Boltzmann Equation *

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Within about a year (1916–1917) Chapman and Enskog independently proposed an important expansion for solving the Boltzmann equation. However, the expansion is divergent or indeterminant in the case of relaxation time $\tau \geq 1$. Since then, this divergence problem has puzzled researchers for a century. Using a modified Möbius series inversion formula, we propose a modified Chapman–Enskog expansion with a variable upper limit of the summation. The new expansion can give not only a convergent summation but also the best-so-far explanation on some unbelievable scenarios occurring in previous practice.

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The Boltzmann equation developed by Ludwig Boltzmann in 1872[1–3] describes the statistical behavior of a thermodynamic system in a non-equilibrium state. To solve the Boltzmann equation, some attempts have been taken to simplify the collision term in the equation. The most popular scheme was proposed by Bhatnagar, Gross and Krook,[2–4] who made the assumption that the effect of molecular collisions is to force a non-equilibrium distribution function at a point in physical space back to a Maxwellian equilibrium distribution function and at the rate that is proportional to the molecular collision frequency. Therefore, the Boltzmann equation can be modified to the equation

$$\frac{\partial f}{\partial t} + \frac{\boldsymbol{p}}{m} \cdot \nabla f + \boldsymbol{F} \cdot \frac{\partial f}{\partial \boldsymbol{p}} = \frac{g - f}{\tau}. \tag{1}$$

Equation (1) is called the Bhatnagar–Gross–Krook (BGK) equation, in which f is the distribution function, $\boldsymbol{F}$ is the external force, m is the mass, $\boldsymbol{v}$ is the velocity field, $p = m\boldsymbol{v}$ is the momentum field, τ is the relaxation time, g is the Maxwellian distribution function. The relaxation time is defined as $\tau \sim \frac{\lambda}{L} K_n$, where λ is the molecular mean free path, L is the characteristic length, $K_n = \lambda/L$ is the Knudsen number.[1–3]

If the force $\boldsymbol{F}$ is not considered, Eq. (1) will reduce to

$$g(t) = f(t) + \tau \frac{Df}{Dt}, \tag{2}$$

where the operator $\frac{D}{Dt} = \frac{\partial}{\partial t} + \boldsymbol{v} \cdot \nabla$.

Assume that the Maxwellian distribution function $g(t)$ is given. Following from Eq. (2), the distribution function $f(t)$ can be constructed in terms of $g(t)$ using formal expansion,

$$\begin{aligned} f(t) &= g(t) - \tau \frac{Df}{Dt} \\ &= g - \tau \frac{D}{Dt}(g - \tau \frac{Df}{Dt}) \\ &= g - \tau \frac{Dg}{Dt} + \tau^2 \frac{D^2 g}{Dt^2} - \ldots, \end{aligned} \tag{3}$$

or equivalently

$$f(t) = \sum_{n=0}^{\infty} (-1)^n \tau^n \frac{D^n}{Dt^n} g(t). \tag{4}$$

This expansion is called the Chapman–Enskog expansion proposed by Enskog and Chapman independently.[3,2]

Unfortunately, the summation in Eq. (4) is divergent or indeterminate under $\tau \geq 1$, hence the Chapman–Enskog expansion is just a formal solution which does not guarantee the convergence. To ensure the convergence in different parameter regimes, many efforts have been made but significant results for a unified approach are far from satisfactory.[2–6]

In mathematics, a divergent series is an infinite series that is not convergent, implying that the infinite sequence of the partial sums of the series does not have a finite limit. If a series converges, the individual terms in the series must approach zero. Thus any series in which the individual terms do not approach zero will diverge. With this understanding, if assume that the derivative $\lim\limits_{n\to\infty} \frac{D^n}{Dt^n} g(t)$ is bounded, then $\sum\limits_{n=0}^{\infty} (-1)^n \tau^n \frac{D^n}{Dt^n} g(t)$ will be divergent or indeterminate under $\tau \geq 1$. To handle the divergence in the case of $\tau \geq 1$, the summation should not be taken up to infinity instead of a finite number of terms, namely,

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the series summation must be truncated at a finite number of terms. For a divergent series, the question is how to determine the finite number of truncated terms. From convergence study of an infinite series, we know that the convergence is dependent on not only the independent expansion variable τ but also its maximum $\tau_{\max}$, and is related to their ratio $\tau_{\max}/\tau$ as well.

To utilize the well-known Möbius inversion, let us consider τ as an independent variable rather than a fixed scalar, Eq. (2) can be revised as

$$g(\tau,t)=f(\tau,t)+\tau\frac{D}{Dt}f(\tau,t). \tag{5}$$

Then a modified Möbius series inversion theorem can be proposed as follows:[7–10] If

$$g(\tau,t)=\sum_{n=0}^{[\tau_{\max}/\tau]} r(n)\tau^n\frac{D^n}{Dt^n}f(\tau,t), \tag{6}$$

then its exact inversion can be given by

$$f(\tau,t)=\sum_{n=0}^{[\tau_{\max}/\tau]} r^{-1}(n)\tau^n\frac{D^n}{Dt^n}g(\tau,t), \tag{7}$$

where the $r(n)$ satisfies

$$\sum_{m+n=k} r^{-1}(n)r(m)=\delta_{k,0}. \tag{8}$$

Note that $\tau_{\max}$ represents the maximum relaxation time under consideration, the change of the upper limit of the sums in Eqs. (6) and (7) suggests that

$$f(\tau,t)|_{\tau>\tau_{\max}}=0,\quad g(\tau,t)|_{\tau>\tau_{\max}}=0. \tag{9}$$

Equations (6) and (7) are true under the condition (8). Proof of Eq. (7) can be simply given in the following.

Substituting Eq. (6) into the right-hand side of Eq. (7), we obtain

$$\begin{aligned}
&\sum_{n=0}^{[\tau_{\max}/\tau]} r^{-1}(n)\tau^n\frac{D^n}{Dt^n}g(\tau,t)\\
&=\sum_{n=0}^{[\tau_{\max}/\tau]} r^{-1}(n)\tau^n\frac{D^n}{Dt^n}\Big(\sum_{m=0}^{[\tau_{\max}/\tau]} r(m)\tau^m\frac{D^m}{Dt^m}f(\tau,t)\Big)\\
&=\sum_{k=0}^{[\tau_{\max}/\tau]}\Big\{\sum_{n+m=k} r^{-1}(n)r(m)\tau^{n+m}\frac{D^{n+m}}{Dt^{n+m}}f(\tau,t)\Big\}\\
&=\sum_{k=0}^{[\tau_{\max}/\tau]}\delta_{k,0}\tau^k\frac{D^k}{Dt^k}f(\tau,t)\\
&=\tau^0\frac{D^0}{Dt^0}f(\tau,t)\\
&=f(\tau,t).
\end{aligned} \tag{10}$$

In order to apply the above result to Eq. (5), the function $r(n)$ must be

$$r(n)=\begin{cases}1, & n\le 1,\\ 0, & n>1.\end{cases} \tag{11}$$

Based on Eq. (8), we can obtain

$$r^{-1}(n)=(-1)^n. \tag{12}$$

This means that the solution to Eq. (5) can be expressed as

$$f(\tau,t)=\sum_{n=0}^{[\tau_{\max}/\tau]}(-1)^n\tau^n\frac{D^n}{Dt^n}g(\tau,t). \tag{13}$$

This is the modified Chapman–Enskog expansion which improves the traditional one given by Eq. (4).

It is easy to see that there is an essential difference between Eq. (13) and Eq. (4). The conventional summation in Eq. (4) is performed up to infinity, however the modified summation in Eq. (13) is up to a finite number $[\tau_{\max}/\tau]$. The summation over infinite terms leads to divergence, however the controllable finite terms of summation bring a convergence since the number of summation is a function of the ratio $[\tau_{\max}/\tau]$. In the case of $\tau>\tau_{\max}$, namely, $\tau_{\max}/\tau<1$, both $g(\tau,t)$ and $f(\tau,t)$ will no longer exist in Eq. (13), owing to the fact that $[\tau_{\max}/\tau]=0$.

The modified Chapman–Enskog expansion in Eq. (13) can be viewed as an extension from a function[7] to a differential operator.

Obviously, the new general solution to Eq. (13) can completely get rid of the divergence problem and is valid as long as τ is within $(0,\tau_{\max}]$.

For example, set relaxation time range as $\tau\in[0.1,10]$, it is natural to take $\tau_{\max}=10$. The solutions to Eq. (13) are changing as τ such as in Table 1.

Table 1. $f(\tau,t)=\sum_{n=0}^{[\tau_{\max}/\tau]}(-1)^n\tau^n\frac{D^n}{Dt^n}g(\tau,t)$.

τ	$\frac{\tau_{\max}}{\tau}$	$\left[\frac{\tau_{\max}}{\tau}\right]$	Expression
$\tau=6$	1.67	1	$f(\tau,t)=g(t)-\tau\frac{Dg}{Dt}$
$\tau=4$	2.5	2	$f(\tau,t)=g(t)-\tau\frac{Dg}{Dt}+\tau^2\frac{D^2g}{Dt^2}$
$\tau=2$	5	5	$f(\tau,t)=g(t)-\tau\frac{Dg}{Dt}+\tau^2\frac{D^2g}{Dt^2}$ $-\tau^3\frac{D^3g}{Dt^3}+\tau^4\frac{D^4g}{Dt^4}-\tau^5\frac{D^5g}{Dt^5}$
$\tau=1$	10	10	$f(\tau,t)=g(t)-\tau\frac{Dg}{Dt}+\tau^2\frac{D^2g}{Dt^2}$ $-\tau^3\frac{D^3g}{Dt^3}+\cdots+\tau^{10}\frac{D^{10}g}{Dt^{10}}$
$\tau=0.1$	100	100	$f(\tau,t)=g(t)-\tau\frac{Dg}{Dt}+\tau^2\frac{D^2g}{Dt^2}$ $-\tau^3\frac{D^3g}{Dt^3}+\cdots+\tau^{100}\frac{D^{100}g}{Dt^{100}}$

The above solution is for a global range of relaxation time, if only "local" relaxation time is required, then $\tau_{\max}=\tau$ could be used, and only two terms will be involved in Eq. (13). The choice of $\tau_{\max}$ should be determined by the physics of practical problems. However, the divergence problem has been overcome. The compatibility of Eq. (13) in all the range of relaxation time indicates that there is a possibility to express a multi-scale flow in a unified way.

Having the modified Chapman–Enskog expansion in Eq. (13), we can have a new perspective on the following scenarios.

Multi-scale scenario: In gas dynamics,[1] in association with τ, different scales of Knudsen number K_n correspond to different equations, for example, $K_n \sim 0$ is related to Euler's equation, $K_n < 0.01$ to the Navier–Stokes equation without slipping boundary, $K_n \in [0.01, 0.1]$ to the Navier–Stokes equation with slipping boundary, $K_n \in [0.1, 1]$ belongs to the transition region and $K_n > 10$ is related to the Boltzmann equation for free-molecular motion. Then, for different scales τ corresponding to different K_n, one has to adopt different Chapman–Enskog expansions. Now the solution to Eq. (13) provides a unified expression for multi-scale of relaxation time τ.

Truncated series summation scenario: In practical computations, it is frequent to expand the first two terms in Eq. (3). It seems surprising that in this case the approximation solution is quite accurate with a reasonably large range of τ.

For instance, if the $\tau_{\max}$ is defined as $\tau \le \tau_{\max} < 2\tau$, or in ratio $1 \le \tau_{\max}/\tau < 2$, which leads to $[\tau_{\max}/\tau] = 1$, we will have

$$f(\tau,t) = \sum_{n=0}^{[\tau_{\max}/\tau]} (-1)^n \tau^n \frac{D^n}{Dt^n} g(\tau,t)$$
$$= \sum_{n=0}^{1} (-1)^n \tau^n \frac{D^n}{Dt^n} g(\tau,t) = g(\tau,t) - \tau \frac{Dg}{Dt}. \quad (14)$$

The highlights of the present study are listed in Table 2.

Table 2. The Chapman–Enskog expansion and its modification.

Expansion	Formulation
Chapman–Enskog	$f(t) = \sum_{n=0}^{\infty} (-1)^n \tau^n \frac{D^n}{Dt^n} g(t)$
Modified Chapman–Enskog	$f(\tau,t) = \sum_{n=0}^{[\tau_{\max}/\tau]} (-1)^n \tau^n \frac{D^n}{Dt^n} g(\tau,t)$

Equation (13) could be considered as a more promising modification of the Chapman–Enskog expansion for future computations. It is an interesting coincidence that the present modification is proposed in the centenary of the Chapman–Enskog expansion. The application of this modified Chapman–Enskog expansion to other topics is remained for further study.

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