REVIEW

Modified Chapman–Enskog expansion: A new way to treat divergent series

Zhen-Su She(佘振苏)†

State Key Laboratory for Turbulence and Complex Systems and the Department of Mechanics and Engineering Sciences, College of Engineering, Peking University, Beijing 100871, *China*

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The resolution by Chen and Sun of divergent Chapman–Enskog expansion problem will not only build a unified foundation for non-equilibrium dynamics modeling at all Mach number and Knudsen number, but also shed light to a large class of difficult theoretical problems involving divergent expansion on strong nonlinearity.

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Non-equilibrium statistical mechanics is profoundly built upon the Boltzmann equation, which governs nearly all flows ranging from dense to rarefied gases and from low to high speed. Solution to the Boltzmann equation such as the Hilbert[1] and Chapman–Enskog[2–4] expansion is not only the milestone in the theoretical study of the subject, but also the current guide in the computational modeling of practical problems. Despite tremendous success of the Chapman–Enskog expansion, two physical regimes remain a great challenge: one with speed largely exceeding the sound speed and another with low density such that the mean free path is of the order of the system size. The first regime is characterized by large Mach number ($Ma > 5$) and the second with order one Knudsen number ($Kn > 1$). In these two cases, the standard Navier–Stokes equation (which is a truncated Chapman–Enskog expansion to the second order) is expected to be inaccurate. Interestingly, a simple extension to third or higher orders of the Chapman–Enskog expansion with inclusion of the so-called Burnett or super-Burnett terms does not seem to produce satisfactory results. In other words, the long-standing Chapman-Enskog expansion may not seem to be the "right" one for a unified kinetic description of non-equilibrium Boltzmann dynamics, owing possibly to its divergence.

Exactly one hundred years later, Chen and Sun[5] have introduced a modified Chapman–Enskog expansion, which may offer a promising resolution of the issue mentioned above. The success stems from using a rigorous Mobius inversion theorem relating two series which mirror one with each other. In an earlier work,[6] Chen generalized the Mobius inversion theorem — a number-theoretical result — to a class of continuous functions describing the distribution functions of oscillators such as phonon and radiation. Here, by proving that a truncated Chapman–Enskog expansion has a more exact correspondence with the original BGK–Boltzmann equation, Chen and Sun discovered a modified Chapman–Enskog expansion by introducing a parameter $\tau_{\max}$, the upper limit for a convergent Chapman–Enskog expansion. The new expansion remains convergent for all cases, since no infinite summation is involved by definition, and thus the difficulty of divergence of the original Chapman–Enskog expansion finds a resolution.

Often, the resolution of a difficult physical problem must bring in a new physics concept which is previously unseen. Here, the new physics concept seems to be related to the quantity $\tau_{\max}$, which has not yet been fully explored in this Express Letter.[5] It might be helpful to offer a discussion: why is $\tau_{\max}$ so important?

As mentioned above, the study of non-equilibrium dynamics encounters great obstacles in the so-called continuum transition regime (with large Ma and Kn), where the statistical and continuum descriptions are themselves put in doubt, owing to the divergence of the Chapman–Enskog expansion in the transition regime of interest. A common practice in dealing with divergent series is to make a truncation, which is subtle in deciding how many terms are appropriate. On the other hand, keeping only two terms often yields reasonable outcome, when compared to empirical data. Thus, it is strongly desirable to justify the truncation, and more importantly to find systematic way to treat divergent series for difficult problems mostly involving strong nonlinearity.

The introduction of parameter $\tau_{\max}$ sheds new light on the problem. A finite $\tau_{\max}$ implies that for all $\tau < \tau_{\max}$, the Chapman–Enskog expansion is convergent, with a smooth non-equilibrium distribution function f, expressible in terms of the equilibrium distribution function g and its spatial-temporal derivatives. Let us try to reverse the logic in order to appreciate the new result: assume that for all interested non-equilibrium

†Corresponding author. E-mail: she@pku.edu.cn

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regimes (including in particular the transition regime) with given τ, there always exists a macroscopic state with well-behaved distribution function f (which must be true by physical intuition, since such state can be directly observed), then, one can always find a $\tau_{\max} > \tau$ such that the well-behaved non-equilibrium distribution f can be expressed in terms of the spatial and temporal derivatives of the equilibrium (Maxwellian) distribution (g, Dg, D^2g, etc.). With this reversed logic in mind, then the Chen–Sun's basic setting become understandable: for all physically sound regimes in which f and g both exist, there must exist a "symmetric way" to express f in terms of g just like the other way around, each containing $[\tau_{\max}/\tau]+1$ terms (i.e., Eqs. (6) and (7) in Ref. [5]). Then, the Mobius inversion theorem allows one to derive rigorously the modified Chapman–Enskog expansion (i.e., Eq. (13)) as an explicit expression of f in terms of g and its derivatives up to a finite order (i.e., $[\tau_{\max}/\tau]$).

How does this understanding help us to solve the hard problem of a unified description of non-equilibrium regimes, in particular for large Kn (i.e., large mean free path) or large Ma with sharp transition across shock. In Ref. [5], Chen and Sun have displayed a table of the solution with fixed $\tau_{\max} = 10$ but varying τ, to illustrate how the new solution (with modified Chapman–Enskog expansion) can be τ-dependent. Note that setting $\tau_{\max} = 10$ is rather inspiring, since often one believes that the Chapman-Enskog expansion would diverge for $\tau \geq 1$; Chen & Sun's seemingly artificial example suggests a way to define meaningful solution beyond $\tau > 1$, which may only be valid locally, hence serves as the basis for computational modeling. Since τ is the parameter to characterize how fast the (actual) non-equilibrium distribution (e.g., f) relaxes to local equilibrium distribution (e.g., g), and is related to Kn and Ma, finding a schema to determine $\tau_{\max}$ will be the key to derive a unified solution for arbitrary Kn and Ma (or a unified formalism for modeling rarefied gases at arbitrary density).

Chen and Sun have addressed this critical issue by proposing two scenarios, one called "multi-scale scenario" and the other "truncated series summation scenario". The first attempts to link Eq. (13) to solutions at various Kn, while the second yields an expression directly applicable to transition regime where a severe truncation occurs. The second scenario seems to have already gained support in the study of shock structure in high-speed flows. Xu[9] has shown that using the Navier–Stokes solver (i.e., truncated Chapman–Enskog expansion) with a regularized τ^*, the right shock structure is captured. It is my understanding that equations (13) and (14) in Ref. [5] provide a theoretical basis for Xu's model, and the regularized τ^* introduced by Xu can be regarded as a specific $\tau/\tau_{\max}$ effect, whose further clarification would be intriguing.

Then, we arrive at a rational answer to why the Navier–Stokes solver is uniformly good: in the continuum limit ($\tau/\tau_{\max} \to 0$), two leading terms are good enough because the series is convergent, and in the transition regime ($\tau/\tau_{\max} \to 1^-$), it is still good, because the series must be truncated up to $[\tau_{\max}/\tau] = 1$. In other words, the existence of $\tau_{\max}$ reveals the fact that not all truncations of the Chapman–Enskog expansion are allowed, which explains why Burnett and super-Burnett terms often do not improve the description of the physics for certain high-speed flows. We may further speculate that physics of supersonic and hypersonic flows are such that different $\tau_{\max}$ appears in different parameter regime, even in different regions of the space (i.e., in shocks). The exploration of the $\tau_{\max}$ effects for these physical systems will become important in future studies, for which the work of Ref. [5] provides a theoretical guide;[10] thus, a new chapter in the study of non-equilibrium physics may begin.

In addition, reference [5] raises a general issue from the applied mathematics point of view. It is a common practice that one keeps one or two terms in an infinite series expansion resulted from an iterative perturbation, and interestingly the truncated expansion often behaves well, justified by comparison with data, at large perturbations such the series is divergent. Then, the intriguing question is why such practice is reasonable, and what is the nature behind the validity of the truncated description. Reference [5] provides an answer for at least the former question. By introducing $\tau_{\max}$, reference [5] suggests that, for a special class of divergent series expressing one function (e.g., f) in terms of the other (e.g., g) and its derivatives, the application of the Mobius inversion theorem yields rigorously a series with finite number of terms (i.e., $[\tau_{\max}/\tau]+1$), which may be a truncation involving only two terms ($\tau \to \tau_{\max}^-$). Thus, the common practice of a short truncation may sometimes be rigorously justified. Chapman–Enskog expansion is just an example of this category.

Then, would it be nice to find other difficult problem of strong nonlinearity which can be solved in the same way? Turbulence is a well-known problem of the same nature: strong nonlinearity makes the representation of the solution by divergent series. Now, the question is: whether can such divergent series be regularized by the application of the Mobius theorem? The theory of renormalization group (RNG) of Yakhot and Orszag[11] expresses fluctuating velocity of a homogeneous isotropic turbulence in terms of a Gaussian velocity field by a divergent series; remarkably, the eddy viscosity evaluated from a second-order truncation of the infinite series has led to an effective model (i.e., the RNG k–ε model) widely used in engineering applications. Is it possible to find an inversion theorem such that the truncation in the RNG theory can be justified? Even further, is it possible to construct a self-consistent (instead of the current *ad hoc*) RNG theory of turbulence, based on the Mobius inversion theorem?

We would like to further ask: what would make the Mo-

bius inversion theorem applicable? This difficult and somewhat abstract question may not easily find an answer, but this inquiry is worthy to be mentioned in the light of Chen & Sun's success, since it might inspire the resolution of a large-class of large-perturbation problem. We will attempt to adopt the reversed logic mentioned earlier to respond to this inquiry. The key seems to recognize that any practical problem of interest must have, physically speaking, some kind of well-defined, even analytically smooth form, since the empirical data suggest it, no matter how large is the expansion parameter; the latter is, in general, subjectively chosen. Often, the appearance of such an analytic form comes as a surprise, if the problem has been stuck too long. An example is the recently proposed Lie-group description of the universal wall function in turbulent boundary layer,[12] a century-old problem since Prandtl first posed it in 1904.

Empirical data suggest that the wall function for canonical turbulent boundary layers exists and is universal, but the Taylor expansion in y (distance from the wall) diverges quickly for y above certain distance. However, by employing an argument of invariance under dilation group transformation in y, which is the only invariant group left for the Navier–Stokes equation in the presence of a solid (no-slip) wall, analytic expression of the so-called mixing length can be derived,[12] validated by experimental and numerical simulation data over the entire domain of the inner region near the wall. Here, the resolution of the divergent series is by direct application of the group symmetry (or invariance) on the appropriately chosen variable (i.e. the mixing length), which is in fact discovered under a general theory extending Landao's idea of order parameters to non-equilibrium situations.[13]

The application of the Mobius inversion theorem in Ref. [5] is based on an additive semi-group; it is likely that for each physical problem, there exists a symmetry group which is the most relevant one to govern the actual variation. If so, identifying such symmetry group becomes the most important task for the successful description of any difficult problem of strong nonlinearity.

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