Notes on kinetic-equation approach of fluid-dynamic equations

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Yoshio Sone
230-133 Iwakura-Nagatani-cho Sakyō-ku Kyoto 606-0026 Japan

Abstract
Kinetic-equation approach of numerical study of fluid-dynamic equations is discussed. A method constructing a kinetic equation replacing the fluid-dynamic-type equation exactly is proposed. On the basis of this method, the validity or improvement of heuristic numerical kinetic-equation systems is discussed.

1 Introduction
There is a recent trend to make use of kinetic-type equation in obtaining numerical solutions of the Euler or Navier-Stokes set of equations (e.g., [1], [2], [3]). The way of computation is different among the authors, but they noticed the simple linear form of the differential term of the kinetic equation and try to avoid some difficulties in numerical analysis of the Euler or Navier-Stokes set (e.g., instability problems in shock wave computations, the pressure term in the incompressible Navier-Stokes set, preference of quick computation of complex problems to detailed precise one). They made some success in various problems.

One of the direction of this trend is by Vasseur's. He uses the simplest part of kinetic equation, that is, the Boltzmann equation without collision term but, instead, modifies the velocity distribution function at each time step. For this scheme he developed the mathematical theory, though it is limited to the case where the ratio of the specific heats is equal to three. Kun Xu's approach is also in this direction, although he uses the BK W equation and introduces some technique to treat the discontinuity (shock wave or contact discontinuity) in the flow field. He investigated many problems by his method.[4]

In the present brief notes, we propose a simple way to construct a kinetic system of equation and initial condition from a set of partial differential equation of a conservation form (e.g., Euler and Navier-Stokes sets) in such a way that some moments of the solution of the kinetic system satisfy the set of partial differential equations exactly. On the basis of this kinetic system, we discuss the numerical scheme of Vasseur type as an example. This type of discussion has wide application to construction of efficient schemes and evaluation of their validity.
2 Exact kinetic-equation approach

Let \( x_i; \eta_i \) and \( t \) be independent variables, and \( f(x_i; \eta_i; t) \) be a dependent variable (or the velocity distribution function). The (macroscopic) variables \( \eta^r \) \((r = 0; 1; \ldots; 4)\) are defined as follows:

\[
Z_{\eta^r} = \eta^r f d\eta_1 d\eta_2 d\eta_2;
\]

(1)

where

\[
\eta_0 = 1; \quad \eta_i = \eta_i; \quad \eta_4 = \eta^2;
\]

(2)

and the fluxes \( \mathcal{H}_i^r \) of the macroscopic variables are defined as follows:

\[
Z_{\mathcal{H}_i^r} = \eta^r f d\eta_1 d\eta_2 d\eta_2;
\]

(3)

Take a velocity distribution function \( f_c \) of Chapman-Enskog type where the space and time variables enter only through the macroscopic variables or their space variables:

\[
f(x_i; \eta_i; t) = f_c(\eta^r; \eta^2; \eta^2);
\]

(4)

where \( r \) is the representative of a collection of the derivatives \( \partial = \partial_{\eta^0}, \ldots, \partial_{\eta^4} \).

Naturally,

\[
Z_{\eta^r} = \eta^r f_c(\eta^r; \eta^2; \eta^2) d\eta_1 d\eta_2 d\eta_2;
\]

The fluxes \( \mathcal{H}_i^r \) corresponding to the velocity distribution function \( f_c(\eta^r; \eta^2; \eta^2) \) of Chapman-Enskog type is denoted by \( \mathcal{H}_i^r \); that is,

\[
\mathcal{H}_i^r(\eta^r; \eta^2) = \eta^r f_c(\eta^r; \eta^2; \eta^2) d\eta_1 d\eta_2 d\eta_2;
\]

(5)

Now, choosing a function \( f_c(\eta^r; \eta^2; \eta^2) \) of Chapman-Enskog type, we discuss a solution of the following functional equation:

\[
\frac{\partial f_c}{\partial t} + \eta^r \frac{\partial f_c}{\partial \eta_i} = \theta_c \left( \frac{\partial^2 f_c}{\partial \eta^2_{\eta^2}} \right) \frac{\partial f_c}{\partial \eta^2} + \frac{\partial^2 \eta^r}{\partial \eta^2 \partial \eta_i} \frac{\partial f_c}{\partial \eta^2} + \left( \frac{\partial^2 f_c}{\partial \eta^2_{\eta^2}} \right) \frac{\partial f_c}{\partial \eta^2} \left( \frac{\partial^2 \eta^r}{\partial \eta^2 \partial \eta_i} \right);
\]

(6)

with the initial condition:

\[
f(x_i; \eta_i; t) = f_c(\eta^r; \eta^2; \eta^2) \quad \text{at} \quad t = t_0;
\]

(7)
This equation has the same form of conservation equation as the equation without the right-hand side terms:

\[
\frac{\partial \frac{\varphi}{\varphi}}{\partial t} + \frac{\partial H}{\partial x} = 0;
\]  

(8)

This is derived from the following manipulation of the right-hand side:

\[
Z \int_{\sigma_{1i}} \int_{\sigma_{2i}} \int_{\sigma_{2i}} d\sigma_{1} d\sigma_{2} =
\]

\[
\frac{\partial \frac{\hat{\varphi}}{\hat{\varphi}}}{\partial t} + \frac{\partial \hat{H}}{\partial x} = 0;
\]  

(9)

with the initial condition

\[
\frac{\varphi}{\varphi} = \frac{\varphi}{\varphi} \text{ at } t = t_{0};
\]  

(10)
Proof: Take a function

\[ f(x_i; \eta; t) = f_c(\frac{1}{2}\phi(x_i; t); r \frac{1}{2}\phi(x_i; t); \eta); \]

where \( \frac{1}{2}\phi(x_i; t) \) is the solution of the following partial differential equations:

\[ \frac{\partial^2}{\partial x_i^2} + \frac{\partial^2}{\partial \phi^2} = 0; \]

with the initial condition

\[ \frac{1}{2}\phi = \frac{1}{2} \quad \text{at} \quad t = t_0; \]

Then

\[ \frac{1}{2}\phi(x_i; t) = \frac{1}{2}\phi(x_i; t); \]

\[ \frac{\partial^2}{\partial x_i^2} + \frac{\partial^2}{\partial \phi^2} = 0; \]

and

\[ \frac{1}{2}\phi = \frac{1}{2} \quad \text{at} \quad t = t_0; \]

Thus, the function \( f \) defined by Eq. (11) with the subsidiary conditions (12) and (13) is a solution of the initial-value problem (6) with (7). From the uniqueness,
the set of the macroscopic variables \( \frac{1}{2} \) obtained the solution \( f \) of the initial-value problem is the solution of the partial differential equations (9) with the initial condition (10).

As the first example, take the Maxwellian distribution
\[
f_c = \frac{\frac{1}{2}}{(2\sqrt{RT})^{3/2}} \exp \left( -\left( \frac{\chi_i - u_i}{2RT} \right)^2 \right); \tag{14}
\]
as a velocity distribution function of Chapman-Enskog type, where the macroscopic variables \( \frac{1}{2} \) are related to the parameters \( \frac{1}{2} u_i \); and \( T \) in the Maxwellian as
\[
\frac{1}{2} = \frac{1}{2}; \quad \frac{1}{2} = \frac{1}{2} u_i; \quad \frac{1}{4} = \frac{1}{4} (3RT + u_i^2); \tag{15}
\]
and the \( \dot{v}_i \) for the Maxwellian are given by
\[
\frac{\dot{v}_i}{\dot{v}_i} = \frac{\chi_i}{\dot{v}_i} = \frac{1}{2} u_i; \quad \frac{\dot{v}_i}{\dot{v}_i} = \frac{1}{2} (3RT + u_i^2); \tag{16}
\]
The macroscopic variables \( \frac{1}{2} \) (or \( \frac{1}{2} u_i \); and \( T \)) derived from the solution of this kinetic equation satisfy the Euler set of equation:
\[
\frac{\partial \frac{1}{2}}{\partial t} + \frac{\partial \frac{1}{2} u_i}{\partial x} = 0; \tag{17a}
\]
\[
\frac{\partial \frac{1}{2} u_i}{\partial t} + \frac{\partial \frac{1}{2} u_i u_j}{\partial x} + \frac{\partial \frac{1}{2} RT}{\partial x} = 0; \tag{17b}
\]
\[
\frac{\partial \frac{1}{4} (3RT + u_i^2)}{\partial t} + \frac{\partial \frac{1}{2} (5RT + u_i^2)}{\partial x} = 0; \tag{17c}
\]
As the second example, take the distribution function:
\[
f_c = \frac{\frac{1}{2}}{(2\sqrt{RT})^{3/2}} \exp \left( -\left( \frac{\chi_i - u_i}{2RT} \right)^2 \right) \exp \left( \frac{a(T; \frac{1}{2} \frac{\chi_i}{\dot{v}_i} \frac{\chi_i}{\dot{v}_i} \frac{5}{2}}{(2RT)^{3/2}} \right); \tag{18}
\]
where
\[
\chi_i = \frac{\chi_i}{(2RT)^{1/2}}; \tag{19}
\]
and \( a(T; \frac{1}{2} \frac{\chi_i}{\dot{v}_i} \frac{\chi_i}{\dot{v}_i} \frac{5}{2}) \) are functions of \( T \) and \( \frac{1}{2} \) which can be chosen according to our convenience. The macroscopic variables \( \frac{1}{2} \) are related to the parameters \( \frac{1}{2} u_i \); and \( T \) in the distribution function (18) as
\[
\frac{1}{2} = \frac{1}{2}; \quad \frac{1}{2} = \frac{1}{2} u_i; \quad \frac{1}{4} = \frac{1}{4} (3RT + u_i^2); \tag{20}
\]
and the ³uxes \( \mathbf{H}^i \) are given by

\[
\mathbf{H}^0 = \frac{1}{2} \mathbf{u}_i; \tag{21a}
\]

\[
\mathbf{H}^1 = \frac{1}{2} \mathbf{u}_i \mathbf{u}_j + RT \mathbf{d}_i \mathbf{b}(T; \beta(R^\beta T)) \frac{\mu}{\mathbf{G}_j} + \frac{\mu}{\mathbf{G}_i} \ i \ \frac{2 \mathbf{G}_k \mathbf{d}_j}{3 \mathbf{G}_k} \ ; \tag{21b}
\]

\[
\mathbf{H}^4 = \frac{1}{2} \mathbf{u}_i (5RT + \mathbf{u}_j^2) \mathbf{b}(T; \beta(R^\beta T)) \frac{\mu}{\mathbf{G}_j} + \frac{\mu}{\mathbf{G}_i} \ i \ \frac{2 \mathbf{G}_k \mathbf{d}_j}{3 \mathbf{G}_k} \ + \ \frac{5a(T; \beta(R^\beta T)) \mathbf{G}_j}{2} \ ; \tag{21c}
\]

The macroscopic variables \( \mathbf{\dot{u}} \) (or \( \mathbf{\dot{\mathbf{u}}}; \mathbf{u}_i \); and \( T \)) derived from the solution of this kinetic equation satisfy the Navier-Stokes set of equations:

\[
\frac{\partial \mathbf{\dot{u}}}{\partial t} + \frac{\partial \mathbf{\dot{u}}}{\partial x} \mathbf{u}_i = 0; \tag{22a}
\]

\[
\frac{\partial \mathbf{\dot{u}}}{\partial t} + \frac{\partial \mathbf{\dot{u}}}{\partial x} \mathbf{u}_i + \frac{\partial \mathbf{\dot{u}}}{\partial x} \mathbf{S} = \frac{\partial}{\partial x} \mathbf{b}(T; \beta(R^\beta T)) \frac{\mu}{\mathbf{G}_j} + \frac{\mu}{\mathbf{G}_i} \ i \ \frac{2 \mathbf{G}_k \mathbf{d}_j}{3 \mathbf{G}_k} \ ; \tag{22b}
\]

\[
\frac{\partial \mathbf{\dot{u}}}{\partial t} + \frac{\partial \mathbf{\dot{u}}}{\partial x} (3RT + \mathbf{u}_j^2) + \frac{\partial \mathbf{\dot{u}}}{\partial x} (5RT + \mathbf{u}_j^2)
\]

\[
= \frac{\partial}{\partial x} \mathbf{b}(T; \beta(R^\beta T)) \mathbf{u}_i \frac{\mu}{\mathbf{G}_j} + \frac{\mu}{\mathbf{G}_i} \ i \ \frac{2 \mathbf{G}_k \mathbf{d}_j}{3 \mathbf{G}_k} \ + \ \frac{5a(T; \beta(R^\beta T)) \mathbf{G}_j}{2} \ ; \tag{22c}
\]

These are the Navier-Stokes set of equations with viscosity \( \mathbf{b}(T; \beta(R^\beta T)) \) and thermal conductivity \( 5a(T; \beta(R^\beta T)) \). Thus choosing \( a(T; \beta) \) and \( b(T; \beta) \) properly, we obtain the Navier-Stokes set with arbitrary viscosity and thermal conductivity. It should be noted that the form (18) of \( f_c \) is not necessary to be taken to be the same distribution function of the Chapman-Enskog expansion that gives the Navier-Stokes set with the same viscosity and thermal conductivity.

In the examples, the function \( f_c \) is somehow resembled with the Chapman-Enskog expansion, but it is not required to be so. We can choose freely according to the request that the function gives the required set of equations. Equation (14) or (18) is just an example giving the Euler set or Navier-Stokes set.

3 Discussion on numerical systems

In the previous section, a kinetic-equation system that describes fluid-dynamic equations exactly is presented. In the present section, we discuss the validity of heuristic numerical kinetic-equation systems. The kinetic-equation approach which is interested in here is the following one or its variant: The solution of an initial-value problem of the Euler set of equations is discussed by the following
kinetic equation in place of solving the Euler set directly. That is, the solution of Eq. (23) in a continuous series of intervals \((t_0; t_1); (t_2; t_3); \ldots\)

\[
\frac{\partial f}{\partial t} + \nabla \cdot (f u) = 0; \tag{23}
\]

under the initial condition of each interval

\[
f = \frac{\frac{1}{2} \rho (m)}{(2\sqrt{RT_m})^3} \exp \left( i \frac{(\kappa_i u_i(m))^2}{2RT_m} \right) \text{ at } t = t_m; \tag{24}
\]

where \(\frac{1}{2} \rho_0; u_i(0); T(0)\) are the real initial value at \(t = t_0\) for the Euler set, and \(\frac{1}{2} \rho_m; u_i(m); T(m)\) \((m \neq 0)\) are \(\frac{1}{2} u_i; \) and \(T\) calculated from \(f\) at \(t = t_m\) obtained as the solution of Eq. (23) in the interval \((t_{m+1}; t_m)\); The \(\frac{1}{2} u_i; \) and \(T\) of the solution \(f\) at arbitrary time is taken the solution of the corresponding initial-value problem of the Euler set.

The above system being compared with the exact system corresponding to Eq. (14) in the previous system, the difference of the kinetic equations is that on their right-hand side, which is of the order of unity. With the same initial condition, the error of the velocity distribution function \(f\) is order of \(t_{m+1} i t_m\) in the interval \((t_m; t_{m+1})\); that is, \(|f_i f_j| = O(t_{m+1} i t_m)\); our interest is the error of the variables \(\frac{1}{2} u_i; \) and \(T\); These variables or their equivalents \(\frac{1}{2}\) satisfy the conservation equations

\[
\frac{\partial \frac{1}{2}}{\partial t} + \frac{\partial \left( \frac{1}{2} u_i \right)}{\partial x_i} = 0; \tag{25}
\]

and the variables \(\frac{1}{2}; u_i; \) and \(T\) (or \(\frac{1}{2}\)) satisfy

\[
\frac{\partial \frac{1}{2}}{\partial t} + \frac{\partial \left( \frac{1}{2} u_i \right)}{\partial x_i} = 0; \tag{26}
\]

The differences between \(u_i x e s H_i f\) and \(H_i f^c (\frac{1}{2}; r \frac{1}{2})\) are bounded by the difference between \(f\) and \(f^c\) by definition [see Eqs. (3) and (5)], that is,

\[
j H_i f = O(|f_i f_j|) = O(t_{m+1} i t_m); \tag{27}
\]

Thus from Eqs. (25) and (26),

\[
j \frac{1}{2} i \frac{1}{2} j = O((t_{m+1} i t_m)^2); \tag{28}
\]

The the initial distribution function \(f_{m+1}\) at \(t = t_{m+1}\):

\[
f_{m+1} = \frac{\frac{1}{2} \rho_{m+1}}{(2\sqrt{RT_{m+1}})^3} \exp \left( i \frac{(\kappa_i u_i(m+1))^2}{2RT_{m+1}} \right) \tag{29}
\]

differ from \(f^c\) at \(t = t_{m+1}\) only by \(O((t_{m+1} i t_m)^2)\); Continuing the discussion to the next interval, we obtain the same error estimate with the subscripts \((m + 1)\) and \((m)\) shifted by unity. Thus, the errors of the distribution function
f and the macroscopic variables $\frac{1}{2}$ at a finite time $t$ from $f^c$ and $\frac{1}{2}$ are of the order of $\max_j t_{(m+1)} - t_{(m)}$: That is, by modifying the distribution function $f$ to the corresponding Maxwellian $f_{(m)}$ at every end $t_{(m)}$ of time interval, we can limit the error within the order of the maximum length of divided time intervals. Thus, the kinetic system described at the beginning of this section (say, system of free molecular type) is an appropriate one to obtain the solution of the Euler set of equations (the first order system). By choosing an appropriate term on the right-hand side of Eq. (23), we can construct a higher-order system.

By a similar discussion, we nd that the solution of the Navier-Stokes set of equations is obtained by the kinetic system of free molecular type with modification of the initial condition at the beginning of every interval to the function $f^c$ given by Eq. (18). For the rst-order system, the kinetic system of free molecular type is sufficient. It often happen that the viscous and thermal conduction terms [a and b in Eq. (18)] are small corrections and that we would like to obtain the solution correct up to that order. Then, for a reasonable computation avoiding too small time step, we should choose the right hand side of Eq. (6) with $f_c$ given by Eq. (14) as the right-hand side of Eq. (23).

The direct simulation Monte-Carlo (DSMC method) developed by Bird[5] is widely used in engineering problems of a rarefied gas ow. The hybrid-method that combines the DSMC and uid-dynamic (Euler or Navier-Stokes) schemes is developed by several authors (e.g., [6], [7], and references there) to save the computing time of the DSMC computation in the uid-dynamic region, where the effective Knudsen number (the local mean free path divided by the local characteristic length scale of variation of the variables) is small. The main difference among various works is the technique of transition to one region to the other between two quite different schemes. Vasseur's method of kinetic-equation approach reminds us the direct simulation DSMC method in the way: Free molecular computation corresponds to free motion of the particles in DSMC, and modification of the distribution function to Maxwellian in each time step corresponds to changing the velocities of some particles by statistical collision simulation. If the second process of the DSMC computation to modify particle velocities by the statistical process is replaced by modifying the distribution of the particle to the local Maxwellian (24) or the distribution e.g., of the type by Eq. (18), the DSMC computation can be carried out more efciently in the uid-dynamic region. In combination of the original DSMC method and the DSMC version of Vasseur's approach, the transition is done naturally and can be another candidate to time saving in addition of the existing domain splitting method.

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