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Conservation Laws and a Compact Quasi-Gasdynamic System

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Abstract—Based on the application of conservation laws, a compact quasi-gasdynamic system, which was previously obtained using a kinetic model, is derived. The possibility of using algorithms previously used to solve the Navier–Stokes equations to solve this system is discussed.

Keywords: quasi-gasdynamic system of equations, conservation laws, time between molecules' collisions, boundary layer on a plate

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1. INTRODUCTION

A quasi-gasdynamic system of equations (QSE) is obtained from the kinetic model using a procedure similar to that based on which the equations of gas dynamics are obtained from the Boltzmann equation [1–5]. Moreover, the QSE for modeling the flow of a viscous heat-conducting gas differed from the similar system of Navier–Stokes equations by the terms in the order of magnitude of the second order of smallness in terms of the Knudsen number $O(\mathrm{Kn}^2)$. This important fact was confirmed both by the results of the numerical calculations by comparing the data obtained using the QSE and the Navier–Stokes equations, and by the results of the theoretical analysis of the equations included in the QSE [1, 2, 6–9].

The derivation of the QSE from the kinetic model was explicitly based on the fact that near equilibrium (proximity to the local Maxwell distribution), the one-particle distribution function changes slightly at the mean free path l or in the time of the order of the characteristic time between collisions of molecules τ. This ensures the correctness of the QSE, at least from a physical point of view, and from the very beginning of its appearance in the mid-1980s, made it possible to successfully simulate complex gas-dynamic flows of viscous heat-conducting gas [1, 2].

Recently, another popular feature of the QSE has been the ability to adapt algorithms based on it to the architecture of computing systems with high and ultra-high performance. This possibility, which is relevant when using extra-massive parallelism in the calculations, is associated with the presence of a system of terms with second time derivatives of gas-dynamic parameters in the QSE [10]. We also note that the hyperbolic nature of QSE, associated with the presence of second derivatives with respect to time, makes it possible at the algorithmic level to contribute to solving the fault tolerance problem that is relevant while using large quantities of independent calculators [11].

The disadvantage of the QSE is their more cumbersome appearance compared to the Navier–Stokes equations. This drawback is especially evident for the QSE version of the system for modeling problems of magnetic gas dynamics, in which, in addition to molecular viscosity and thermal conductivity, magnetic viscosity is also taken into account. In addition, the non-standard form of the members of the QSE caused certain difficulties when using algorithms previously developed for solving the Navier–Stokes equations.

In [12, 13] the following compact version of the QSE was proposed:

$$W_i = \frac{\tau}{2\rho}\frac{\partial}{\partial x_k}(\rho u_i u_k + \delta_{ik} p), \tag{1}$$

$$\frac{\partial \rho}{\partial t} + \frac{\tau}{2}\frac{\partial^2 \rho}{\partial t^2} + \operatorname{div}\left[\rho(\overline{u} - \overline{w})\right] = 0, \tag{2}$$

$$\frac{\partial \rho \overline{u}}{\partial t} + \frac{\tau}{2}\frac{\partial^2 \rho \overline{u}}{\partial t^2} + \operatorname{div}\left[\rho(\overline{u} - \overline{w}) \otimes \overline{u}\right] + \nabla p = \operatorname{div} P_{NS}, \tag{3}$$

$$\frac{\partial E}{\partial t} + \frac{\tau}{2}\frac{\partial^2 E}{\partial t^2} + \operatorname{div}\left[(E + p)(\overline{u} - \overline{w})\right] = \operatorname{div} \overline{q} + \operatorname{div}(P_{NS}\overline{u}). \tag{4}$$

Here t is time, x_k is the spatial coordinate, $k = 1,2,3$, ρ is density, $\overline{u}$ is speed, p is pressure, E is total energy, $\overline{q}$ is the heat flux vector

$$q_k = \kappa \frac{\partial T}{\partial x_k}, \tag{5}$$

κ is the coefficient of thermal conductivity, and P_{NS} is the viscous stress tensor in the Navier–Stokes equations.

This system (1)–(4) was obtained from the initial quasi-gasdynamic system by estimating by order the magnitude of its members. In this work, system (1)–(4) will be obtained directly from the conservation laws subject to a time limit τ from below between collisions of molecules per time interval Δt.

2. THE CONTINUITY EQUATION OF THE QSE

One of the main differences between the QSE and the gas dynamics equations is the presence of second time derivatives of the gas-dynamic parameters and the appearance of a dissipative term in the continuity equation. Their appearance is due to the fact that in a discrete kinetic model the minimum time scale is the time between collisions τ. Once again, we describe this model [1, 2].

Assume that at a point in time $t = t^j$ the single-particle distribution function of the molecules has the local Maxwell form:

$$f(t^j, x, \overline{\xi}) = f_0 = \frac{\rho(t, \overline{x})}{\left(2\pi RT(t,x)\right)^{3/2}} l \frac{-\left(\xi_i - u_i(t,x)\right)^2}{2RT}. \tag{6}$$

Here, the following notation was additionally used: R is the gas constant and $\overline{\xi}$ is the velocity vector of molecules.

Over time $t^{j+1} - t^j = \tau$, assume that the gas molecules undergo collisionless expansion. Then at time $t = t^{j+1}$, an instantaneous process of the collision of the molecules occurs and the distribution function again becomes locally Maxwellian. After that, the process is repeated. We again draw attention to the fact that in our reasoning the time scales smaller than τ are not considered.

The relationship between the value of the distribution function before maxwellization at time t^{j+1} and the value of the local-Maxwell function at time t^j is expressed by the ratio[1]

$$f(t^{j+1}, \overline{x}, \overline{\xi}) = f_0(t^j, \overline{x} - \overline{\xi}, \tau, \overline{\xi}). \tag{7}$$

We expand the right-hand side of (7) in a Taylor series up to terms of the third order of smallness in magnitude $|\xi|\tau$:

$$f(t^{j+1}, \overline{x}, \overline{\xi}) - f_0(t^j, \overline{x}, \overline{\xi}) = -\tau \xi_i \frac{\partial f_0}{\partial x_i} + \frac{\partial}{\partial x_k}\frac{\tau}{2}\xi_i \xi_k \frac{\partial f_0}{\partial x_i}. \tag{8}$$

Multiply the left and right side of (8) by the adder invariant m, the mass of the molecule, and integrate similarly to obtaining the continuity equation from the Boltzmann equation for the velocities of the molecules. Given that

$$\int f \varphi(\xi) d\xi = \int f_0 \varphi(\xi) d\xi, \tag{9}$$

[1] Here, for simplicity, we assume that the field of external forces affectin the change $\overline{\xi}$ is absent.

where $\varphi(x)$ are adder invariants $\varphi(x) = m, m\bar{\xi}, (m\xi^2/2)$, we get

$$\rho^{j+1} - \rho^j = -\tau \operatorname{div} \rho\bar{u} + \frac{\partial}{\partial x_k}\frac{\tau}{2}\frac{\partial}{\partial x_i}(\rho u_i u_k + \delta_{ik} p). \tag{10}$$

Expanding the left side of (10) in a Taylor series, we finally arrive at the equation:

$$\frac{\partial \rho}{\partial t} + \frac{\tau}{2}\frac{\partial^2 \rho}{\partial t^2} + \operatorname{div} \rho\bar{u} = \frac{\partial}{\partial x_k}\frac{\tau}{2}\frac{\partial}{\partial x_i}(\rho u_i u_k + \delta_{ik} p). \tag{11}$$

This equation is different from the classic continuity equation.

$$\partial\rho/\partial t + \operatorname{div} \rho\bar{u} = 0, \tag{12}$$

$$\text{on the totality of members } \frac{\tau}{2}\frac{\partial^2 \rho}{\partial t^2} - \frac{\partial}{\partial x_k}\frac{\tau}{2}\frac{\partial}{\partial x_i}(\rho u_i u_k + \delta_{ik} p), \tag{13}$$

which in total amount to an order of magnitude $O(\mathrm{Kn}^2)$ [1, 2, 9].

Thus, the discrete kinetic model under consideration, in which the minimum time scale is τ, led to the continuity equation (11), which differs from the classical equation (12) by the sum of the terms in the order of magnitude $O(\mathrm{Kn}^2)$. The same order of the difference between the QSE and the Navier–Stokes equations is observed for equations describing the change in momentum and total energy E and entropy [8, 9]. Recall that the Navier–Stokes equations themselves are obtained from the Boltzmann kinetic equation using the Chapman-Enskog procedure with the same accuracy $O(\mathrm{Kn}^2)$ [3–5].

We now consider the method of obtaining Eq. (2.6), remaining within the traditional methods used in continuum mechanics. Moreover, from the kinetic models, we use only the lower bound for time τ of the interval Δt in which there is a change in the gas-dynamic parameters.[2]

3. THE TRADITIONAL METHOD OF OBTAINING THE CONTINUITY EQUATION OF QSE

Consider the changes in mass in the final volume Ω during $\Delta t = t^{j+1} - t^j$

$$M^{j+1} - M^j \int_\Omega \rho^{j+1} dx - \int_\Omega \rho^j dx = -\int_{t^j}^{t^{j+1}} \oint_S \rho\bar{u} ds, \tag{14}$$

where S is the surface limiting volume Ω and M is the mass of volume Ω.

In contrast to the generally accepted method for obtaining the continuity equation, we consider the final time interval over which the mass of volume changes $\bar{\Omega}$: $\Delta t = t^{j+1} - t^j = \tau$.

Imagine the momentum $\rho\bar{u}$ on the segment $t \in [t^j, t^j + \tau]$ as

$$\rho u(t) = \rho u^j + \tau\frac{\partial \rho u^j}{\partial t} + O(\Delta t^2). \tag{15}$$

We substitute (15) into the right-hand side of (14), integrate over time over the interval $[t^j, t^{j+1}]$, and use the Gauss–Ostrogradsky theorem. As a result, we get

$$\rho^{j+1} - \rho^j = -\tau \operatorname{div}\left(\rho u^j + \frac{\tau}{2}\frac{\partial \rho u^j}{\partial t}\right) + O(\Delta t^2). \tag{16}$$

We represent the left side of expression (16) as

$$\rho^{j+1} - \rho^j = \tau\frac{\partial \rho^j}{\partial t} + \frac{\tau^2}{2}\frac{\partial^2 \rho^j}{\partial t^2} + O(\tau^2), \tag{17}$$

and we use the expression

[2] The choice τ as the minimum scale Δt is not accidental, since the establishment of gas-dynamic parameters occurs in a time period that is not smaller than the characteristic time between molecular collisions τ.

$$\frac{\partial \rho u_i}{\partial t} = -\frac{\partial (\rho u_i u_k + \delta_{ik} p)}{\partial x_k}, \tag{18}$$

to find $(\partial \rho u / \partial t)$; the equality holds exactly for an equation describing the change in momentum in an ideal gas. In a non-ideal gas, this expression is accurate to the terms describing the viscous stress, i.e., $O(\tau)$.

Combining (16)–(18), we finally obtain

$$\frac{\partial \rho}{\partial t} + \frac{\tau}{2}\frac{\partial^2 \rho}{\partial t^2} + \operatorname{div}(\rho \overline{u}) = \frac{\partial}{\partial x_i}\frac{\tau}{2}\frac{\partial}{\partial x_k}(\rho u_i u_k + \delta_{ik} p), \tag{19}$$

which exactly coincides with Eq. (11) obtained based on a discrete kinetic model.

Thus, the introduction of a lower limit on the admissible time interval leads, both in the discrete kinetic model and the macroscopic description, to the appearance of additional terms in the continuity equation. In total, these additional terms amount to an order of magnitude $O(\mathrm{Kn}^2)$, i.e., significantly fewer dissipative viscous and heat-conducting members of the Navier–Stokes system, whose order of magnitude $O(\mathrm{Kn})$. The time smoothing procedure was previously carried out in [14] without the time relation τ with a characteristic time between collisions of molecules. In addition, in the analogue of Eq. (19) obtained in [14], there is no term with the second time derivative $(\tau/2)(\partial^2 \rho / \partial t^2)$.

We represent Eq. (19) in the form

$$\frac{\partial \rho}{\partial t} + \frac{\tau}{2}\frac{\partial^2 \rho}{\partial t^2} + \operatorname{div}\left(\rho(\overline{u} - \overline{w})\right) = 0, \tag{20}$$

$$\text{where } \rho \overline{w} = \frac{\tau}{2}\frac{\partial}{\partial x_k}(\rho u_i u_k + \delta_{ik} p) \tag{21}$$

is the additional impulse arising when taking the lower limit on the minimum change scale Δt into account.

The presence of this impulse and the second derivatives with respect to time associated with a restriction from below to Δt is the main difference between the QSE and the Navier–Stokes system of equations.

A characteristic feature of this impulse is that it can be considered as an integral part of the total impulse $\rho(\overline{u} - \overline{w})$, which affects the change in density (20).

We take into account the presence of speed $\overline{w}$ associated with this additional momentum in the construction of other equations of gas dynamics. Thus, when deriving the momentum balance, we will take into account the kinetic pressure of the gas, the viscous stress tensor P_{NS}, and the generalized momentum $\rho(\overline{u} - \overline{w})$.

Just as for density, we write the change in momentum over time τ in the form

$$(\rho u)^{j+1} - (\rho u)^j = \frac{\partial \rho u^j}{\partial t} + \frac{\tau}{2}\frac{\partial^2 \rho u^j}{\partial t^2} + O(\tau^2) t^{j+1} - t^j = \tau.$$

As a result, the equation for the momentum transfer is written as follows:

$$\frac{\partial \rho u}{\partial t} + \frac{\tau}{2}\frac{\partial^2 \rho u}{\partial t^2} + \operatorname{div}\left[\rho(\overline{u} - \overline{w}) \otimes \overline{u}\right] + \nabla p = \operatorname{div} P_{NS}. \tag{22}$$

Similarly, when deriving the balance for the full energy E,we take into account the energy transfer due to speed $\overline{u} - \overline{w}$, heat flow vectors $\overline{q}$ (5), and the work of viscous forces $P_{NS}\overline{u}$:

$$\frac{\partial E}{\partial t} + \frac{\tau}{2}\frac{\partial E}{\partial t^2} + \operatorname{div}\left[(E + p)(\overline{u} - \overline{w})\right] = \operatorname{div} \overline{q} + \operatorname{div}(P_{NS}\overline{u}). \tag{23}$$

Combining Eqs. (19), (22), and (23), we arrive at the compact QSE (1)–(4).

A similar anlaysis for problems of magnetic gas dynamics will lead to the corresponding compact quasi-gasdynamic equations of magnetic gas dynamics:

$$W_k = \frac{1}{\rho}\frac{\partial}{\partial x_i}\left[\left(p + \frac{B^2}{8\pi}\right)\delta_{ik} + \rho u_i u_k - B_i B_k\right], \tag{24}$$

$$\frac{\partial \rho}{\partial t} + \frac{\tau}{2}\frac{\partial^2 \rho}{\partial t^2} + \operatorname{div}\left[\rho\left(\overline{u} - \overline{w}\right)\right] = 0, \tag{25}$$

$$\frac{\partial \rho \overline{u}}{\partial t} + \frac{\tau}{2}\frac{\partial^2 \rho \overline{u}}{\partial t^2} + \operatorname{div}\left[\rho(\overline{u} - \overline{w}) \otimes \overline{u} + B_i B_k\right] + \nabla\left(p + \frac{B^2}{8\pi}\right) = \operatorname{div} P_{NS}, \tag{26}$$

$$\frac{\partial E}{\partial t} + \frac{\tau}{2}\frac{\partial^2 E}{\partial t^2} + \operatorname{div}\left[\left(E + p + \frac{B^2}{8\pi}\right)(\overline{u} - \overline{w})\right] = \operatorname{div} \overline{q} + \operatorname{div} P_{NS}\overline{u}, \tag{27}$$

$$\frac{\partial B}{\partial t} + \frac{\tau_m}{2}\frac{\partial^2 B}{\partial t^2} = \operatorname{rot}\left[(\overline{u} - \overline{w}) \otimes B + \nu_m \operatorname{rot} B\right], \tag{28}$$

$$\operatorname{div} \overline{B} = 0\ . \tag{29}$$

Here, the following notation was additionally used: $\overline{B}$ is the vector of the tension of the magnetic field and ν_m is the magnetic viscosity.

Equations (24)–(27) can be obtained using a procedure similar to obtaining equations of compact QSE (1)–(4). Equations (28) and (29) were obtained using the complex-valued function [7, 15]

$$f_{OM} = \frac{\rho}{(2\pi RT)^{3/2}} \exp\left[-\left(\xi_k - u_k - i\left(B\Big/\sqrt{4\pi\rho}\right)\right)^2 \Big/ 2RT\right] \tag{30}$$

(here $k = 1,2,3$; i is an imaginary unit) and the subsequent use of the discrete kinetic model, which led to a balance equation similar to (8) [15]:

$$\frac{\partial f_{OM}}{\partial t} + \frac{\tau_m}{2}\frac{\partial^2 f_{OM}}{\partial t^2} + \tau_m \operatorname{div}(\xi f_{OM}) = \frac{\partial}{\partial x_k}\tau_m \xi_i \xi_k \frac{\partial f_{OM}}{\partial x_i}. \tag{31}$$

Time τ_m is the characteristic time of equilibrium in the aggregate ensemble consisting of neutral and charged particles, and the magnetic field $\overline{B}$ can be determined using magnetic viscosity ν_m:

$$\tau_m = \frac{2\rho\nu_m}{p + \left(B^2\Big/(8\pi)\right)}\ . \tag{32}$$

In other words, τ_m is defined similarly to τ through the ratio of viscosity and the total gas kinetic and magnetic pressure.

4. COMPUTATIONAL ALGORITHMS FOR COMPACT QSE

Over the decades of the existence and development of computational hydro- and gas dynamics, a large number of algorithms have been developed with these or other properties. Let us see how these algorithms can be adapted to solve the compact QSE (1)–(4).

First, we consider the approximation of spatial derivatives included in system (1)–(4). Value W_k (1), accurate to the factor $\tau/(2\rho)$, coincides with the spatial derivatives included in the equation describing the change in momentum in the Euler system of equations. After finding $\overline{W}$, determine the speed $\overline{u} - \overline{w} = \overline{v}$. Subsequently, to approximate the spatial derivatives included in system (2)–(4), we can use the algorithms used to solve the Navier–Stokes equations.

Thus, for approximation with respect to spatial variables in a compact quasi-gasdynamic system, we can use the whole arsenal of methods previously accumulated for modeling the Navier–Stokes equations.

Equations (2)–(4) can be written as

$$\frac{\partial \overline{Q}}{\partial t} + \frac{\tau}{2}\frac{\partial^2 \overline{Q}}{\partial t^2} = \operatorname{div} \overline{S}_{\overline{Q}}. \tag{33}$$

Here $\overline{Q}$ is the vector of gas-dynamic variables, $\overline{Q} = \rho, \rho\overline{u}$, and E and $\overline{S}_{\overline{Q}}$ is the flow dependent on Q.

The simplest approximation is a three-layer explicit scheme:

$$\frac{\overline{Q}^{j+1} - \overline{Q}^{j-1}}{2\Delta t} + \frac{\tau^*}{2}\frac{\overline{Q}^{j+1} - 2\overline{Q}^{j} + \overline{Q}^{j-1}}{\Delta t^2} = \operatorname{div} S^j_{\overline{Q}}. \tag{34}$$

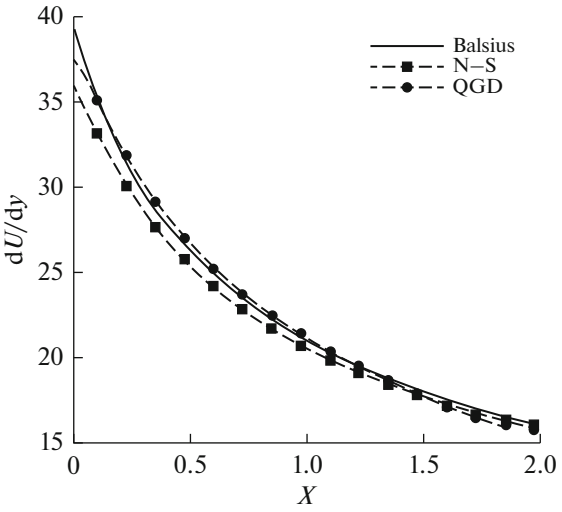

Fig. 1.

To obtain the computational effect of using the second time derivative instead of τ choose a large value τ^*. τ^* is optimal by the order of magnitude, coinciding with the ratio of the characteristic grid pitch h to the characteristic speed υ:

$$\tau^* \sim h/\upsilon. \tag{35}$$

With this value τ^* the necessary condition

$$\left[\frac{\tau^*}{2}\frac{\partial^2\bar{Q}}{\partial t^2}\right] \ll \left[\frac{\partial\bar{Q}}{\partial t}\right], \tag{36}$$

is satisfied and the stability of the three-layer scheme is ensured with the following restriction on the time step Δt [17]:

$$\Delta t \lesssim h^{3/2}. \tag{37}^3$$

The aim of this work is to analyze and identify the capabilities of a compact QSE rather than modeling specific gas-dynamic flows. Therefore, to illustrate the capabilities of system (1)–(4), we use the results of the calculations of a homogeneous viscous gas flow around a flat plate with the Mach number $M = 0.2$ and Reynolds number $Re = 10^5$ taken from [13].

Figure 1 shows the stress of friction $\partial u/\partial y$ along a flat plate. The results obtained using the Blasius solution [17], the solution obtained using the Navier–Stokes equations, and the compact QSE were compared.

It can be seen that all three solutions are close to each other when moving away from the edge of the plate. Nevertheless, near the edge, the solution based on the Navier–Stokes equations differs more from the Blasius solution than the solution based on the QSE. This is due to the fact that near the edge the effective Knudsen number increases. In contrast to the Navier–Stokes equations, the QSE, make it possible to correctly describe the gasdynamic parameters at much larger Knudsen numbers [1, 18].

CONCLUSIONS

Based on the conservation laws and taking into account the presence of a minimum time scale, a method for obtaining a compact quasi-gas-dynamic system is described. Thus, a relationship is realized between the kinetic and macroscopic methods of deriving both a quasi-gas-dynamic system and its compact version. The obvious advantage of the compact version of the QSE under consideration lies in their ability to adapt the algorithms used to solve them to the architecture of ultra-high performance computing

[3] The advantages of condition (37) over the stability condition for explicit schemes for parabolic equations ($\Delta t \lesssim h^2$) are especially evident with detailed spatial approximations (small h), which are implemented on high-performance computing systems.

systems. In addition, a simple transfer of previously developed algorithms for modeling viscous gas flows to the solution of compact QSE is possible.

CONFLICT OF INTEREST

The authors declare that they have no conflicts of interest.

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