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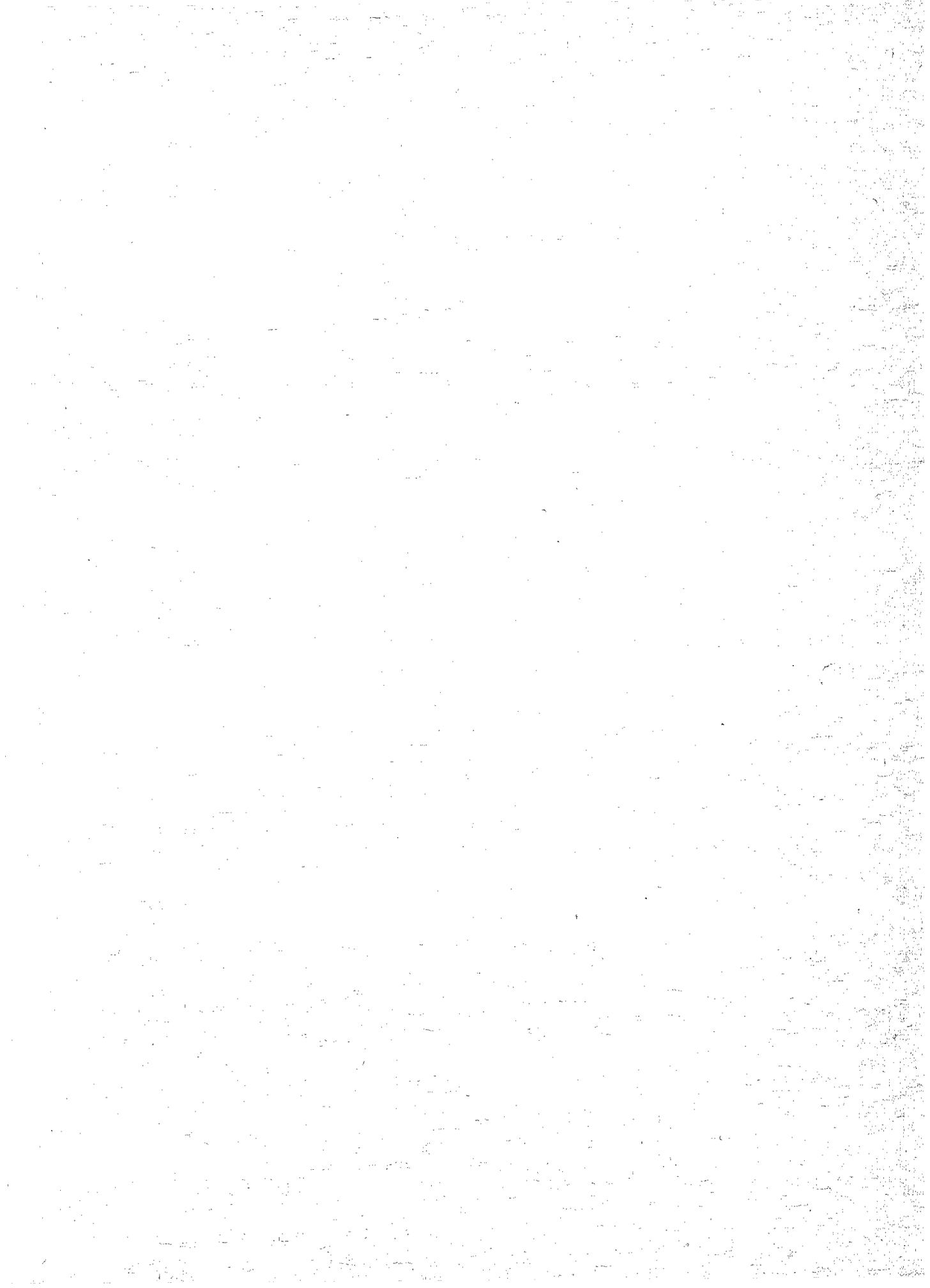
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# The Piecewise Ergodic Problem for Gas Systems

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Abstract: To inform ourselves and others about the innate relaxation structures of nonequilibrium theory, we present in this report a brief outline of the piecewise ergodic problem of organizing and ordering the various relaxation processes of a gas system. Our outline follows the development of G. E. Uhlenbeck.

The central problem stimulating this work is loosely described: What are the connections and relations between the coarse phenomenological laws of gas dynamics and the fine detailed laws of classical mechanics governing a molecular system?

Phenomenologically, the physical gas can be described very well using the concepts of temperature, pressure, viscosity, *etc.* without exact knowledge of the intermolecular forces and without constant referral to the molecular behavior. Of course, less information about the system is stored in this form of description than is stored in the exact knowledge of the motions of all individual molecules; however, the latter description presents a formidable problem of extracting information.

Several descriptions are available with different levels of information and simpler methods of information retrieval. The information level is essentially determined by the choice of "state variables" used to describe the system; *i.e.*, the choice of phase space. The choice of state variables is imposed by the particular experimental phenomena which is studied.

As emphasized by Uhlenbeck [1], a given set of state variables will be useful for the extraction of information provided it is (a) closed, meaning we can ignore the phase spaces of the descriptions with greater information, and (b) causal, meaning we can make predictions from initial data.

The most detailed (in fact, totally exact) description is made using the instantaneous assignment of position  $x$  and velocity  $v$  coordinates to each of the  $N$  molecules; so that, a state variable on this information level is a point  $p = (x_1, v_1), \dots, (x_n, v_n)$  in  $6N$  space. The motion of the point  $p(t)$  in the phase space is governed by the associated Hamiltonian system of equations: For unit mass points interacting through additive central forces with a common interaction potential and no outside forces, the given Hamiltonian of the system is [1a]

$$H(p) = \sum_{i=1}^N \frac{v_i^2}{2} + \sum_{i < j} \phi(|x_i - x_j|), \quad (1)$$

and the equations of motion for the spatial and velocity coordinates are

$$\dot{x}_i = \frac{\partial H}{\partial v_i}, \quad 1 \leq i \leq N, \quad (2a)$$

$$\dot{v}_i = -\frac{\partial H}{\partial x_i}, \quad 1 \leq i \leq N. \quad (2b)$$

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The system can also be described exactly using the (dual) Liouville equation governing the evolution of the distribution function  $\mathcal{W}(t,p)$  for the system to be found in the state  $p$  at time  $t$ . The distribution function  $\mathcal{W}(t,p)$  is a closed and causal state variable.

A second description with less information and incorporating less detail is made using the "molecular" distribution function  $F(t,x,v)$  for the number of molecules in an elementary volume of the six-dimensional phase space for a single molecule.

Classically, the evolution of  $F$  for a dilute gas is governed by the famous integral-differential equation of Boltzmann [2a]:

$$\frac{\partial F}{\partial t} = -v \cdot \text{grad}_x F + \int dv_1 \int d\Omega g I(g,\theta) (F'F'_1 - FF_1), \quad (3)$$

where the indices on  $F$  indicate the four velocity variables describing a binary collision, namely,  $(v,v_1) \rightarrow (v,v'_1)$ ; where  $g = |v' - v_1| = |v' - v'_1|$  is the magnitude of the relative velocity, which is rotated through an angle  $\theta$  in the collision plane by a collision; and where  $I(g,\theta)$  is the differential collision cross section (probability) for a  $(g,\theta)$  collision in unit time and is determined from the known intermolecular potential  $\phi$ .

If we assume  $F$  is defined by Eq. (3), then  $F$  is a closed-state variable, since Eq. (3) requires no knowledge of the molecular background except qualitative features of  $\phi$ . However, the determination of  $I(g,\theta)$ , using classical mechanics, requires a referral to the molecular description.  $F$  is also apparently causal, since its solutions of Eq. (3) are uniquely determined by their initial values  $F(0,x,v)$ .

Again a coarser description is made using the experimental quantities

$$\begin{aligned} \rho &= \text{mass density,} \\ Q &= \text{thermal energy density,} \\ \bar{u}_i &= \text{average velocity vector,} \\ P_{ij} &= \text{pressure tensor,} \\ q_i &= \text{thermal flow density vector.} \end{aligned}$$

If these quantities are related to various moments of the molecular distribution function  $F$ , giving

$$\rho = \int F dv, \quad (4a)$$

$$Q = \frac{\rho}{2} \int |U|^2 F dv, \quad (4b)$$

$$\bar{u}_i = \int v_i F dv, \quad (4c)$$

$$U_i = v_i - \bar{u}_i, \quad (4d)$$

$$P_{ij} = \rho \int U_i U_j F dv, \quad (4e)$$

$$q_i = \frac{\rho}{2} \int U_i |U|^2 F dv, \quad (4f)$$

then it is possible to derive the conservation laws [2b]:

$$\frac{\partial P}{\partial t} + \text{div}(\rho \bar{u}) = 0, \quad (5a)$$

$$\rho \frac{D}{Dt} \bar{u}_i = - \sum_{j=1}^3 \frac{\partial P_{ij}}{\partial x_j}, \quad 1 \leq i \leq 3, \quad (5b)$$

$$\rho \frac{D}{Dt} Q + \sum_{j=1}^3 \frac{\partial q_j}{\partial x_j} = - \frac{1}{2} \sum_{i,j=1}^3 P_{ij} D_{ij}, \quad (5c)$$

where

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \sum_{j=1}^3 \bar{u}_j \frac{\partial}{\partial x_j},$$

$$D_{ij} = \frac{1}{2} \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right).$$

The state variables  $\rho$ ,  $Q$ ,  $\bar{u}$ ,  $P$ , and  $q$  are closed relative to the molecular background; however, they are not closed relative to the "kinetic" background determined by Eq. (3). The conservation Eqs. (5) contain too many unknowns.

A still coarser description is made on the "fluid" level by choosing the mass density  $\rho$ , thermal energy density  $Q$ , and average thermal velocity  $\bar{u}$  as the principle state variables. Classically they are related through the Navier-Stokes equations of hydrodynamics, which can be obtained from Eqs. (5) by using the Newton and Fourier laws [2c], with known viscosity  $\mu$  and heat conduction  $\kappa$  coefficients, to calculate the pressure tensor  $P_{ij}$  and heat flux  $q_i$ :

$$P_{ij} = \frac{2}{3} Q \delta_{ij} - 2\mu \left( D_{ij} - \frac{1}{3} \sum_l D_{ll} \delta_{ij} \right), \quad (6a)$$

$$q_i = \kappa \frac{\partial Q}{\partial x_i}. \quad (6b)$$

Labeling the first of the descriptions as dynamic ( $W$ ), the second as kinetic ( $F$ ), and the third as hydrodynamic ( $\rho, Q, \bar{u}$ ), Uhlenbeck [3] posed the following problem: try to follow the gas to thermal equilibrium through the various descriptive levels; dynamic to kinetic, kinetic to hydrodynamic, and hydrodynamic to thermal equilibrium.

Many researchers have studied the connective relations between the different levels of description: Bogoliubov [4], Frieman [5], Sandri [6], McCune, Sandri, and Frieman [7], Kirkwood [8], and Prigogine and Balescu [9]. A paper by Cohen [10], gives a comparison of several methods and contains an extended bibliography. Of course the original works of Boltzmann [11] are an indispensable foundation.

Let us concentrate on a connection between the kinetic and hydrodynamic descriptions.

Suppose  $F$  is a solution of the Boltzmann equation, Eq. (3), and define the mass density  $\rho$ , thermal energy density  $Q$ , and average thermal velocity  $\bar{u}$  using Eqs. (4a) through (4c). These are chosen as the principle state variables for a hydrodynamic description, since they are less sensitive to collisions than  $P$  and  $q$ . Since the conservation equations, Eqs. (5), derived from Eq. (3) by simply taking velocity moments, contain the pressure tensor  $P$  and thermal flow

density vector  $\mathbf{q}$ , the state variables  $\rho$ ,  $Q$ , and  $\bar{u}$  are generally not closed, being tied to the kinetic background  $F$  through  $P$  and  $\mathbf{q}$ . Curiously, Maxwell [12] found that, after a certain relaxation time,  $P$  and  $\mathbf{q}$  attain quasi-equilibrium values which depend only on the gradients of the hydrodynamic variables and not on the initial values of  $P$  and  $\mathbf{q}$ .

This suggests that the stress tensor  $P$  and thermal flow density vector  $\mathbf{q}$  can be eliminated from Eqs. (5) by expressing them as gradients of the hydrodynamic variables. If this is true, then the consequent closed conservation equations for  $\rho$ ,  $Q$ , and  $\bar{u}$  would possibly determine them from their initial values. As a result the classical Navier-Stokes equations would then become an approximation to the true conservation equations for  $\rho$ ,  $Q$ , and  $\bar{u}$  and the Newton-Fourier laws would become an approximation to the true expressions of  $P$  and  $Q$  as gradients of  $\rho$ ,  $Q$ , and  $\bar{u}$ . However, we must recall the existence of solutions of the Boltzmann equation with nonzero stresses and zero gradients of the hydrodynamic variables.

Hilbert, Chapman, Enskog and others have formulated methods for extracting information about  $\rho$ ,  $Q$ , and  $\bar{u}$  from  $F$ . A paper of Grad [13] contains a useful comparison of the Hilbert and Chapman-Enskog methods. In essence, these methods develop algorithms for constructing special (Hilbert) solutions  $F$  for which  $P$  and  $\mathbf{q}$  can be determined using gradients of  $\rho$ ,  $Q$ , and  $\bar{u}$ .

Grad [13] has developed an asymptotic theory relating the formal Hilbert solutions of the Hilbert and Chapman-Enskog algorithms to actual solutions of the Boltzmann equation. McCune, Morse, and Sandri [14] have developed an asymptotic analysis of the transient behavior of the stress tensor  $P$  and thermal vector  $\mathbf{q}$  as the gas relaxes to its fluid description.

Most, if not all, of the past work focused on developing methods for extracting the desired information contained in the distribution function  $F$ , assuming the necessary relaxation structure existed. As a rule the required relaxation parameters are developed and introduced in the context of the molecular background and not as characteristic parameters of the equation.

Recently, McKean [15] developed a characterization of the Hilbert solutions and showed the relationship to ordinary solutions for a linear two-state system, corresponding to the linearization about an equilibrium state in a two-state nonlinear system with either colinear or uniform scattering laws. This work and my personal association with McKean, while visiting Rockefeller University (1966-1968), prompted the investigations I am undertaking.

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