Boltzmann's Equation and Classical Hydrodynamic Models Based on Maximum Entropy Principle

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1/15/2010

Abstract

The Liouville equation describes the time evolution of a phase-space distribution function. L. Boltzmann formulated his equation in 1872 for a nonequilibrium system of many particles in dilute gases by analyzing the elementary collision processes between pairs of particles. A tremendous amount of hydrodynamic (HD) models have been derived since then by means of the moment method which raises many practical problems of the models associated with the so-called closure problem of the method. In 1996, C. Levermore has derived the HD models based on the maximum entropy principle which sets the derivation of classical HD and quantum HD models on a clear physical and mathematically rigorous basis. These topics will be briefly presented here with the 1D Euler equations of an ideal gas as an illustrative example.

The Single-Particle Liouville Equation

We first consider a particle of constant mass m moving in a conservative force field for which the total energy E of the particle is

$$E = K + V = \text{constant} \tag{1}$$

where $K(t, \mathbf{x})$ is the kinetic energy and $V(\mathbf{x})$ is the potential energy. The particle is associated with the position vector $\mathbf{x} = (x_1, x_2, x_3) \in R^3_{\mathbf{x}}$, the velocity vector $\mathbf{v} = (v_1, v_2, v_2) \in R^3$, and the momentum vector $\mathbf{p} = m\mathbf{v} = (p_1, p_2, p_2) \in R^3_{\mathbf{p}}$. Then the force $\mathbf{F}$ acting on the particle is given by

$$\mathbf{F} = m\frac{d\mathbf{v}}{dt} = -\nabla_{\mathbf{x}} V. \tag{2}$$

25 January 2010

From this equation, we obtain the system of ordinary differential equations

$$\frac{d\mathbf{x}}{dt} = \mathbf{v} \tag{3}$$

$$\frac{d\mathbf{p}}{dt} = -\nabla_{\mathbf{x}} V = \mathbf{F} \tag{4}$$

which describes the trajectories of the particle in the phase (position-momentum) space, i.e., in the 6 dimensional $(\mathbf{x}, \mathbf{p})$-space. Together with a given initial state $\mathbf{x}(t=0) = \mathbf{x}_0$, $\mathbf{p}(t=0) = \mathbf{p}_0$ this system constitutes an initial value problem for the trajectory $(\mathbf{x}(t), \mathbf{p}(t))$ passing through $(\mathbf{x}_0, \mathbf{p}_0)$. Instead of the precise initial state $(\mathbf{x}_0, \mathbf{p}_0)$, we assume that the particle is represented by *probability density (distribution) function* $f(t, \mathbf{x}, \mathbf{p}) \geq 0$ such that its initial state is expressed by

$$\iint f(0, \mathbf{x}, \mathbf{p}) d\mathbf{x} d\mathbf{p} = 1 \tag{5}$$

which means that at $t = 0$ the particle exists in the whole $(\mathbf{x}, \mathbf{p})$-space (the probability to locate it is 1). Thus, $P(t, B) = \iint_B f(t, \mathbf{x}, \mathbf{p}) d\mathbf{x} d\mathbf{p}$ means the probability to find the particle in a subset B of $(\mathbf{x}, \mathbf{p})$-space at the time t. It is reasonable to postulate that $f(t, \mathbf{x}, \mathbf{p})$ does not change along the trajectories of the particle (the shape of the distribution function of the particle does not change), i.e., we assume

$$f(t, \mathbf{x}, \mathbf{p}) = f(0, \mathbf{x}, \mathbf{p}) \quad \forall \mathbf{x}, \mathbf{v} \text{ and } \forall t \geq 0. \tag{6}$$

Differentiating (6) with respect to t gives

$$\begin{aligned}
0 &= \frac{df(0, \mathbf{x}, \mathbf{p})}{dt} = \frac{df(t, \mathbf{x}, \mathbf{p})}{dt} && (7)\\
&= \frac{\partial f}{\partial t} + \sum_{i=1}^{3} \left(\frac{\partial f}{\partial x_i} \frac{dx_i}{dt} + \frac{\partial f}{\partial p_i} \frac{dp_i}{dt} \right) && (8)\\
&= \frac{\partial f}{\partial t} + \frac{d\mathbf{x}}{dt} \cdot \nabla_{\mathbf{x}} f + \frac{d\mathbf{p}}{dt} \cdot \nabla_{\mathbf{p}} f && (9)\\
&= \frac{\partial f}{\partial t} + \frac{d\mathbf{x}}{dt} \cdot \nabla_{\mathbf{x}} f - \nabla_{\mathbf{x}} V \cdot \nabla_{\mathbf{p}} f && (10)
\end{aligned}$$

which is the classical *Liouville* (or *transport*) equation governing the evolution of the distribution function of a particle in a force field.

Boltzmann's Equation

For a system of M particles (an *ensemble* of M interacting particles), the single-particle distribution function $f(t, \mathbf{x}, \mathbf{p})$ in (5) is generalized to the many-particle distribution function as

$f(t, \mathbf{x}, \mathbf{p})$ denotes the number of particles per unit volume in $d\mathbf{x}d\mathbf{p}$,
(f is a *microscopic* variable) (11)

with $\mathbf{x} \in R^3_{\mathbf{x}}$ and $\mathbf{p} \in R^3_{\mathbf{p}}$ such that

$$\iint f(t, \mathbf{x}, \mathbf{p}) d\mathbf{x}d\mathbf{p} = M. \tag{12}$$

If the rate of change of the particle ensemble due to the convection caused by the force field vanishes along its trajectories when collisions are neglected, we have a similar equation as (10), i.e.,

$$\left(\frac{df}{dt}\right)_{\text{conv}} := \frac{\partial f}{\partial t} + \frac{d\mathbf{x}}{dt} \cdot \nabla_{\mathbf{x}} f - \nabla_{\mathbf{x}} V \cdot \nabla_{\mathbf{p}} f = 0. \tag{13}$$

L. Boltzmann postulated in *1872* that for a nonequilibrium system of many particles (dilute gases) it is reasonable to assume that the rate of change of the ensemble due to convection and the rate of change due to collisions balance, i.e.,

$$\left(\frac{df}{dt}\right)_{\text{conv}} = \left(\frac{df}{dt}\right)_{\text{coll}}. \tag{14}$$

The Boltzmann equation hence reads as

$$\frac{\partial f}{\partial t} + \frac{d\mathbf{x}}{dt} \cdot \nabla_{\mathbf{x}} f - \nabla_{\mathbf{x}} V \cdot \nabla_{\mathbf{p}} f = C(f), \tag{15}$$

where C is the *collision operator* representing the short range collisions of the particles with other particles and with their environment. The operator is defined by

$$\left(\frac{df}{dt}\right)_{\text{coll}} := C(f) = \int \left[s(\mathbf{x}, \mathbf{p}', \mathbf{p}) f'(1 - f) - s(\mathbf{x}, \mathbf{p}, \mathbf{p}') f(1 - f')\right] d\mathbf{p}' \tag{16}$$

where $f' := f(t, \mathbf{x}, \mathbf{p}')$, the integral represents the 'sum' of rates of particles being scattered from all possible states $(\mathbf{x}, \mathbf{p}')$ into the state $(\mathbf{x}, \mathbf{p})$ at time t minus the sum of the rates of the particles being scattered from $(\mathbf{x}, \mathbf{p})$ into $(\mathbf{x}, \mathbf{p}')$, $(1 - f)$ is the probability that the state $(\mathbf{x}, \mathbf{p})$ is not occupied, and $s(\mathbf{x}, \mathbf{p}', \mathbf{p})d\mathbf{p}'$ is the transition (scattering) rate for a particle with position vector $\mathbf{x}$ to change its velocity $\mathbf{p}'$ belonging to the volume $d\mathbf{p}'$ (around $\mathbf{p}'$) to $\mathbf{p}$.

The Moment Method

The computational cost for solving the Boltzmann (integro-differential) equation (15) in 7 dimensional $(t, \mathbf{x}, \mathbf{p})$-space is *extremely expensive* albeit its physical accuracy. It also provides *too much* information than necessary. In applications, we are usually interested in a *few macroscopic quantities* that can be

experimentally observed, for example, the macroscopic variables of particle density $\rho(t,\mathbf{x})$, particle mean (averaged) velocity $\mathbf{u}(t,\mathbf{x})$, and particle mean temperature $T(t,\mathbf{x})$.

We introduce the *moment functions* $\psi_j(\mathbf{p})$ and the corresponding *moments*

$$\mu_j := \langle f, \psi_j \rangle := \int_{R^3_{\mathbf{p}}} f(t,\mathbf{x},\mathbf{p})\psi_j(\mathbf{p})d\mathbf{p}, \quad j = 1, \cdots m. \tag{17}$$

As the most important moments (*macroscopic variables*), we mention

$$\mu_1 := \rho = \langle f, \psi_1 \rangle = \langle f, 1 \rangle \quad \text{(mass density)} \tag{18}$$
$$\mu_2 := \rho\mathbf{u} = \langle f, \psi_2 \rangle = \langle f, \mathbf{p} \rangle \quad \text{(momentum density)} \tag{19}$$
$$\mu_3 := E = \langle f, \psi_3 \rangle = \left\langle f, \frac{1}{2}|\mathbf{p}|^2 \right\rangle \quad \text{(energy density)} \tag{20}$$

Multiplying (15) by a moment function $\psi(\mathbf{p})$ and integrating over the momentum space $R^3_{\mathbf{p}}$, we have

$$\int \psi(\mathbf{p}) \left[\frac{\partial f}{\partial t} + \mathbf{p} \cdot \nabla_{\mathbf{x}} f - \nabla_{\mathbf{x}} V \cdot \nabla_{\mathbf{p}} f \right] d\mathbf{p} = \int \psi(\mathbf{p}) C(f) d\mathbf{p} \tag{21}$$

$$\frac{\partial \mu}{\partial t} + \sum_{i=1}^{3} \left(\frac{\partial \langle f, p_i \psi \rangle}{\partial x_i} + \left\langle \frac{\partial f}{\partial p_i}, F_i \psi \right\rangle \right) = \langle C(f), \psi \rangle \tag{22}$$

The *conservation laws* of *mass*, *momentum*, and *energy* imply that

$$\left\langle C(f), \begin{bmatrix} 1 \\ \mathbf{p} \\ \frac{1}{2}|\mathbf{p}|^2 \end{bmatrix} \right\rangle = 0 \tag{23}$$

where the moment functions in (21) are chosen as in (18)-(20). We now derive the first equation of (21) via (23). By the *divergence theorem*, we observe from (21) and $\psi_1(\mathbf{p}) = 1$ that

$$\begin{aligned}
\int_{\Omega_{\mathbf{p}}} \psi_1(\mathbf{p}) \mathbf{F} \cdot \nabla_{\mathbf{p}} f d\mathbf{p} &= \sum_{i=1}^{3} F_i \int_{\Omega_{\mathbf{p}}} \psi_1(\mathbf{p}) \frac{\partial f}{\partial p_i} d\mathbf{p} \\
&= \sum_{i=1}^{3} F_i \left(\int_{\partial\Omega_{\mathbf{p}}} \psi_1 f n_i d\mathbf{p} - \int_{\Omega_{\mathbf{p}}} f \frac{\partial \psi_1}{\partial p_i} d\mathbf{p} \right) \\
&= -\sum_{i=1}^{3} F_i \int_{\Omega_{\mathbf{p}}} f \frac{\partial \psi_1}{\partial p_i} d\mathbf{p} \qquad (24) \\
&= -\int_{\Omega_{\mathbf{p}}} f \mathbf{F} \cdot \nabla_{\mathbf{p}} \psi_1 d\mathbf{p} = 0 \qquad (25)
\end{aligned}$$

where $\mathbf{n} = (n_1, n_2, n_3)$ is a unit outward vector on the boundary $\partial\Omega_{\mathbf{p}}$ of an arbitrary open set $\Omega_{\mathbf{p}}$ of $R^3_{\mathbf{p}}$ where we assume that f vanishes. By (18), we thus obtain the *continuity equation* (the conservation of mass)

$$\frac{\partial \rho}{\partial t} + \nabla_{\mathbf{x}} \cdot (\rho \mathbf{u}) = 0. \tag{26}$$

Note that in this derivation process we have already introduced another (*extra*) unknown variable $\mathbf{u}$. Together with the unknown variable ρ, we need to have one more equation to determine the two variables ($\mu_1 = \rho, \mu_2 = \mathbf{u}$) uniquely. We then do a similar derivation from (21) by choosing the second moment $\psi_2 = \mathbf{p}$ to get the extra equation of conservation of momentum (see below). However, once we obtain the second equation, we will encounter a similar problem, i.e., one more unknown variable will be introduced. This means that there always exists one more next equation waiting to be derived or the last unknown variable has to be determined (*closed*) by some formula which is frequently based on a heuristic physical or mathematical way. This is the so-called the *closure problem* in the moment-based literature for deriving hydrodynamic models from Boltzmann's equation. In the literature, we may have as many as *35-moment equations*. The more moment equations we have the more accurate physical results we get with of course the more computational cost that we must pay.

The Maximum Entropy Principle

Since Levermore's 1996 paper [1], there has been a great deal of work on the development of classical and quantum hydrodynamic (HD) models based on the maximum entropy principle (MEP) "à la Levermore" [2,3]. This approach stands upon a clear physical basis and mathematical rigorousness. It has been shown to be robust and flexible in formulating various HD models in applications.

The MEP is a *postulate* stating that if a certain number of moments μ_j, $j = 1, \cdots m$, are given, then there exists a distribution function f_{ME} that maximizes the entropy functional

$$H(f) = -\int (f \ln f - f)\, d\mathbf{p} \tag{27}$$

under the constraints

$$\mu_j = \int f \psi_j(\mathbf{p}) d\mathbf{p}. \tag{28}$$

Introducing the Lagrange multipliers λ_j, this contrained optimization problem is equivalent to maximize the following Lagrange functional without constraints

$$L(f) = H(f) + \boldsymbol{\lambda} \cdot \left(\int f \boldsymbol{\psi}(\mathbf{p}) d\mathbf{p} - \boldsymbol{\mu} \right) \tag{29}$$

where $\boldsymbol{\lambda}$, $\boldsymbol{\mu}$, and $\boldsymbol{\psi}$ are m-component vectors. The necessary condition that all directional derivatives vanish at the maximizer f_{ME} leads to

$$\begin{aligned} 0 &= \frac{dL}{df} = -\int \ln f d\mathbf{p} + \boldsymbol{\lambda} \cdot \int \boldsymbol{\psi}(\mathbf{p}) d\mathbf{p} \\ &= \int \left(\ln f + \boldsymbol{\lambda} \cdot \boldsymbol{\psi}\right) d\mathbf{p} \end{aligned} \tag{30}$$

so that

$$\ln f_{\mathrm{ME}} + \boldsymbol{\lambda} \cdot \boldsymbol{\psi} = 0 \Longrightarrow f_{\mathrm{ME}} = \exp\left(\boldsymbol{\lambda} \cdot \boldsymbol{\psi}\right) \tag{31}$$

where the Lagrange multipliers $\boldsymbol{\lambda}$ have to be chosen in such a way that the moment constraints (28) are satisfied, i.e.,

$$\mu_j = \int \exp\left(\boldsymbol{\lambda} \cdot \boldsymbol{\psi}\right) \psi_j(\mathbf{p}) d\mathbf{p}. \tag{32}$$

Suppose that we are given the three moments $\boldsymbol{\mu}$ associated with the three moment functions $\boldsymbol{\psi}$ as that in (18)-(20), i.e.,

$$\boldsymbol{\mu} = \begin{bmatrix} \mu_1 \\ \mu_2 \\ \mu_3 \end{bmatrix} = \begin{bmatrix} \rho \\ \rho \mathbf{u} \\ E = \frac{1}{2}\rho \left|\mathbf{u}\right|^2 + \frac{3}{2}\rho T \end{bmatrix}, \quad \boldsymbol{\psi} = \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{bmatrix} = \begin{bmatrix} 1 \\ \mathbf{p} \\ \frac{1}{2}\left|\mathbf{p}\right|^2 \end{bmatrix}, \tag{33}$$

it is shown [2] that the maximizer distribution function f_{ME} of the entropy maximization problem (29) is the Maxwellian

$$f_{\mathrm{Max}} = \frac{\rho}{\left(2\pi T\right)^{3/2}} \exp\left(-\frac{\left|\mathbf{p} - \mathbf{u}\right|^2}{2T}\right) \tag{34}$$

which satisfies

$$\int f_{\mathrm{Max}} \begin{bmatrix} 1 \\ \mathbf{p} \\ \frac{1}{2}\left|\mathbf{p}\right|^2 \end{bmatrix} dp = \begin{bmatrix} \rho \\ \rho \mathbf{u} \\ \frac{1}{2}\rho \left|\mathbf{u}\right|^2 + \frac{3}{2}\rho T \end{bmatrix}. \tag{35}$$

By this equation, we thus now *close* the moment system (21) and obtain the *Euler* equations of gas dynamics

$$\frac{\partial}{\partial t} \begin{bmatrix} \rho \\ \rho \mathbf{u} \\ \frac{1}{2}\rho \left|\mathbf{u}\right|^2 + \frac{3}{2}\rho T \end{bmatrix} + \nabla_{\mathbf{x}} \cdot \begin{bmatrix} \rho \mathbf{u} \\ \rho \mathbf{u} \otimes \mathbf{u} + \rho T \mathbf{Id} \\ \left(\frac{1}{2}\rho \left|\mathbf{u}\right|^2 + \frac{5}{2}\rho T\right) \mathbf{u} \end{bmatrix} = \begin{bmatrix} 0 \\ -\rho \nabla_{\mathbf{x}} V \\ \rho \mathbf{u} \cdot \nabla_{\mathbf{x}} V \end{bmatrix}. \tag{36}$$

With the pressure $p = \rho T$ and without external force, the 1D Euler equations of an ideal gas are

$$\frac{\partial}{\partial t}\begin{bmatrix} \rho \\ \rho u \\ \frac{1}{2}\rho u^2 + \frac{3}{2}p \end{bmatrix} + \frac{\partial}{\partial x}\begin{bmatrix} \rho u \\ \rho u^2 + p \\ \left(\frac{1}{2}\rho u^2 + \frac{5}{2}p\right) u \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}. \tag{37}$$

References

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[3] P. Degond, S. Gallego, F. Méhats, and C Ringhofer, Quantum hydrodynamic and diffusion models derived from the entropy principle, in Lecture Notes in Math., Springer-Verlag, 1946 (2008) 111-168.