Tai-Ping Liu

Academia Sinica, Taiwan
Stanford University

Newton Institute, September 28, 2010
Hilbert Sixth Problem: Mathematical Treatment of the Axioms of Physics.

The investigations on the foundations of geometry suggest the problem: To treat in the same manner, by means of axioms, those physical sciences in which mathematics plays an important part; in the first rank are the theory of probabilities and mechanics.

As to the axioms of the theory of probabilities, it seems to me desirable that their logical investigation should be accompanied by a rigorous and satisfactory development of the method of mean values in mathematical physics, and in particular in the kinetic theory of gases.
Important investigations by physicists on the foundations of mechanics are at hand; I refer to the writings of Mach, Hertz, Boltzmann and Volkmann. It is therefore very desirable that the discussion of the foundations of mechanics be taken up by mathematicians also. Thus Boltzmann’s work on the principles of mechanics suggests the problem of developing mathematically the limiting processes, there merely indicated, which lead from the atomistic view to the laws of motion of continua.
Kinetic Theory

\[ f(x, t, \xi), \text{ density distribution function} \]

\( x \in \mathbb{R}^3 \) space, \( t \) time,
\( \xi \in \mathbb{R}^3 \) microscopic velocity.

Macroscopic variables

\[
\begin{cases}
\rho(x, t) \equiv \int_{\mathbb{R}^3} f(x, t, \xi) d\xi, \text{ density,} \\
\rho \mathbf{v}(x, t) \equiv \int_{\mathbb{R}^3} \xi f(x, t, \xi) d\xi, \text{ momentum,}
\end{cases}
\]

\[
\begin{cases}
\rho E(x, t) \equiv \int_{\mathbb{R}^3} \frac{|\xi|^2}{2} f(x, t, \xi) d\xi, \text{ total energy.} \\
\rho e(x, t) \equiv \int_{\mathbb{R}^3} \frac{|\xi - \mathbf{v}|^2}{2} f(x, t, \xi) d\xi, \text{ internal energy,}
\end{cases}
\]

\[ \rho E = \rho e + \frac{1}{2} \rho |\mathbf{v}|^2. \]
Hilbert Sixth Problem

Macroscopic variables

\[
\begin{align*}
p_{ij}(x, t) & \equiv \int_{\mathbb{R}^3} (\xi_i - v_i)(\xi_j - v_j) f(x, t, \xi) d\xi, \\
p & \equiv \frac{p_{11} + p_{22} + p_{33}}{3} = \frac{1}{3} \int_{\mathbb{R}^3} |v - \xi|^2 f(x, t, \xi) d\xi, \text{ pressure,} \\
P & = (p_{ij})_{1 \leq i, j \leq 3}, \text{ stress tensor,} \\
q_i(x, t) & \equiv \int_{\mathbb{R}^3} (\xi_i - v_i) \frac{|v - \xi|^2}{2} f(x, t, \xi) d\xi, \text{ heat flux.}
\end{align*}
\]

1. Fluid dynamics equations, such as the Navier-Stokes and Euler equations, are systems of partial differential equations for the macroscopic variables.

2. In the kinetic theory, the macroscopic variables are derived quantities, the mean values of the distribution function.

3. "the method of mean values in mathematical physics."

Tai-Ping Liu
Boundary condition

1. For fluid dynamics, the boundary conditions are, naturally, prescribed for the macroscopic variables. There are conditions such as the Dirichlet, Neumann and other usual PDE boundary conditions. As is well-known, these conditions often give rise to paradox.

2. For the kinetic theory, it is possible to prescribe physically more realistic boundary conditions, such as diffuse reflection, specular reflection, Maxwell-types, complete condensation, ···, boundary conditions. This allows for the modeling and study of new physical phenomena.
Hilbert Sixth Problem

Boltzmann equation

\[ \partial_t f + \xi \cdot \partial_x f = \frac{1}{k} Q(f, f). \]

Transport: \( \partial_t f + \xi \cdot \partial_x f \)

Collision operator:

\[ Q(f, f)(\xi) \equiv \int_{\mathbb{R}^3} \int_{S^2_+} [f(\xi')f(\xi_{*}) - f(\xi)f(\xi_{*})]B(|\xi - \xi_{*}|, \theta) d\Omega d\xi_{*}. \]

\[ \begin{align*}
\xi' &= \xi - [(\xi - \xi_{*}) \cdot \Omega] \Omega, \\
\xi'_{*} &= \xi_{*} + [(\xi - \xi_{*}) \cdot \Omega] \Omega.
\end{align*} \]

Hard sphere models \( B = |(\xi - \xi_{*}) \cdot \Omega| = |\xi - \xi_{*}| \cos \theta. \)
Hilbert Sixth Problem

Boltzmann equation

\[
\partial_t f + \xi \cdot \partial_x f = \frac{1}{k} \int_{\mathbb{R}^3} \int_{S^2_+} [f(\xi')f(\xi_*) - f(\xi)f(\xi_*)] B(|\xi - \xi_*|, \theta) d\Omega d\xi_*.
\]

1. Transport in space-time \((x, t)\); collision in microscopic velocity \(\xi\). Thus Boltzmann equation is time irreversible.

2. Collision operator is functional of binary collisions, expressed as the products \(f(\xi')f(\xi_*) - f(\xi)f(\xi_*)\). Thus it is for rarefied gases and under the molecular chaos hypothesis.

3. The Boltzmann equation is taken as limit of Newtonian particle systems for fixing the mean free path \(k\) in the Boltzmann-Grad limit of the number \(N\) of particles, the diameter \(d\) of each particles satisfying \(N \to \infty, d \to 0\), \(Nd^2 = 1/k\) fixed.
Hilbert Sixth Problem

Boltzmann equation

\[ \begin{cases} \partial_t f + \xi \cdot \partial_x f = \frac{1}{k} Q(f, f), \\ Q(f, f) = \int_{\mathbb{R}^3} \int_{S^2_+} [f(\xi')f(\xi_*) - f(\xi)f(\xi_*))]B(|\xi - \xi_*|, \theta) d\Omega d\xi_. \end{cases} \]

Conservation Laws

\[ \int_{\mathbb{R}^3} \begin{pmatrix} 1 \\ \xi \\ \frac{1}{2}|\xi|^2 \end{pmatrix} Q(f, f) d\xi = 0, \quad \begin{pmatrix} \text{mass} \\ \text{momentum} \\ \text{energy} \end{pmatrix}. \]

H-Theorem

\[ \int_{\mathbb{R}^3} \log fQ(f, f) d\xi = \frac{1}{4} \int_{\mathbb{R}^3} \int_{S^2_+} \log \frac{ff_*}{f'f'_*} [f'f'_* - ff_*]Bd\Omega d\xi_* d\xi \leq 0. \]
Conservation laws

\[ \partial_t \rho + \partial_x \cdot (\rho \mathbf{v}) = 0, \text{ mass}, \]
\[ \partial_t (\rho \mathbf{v}) + \partial_x \cdot (\rho \mathbf{v} \times \mathbf{v} + \mathbf{P}) = 0, \text{ momentum}, \]
\[ \partial_t (\rho E) + \partial_x \cdot (\rho \mathbf{v} E + \mathbf{P} \mathbf{v} + \mathbf{q}) = 0, \text{ energy}. \]

H-Theorem

\[ \partial_t H + \partial_x \cdot \mathbf{H} = \frac{1}{4k} \int_{\mathbb{R}^3} \int_{S^2_+} \log \frac{ff_*}{f'f'_*} [f'f'_* - ff_*] Bd\Omega d\xi_* d\xi \leq 0, \]
\[ H \equiv \int_{\mathbb{R}^3} f \log f d\xi, \quad \mathbf{H} \equiv \int_{\mathbb{R}^3} \xi f \log f d\xi. \]

Irreversibility
Paradox and controversy of deriving the Boltzmann equation from the Newtonian particle system.

1. **Poincare Recurrence Theorem**: A volume-preserving systems with bounded orbits (e.g. Hamiltonian system with finite energy) will, almost surely and after a sufficiently long time, return to a state very close to the initial state. The **Poincar recurrence time** is the length of time elapsed until the recurrence.

2. The **Boltzmann-Grad limit**

   \[ N \rightarrow \infty, \quad d \rightarrow 0, \quad Nd^2 = \text{constant} \]

   is for rarefied gases; it will push the ergodicity and the recurrence time beyond infinity. So the molecular chaos hypothesis at the initial time would propagate into the solution at full force for all future time.

3. Boltzmann reportedly said to Poincare: ”But you would have to wait for a long time.”
Hilbert Sixth Problem, Part I: Newton to Boltzmann

Liouville equation

\[ \partial_t f^N + \sum_{i=1}^N \xi_i \cdot \partial_{x_i} f^N + \sum_{i=1}^N F^i \cdot \partial_{\xi_i} f^N = 0. \]

\( f^N (x^1, \ldots, x^N, \xi^1, \ldots, \xi^N, t) \): distribution function for the i-th particle at \((x^i, \xi^i)\). \( F^i \): force on the i-th particle.

The interacting force \( F^i = \sum_{j \neq i} F_{i,j} \). Textcolorbluefinite range force: \( F_{i,j} = 0 \) for \(|x^i - x^j| > d\), the diameter of the molecular.

\( \Omega_1 \equiv \{|x^1 - x^j| > d, j > 1\} \), \( \Omega_{12} \equiv \{|x^1 - x^j| > d, j > 2\} \).

\[ f^1 (x^1, \xi^1, t) \equiv \int_{\Omega_1} f^N dx^2 \cdots dx^N d\xi^2 \cdots d\xi^N, \]

\[ f^2 (x^1, x^2, \xi^1, \xi^2, t) \equiv \int_{\Omega_{12}} f^N dx^3 \cdots dx^N d\xi^3 \cdots d\xi^N, \cdots \]
BBGKY hierarchy:

\[
\begin{aligned}
\partial_t f^1 + \xi^1 \cdot \partial_{x^1} f^1 &= (N - 1) \int_{\partial S_{12}} (\xi^2 - \xi^1) \cdot n_1^2 f^2 d^2 x^2 d\xi^2,
\partial_t f^2 + \xi^1 \cdot \partial_{x^1} f^2 + \xi^2 \cdot \partial_{x^2} f^2 + F_{1,2} \partial_{\xi^1} f^2 + F_{2,1} \partial_{\xi^2} f^2 \\
&= (N - 2) \int_{S_{13}} (\xi^3 - \xi^1) \cdot n_1^3 f^3 d^2 x^3 d\xi^3 + \cdots,
\end{aligned}
\]

\[
S_{12} \equiv \{ x^2 : |x^2 - x^1| < d, \}
\]

\[
S_{13} \equiv \{ x^3 : |x^3 - x^1| < d, \}
\]

1. Lanford, Oscar E., III (1974): Liouville equation → Boltzmann equation for $\frac{1}{5}$ mean free time $T$.

2. Strong molecular chaos hypothesis of complete factorization at initial time:

$$f^N(x^1, \ldots, x^N, \xi^1, \ldots, \xi^N, t) = \prod_{i=1}^N f^1(x^i, \xi^i, t), \ t = 0.$$ 

3. Convergence and uniqueness of the full BBGKY hierarchy by Cauchy-Kowalevsky-type analysis for time up to $1/5$ the mean free time, $0 \leq t \leq \frac{1}{5} T$.

4. The limiting infinite BBGKY hierarchy coincides with the Boltzmann hierarchy.

OPEN PROBLEMS:

1. Show that the molecular chaos hypothesis

\[ f^2(x^1, x^2, \xi^1, \xi^2, t) = f^1(x^1, \xi^1, t)f^1(x^2, \xi^2, t) \]

at the initial time \( t = 0 \) would propagate to later time \( t > 0 \) in the Boltzmann-Grad limit, at least for the time period when the Boltzmann solution exists and smooth, so that the limiting equation is the Boltzmann equation.

2. The Boltzmann equation has been derived for finite range inter-molecular force between particles under the molecular chaos hypothesis. There is no definite derivation of the Boltzmann equation for inter-molecular forces with infinite range. This is a fundamental question on the validity of the Boltzmann theory.
H-Theorem

$$\partial_t H + \partial_x \cdot \vec{H} = \frac{1}{4k} \int_{\mathbb{R}^3} \int_{S^2_+} \log \frac{f f_*}{f' f'_*} [f' f'_* - f f_*] B d\Omega d\xi_* d\xi \leq 0,$$

= 0 if and only if $f(\xi)f(\xi_*) = f(\xi')f(\xi'_*)$, or,

$$f(x, t, \xi) = \frac{\rho(x, t)}{(2\pi R \theta(x, t))^{3/2}} e^{-\frac{|\xi - v(x, t)|^2}{2 R \theta(x, t)}} \equiv M(\rho, v, \theta),$$

Maxwellian, thermo-equilibrium states, $Q(M, M) = 0$. 
Conservation laws

\[ \partial_t \rho + \partial_x \cdot (\rho \mathbf{v}) = 0, \text{ mass}, \]
\[ \partial_t (\rho \mathbf{v}) + \partial_x \cdot (\rho \mathbf{v} \times \mathbf{v} + \mathbf{P}) = 0, \text{ momentum}, \]
\[ \partial_t (\rho E) + \partial_x \cdot (\rho \mathbf{v} E + \mathbf{P} \mathbf{v} + \mathbf{q}) = 0, \text{ energy}. \]

1. More (14) unknowns than (5) equations. Need to know the dependence on microscopic velocity to compute the stress tensor \( \mathbf{P} \) and heat flux \( \mathbf{q} \).

2. Boltzmann equation is equivalent to a system of infinite PDEs.
Boltzmann equation

\[ \partial_t f + \xi \cdot \partial_x f = \frac{1}{k} Q(f, f). \]

At thermo-equilibrium, \( f = M, \quad Q(M, M) = 0 \), the stress tensor \( P = \rho I \) is the pressure \( \rho = (3/2)e \) and heat flux become zero, \( q = 0 \), and the conservation laws become the self-sufficient Euler equations in gas dynamics:

\[
\begin{align*}
\partial_t \rho + \partial_x \cdot (\rho \mathbf{v}) &= 0, \\
\partial_t (\rho \mathbf{v}) + \partial_x \cdot (\rho \mathbf{v} \times \mathbf{v} + pI) &= 0, \\
\partial_t (\rho E) + \partial_x \cdot (\rho \mathbf{v} E + \rho \mathbf{v}) &= 0.
\end{align*}
\]
Assume the stress tensor $P$ and the heat flux $q$ as functions of the basic variables $(\rho, \rho v, \rho E)$ and their differentials.

**Euler equations:**

$$P_{ij} = \rho I, \quad q = 0,$$

the stress tensor is the pressure and no heat flux.

**Navier-Stokes equations:**

$$P_{ij} = p\delta_{ij} - \mu \left( \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} - \frac{3}{2} \frac{\partial v_k}{\partial x_k} \delta_{ij} \right) - \nu \frac{\partial v_k}{\partial x_k},$$

the stress tensor is the pressure plus shear stresses;

$$q_i = -\lambda \frac{\partial \theta}{\partial x_i},$$

the heat flux is the heat conductivity.
Hilbert Sixth Problem, Part II: Boltzmann to Fluid Dynamics

Boltzmann equation

$$\partial_t f + \xi \cdot \partial_x f = \frac{1}{k} Q(f, f).$$

Open Problem: As the mean free path $k \to 0$, $Q(f, f) \to 0$ and so $f \to M$ and Boltzmann solutions converge to an Euler solution.

Difficulty: The Euler solutions in general contain shock waves, and the limit is highly singular. As the shock waves, though of lower dimensional, can be dense; thus the above convergence should be an almost everywhere convergence to the weak solutions of the Euler equations.
Boltzmann shock waves,

\[
\begin{cases}
  f(x, t, \xi) = \phi(\eta, \xi), \ \eta = \frac{x_1 - st}{k}, \\
  \partial_\eta \phi + \xi_1 \partial_\eta \phi = Q(\phi, \phi).
\end{cases}
\]

Shock wave theory


\[ \partial_t u + \partial_x f(u) = 0 \]

The Glimm scheme, global estimates on total variation.

2. Bianchini, Stefano; Bressan, Alberto (2005): *Zero dissipation limit*, \( \varepsilon \to 0 \), for system with artificial viscosity:

\[ \partial_t u + \partial_x f(u) = \varepsilon u_{xx}. \]

Generalized Glimm scheme.
The Boltzmann shock $f(x, t, \xi) = \phi(\eta, \xi)$, with the self-similar variable $\eta = (x_1 - st)/k$, has width of the order of the mean free path $k$, same as the Navier-Stokes shocks. On the other hand, the derivation, via Chapman-Enskog expansion, of the Navier-Stokes equations in gas dynamics is under the hypothesis that the solutions have slow variation over the distance of the mean free path $k$. Thus, viewing from the kinetic theory, the systems of the Navier-Stokes equations and the Euler equations in gas dynamics are equivalent. In fact, the Navier-Stokes approximation is accurate only for small variation of the solutions. The approximation is exact time-asymptotically for dissipation over a global Maxwellian.

Kawashima, Shuichi; Matsumura, Akitaka; Nishida, Takaaki (1979): Time-asymptotic equivalence of Boltzmann equation and compressible Navier-Stokes equations.
To derive the "Incompressible" Navier-Stokes equations, one need to take weakly nonlinear perturbation, \( f = M + kg \) of a global Maxwellian \( M \), and the large-time limit:

\[
k \partial_t f + \xi \cdot \partial_x f = \frac{1}{k} Q(f, f)
\]

as the mean free path goes to zero, \( k \to 0 \). Hilbert expansion:

\[
g = g_0 + kg_1 + k^2 g_2 + \cdots , \text{ distribution function,}
\]

\[
\rho = \rho_0 + k\rho_1 + k^2 \rho_2 + \cdots , \text{ density,}
\]

\[
p = p_0 + kp_1 + k^2 p_2 + \cdots , \text{ pressure,}
\]

\[
\theta = \theta_0 + k\theta_1 + k^2 \theta_2 + \cdots , \text{ temperature,}
\]

\[
\mathbf{v} = k\mathbf{v}_1 + k^2\mathbf{v}_2 + \cdots , \text{ velocity.}
\]
Hilbert Sixth Problem, Part II: Boltzmann to Fluid Dynamics

Hilbert expansion

1. $\partial_x p_1 = 0,$

2. \[
\begin{cases}
\partial_x \cdot \mathbf{v}_1 = 0, \\
\partial_t \mathbf{v}_1 + \mathbf{v}_1 \cdot \partial_x \mathbf{v}_1 + \frac{1}{2} \partial_x p_2 = \gamma \Delta \mathbf{v}_1.
\end{cases}
\]

This is of the form of incompressible Navier-Stokes equations, involving the pressure $p_2$ and not $p_1 = \rho_1 + \theta_1$. The determination of $p_1$ requires the energy equation for compressible fluid involving the work done by the pressure $P_1$: \[
\frac{5}{2} \partial_t \tau_1 - \partial_t p_1 + \frac{5}{2} \mathbf{v}_1 \partial_x \tau_1 = \gamma' \Delta \tau_1,
\] thereby changing the density $\rho_1$.

Concluding Remarks

1. The kinetic theory yields understanding of key physical phenomena beyond the classical fluid dynamics theory. These phenomena, the thermal creep, ghost effects, bifurcation of transonic condensation/evaporation, etc, originate in no small part from the boundary effects that only the kinetic theory can model. *Modern Fluid Dynamics*: Sone, Yoshio: *Molecular Gas Dynamics*. Birkhauser, (2007).

2. The study of the validity of the Boltzmann theory is a mathematical problem. The Boltzmann equation is the most basic equation in the kinetic theory. Exact analysis of the Boltzmann equation is therefore of fundamental importance. Hilbert’s problem of going from *the atomistic view to the laws of motion of continua* remains an exciting challenge that is largely unsolved.