Thermodynamic Theory of Incompressible Hydrodynamics

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The grand potential for open systems describes thermodynamics of fluid flows at low Mach numbers. A new system of reduced equations for the grand potential and the fluid momentum is derived from the compressible Navier-Stokes equations. The incompressible Navier-Stokes equations are the quasistationary solution to the new system. It is argued that the grand canonical ensemble is the unifying concept for the derivation of models and numerical methods for incompressible fluids, illustrated here with a simulation of a minimal Boltzmann model in a microflow setup.

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The classical incompressible Navier-Stokes equation (INS) is a mechanical description of fluid flows at low Mach numbers (Mach number, $\mathrm{Ma} = U_0/c_s$, is the ratio of the characteristic flow velocity U_0 to the isentropic sound speed c_s defined at some reference temperature $\overline{T}$ and density $\overline{\rho}$). The INS equation can be written in the Eulerian coordinate system as

$$\partial_t u_\alpha + u_\beta \partial_\beta u_\alpha + \partial_\alpha P = \frac{1}{\mathrm{Re}} \partial_\beta \partial_\beta u_\alpha, \qquad \partial_\alpha u_\alpha = 0, \quad (1)$$

where $\mathbf{u}$ is the fluid velocity, P is the pressure, and Re the Reynolds number, which characterizes the relative strength of the viscous and the inertial forces [1]. The pressure in (1) is not an independent thermodynamic variable but is rather determined by the condition of the incompressibility

$$\partial_\beta \partial_\beta P = -(\partial_\beta u_\alpha)(\partial_\alpha u_\beta). \quad (2)$$

Thus, in order to obtain the pressure at a point, one has to solve the Laplace equation (2) in a domain, and the relationship between the pressure and the velocity becomes highly nonlocal. The physical meaning of (2) is that in a system with infinitely fast sound propagation, any pressure (and thus density) disturbance induced by the flow is instantaneously propagated into the whole domain.

A textbook justification for the thermodynamics of the INS description is usually based on the isentropic flow assumption. If this assumption is valid for all times (the entropy density is simply convected by the flow), then the thermodynamic pressure depends only on the acoustic (density) variations. For low Mach number flows, these variations adjust to the flow on every spatial scale in the long time dynamics [1]. The way this adjustment takes place is nontrivial, and it was given considerable attention recently [2,3]. In particular, it was proved that weak solutions of the isentropic compressible Navier-Stokes equations converge to that of the INS equation for some special boundary conditions (adiabatic absorbing walls). However, it remains a challenge to give a thermodynamic derivation of the incompressibility without the isentropic flow assumption. Such a thermodynamic derivation goes far beyond academic interest. Indeed, as is well known, the INS equations are extremely hard to study, both analytically and numerically. Therefore, an extended system where the flow is coupled to a dynamic equation for a scalar thermodynamic variable provides a better starting point for numerical and theoretical studies of the incompressible hydrodynamics. Indeed, in the computational fluid dynamics, at least two undeniably successful routes to avoid the "elliptic solver problem", that is, avoiding the nonlocality of the pressure (2) are well known. The first is the so-called artificial compressibility method [4,5], where an evolution equation for the pressure is postulated instead of the constraint (2). The second route is kinetic-theory models such as the lattice Boltzmann method. The thermodynamics of the lattice Boltzmann method was clarified [6], and the method enjoys a thermodynamically sound derivation from the Boltzmann equation [7]. Can the compressibility methods be modified in a way to make them physical models?

In this Letter, we present the thermodynamic description of incompressible fluid flows. In step one, we will argue that the grand potential is the proper thermodynamic potential to study the onset of incompressibility. Use of the grand potential instead of the entropy enormously simplifies the equations of compressible hydrodynamics in the low Mach number limit. We show that after a short time dynamics during which acoustic waves are damped by viscosity, the fast dynamics of the grand potential becomes singularly coupled to the slow dynamics of momentum, and *reduced* compressible Navier-Stokes equations are derived (RCNS). The incompressible Navier-Stokes equation is the quasistationary solution of the RCNS, when the Mach number tends to zero. Finally, by writing the grand potential for the Boltzmann equation, we show that the present constructions leads to the entropic lattice Boltzmann method. Correctness of the present almost-incompressible description is illustrated with a simulation of a microflow setup.

A low Mach number flow is a setup where only small spatial deviations of the entropy and the density from the equilibrium value exist. The grand potential is the natural thermodynamic variable to describe such a setup. This happens because the balance laws (compressible Navier-Stokes equations or the Boltzmann equation) are always written for a sufficiently small volume element in the Eulerian frame of reference (i.e., the volume element is fixed in space). From a thermodynamic standpoint, this volume element is an open system. The thermodynamic equilibrium is conveniently described in terms of the grand potential $\Omega(\psi, T)$, where ψ is chemical potential, and T is the temperature.

Now, we shall find the expression for the grand potential in the Eulerian coordinate system for a volume element δV, in thermodynamic equilibrium. In the comoving system, the grand potential is written as $\Omega_{\rm L}(\psi, T) = -P(\psi, T)\delta V$, where P is the pressure. The transition to the Eulerian (fixed) system is done by fixing the momentum, $\Omega_{\rm E}(\psi, T, \mathbf{m}) = -P\delta V + \lambda_\alpha m_\alpha \delta V$, where λ_α are Lagrange multipliers, and $\mathbf{m}$ is the momentum density. For small values of momentum, the Lagrange multipliers can be specified by noting that the energy in the Eulerian coordinate system is $[\epsilon + (m^2/2\rho)]\delta V$, where ϵ is the internal energy density. Using the relationship between the energy and the grand potential for the thermodynamic equilibrium, we find that $\lambda_\alpha = m_\alpha/2\rho + O(m^3)$. Thus, in the Eulerian coordinate system, the grand potential, up to the higher-order terms in momentum, is written as

$$\Omega_{\rm E} = \left(-P + \frac{m^2}{2\rho}\right)\delta V. \tag{3}$$

The difference of the pressure and the kinetic energy is the (negative of) density of the grand potential, and it will be used below as the natural thermodynamic potential for the low Mach number flows

$$\mathcal{G} = P - \frac{m^2}{2\rho}. \tag{4}$$

Dynamic equations for the set of variables ρ, $\mathbf{m}$, and $\mathcal{G}$ are written using the standard compressible Navier-Stokes equations (CNS) for Newtonian fluids [1]. Note that CNS are usually written in terms of a different set of variables (for example, in terms of the entropy density S instead of $\mathcal{G}$). The recomputation from either form of the CNS equations to the present set of variables poses no difficulties, and we here write the final result:

$$\begin{aligned}
&\partial_t\rho + \partial_\alpha m_\alpha = 0,\\
&\partial_t m_\alpha + \partial_\beta\left[\left(\mathcal{G} + \frac{m^2}{2\rho}\right)\delta_{\alpha\beta} + \frac{m_\alpha m_\beta}{\rho} + \Pi_{\alpha\beta}\right] = 0,\\
&\partial_t\mathcal{G} + \rho\frac{\partial P}{\partial\rho}\bigg|_S \partial_\alpha\left(\frac{m_\alpha}{\rho}\right) - \partial_\alpha\left[m_\alpha\left(\frac{m^2}{2\rho^2}\right) + \frac{m_\beta}{\rho}\Pi_{\alpha\beta}\right] +\\
&\left(1 + \frac{1}{\rho C_{\rm V}}\frac{\partial P}{\partial T}\bigg|_\rho\right)\Pi_{\alpha\beta}\partial_\alpha\left(\frac{m_\beta}{\rho}\right) = \frac{1}{\rho C_{\rm V}}\frac{\partial P}{\partial T}\bigg|_\rho \partial_\alpha(\kappa\partial_\alpha T),
\end{aligned} \tag{5}$$

where $\Pi_{\alpha\beta}$ is the stress tensor of a Newtonian fluid

$$\Pi_{\alpha\beta} = -\mu\left[\partial_\alpha\left(\frac{m_\beta}{\rho}\right) + \partial_\beta\left(\frac{m_\alpha}{\rho}\right) - \delta_{\alpha\beta}\left(\frac{2}{D} - \lambda\right)\partial_\gamma\left(\frac{m_\gamma}{\rho}\right)\right],$$

with D the spatial dimension, μ the shear viscosity, and λ the ratio of bulk to shear viscosity. In (5), κ is the thermal conductivity, $C_{\rm V}$ is the specific heat at constant volume, and the temperature T is known from the equation of state. Variations of material parameters such as viscosity μ will be ignored in the further discussion. Note that Eqs. (5) are "exact" in the sense that they are just the standard CNS equations written for ρ, $\mathbf{m}$, and the function $\mathcal{G}$ (4). However, the physical meaning of the function $\mathcal{G}$ (4) as the density of the grand potential is valid only up to the lowest order in momentum.

Since the speed of sound, $c_{\rm s} = \sqrt{\partial P/\partial\rho|_S}$, contributes to the dynamic equation for the grand potential, it is instructive to rewrite (5) as:

$$\partial_t\mathcal{G} + \partial_\alpha(c_{\rm s}^2 m_\alpha) - \frac{m_\alpha}{\rho}\partial_\alpha(\rho c_{\rm s}^2) - \ldots \tag{6}$$

We expect the following scenario of the onset of incompressibility, as it can be inferred from (6): If the speed of sound is "large", then, after a "short-time" dynamics of the density leading to $\rho \approx$ const, the third term in (6) can be neglected, whereas the second term becomes the dominant contribution to the time derivative of $\mathcal{G}$. The dynamic equation for the grand potential becomes then singularly perturbed, and represents the "fast" mode coupled to the "slow" dynamics of momentum. The contributions to the time derivative of the grand potential not displayed in (6) are responsible for corrections to the incompressibility. We now proceed with quantifying these statements.

For small deviations from the no-flow situation, ($|m_\alpha m_\beta| \ll P\rho$, which implies Ma $\ll 1$), we are interested in the long time solutions of the CNS equations (times of the order of the momentum diffusivity time $t_{\rm md} \sim \overline{\rho}L^2/\mu$, where L is a characteristic length associated with the flow). We define a dimensionless number, $\mathrm{Kn} = \mu/(\rho c_{\rm s} L)$, the ratio of the sound propagation time $L/c_{\rm s}$, and the momentum diffusivity time, as the Knudsen number for a general fluid, and we are considering Kn $\ll$ Ma $\ll 1$. For the sake of simplicity, we assume that the Prandtl number Pr$\sim$1 in the subsequent analysis. The *short-time* dynamics is isentropic and linear, and it is well known that, away from boundaries, any density perturbation at a distance r away from the disturbance source decays as (see [1], p. 300)

$$\delta\rho(r,t) \propto (\mathrm{La}\, rL)^{-1/2} \exp\left(-\frac{(r-c_s t)^2}{2\mathrm{La} rL}\right). \tag{7}$$

Here a new dimensionless number La is defined as:

$$\mathrm{La} = \mathrm{Kn}\left(2 - \frac{2}{D} + \lambda\right) + \frac{\mathrm{Kn}(\gamma-1)}{\mathrm{Pr}}, \tag{8}$$

where γ the ratio of specific heat at constant pressure and volume. La generalizes the notion of a Knudsen number for an arbitrary fluid (we call it the Landau number; see [1], p. 300). Thus, the short term hydrodynamics reveals the following length scale L_a and the time scale t_a (since we assume Pr$\sim$1, we need not distinguish between La and Kn for the present purpose):

$$t_a \sim \sqrt{\mathrm{Kn}}\left(\frac{L}{c_s}\right), \qquad L_a \sim \sqrt{\mathrm{Kn}} L, \tag{9}$$

At the time scale larger than t_a, and on the spatial scale larger than L_a, the density of the fluid can be safely treated as a constant (in the usual isentropic theory, the characteristic time for the onset of incompressibility is of the order $L/c_s \gg t_a$). Note that the length scale L_a was also found in the derivation of the subgrid model from kinetic theory [8]. On the time-space scale larger than (9), we can neglect the density variation, and the temperature variation δT (from the globally uniform value $\overline{T}$), becomes a function of the grand potential,

$$\delta T \approx \frac{\partial T}{\partial P}\bigg|_{\rho}\left(\mathcal{G} + \frac{m^2}{2\rho}\right).$$

Once the time and space scales (9) are identified, we complete the reduction of the CNS equations (5) by merely rescaling the variables. The momentum is scaled by the characteristic momentum $\overline{\rho}U_0$ (known from the initial or boundary condition), $\mathbf{j} = \mathbf{m}/(\overline{\rho}U_0)$, and we introduce the reduced grand potential density, $\Theta = \mathcal{G}/(\overline{\rho}U_0^2)$. Making time dimensionless with t_a, space with L_a ($t \to t/t_a$, $\mathbf{x} \to \mathbf{x}/L_a$), neglecting variations of the density, and taking into account the thermodynamic relation for the temperature mentioned above, the two last equations in (5) reduce to the following scale-independent closed set of equations for the dimensionless grand potential and momentum:

$$\begin{aligned}
\partial_t j_\alpha &= -\mathrm{Ma}\,\partial_\beta\left[j_\alpha j_\beta + \delta_{\alpha\beta}\left(\Theta + \frac{j^2}{2}\right)\right] + \sqrt{\mathrm{Kn}}\left(1+\lambda-\frac{2}{D}\right)\partial_\alpha\partial_\beta j_\beta + \sqrt{\mathrm{Kn}}\,\partial_\beta\partial_\beta j_\alpha,\\
\partial_t\Theta &= -\frac{1}{\mathrm{Ma}}\partial_\alpha\left[j_\alpha\left(1-\frac{\mathrm{Ma}^2 j^2}{2}\right)\right] + \sqrt{\mathrm{Kn}}\left[\frac{\gamma}{\mathrm{Pr}}\partial_\alpha\partial_\alpha\Theta + \left(\frac{\gamma}{\mathrm{Pr}}-1\right)\partial_\alpha\partial_\alpha\frac{j^2}{2} + (\partial_\alpha j_\beta)(\partial_\alpha j_\beta)\right.\\
&\quad \left. + \frac{\partial P}{\partial T}\bigg|_{\overline{\rho}}\frac{1}{2C_V}(\partial_\alpha j_\beta + \partial_\beta j_\alpha)(\partial_\alpha j_\beta + \partial_\beta j_\alpha) - \left(1+\lambda-\frac{2}{D}\right)\partial_\beta(j_\beta\partial_\alpha j_\alpha)\right].
\end{aligned} \tag{10}$$

Note that all "material parameters" appearing in (10) (C_V, γ, λ, κ) are evaluated at equilibrium at $\overline{\rho}$ and $\overline{T}$.

The *reduced* set of compressible Navier-Stokes Eqs. (10) is valid for Kn $\ll$ Ma $\ll$ 1, and, as we explained above, on the scales larger than acoustic scales (9). Roughly speaking, (10) is what survives from the compressible Navier-Stokes equations just before the incompressibility sets on. Indeed, the time derivative of Θ becomes singularly perturbed as the Mach number tends to zero, and we recover the incompressibility condition, $\partial_\alpha j_\alpha = 0$, as the quasistationary solution of the system (10). This solution, when substituted in the momentum equation, recovers the INS equation (1) with the usual accuracy of the order $O(\mathrm{Ma}^2)$. Note that the velocity in the INS equations recovered from (10) is $\mathbf{u} = \mathbf{j}/\overline{\rho}$. Corrections to the quasistationary solution can be found in a systematic way [9], and we do not address this here. The following point needs to be stressed: The dissipation terms (proportional to $\sqrt{\mathrm{Kn}}$) *cannot* be neglected in the equation for the grand potential (10) and simultaneously kept in the momentum equation. This is at variance with the artificial compressibility method [4,5]. In other words, the RCNS is *the minimal thermodynamic system* for incompressible hydrodynamics.

In this Letter, we reported a new basic physical fact of fluid dynamics: Grand potential (3) for low Mach number flows gives the thermodynamic description of the incompressible phenomena. The resulting system (10) includes a *local* (nonadvected) equation for the scalar thermodynamic field. What follows from this fact? Let us list some of the consequences:

(i) With the corrections mentioned above, the numerical schemes of the artificial compressibility kind become a firm status of physical models.

(ii) The structure of the coupling between the flow and the thermodynamic variable hints at the fact that the true incompressible flows are attractors of system (10), with the INS as the leading-order approximation. It may be easier to study attractors of (10), rather than of the INS equations.

(iii) System (10) can be a starting point for a systematic derivation of nonlinear models for heat transport in the nearly-incompressible fluids such as multiphase fluids, polymeric liquids, and melts, etc.

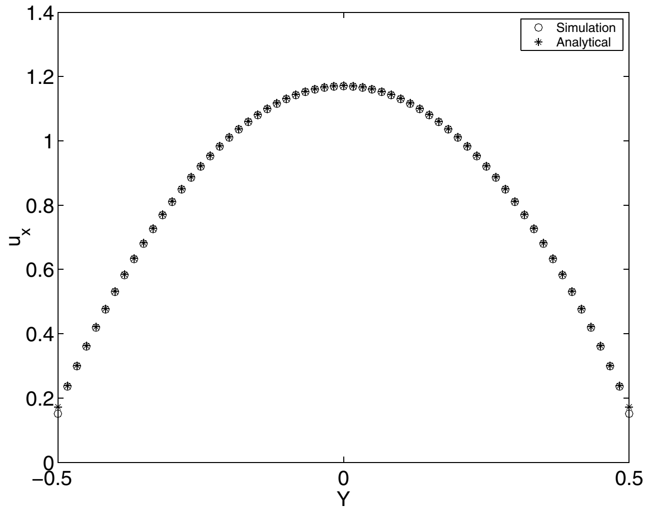

FIG. 1. Velocity profile of the 2D body-force driven Poiseuille flow at Kn = 0.035 and Ma = 0.01.

(iv) In the celebrated Kolmogorov theory, the equation for the kinetic energy is used to make predictions about the structure of the fully developed turbulence. The present thermodynamic approach unambiguously delivers the density of the grand potential as the scalar field associated with the incompressible fluid flow, and thus can be relevant to develop theories of turbulence through studying the resulting balance equation.

Let us dwell on the use of (10) for numerical simulation of incompressible flows. Recall that the spectral methods [10] for the INS (1) are very efficient for high Reynolds number flows in simple geometries. On the other hand, thanks to a relatively simple structure of the system (10), it can be addressed by a host of discretization methods. The system (10) can be useful for simulation of flows in complex geometries and especially nonstationary problems. Note that the system (10) contains terms of different orders of magnitude. This situation is typical for all relaxational schemes and we do not discuss here how to deal with this issue numerically (see, e.g., [6,7]). Note, however, the important smoothing effect of the diffusion term (inversely proportional to the Prandtl number) in the equation for Θ which makes the physical system (10) more amenable to numerics.

We conclude this Letter with a more general statement that the grand potential (and the relevant grand canonical ensemble) can be implemented for, eventually, any more microscopic setup. This viewpoint provides a unified setting for derivations of a variety of mesoscopic or molecular dynamics models for numerical simulation of incompressible and nearly-incompressible flows. As an illustration here, let us assume Boltzmann's description with the one-particle distribution function $f(\mathbf{v}, \mathbf{x}, t)$. Starting from the general form of the grand potential $\mathcal{G}(f, \alpha, \beta, \boldsymbol{\lambda}) = \int f[\ln f + \alpha + \lambda_\alpha v_\alpha + \beta v^2] d\mathbf{v}$, it is easy to show that at equilibrium $f^{\rm eq}(\mathbf{v}, \alpha, \beta, \boldsymbol{\lambda})$ (defined from $\delta\mathcal{G} = 0$), we have $\mathcal{G}(f^{\rm eq}) = \mathcal{G}^{\rm eq}(\alpha, \beta) + (\lambda^2/2) \int f^{\rm eq}(\mathbf{v}, \alpha, \beta, 0) \times (v^2/2) d\mathbf{v}$ for small λ. When the velocity integral $\mathcal{G}(f, \alpha, \beta, \boldsymbol{\lambda})$ is evaluated with the Gauss-Hermit quadrature with the weight $\exp(\beta v^2)$ at fixed β, one obtains the entropy function of the lattice Boltzmann method [6,7]. The present alternative derivation based on the grand potential is new. Thus, the entropic lattice Boltzmann method can be used for finite, but small, Knudsen low Mach number flow problems often encountered in the microflows [11]. In Fig. 1 we present an excellent comparison between the analytical solution to the Bhatnagar-Gross-Krook (BGK) kinetic equation [12] and the entropic lattice Boltzmann simulation for the body-force driven 2D Poiseuille microflow.

While this Letter was in the revision process, we learned about a very recent Letter [13] which states the usefulness of the grand potential in the context of plasma turbulence simulations.

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