Phase-space Lagrangian dynamics of incompressible thermofluids

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Abstract

Phase-space Lagrangian dynamics in ideal fluids (i.e., continua) is usually related to the so-called ideal tracer particles. The latter, which can in principle be permitted to have arbitrary initial velocities, are understood as particles of infinitesimal size which do not produce significant perturbations of the fluid and do not interact among themselves. An unsolved theoretical problem is the correct definition of their dynamics in ideal fluids. The issue is relevant in order to exhibit the connection between fluid dynamics and the classical dynamical system, underlying a prescribed fluid system, which uniquely generates its time-evolution.

The goal of this paper is to show that the tracer-particle dynamics can be exactly established for an arbitrary incompressible fluid uniquely based on the construction of an inverse kinetic theory (IKT) (Tessarotto \textit{et al.}, 2000-2008). As an example, the case of an incompressible Newtonian thermofluid is here considered.

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1 Introduction

A basic aspect of fluid dynamics is related to the definition of the Lagrangian dynamics which characterizes both compressible and incompressible fluids. The customary approach to the Lagrangian formulation is based typically on a configuration-space description, i.e., on the introduction of the (configuration-space) Lagrangian path, \( r(t) \), spanning the configuration space (fluid domain) \( \Omega \). Here \( r(t) \) denotes the solution of the initial-value problem \( \frac{D}{Dt} r = V(r, t) \), with \( r(t_0) = r_o \). Here \( \frac{D}{Dt} \equiv \frac{\partial}{\partial t} + \mathbf{V} \cdot \nabla \) denotes the so-called "fluid" convective derivative, \( r_o \) an arbitrary vector belonging to \( \overline{\Omega} \) and \( \mathbf{V}(r, t) \) the velocity fluid field, to be assumed continuous in \( \overline{\Omega} \) (closure of \( \Omega \)) and suitably smooth in \( \Omega \). However, in turbulence theory the statistical formulation for the associated joint probability density for velocity increments requires the introduction of a phase-space representation of suitable type \([1]\), in which usually the phase-space is identified with \( \Gamma = \Omega \times \mathbb{R}^3 \) (with closure \( \Gamma = \overline{\Omega} \times \mathbb{R}^3 \)), here denoted as restricted phase-space. Therefore it is natural to seek possible phase-space representations of this type for fluid systems. The goal of this investigation is concerned with the formulation of restricted-phase-space Lagrangian dynamics in such a way that the phase-space \( \Gamma \) coincides with the direct product space \( \Gamma = \Omega \times V \), \( \Omega \) being the fluid domain and \( V \) (velocity space) the set \( \mathbb{R}^3 \).

In particular in this paper, extending the formulation previously developed (Cremaschini et al. \([2]\) and Marco Tessarotto et al. \([3, 4]\)), we shall adopt for this purpose a so-called phase-space inverse kinetic theory (IKT) (see also Tessarotto et al., 2000-2008 \([5, 6, 7, 8, 9, 10]\)). Basic feature (of such an approach) it that is relies on first principles, i.e., classical statistical mechanics and a prescribed complete set of fluid equation. This permits us to advance in time the relevant fluid fields by means of phase-space Lagrangian equations defined by the vector field \( \mathbf{X}(x, t) \), namely

\[
\begin{align*}
\frac{dx}{dt} &= \mathbf{X}(x, t), \\
x(t_0) &= x_o,
\end{align*}
\]

where \( x_o \) is an arbitrary initial state of \( \Gamma \) (closure of the phase-space \( \Gamma \)). The result appears relevant in particular for the following reasons: 1) the Lagrangian dynamics here determined permits to advance in time self-consistently the fluid fields, i.e., in such a way that they satisfy identically the required set of fluid equations. For isothermal fluids, this conclusion is consistent with the results indicated previously \([7]\); 2) the Lagrangian dynamics takes into account the specific form of the phase-space distribution function which advances in time the fluid fields; 3) the theory permits an exact description of the motion of those particles immersed in the fluid which follow the Lagrangian dynamics (classical molecules).
Phase-space Lagrangian dynamics and particle dynamics in ideal fluids are closely related issues. In fact both must be uniquely described via a suitable complete set of fluid fields \{Z(\mathbf{r}, t)\} which define the fluid state. This refers, in particular, to the so-called ideal tracer particles, for which both self-interaction produced by the perturbations of the fluid fields generated by the same particles and binary collisions among them are negligible (in this sense they can therefore be intended also as "collisionless"). It is well known, however, that in customary approaches (see for example Maxey and Riley, 1982 [11]) the equations of motion for ideal tracer particle are only known in some approximate sense and therefore do not reproduce exactly the correct fluid dynamics.

The purpose of this paper is to show that an exact solution can be reached for phase-space Lagrangian dynamics, and in particular for the conventional tracer dynamics, based on the formulation of a suitable IKT. By definition, an IKT must provide the complete set of fluid equations describing the fluid, by means of velocity moments of an appropriate phase-space probability density function (pdf). We intend to show that such a theory can be uniquely determined in the framework of classical statistical mechanics by invoking suitable statistical assumptions on the IKT. In particular, we present here a theory which applies to incompressible Newtonian fluids, including both isothermal and non-isothermal fluids [2, 3, 4]. In the following we intend to show that customary tracer-dynamics equations due to several authors - including Tchen (1947 [12]), Corrsin and Lumley (1956 [13]), Buevich (1966 [14]) and Riley (1971 [15]) and Maxey and Riley (1982 [11]) - are incompatible with the exact phase-space Lagrangian formulation here obtained.

In detail the plan of the paper is as follows. First, in Section 2 previous approaches to ideal tracer particle dynamics are summarized. Second in Sec. 3 a comparison between Eulerian and Lagrangian phase-space approaches is provided. Furthermore, in Sec. 4 the IKT for incompressible thermodynamics is presented. This permits us to determine the appropriate form of the vector field \mathbf{X}(\mathbf{x}, t). Next, in Section 5 the Lagrangian formulation of IKT is discussed in detail. The new set of phase-space Lagrangian equations are shown to advance uniquely in time the relevant fluid fields of an incompressible thermodynamics. As a basic consequence, in Section 6 we will derive the exact dynamics of ideal tracer particles (see below for definition), comparing it with previous results.

2 Previous approaches to tracer particle dynamics

The motion of small particles (such as solid particles or droplets, commonly found in natural phenomena and industrial applications) which can be injected in a fluid with arbitrary initial velocity, in practice, may be very different from that of the fluid. The accurate description of particle dynamics,
as they are pushed along erratic trajectories by binary collisions (in real fluids) and by fluctuations of the fluid fields (in ideal fluids), is fundamental to transport and mixing in turbulence [1]. It is essential, for example, in combustion processes [16], in the industrial production of nanoparticles [17] as well as in atmospheric transport, cloud formation and air-quality monitoring of the atmosphere [18, 19]. The Lagrangian approach - denoted as Lagrangian turbulence (LT) - has been fruitful in advancing the understanding of the anomalous statistical properties of turbulent flows [20]. In particular, the dynamics of particle trajectories has been used successfully to describe mixing and transport in turbulence [16, 21]. Nevertheless, issues of fundamental importance remain unresolved (see for example Refs. [22, 23] for recent results regarding the Lagrangian view of passive scalar turbulence). In the past, the treatment of Lagrangian dynamics in turbulence was based on stochastic models of various nature, pioneered by the meteorologist Richardson [24] (see also [22, 23]). These models, which are based on tools borrowed from the study of random dynamical systems, typically rely - however - on experimental verification rather than on first principles. However, in most cases there remains a lack of experimental data to verify the reliability of such models [22]. Verification can be based, in particular, on the measurement of fluid particle trajectories, obtained by seeding a turbulent flow with a small number of tracer particles and following their motions with an imaging system. On the other hand, the accurate evaluation of the Lagrangian velocity in laboratory turbulence experiments requires measurements of positions of tracer particle by using a suitable tracking system able to resolve very short time (and spatial) scales. In practice this can be a very challenging task since particle motions must be measured on very short time scales.

As for the theory itself, rigorous results have been scanty, probably because of the subject complexity. In the case of ideal or dilute real fluids, however, particle motion is necessarily collisionless (in the sense specified above) while the dynamics of ideal tracer particles is controlled by the force produced on them only by the unperturbed fluid fields. Several authors have tried in the past to derive, based on phenomenological arguments, an approximate equation for the ideal tracer-particle dynamics, describing the motion of a particle suspended in a non-uniform flow. Since the original Basset-Boussinesq-Oseen (BBO) equation [25, 26, 27], formulated in the case of a uniform flow, several papers have appeared proposing modifications or corrections of the same equation for non-uniform flows (for a review see [11]). The first attempt at a generalization of this type is due to Tchen, (1947 [12]), who considered the motion of a rigid sphere in an incompressible isothermal Navier-Stokes (NS) fluid. Tchen [12] derived an approximate equation of motion for a finite-size spherical particle of radius $a$ and mass $m_P$ describing its dynamics in terms of the Newtonian state of its center of mass $\{r(t), \nu(t)\}$. His equation was later modified by Corrsin and Lumley (1956 [13]), to take into account contributions due to pressure gradients previously ignored, and by Buevich (1966
in order to consider also the effect of viscous stress. The version of the equation currently adopted by some authors (see for example Gui et al., 2008 where it was used to investigate modifications of turbulence) is, however, the one later developed by Maxey and Riley (1982) in which also the buoyancy contribution produced by the volume displaced by the particle was taken into account. In the approximation in which perturbations of the fluid fields produced by the particle are negligible the equation of motion developed by Maxey and Riley reduces to:

$$m_P \frac{d}{dt} \mathbf{v}(t) = m_F \frac{d \mathbf{V}(\mathbf{x}, t)}{dt} \bigg|_{\mathbf{x} = \mathbf{r}(t)} - \frac{1}{2} m_F \frac{d}{dt} \left\{ \mathbf{v}(t) - \mathbf{V}(\mathbf{r}(t), t) \right\} \bigg|_{\mathbf{x} = \mathbf{r}(t)}$$

(2)

(M-R equation), where the last contribution on the r.h.s. denotes the so-called buoyancy effect. Here the notation is standard. Thus, \(\{\mathbf{V}(\mathbf{r}, t), p(\mathbf{r}, t)\}\) are respectively the fluid velocity and pressure, \(\mathbf{f}\) the volume force density and finally \(\rho_0, \nu > 0\) the constant mass density and kinematic viscosity (with \(\nu\) related to the dynamic viscosity \(\mu\) by the identity \(\nu = \mu/\rho_0\)). In particular, \(\mathbf{f}\) can be written \(\mathbf{f} = -\nabla \phi + \mathbf{f}_R\), with \(\rho_0 \mathbf{g} = -\nabla \phi\), where \(\mathbf{g}\) is the constant local gravity acceleration, \(\phi = \rho_0 gz\) the gravitational potential (hydrostatic pressure) and \(\mathbf{f}_R\) a possible non-potential force density. Moreover, \(m_F\) is the mass of the fluid displaced by the sphere, \(\frac{d}{dt} \equiv \frac{\partial}{\partial t} + \mathbf{v}(t) \cdot \nabla\) the ”particle” convective derivative and \(\mathbf{V}(\mathbf{r}(t), t)\) and \(\mathbf{v}(t) - \mathbf{V}(\mathbf{r}(t), t)\) are respectively the fluid and particle relative velocities evaluated at the position of the particle center of mass. It should be noted, however, that also this equation is still unsatisfactory. In fact, it is obtained by requiring that the particle velocity remains always suitably close to the fluid one, so that contributions due to the relative velocity - i.e., proportional to the particle relative velocity \(\mathbf{u}(t) \equiv \mathbf{v}(t) - \mathbf{V}(\mathbf{r}(t), t)\) - are actually ignored in Eq.(2), requiring that for all \(\{\mathbf{r}(t), \mathbf{v}(t)\}\) there results:

$$|\mathbf{u}(t)| \ll |\mathbf{V}(\mathbf{r}(t), t)|.$$  

(3)

The limitation appears serious because the actual dynamics (i.e., both the velocity and the acceleration) of ideal tracer particles may be in principle very different from that of the fluid elements. In addition, the accurate description of ideal particle dynamics is essential both in LR and in environmental fluid dynamics (dynamics of anthropogenic pollutants in the atmosphere, diffusion of dusty particles, droplets, aerosol particles, etc.). This involves, in fact, the ability to simulate tracer dynamics in a variety of different physical conditions and in fluid flows characterized by a turbulent behavior. Therefore, an open issue remains the very definition of the dynamics of tracer particles which may be injected in an ideal fluid with arbitrary initial velocities. Clearly, such a formulation - if achievable at all - should rely exclusively on first principles, i.e., in particular the exact validity of the fluid equations. This
problem is closely related to the formulation of phase-space approaches for fluid systems, based on the introduction of suitable phase-space representations of classical fluid dynamics in terms of an appropriate phase-space pdf. By construction, the dynamics of a fluid is completely described by the time-evolution of its fluid fields (which, in turn, are assumed as classical solutions of a well-posed initial-boundary value problem defined by a complete set of fluid equations). Therefore, unless suitable restrictions are posed, phase-space dynamics remains intrinsically non-unique. This is true, in particular, due to the arbitrariness in the choice of the possible phase-space and the definition of the evolution equation for the pdf.

3 Eulerian and Lagrangian phase-space approaches

As it is well known, phase-space descriptions of fluids can be achieved in principle choosing either an Eulerian or a Lagrangian point of view. Based on the IKT approach for incompressible fluids earlier developed \([5, 6, 7, 8, 9]\) such a connection can be uniquely established. IKT is based on the identification of the complete set of fluid fields (which describe the fluid) with velocity-moments of a suitably-defined kinetic distribution function \(f(x,t)\). The pdf is assumed to satisfy the basic principles of classical statistical mechanics, which include in particular:

1. *the principle of conservation of probability*;
2. a suitable *correspondence principle* (Ellero et al., 2005 \([7]\)) whereby appropriate (velocity-) moments of the pdf can be identified with the relevant fluid fields;
3. *the principle of entropy maximization* (PEM, Jaynes, 1957 \([29]\));
4. and *an entropic principle assuring that the statistical entropy cannot decrease in time* (Tessarotto, 2008 \([3]\)).

The first axiom implies that the pdf must satisfy a Liouville equation, i.e., a Vlasov-type *inverse kinetic equation* (IKE, Ellero et al. \([7]\)). As it is well-known, this type of kinetic equation is, in fact, appropriate for the statistical description of particles subject solely to mean-field interactions. This is consistent with the assumption of an ideal fluid, i.e., a continuum in which the fluid elements are, by definition, subject only to mean-field interactions. In such a case, the time-evolution of the pdf is determined by the *Eulerian IKE*

\[
Lf(x,t) = 0. \tag{4}
\]

Here \(f(x,t)\) denotes the Eulerian representation of the pdf, \(L\) is the streaming operator \(Lf \equiv \frac{\partial}{\partial t}f + \frac{\partial}{\partial x} \cdot \{X(x,t)f\}\), \(X(x,t) \equiv \{v, F(x,t)\}\) a suitably smooth vector field, while \(v\) and \(F(x,t)\) denote respectively the velocity and an appro-
appropriate "mean-field" acceleration vector field. The implications of the principle of maximum entropy \[29\] and of the entropic principle, both involving the assumption that the Boltzmann-Shannon (B-S) entropy functional

\[
S(t) \equiv S(f(x,t)) = -\int_{\Gamma} dx f(x,t) \ln f(x,t)
\]  

exists, have been discussed elsewhere \[2, 3\] (see also Tessarotto et al., 2007 \[9\]). In particular this provides a well-defined initial condition for the pdf, \(f(x,t_0) = f_M(x,t_0)\) [see below Eq. (14)] and also a (generally non-unique) representation for the streaming operator \(L\) (Tessarotto et al., 2006 \[8\]). As a main consequence the same approach can in principle be used to determine in a rigorous way the Lagrangian formulation for arbitrary complex fluids. Although the choice of the phase-space \(\Gamma\) is in principle arbitrary, in the case of incompressible isothermal fluids, it is found \[6\] that it can always be reduced to the direct-product space \(\Gamma = \Omega \times V\) (restricted phase-space), where \(\Omega, V \subseteq \mathbb{R}^3\), \(\Omega\) is an open set denoted as configuration space of the fluid (fluid domain) and \(V\) is the velocity space.

4 The case of an incompressible thermofluid

Let us consider for definiteness an incompressible, viscous and generally non-isentropic thermofluid (which comprises as a particular case also the treatment of incompressible isothermal fluids earlier developed in Ref.\[4\]). This is described by the fluid fields \(\{Z\} \equiv \{\rho \geq 0, V, p \geq 0, T > 0, S_T\}\), to be identified respectively with the mass density, the fluid velocity, pressure, temperature and thermodynamic entropy. In the open set \(\Omega\) they are assumed to satisfy the so-called incompressible Navier-Stokes-Fourier equations (INSFE), i.e.,

\[
\rho = \rho_0 > 0,
\]

\[
\nabla \cdot V = 0,
\]

\[
\frac{D}{Dt} V = F_H - \frac{1}{\rho_0} [\nabla p - f] + \nu \nabla^2 V,
\]

\[
\frac{D}{Dt} T = \chi \nabla^2 T + \frac{\nu}{2c_p} \left( \frac{\partial V_i}{\partial x_k} + \frac{\partial V_k}{\partial x_i} \right)^2 + \frac{1}{\rho_0 c_p} J \equiv K,
\]

\[
\frac{\partial}{\partial t} S_T \geq 0,
\]

where \(\rho_0\) is a constant,

\[
F_H \equiv -\frac{1}{\rho_0} [\nabla p - f] + \nu \nabla^2 V
\]  

7
is the fluid acceleration and $\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{V} \cdot \nabla$ the convective derivative. These equations are assumed to satisfy a suitable initial-boundary value problem (INSFE problem) so that a smooth (strong) solution exists for the fluid fields $\{Z\}$. Here the notation is standard [3]. Thus, Eqs. (6)-(8) together are denoted incompressible Navier-Stokes equations (INSE) [with Eqs. (6) and (7) representing respectively the so-called incompressibility and isochoricity conditions and Eq. (8) the forced Navier-Stokes equation written in the Boussinesq approximation], while Eq. (9) is the Fourier equation. Finally (1) denotes the entropy inequality which defines the second principle of thermodynamics. As a consequence, in such a case the force density $\mathbf{f}$ reads $\mathbf{f} = \rho_0 \mathbf{g} (1 - k_{\rho_0} T) + \mathbf{f}_1$, where the first term represents the (temperature-dependent) gravitational force density, while the second one ($\mathbf{f}_1$) the action of a possible non-gravitational externally-produced force. Hence $\mathbf{f}$ can be written also as $\mathbf{f} = -\nabla \phi + \mathbf{f}_R$, where $\phi = \rho_0 g z$ and $\mathbf{f}_R = -\rho_0 g k_{\rho_0} T + \mathbf{f}_1$ denote respectively the gravitational potential (hydrostatic pressure) and the non-potential force density. Moreover, in Eq. (9) $K$ and $J$ are the quantities of heat generated per unit volume and unit time by all sources and, respectively, only by the external sources. In particular, the inequality (10) defines the so-called 2nd principle for the thermodynamic entropy $S_T$. For its validity in the following we shall assume that there results everywhere in $\overline{\Omega} \times T$

$$\int_{\Omega} dr \left( \chi \nabla^2 T + \frac{1}{\rho_0 c_p} J \right) \geq 0, \quad (12)$$

which defines a so-called externally heated thermofluid. In these equations $g, k_{\rho_0}, \nu, \chi$ and $c_p$ are all real constants which denote respectively the local acceleration of gravity, the density thermal-dilatation coefficient, the kinematic viscosity, the thermometric conductivity and the specific heat at constant pressure. Thus, by taking the divergence of the N-S equation (8), there it follows the Poisson equation for the fluid pressure $p$, namely $\nabla^2 p = -\rho_0 \nabla \cdot (\mathbf{V} \cdot \nabla \mathbf{V}) + \nabla \cdot \mathbf{f}$, with $p$ to be assumed non negative and bounded in $\overline{\Omega} \times T$.

4.1 Functional uniqueness of IKT

Let us now assume that $f(x,t)$ is a solution of the Eulerian kinetic equation (1) defined in a suitable extended phase-space $\Gamma \times I$, where $I \subseteq \mathbb{R}$ is a suitable time interval. In such a case, we intend to show that $f(x,t)$ [to be assume strictly positive] can be defined in such a way that the fluid fields $\mathbf{V}, p_1$ and $S_T$ can be identified with its velocity moments $\int d\mathbf{v} G(x,t) f(x,t)$, where respectively $G(x,t) = \mathbf{v}, \rho_0 u^2 / 3, -\ln f(x,t), \mathbf{u} \equiv \mathbf{v} - \mathbf{V}(r,t)$ is the relative velocity and $p_1$ the kinetic pressure defined as:

$$p_1 = p_0(t) + p - \phi + \frac{\rho_0}{m_p} T. \quad (13)$$
Here $p_0(t)$ (to be denotes as *pseudo-pressure*) is an arbitrary strictly positive and suitably smooth function defined in $I$. Moreover, $m_P > 0$ is a constant mass, whose value remains in principle arbitrary. In particular it can be identified with the average mass of the molecules forming the fluid. Finally, the thermodynamic entropy $S_T$ can be identified with the Shannon statistical entropy functional $S(f(x,t))$, provided the function $p_0(t)$ is a suitably prescribed function and $f(x,t)$ is strictly positive in the whole set $\Gamma \times I$. To reach the proof, let us first show that, by suitable definition of the vector field $F(x,t)$, a particular solution of the IKE (4) is delivered by the Maxwellian distribution function:

$$f_M(x,t) = \frac{1}{\pi^2 v_{Th}^2} \exp \left\{ -\frac{u^2}{v_{Th}^2} \right\},$$

(14)

where $v_{Th} = \sqrt{2p_1(r,t)/\rho_0}$ is the *thermal velocity driven by the kinetic pressure* $p_1(r,t)$. Based on the results earlier obtained for ideal isothermal and incompressible fluids [7, 8, 9] and incompressible therofluids [3] the following theorem is reached:

**Theorem - IKT formulation for INSFE**

Let us assume that the INSFE problem admits a smooth strong solution in $\Omega \times I$, such that the inequality (12) is fulfilled and the fluid fields $\{Z\}$ belong to the "minimal functional setting" (see Ref. [3]). Moreover, let us assume that in $\bar{\Omega} \times I$:

1) the pdf $f(x,t)$ is suitably smooth, strictly positive and admits the velocity moments $G(x,t) = 1, \mathbf{v}, \rho_0 \mathbf{u}_3, \rho_0 \mathbf{u}_3 \mathbf{u}_3, \rho_0 \mathbf{u}_3 \mathbf{u}_3 \mathbf{u}_3$; thus, we denote in particular $Q = \rho_0 \int d^3 \mathbf{v} \mathbf{u}_3 f$ and $\Pi = \rho_0 \int d^3 \mathbf{v} \mathbf{u}_3 \mathbf{u}_3 f$;

2) the B-S entropy integral (5) exists in the time interval $I \subseteq \mathbb{R}$;

3) the inequality (12) is assumed to hold;

4) there results identically (correspondence principle):

$$\int d^3 \mathbf{v} f(x,t) = 1,$$

(15)

$$\int d^3 \mathbf{v} \mathbf{v} f(x,t) = \mathbf{V}(r,t),$$

(16)

$$\rho_0 \int d^3 \mathbf{v} \frac{u^2}{3} f(x,t) = p_1(r,t),$$

(17)

$$S_T(t) = S(f(x,t)).$$

(18)
Then it follows that:

\( T_1 \) the local Maxwellian distribution \( f_M(x, t) \), defined by Eq. (14), is a particular solution of the inverse kinetic equation (14):

\[ f(x, t) = f_M(x, t) \]

\( T_2 \) the mean-field acceleration vector field \( F \) reads

\[ F(x, t) = F_0 + F_1. \] (19)

The functional form of the vector fields \( F_0, F_1 \) is determined uniquely by requiring that they depend only on the velocity moments indicated above. They read respectively:

\[ F_0(x, t) = \frac{1}{\rho_0} \left[ \nabla \cdot \Pi - \nabla p_1 + f_R \right] + D(x, t) + \nu \nabla^2 V, \] (20)

\[ F_1(x, t) = \frac{1}{2} \left\{ \frac{1}{p_1} A + \frac{1}{p_1} \nabla \cdot \Pi - \frac{1}{p_1^2} \nabla \cdot \Pi \right\} + \left( \frac{u^2}{v_{th}^2} - \frac{3}{2} \right). \] (21)

where

\[ D(x, t) = \frac{1}{2} \left\{ \nabla V \cdot u + u \cdot \nabla V \right\}, \] (22)

\[ A = \frac{\partial}{\partial t} (p_0 + p) - V \cdot \left[ \frac{D}{Dt} V - \frac{1}{\rho_0} f_R \nu \nabla^2 V \right] + \frac{\rho_0 K}{m_P} \equiv \frac{D}{Dt} p_1; \] (23)

\( T_3 \) for an arbitrary pdf \( f(x, t) \) fulfilling assumptions 1-3 equations (15)-(22) are fulfilled identically in \( \Omega \times I \).

**PROOF**

Let us, first, prove proposition \( T_1 \). For this purpose, let us assume that a strong solution of the INSFE problem exists which in the set \( \Omega \times I \) satisfies identically Eqs. (6)-(9). In such a case it is immediate to prove that \( f_M(x, t) \) is a particular solution of the inverse kinetic equation (14). This can be proved either: a) by direct substitution of \( f \equiv f_M(x, t) \) in Eq. (4) (Proposition A); b) by direct evaluation of the velocity moments of the same equation for \( G(x, t) = 1, v, u^2/3 \) (Proposition B). Regarding Proposition B, we notice that the first two moment equations coincide respectively with the isochoricity and Navier-Stokes equations [Eqs. (6) and (8)]. Therefore, the third moment equation delivers the Fourier equation [Eq. (9)]. The same proof (Proposition B) is straightforward also if \( f \neq f_M(x, t) \). This is reached again imposing the same constraint equation (15) on first velocity-moment of the distribution function.
f. The proof of $T_2$ and $T_3$ follows in the same way by direct evaluation of the velocity moments of the same equation for $G(x,t) = 1, v, \rho_o u^2, \rho_o u^3, \rho_o uu$. Q.E.D.

5 Lagrangian formulation of IKT

The previous results permit us to formulate in a straightforward way also the equivalent Lagrangian form of IKE [see Eq.(6)]. The Lagrangian formulation is achieved in two steps: a) by identifying a suitable dynamical system, which determines uniquely the time-evolution of the kinetic probability density prescribed by IKT. Its flow defines a family of phase-space trajectories, here denoted as phase-space Lagrangian paths (phase-space LP’s); b) by proper parametrization in terms of these curves of the pdf and the inverse kinetic equation, the explicit solution of the initial-value problem defined by the inverse kinetic equation [4] is determined. First, we notice that - in view of the previous theorem it is obvious that the phase-space LP’s must be identified with the phase-space trajectories $x(t)$ of a classical dynamical system

$$x_o \rightarrow x(t) = T_{t,t_o} x_o \equiv \chi(x_o, t_o, t)$$  \hspace{1cm} (24)

(here denoted as INSFE dynamical system), with $T_{t,t_o}$ the corresponding evolution operator generated by the vector field $X(x,t)$, to be prescribed according to the previous theorem. Hence, the initial-value problem (1) is realized by the equations

$$\begin{align*}
\frac{d}{dt} x(t) &= v(t), \\
\frac{d}{dt} v(t) &= F(x(t), t; f), \\
\frac{d}{dt} x(t_o) &= v_o, \\
\frac{d}{dt} v(t_o) &= v_o,
\end{align*}$$  \hspace{1cm} (25)

where the vector field $F(r(t), t; f)$ is defined by Eq.(19). Here, by construction $v(t)$ and $F(r(t), t; f)$ are respectively the Lagrangian velocity and acceleration, both spanning the vector space $\mathbb{R}^3$. In particular, $F(r(t), t; f)$, which is defined by Eqs.(20)-(21), and depends functionally on the kinetic probability density $f(x,t)$, is the Lagrangian acceleration which corresponds to an arbitrary kinetic probability density $f(x,t)$. From the theorem it follows that in the Lagrangian representation the kinetic equation (Lagrangian IKE) can be written in the form

$$J(x(t), t) f(x(t), t) = f(x_o, t_o) \equiv f_o(x_o),$$  \hspace{1cm} (26)

where $f_o(x_o)$ is a suitably smooth initial pdf and $J(x(t), t)$ is the Jacobian $J(x(t), t) = \left| \frac{\partial x(t)}{\partial x_o} \right|$ of the map $x_o \rightarrow x(t)$ which is generated by Eq.(25). It
follows that the Lagrangian equation (26) is uniquely specified by the proper definition of a suitable family of phase-space LP’s. Eq.(26) also provides the connection between Lagrangian and Eulerian viewpoints. In fact the Eulerian pdf, \( f(x,t) \), is simply obtained from Eq.(26) by letting \( x = x(t) \) in the same equation. As a result, the Eulerian and Lagrangian formulations of IKT, and hence of the underlying moment (i.e., fluid) equations, are manifestly equivalent.

6 The exact dynamics of ideal tracer particles

Let us now analyze in detail the equations of motion for ideal tracer particles immersed in an incompressible thermofluid described by INSFE [Eqs.(6)-(10)]. First, it must be remarked that two types of forces can in principle be present: a) a volume force, acted by the fluid (the same one which is responsible of the phase-space Lagrangian dynamics); b) particle-localized forces, such as the gravitational pull, acting directly on the tracer particle. In particular, regarding the first one, its specific form depends on the assumed pdf to be associated to the fluid. As discussed elsewhere \[30\], its choice depends closely on the type of fluid to be considered, i.e., deterministic or stochastic (as appropriate to describe turbulent flows). In particular, the position \( f \equiv f_M(x,t) \), with \( f_M(x,t) \) defined by Eq.(14) is suitable for the description of deterministic, i.e., non-turbulent flows. In such a case the appropriate form of the equation is obtained from Eqs.(19)-(23). Instead, the general case, in which one allows \( f \neq f_M(x,t) \), is provided by Eqs. (19) with (20) and (21).

Let us now assume that \( m_P \neq m_F \), \( m_F \) denoting the mass of the displaced fluid. In view of the IKT approach the equations of motion depend necessarily on the form of the pdf \( f(x,t) \), and hence describe in this sense the conditional phase-space dynamics. To construct the equation of motion for an ideal tracer particle of arbitrary mass, let us now assume, for definiteness, that the sole particle-localized force acting directly on the tracer particle is produced by the gravitational pull. The equation of motion for an ideal tracer particle of mass \( m_P \) reads simply in such a case:

\[
m_P \left[ \frac{d}{dt} v(t) - g \right] = m_F \left[ F(x,t; f) - g \right].
\] (27)

which describes the conditional dynamics of an ideal tracer particle immersed in an incompressible thermofluid described by a pdf \( f(x,t) \). We stress that the form of the pdf depends on the specific assumptions made on the fluid \[30\]. The interpretation of this equation is as follows. The terms on the l.h.s. represent the ”inertial” and gravitational forces acting on the tracer particle. Instead, all the terms on the r.h.s. represent the volume force acting responsible
for the phase-space Lagrangian motion. The physical interpretation of the various contributions appearing in the volume force [see Eqs. (19), (20) and (21)] is made transparent by representing them in terms of the vector fields \( m_F F_0(x,t; f) \) and \( m_F F_1(x,t; f) \), to be interpreted as mean-field forces. One obtains in fact, in particular:

\[
m_F \left[ F_0(x,t; f) - g - \frac{v_H^2}{2p_1} \nabla p_1 \right] \equiv m_F F_H + m_F D(x,t), \tag{28}
\]

It is immediate to prove that the terms in the first equation take into account the fluid and convective forces \( m_F F_H \) and \( m_F D(x,t) \), with \( F_H \) and \( D(x,t) \) denoting respectively the fluid acceleration \( (11) \) and the convective term defined above [see Eq.(22)]. In a similar way one can show that, in case \( m_P \neq m_F \), Eq.(27) recovers also the buoyancy force density \( (m_P - m_F) g \) pointed out by Maxey and Riley \( (11) \). Finally, for the sake of comparison, let us consider the case of an isothermal fluid and require - consistent with Eq.(3) - that locally in the extended phase-space \( \Gamma \times I \) condition \( (3) \) holds at time \( t = t_o \). The validity of previous tracer-particle equations [i.e., in particular the MR (Maxey-Riley) equation \( (2) \)] requires that the inequality \( (3) \) holds for all times \( (t \in I) \). In particular, one can prove that in such a limit our Eq.(27) agrees with the MR equation \( (2) \). In fact, it yields

\[
m_P \frac{d}{dt} v(t) \cong m_F \frac{D V(x,t)}{D t} \bigg|_{x=r(t)} + m_F F_1 - (m_P - m_F) g, \tag{29}
\]

where, in validity of \( (3) \), it follows that the pressure mean-field force can be approximated as \( m_F F_1 \cong -\frac{1}{2} m_F \frac{d}{dt} \{ v(t) - V(x(t),t) \} \bigg|_{x=r(t)} \). On the other hand, a serious objection to all of the previous tracer-dynamics equations is provided by the possible violation of the asymptotic condition \( (3) \), which may not be uniformly fulfilled in the set \( I \). This occurs, manifestly, if an initial condition of the type \( |u(t_o)| \sim |V(r(t_o),t_o)| \) is imposed on a tracer particle (this requirement is not physically unreasonable since, in principle, tracer particles might be injected in a fluid with arbitrary initial velocities). However, even if initially (at \( t = t_o \)) one requires the validity of \( (3) \) in general it may well be also that \( |u(t)| \sim |V(r(t),t)| \) at some later time \( (t > t_o) \). This can be achieved, for example, even imposing the initial condition \( |u(t_o)| = 0 \). The result is a consequence of Eq.(27). Indeed one can prove that, even imposing the initial condition \( |u(t_o)| = 0 \), generally \( |u(t)| \neq 0 \), with \( |u(t)| \) not satisfying \( (3) \). In other words, ideal tracer particles having initially the same local velocity of the fluid may develop in time a finite relative velocity. This implies that, generally, the full exact tracer-dynamics equation, i.e., Eq.(27), should be used, instead of the asymptotic approximation indicated above [see Eq.(29)].
7 Concluding remarks

In this paper the phase-space Lagrangian dynamics has been determined as appropriate for an incompressible thermodruid described by a suitable set of fluid equations [INSFE, see Eqs.(6)-(10)]. We have shown that, based on the formulation of a restricted phase-space inverse kinetic theory, the phase-space Lagrangian dynamics can be uniquely established. The governing equations which determine the phase-space Lagrangian trajectories (LP’s) are found to depend functionally on the pdf \([f(x, t)]\), to be uniquely associated to the fluid by means of the IKT here adopted. In particular, the theory permits to advance uniquely in time \(f(x, t)\) and in terms of the same pdf also the complete set of fluid fields which describe the fluid. This feature is of fundamental importance in turbulence theory (see [30]).

As a further consequence, the dynamics of ideal tracer particles (i.e., for which the perturbations of the fluid fields produced by the same particles are negligible) is established. Remarkably, this result overcomes limitations of customary ideal tracer-dynamics equations [see in particular the Maxey and Riley equation \([11]\) given by Eq.(2)]. All of these equations are, actually, in disagreement with the present theory for finite particle relative velocities. The basic new result is represented by Eq.(27) which describes, for arbitrary initial velocity, the conditional dynamics of an ideal tracer particle in an incompressible thermodruid described by a suitable pdf \(f\).

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