Time Derivatives in Material and Spatial Description—What Are the Differences and Why Do They Concern Us?

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Abstract This paper has many, albeit mostly didactic objectives. It is an attempt toward clarification of several concepts of continuum theory which can lead and have led to confusion. In a way the paper also creates a bridge between the lingo of the solid mechanics and the fluid mechanics communities. More specifically, an attempt will be made, first, to explain and to interpret the subtleties and the relations between the so-called material and spatial description of continuum fields. Second, the concept of time derivatives in material and spatial description will be investigated meticulously. In particular, it will be explained why and how the so-called material and total time derivatives differ and under which circumstances they turn out to be the same. To that end, material and total time derivatives will be defined separately and evaluated in context with local fields as well as during their use in integral formulations, i.e., when applied to balance equations. As a special example the mass balance is considered for closed as well as open bodies. In the same context the concept of a "moving observation point" will be introduced leading to a generalization of the usual material derivative. When the total time derivative is introduced the distinction between the purely mathematical notion of a coordinate system and the intrinsically physics-based concept of a frame of reference will gain particular importance.

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1 Introduction

There are two fundamentally different approaches for describing the kinematics of continua. One method of observing a structure's motion is based on following individual particles of the body as they move through space and time. It is used for modeling solid matter with various rheological properties (elastic and nonelastic). In the other method motion is described by focusing on a specific location of space through which the structure moves as time passes on. It is mostly used in fluid and gas mechanics as well as in granular media modeling. Following Malvern (1969), we will call the first description *material* and the second one *spatial*.

In order to consider multiphase structures consisting of a solid and fluid phases it is convenient to use the material description for the solid and a modification of the spacial description for fluids. In this case it is very important to understand how the concepts introduced in the different descriptions relate to each other. This holds, in particular, for the time derivatives. The so-called *total derivative in material description* and the *material derivative in spatial description* written in terms of a partial derivative look very similar. Thus it is not surprising that it is a widespread opinion that the total and the material derivatives are different names for the same concept. But as it will be shown further down they are different concepts describing a rate of change of a property of the material point and a rate of change of a property at the space point. Consequently, one aim of the present paper is to give a definition of the total derivative (as an analogue and generalization of the derivative used in the material description), to give a definition of the material derivative (as an analogue and generalization of the derivative used in the spatial description), to make a strict distinction between these concepts, and to investigate the conditions for which they coincide.

In summary, this paper is an attempt to clarify sometimes obscure and confusing statements made in context with the material and spatial description and the associated time derivatives. In this sense it is of didactic value and we only claim to raise awareness of the situation and to provide some comments regarding possible ways out of die-hard conundrums.

2 Total and Material Derivatives in Material and Spatial Descriptions—Literature Review

The main problem with the definition of a *total time derivative* is that the corresponding operator appearing in the laws of continuum theory is not simply a purely mathematical concept. Rather it contains an underlying, definitive physical meaning. In order to clarify the problem we start with a purely mathematical definition. Let $g = \tilde{g}(u(t), v(t), w(t), t)$. The total derivative of $\tilde{g}$ with respect to t (the symbol of the time variable, chosen as a reminder for later purpose) is:

$$\frac{d\tilde{g}}{dt} = \frac{\partial \tilde{g}}{\partial u}\frac{du}{dt} + \frac{\partial \tilde{g}}{\partial v}\frac{dv}{dt} + \frac{\partial \tilde{g}}{\partial w}\frac{dw}{dt} + \frac{\partial \tilde{g}}{\partial t}. \tag{1}$$

Now let the arguments of the function depend on two independent variables, say $u = u_*(s,t)$, $v = v_*(s,t)$, $w = w_*(s,t)$. We can form partial derivatives of $g = g_*(s,t)$ with respect to one of its arguments with the other held constant. Thus in the case of a function of several independent variables (here s and t) every derivative is a partial one. The concept of a total derivative of a function of several independent variables does not exist in mathematics.

In mechanics of continua all quantities characterizing a stress–strain state are functions of several *independent* variables—three spatial coordinates and time. Therefore, introducing the concept of a total derivative with respect to time in a strictly mathematical sense is impossible. An additional physics-based idea postulating what spatial coordinates should be fixed and how to identify them is needed. We will get back to that later.

Within the framework of material description the so-called material points are identified by their position, $\boldsymbol{R}$, in an arbitrary chosen reference configuration. The reference configuration is usually chosen to be fixed in the frame of reference. The total derivative of a vector field, $\boldsymbol{\psi}(\boldsymbol{R}, t)$, is then defined as a partial derivative with respect to t with $\boldsymbol{R}$ held constant, see Dmitrienco (2009):

$$\frac{d\boldsymbol{\psi}}{dt} = \left.\frac{\partial \boldsymbol{\psi}}{\partial t}\right|_{\boldsymbol{R}=\text{const}}. \tag{2}$$

Note that in some cases it makes sense to exclude a rigid body motion from our considerations (e.g., if we are only interested in the (local) deformation, i.e., the displacement, $\boldsymbol{u}$, of the matter of an object, it does not make sense to look at its total motion. Hence, we "take out" the rotation when considering the deformation of a spinning shaft, or the translative/rotative motion of a flying aircraft when bending of its wing becomes an issue, etc.). If a coordinate system comoving with the body is used then the reference position vector depends on time and the definition (2) has to be modified since $\boldsymbol{R} = \hat{\boldsymbol{R}}(t)$.

In a number of books on solid mechanics and nonlinear elasticity the derivative (2) is called material, substitutional, or individual (see, e.g., Ogden 2003; Asaro and Lubarda 2006) and the concept of a total derivative is not introduced. In other books the definition (2) is not given explicitly. Rather the material derivative is defined as a rate of change of a variable, $\boldsymbol{\psi}$, whose arguments are the current position vector of a material particle (the so-called *motion*), $\boldsymbol{r}(\boldsymbol{R}, t)$, and time, t. Then, by virtue of the chain rule of calculus:

$$\dot{\boldsymbol{\psi}} \equiv \frac{D\boldsymbol{\psi}}{Dt} = \left.\frac{\partial \boldsymbol{\psi}}{\partial t}\right|_{\boldsymbol{r}=\text{const}} + \boldsymbol{v}\cdot\nabla\boldsymbol{\psi}, \qquad \nabla = \frac{\partial}{\partial \boldsymbol{r}}, \qquad \boldsymbol{v} = \left.\frac{\partial \boldsymbol{r}(\boldsymbol{R}, t)}{\partial t}\right|_{\boldsymbol{R}=\text{const}}. \tag{3}$$

In these books the definition of the total derivative is either not given at all or it is said that the material derivative coincides with the total one (Milne-Thomson 1960;

Lojtsanskij 1950; Durst 1992). It is interesting to note that in Petrila and Trif (2005), p. 7, the derivative (2) is called "a *local* or *material derivative*," while in the case of (3) it "is designed to be the *total* or *spatial* or *substantive derivative or the derivative following the motion*." Truesdell (1972), p. 104, writes more cautiously:

> The dot operator as defined by (3) is called the *substantial derivative*. [...] We have already agreed to use the dot to denote the time derivative in the substantial and referential descriptions, and the definition (3) has been framed so as to render the two usages consistent with each other.

The symbol of the total derivative appears also in balance equations as a generalization of the theorem on differentiation of an integral with respect to a parameter, see Truesdell (1972). Widely used in continuum mechanics is a volume-related transport theorem of the form:

$$\frac{d}{dt}\int_{V(t)} \boldsymbol{\psi}\, dV = \int_{V(t)} \left(\frac{D\boldsymbol{\psi}}{Dt} + (\boldsymbol{\psi}\nabla)\cdot\boldsymbol{v}\right) dV, \tag{4}$$

which contains symbols of the material and of the total derivatives, D/Dt and d/dt, respectively (Adler 1992; Ogden 2003; Asaro and Lubarda 2006; Gurtin 1981). Note that integration over the volume in (4) does not exclude a dependence of the result of integration from a position vector, since in the case of a nonuniform distribution of the field $\boldsymbol{\psi}$ across the medium varying from subvolume to subvolume, the result depends on the position of a subvolume within the medium. Thus the left part of (4) can be the total derivative of a function of several independent variables, namely time and the location of the subvolume. This might be one reason why Truesdell (1972), p. 105, says:

> More generally, if $\boldsymbol{\Psi}$ denotes a tensor field of any order,
>
> $$\frac{d}{dt}\int_{\mathcal{P}} \boldsymbol{\Psi}\, dM = \frac{d}{dt}\int_{\mathcal{X}(\mathcal{P},t)} \rho\boldsymbol{\Psi}\, dV = \int_{\mathcal{X}(\mathcal{P},t)} \rho\dot{\boldsymbol{\Psi}}\, dV \tag{5}$$
>
> and $\dot{\boldsymbol{\Psi}}$ is to be calculated by an appropriate rule of the type (3). (The central expression, which involves an undefined operation d/dt, is to be regarded only as a suggestive way of writing the left-hand expression.) The commutation formula (5) is used so often in continuum mechanics that it is taken for granted without special reference.

At the same time many authors point out that the transport theorem is used for the calculation of the material derivative over a *material volume*, i.e., a volume that consists of the same matter all the time. For example, we find in Eringen (1980), p. 79[1]:

> The material derivative of any field over a material volume is given by
>
> $$\frac{D}{Dt}\int_{V(t)} \boldsymbol{\varphi}\, dV = \int_{V(t)} (\dot{\boldsymbol{\varphi}} + \boldsymbol{\varphi}\nabla\cdot\boldsymbol{v})\, dV = \int_{V(t)} \left(\frac{\partial\boldsymbol{\varphi}}{\partial t} + \nabla\cdot(\boldsymbol{v}\boldsymbol{\varphi})\right) dV. \tag{6}$$

[1]Eringen's choice of symbols has been adapted to coincide with the ones used in this article.

The derivative $\dot{\boldsymbol{\varphi}}$ in (6) has the same meaning as in (5). The apparent difference between (6) and (5) is due to the fact that the transport theorem in the form (5) is written for specific quantities, $\boldsymbol{\Psi}$.

Analogous formulae can be found in many other books, see, e.g., Malvern (1969), Mase (1970), Fung (1965). However, it is not clear which velocity of what point appears in the convective part of (3) and what $\boldsymbol{r}$ is fixed. Therefore, in that case the operation D/Dt on the left side to the integral is also undefined.

Despite such differences, the material description is presented in the solids-related literature more or less similarly. The situation is quite different with hydrodynamics books. First of all, it should be noted that in fact the material description is also used in many hydrodynamics books, see, e.g., Serrin (1959), Petrila and Trif (2005). However, a consistent presentation of the alternative, so-called spatial description can be found, for example, in Lojtsanskij (1950), Daily and Harleman (1966), Batchelor (1970).

The spatial description is a method of observing a motion that focuses on a specific location in space through which the structure moves as time passes, the so-called *observation point*. The difference between the material and the spatial descriptions is basically as follows. Within the material description there are two configurations—the reference and the current one—, which are determined by the position vectors $\boldsymbol{R}$ and $\boldsymbol{r}(\boldsymbol{R},\ t)$, respectively. $\boldsymbol{R}$ labels the substantial point and $\boldsymbol{r}(\boldsymbol{R},\ t)$ is the basic functional relationship through which all other kinematic characteristics are expressed. The spatial description considers only the current configuration and the position vector $\boldsymbol{r}$ describes the position of a (fixed) point in space so that it does not depend on time and on the evolution of matter. The primary quantity in the spatial description is the velocity of the matter and all other quantities are expressed in terms of $\boldsymbol{v}(\boldsymbol{r},\ t)$.

The concept of a material derivative in hydrodynamics seems to originally stem from Stokes (cf., Granger (1995), Sect. 1.7.3) in order to describe changes in the properties of liquid particles during the time dt, which in the beginning of the interval dt was at a certain point in space. In order to show how the material derivative in spatial description is introduced we present a quote from the book of Adler (1992), p. 55, who uses δt instead dt for designation of the time increment (the equation labels have been adjusted for convenience; note that by "element" Adler means "material element" as he says in a here-not-quoted sentence before):

> At time t, the element is located at position $\boldsymbol{r}$, and at $t + \delta t$, it is located at $\boldsymbol{r} + \boldsymbol{v}\delta t$. Hence a change in the quantity ψ for this particular element can be expressed as
>
> $$\psi(\boldsymbol{r} + \boldsymbol{v}\delta t, t + \delta t) - \psi(\boldsymbol{r}, t) = \left(\frac{\partial \psi}{\partial t} + \boldsymbol{v} \cdot \nabla \psi\right) \delta t. \tag{7}$$
>
> The time derivative of ψ, following the motion of the fluid, can be symbolized by the operator D/Dt called the *material derivative*:
>
> $$\frac{D\psi}{Dt} = \frac{\partial \psi}{\partial t} + \boldsymbol{v} \cdot \nabla \psi. \tag{8}$$

This is the only possible way to introduce the material derivative within the framework of a spatial description and it is presented in many hydrodynamics books, see, e.g., Batchelor (1970), Lamb (1975), Rouse (1959), Lojtsanskij (1950), Landau and Lifshitz (1959), Prandtl and Tietjens (1929). It should be noted that this definition of a material derivative cannot be regarded as a mathematical definition of the function derivative since an increment of argument $\boldsymbol{v}\delta t$ cannot be expressed in terms of function arguments $\boldsymbol{r}$ and t.

Thus, the formally introduced definition of the material derivative as a derivative of a composite function cannot be used in spatial description. Also, it is worthwhile mentioning that in the velocity of (8) we put $\boldsymbol{v}(\boldsymbol{r}, t)$, whereas in (3) it is a function of the reference position vector, $\boldsymbol{v}(\boldsymbol{R}, t)$.

Now let us consider the definition of the material derivative (2) as a derivative following the motion of the fluid. In the spatial description a given region in space is considered. The material element at position $\boldsymbol{r}$ at time t possesses the velocity $\boldsymbol{v}(\boldsymbol{r}, t)$ and moves to the position $\boldsymbol{r} + \boldsymbol{v}dt$. Thus in order to describe the evolution of matter during the infinitesimal period of time dt one may use the material description taking $\boldsymbol{r}$ and $d\boldsymbol{u}(\boldsymbol{x}, t) = \boldsymbol{v}dt$ as the reference position and the infinitesimal displacement correspondingly. As a result, one may apply mathematical methods developed for the material description to the spatial description, taking at every moment of time the current configuration as the reference one and considering a small vicinity of this configuration, see Ilyushin (1971). Fixing the position vector of the material particle at some moment of time and taking it as the reference position vector contradicts the essence of spatial description, thus the definition (2) cannot be used in it.

It should be noted that since there is only the current configuration in the spatial description it is obvious which coordinates should be fixed. The total derivative is defined as a partial derivative with the observation point, $\boldsymbol{r}$, being held constant,

$$\frac{d\boldsymbol{\psi}}{dt} = \left.\frac{\partial \boldsymbol{\psi}}{\partial t}\right|_{\boldsymbol{r}=\text{const}}. \tag{9}$$

In addition to that the balance equations are formulated for a constant volume containing the observation point. As a result a partial derivative operator appears in front of the integral (Milne-Thomson 1960; Landau and Lifshitz 1959). The total derivative is usually not used in classical hydrodynamics at all and all equations are written in terms of the material and partial derivatives.

However, in order to consider more complicated problems (e.g., fluid flow through a deformable solid or porous media) it is convenient to use a moving observation point fixed within the (elementary) volume jointly traversing space at a given velocity.

An expression for the material derivative in the spatial description with a moving observation point was suggested in Altenbach et al. (2003), Zhilin (2012) and contains the total time derivative:

$$\frac{D\boldsymbol{\psi}}{Dt} = \frac{d\boldsymbol{\psi}(\boldsymbol{r}(t), t)}{dt} + \left(\boldsymbol{v}(\boldsymbol{r}(t), t) - \frac{d\boldsymbol{r}(t)}{dt}\right) \cdot \nabla \boldsymbol{\psi}(\boldsymbol{r}(t), t). \tag{10}$$

A similar expression can be found in the literature on porous media, e.g., Hassanizadeh and Gray (1980). A porous medium is viewed as a body consisting of two coexistent continua. The motion of the solid phase is defined by the current position vector $\boldsymbol{r}^s(\boldsymbol{R}^s,\ t)$, the motion of the solid so-to-speak. The time rate of change with respect to the solid phase of a quantity $\boldsymbol{\psi}$ is defined as:

$$\frac{D^s\boldsymbol{\psi}}{Dt} = \left.\frac{\partial\boldsymbol{\psi}(\boldsymbol{R}^s,\ t)}{\partial t}\right|_{\boldsymbol{R}^s=\text{const}} = \left.\frac{\partial\boldsymbol{\psi}(\boldsymbol{r}^s,\ t)}{\partial t}\right|_{\boldsymbol{r}^s=\text{const}} + \boldsymbol{v}^s\cdot\nabla\boldsymbol{\psi}, \tag{11}$$

where $\boldsymbol{v}^s$ is the solid phase velocity. It is obvious that (11) coincides with the definitions of the total derivative in the material description (2), (3). The time rate of change of the quantity $\boldsymbol{\psi}$ with respect to the fluid phase is given by

$$\frac{D^f\boldsymbol{\psi}}{Dt} = \left.\frac{\partial\boldsymbol{\psi}(\boldsymbol{r}^s,\ t)}{\partial t}\right|_{\boldsymbol{r}^s=\text{const}} + \boldsymbol{v}^f\cdot\nabla\boldsymbol{\psi}, \tag{12}$$

where $\boldsymbol{v}^f$ is the fluid-phase velocity field.

Subtraction of Eq. (11) from (12) yields the following relation, see Hassanizadeh and Gray (1980):

$$\frac{D^f\boldsymbol{\psi}}{Dt} = \frac{D^s\boldsymbol{\psi}}{Dt} + (\boldsymbol{v}^f - \boldsymbol{v}^s)\cdot\nabla\boldsymbol{\psi}. \tag{13}$$

By taking into account that $d\boldsymbol{r}(t)/dt$ in (10) corresponds to the velocity of the solid phase one can see that the definitions (13) and (10) coincide.

The moving observation point is also considered in the Arbitrary Lagrangian–Eulerian (ALE) technique. ALE is used to account for the deformation of the fluid domain which arises from the displacement and deformation of the solid structure. The material derivative is defined by the fundamental ALE equation (see all of the references immediately below for details):

$$\frac{D\boldsymbol{\psi}}{Dt} = \left.\frac{d\boldsymbol{\psi}}{dt}\right|_{\boldsymbol{R}=\text{const}} + (\boldsymbol{v} - \hat{\boldsymbol{v}})\cdot\nabla\boldsymbol{\psi}, \tag{14}$$

where $\boldsymbol{v}$ is the velocity of the fluid particle and $\hat{\boldsymbol{v}}$ is referred to indistinctly as the "velocity of the reference point" by Dettmer and Peric (2006) or "velocity of the moving frame" by Del Pin et al. (2007). In fact, it should be called unmistakably "grid velocity" as in Vuong et al. (2015) and Gadala (2004), or "mesh velocity" as in Khoei et al. (2007) or Filipovic et al. (2006). Also note that the concept of a moving grid and of a relative speed inherent to the material derivative was anticipated before ALE became a prominent concept by Müller and Muschik (1983), where $\hat{\boldsymbol{v}}$ was called "mapping velocity." Moreover, d/dt corresponds to the change of the material particle quantity, which is noted by an observer traveling with a point on the reference frame. The definitions (10), (13), and (14) coincide.

However, in some articles, see Dang and Meschke (2014), Preisig and Zimmermann (2011), Sarrate et al. (2001), the material derivative is defined by:

$$\frac{D\boldsymbol{\psi}}{Dt} = \frac{\partial \boldsymbol{\psi}}{\partial t} + \left(\boldsymbol{v} - \hat{\boldsymbol{v}}\right) \cdot \nabla \boldsymbol{\psi}, \tag{15}$$

where the symbol $\boldsymbol{v}$ was used for the fluid velocity and $\hat{\boldsymbol{v}}$ for the so-called "velocity of the moving reference," see Dang and Meschke (2014), or "fluid mesh velocity" as termed by Preisig and Zimmermann (2011) or Sarrate et al. (2001). Even if we ignore differences in the linguistic terminology, Eq. (15) coincides with (14), (10), and (13) only if the partial derivative in (15) is defined with the reference position vector of the observation point held constant. At the same time it is written in Surana et al. (2014)[2]:

> ... the Eulerian description with transport
>
> $$\rho \left(\left.\frac{\partial \boldsymbol{v}}{\partial t}\right|_{\boldsymbol{r}=\mathrm{const}} + \boldsymbol{v} \cdot \nabla \boldsymbol{v} \right) - \nabla \cdot \boldsymbol{\sigma} - \rho \boldsymbol{f} = 0,$$
>
> is converted to ALE form by replacing velocity $\boldsymbol{v}$ (velocity at a fixed location $\boldsymbol{r}$) in the convective terms with convective velocity $\bar{\boldsymbol{C}} = \boldsymbol{v} - \hat{\boldsymbol{v}}$.

It is obvious that in this case the material derivative in Surana et al. (2014) differs from the material derivatives defined by (14), (10), and (13). It is seen that there are different formulae for the operator of a material derivative in modern literature. Some authors distinguish between the total and the material derivatives, but sometimes it is used synonymously, namely as "the total time or the material derivative," cf., Milne-Thomson (1960), Lojtsanskij (1950). Sometimes an operator of material derivative is defined through another operator of material derivative (equations analogously to (13)). It conflicts with the classical interpretation of the material derivative as a derivative following the motion of the specific particle.

In many papers the material derivative is written in a form very similar to the one adopted from the classical textbooks. However, it is not specified what is meant by the partial time derivative. As a result, a comparison of material derivatives used by different authors in order to ensure that they coincide or differ is extremely difficult in some cases. Furthermore, definitions of the used notations are not always provided, and only formulae for calculations are listed.

In summary of our review we have to conclude that we are facing, first, the need for a clear distinction between the concept of a material and a spatial description of fields. Second, a distinction of various time derivatives of these fields is required, namely between one unfortunately called material time derivative, despite the fact that it exists in material *and* in spatial description, as well as the other known as total time derivative. Sometimes both coincide in meaning and sometimes they do not. Following this remark, it is the goal of the present paper to give, first, clear mathematical definitions of the material and of the total time derivatives, which can be used for a moving observation point and for a nonconstant reference vector, and, second, to clarify the physical meaning of these operators.

[2] This is not a verbal quote. For the convenience of the reader it has been adjusted to the symbols used in this paper.

3 Material Description

3.1 Kinematics of Continua

In material description quantities related to material particles are functions of the reference position, $\boldsymbol{R}$, and of time, t, which we will refer to as "referential variables." Any such function $f = f_*(\boldsymbol{R}, t)$ may be replaced by a function of the spatial variables $\tilde{f}(\boldsymbol{r}, t)$, which has the same value, f, at the corresponding position vector: $f = f_*(\boldsymbol{R}, t) = \tilde{f}(\boldsymbol{r}_*(\boldsymbol{R}, t), t)$.

Suppose that the reference position vector does not depend on time. Then the rate of change of a quantity relevant for characterization of the material particle is

$$\frac{\partial f_*}{\partial t} = \lim_{\Delta t \to 0} \frac{f_*(\boldsymbol{R}, t + \Delta t) - f_*(\boldsymbol{R}, t)}{\Delta t}, \tag{16}$$

if it is a function of the referential variables. Otherwise

$$\begin{aligned} \frac{d_r \tilde{f}}{dt} &= \lim_{\Delta t \to 0} \frac{\tilde{f}(\boldsymbol{r}_*(\boldsymbol{R}, t + \Delta t), t + \Delta t) - \tilde{f}(\boldsymbol{r}_*(\boldsymbol{R}, t), t)}{\Delta t} \\ &= \lim_{\Delta t \to 0} \frac{\tilde{f}(\boldsymbol{r}_*(\boldsymbol{R}, t + \Delta t), t + \Delta t) - \tilde{f}(\boldsymbol{r}_*(\boldsymbol{R}, t + \Delta t), t)}{\Delta t} \\ &\quad + \lim_{\Delta t \to 0} \frac{\tilde{f}(\boldsymbol{r}_*(\boldsymbol{R}, t + \Delta t), t) - \tilde{f}(\boldsymbol{r}_*(\boldsymbol{R}, t), t)}{\Delta t} \\ &= \frac{\partial \tilde{f}(\boldsymbol{r}, t)}{\partial t} + \frac{\partial \boldsymbol{r}_*(\boldsymbol{R}, t)}{\partial t} \cdot \nabla \tilde{f}, \qquad \nabla \equiv \frac{\partial}{\partial \boldsymbol{r}}. \end{aligned} \tag{17}$$

The rate of change of a physical quantity should not depend on the choice of variables. Thus

$$\frac{\partial f_*(\boldsymbol{R}, t)}{\partial t} = \frac{d_r \tilde{f}(\boldsymbol{r}, t)}{dt}, \qquad \frac{d_r}{dt} \equiv \left.\frac{\partial}{\partial t}\right|_{\boldsymbol{r}=\text{const}} + \frac{\partial \boldsymbol{r}_*(\boldsymbol{R}, t)}{\partial t} \cdot \nabla. \tag{18}$$

Equation (18)$_1$ is consistent with the chain rule of calculus. The operator d_r/dt defines the total derivative under the condition that the reference position vector is a constant.

Now let $\boldsymbol{R} = \boldsymbol{R}_{*0}(\boldsymbol{R}_0, t)$, where $\boldsymbol{R}_0$ does not depend on time. The velocity vector is thus defined by

$$\begin{aligned} \boldsymbol{v} &= \lim_{\Delta t \to 0} \frac{\boldsymbol{r}_*(\boldsymbol{R}_{*0}(\boldsymbol{R}_0, t + \Delta t), t + \Delta t) - \boldsymbol{r}_*(\boldsymbol{R}_{*0}(\boldsymbol{R}_0, t), t)}{\Delta t} \\ &= \frac{\partial \boldsymbol{r}_*(\boldsymbol{R}, t)}{\partial t} + \frac{\partial \boldsymbol{R}}{\partial t} \cdot \overset{\circ}{\nabla} \boldsymbol{r} \equiv \frac{d^\circ \boldsymbol{r}}{dt}, \\ \overset{\circ}{\nabla} &\equiv \frac{\partial}{\partial \boldsymbol{R}}, \qquad \frac{d^\circ}{dt} \equiv \left.\frac{\partial}{\partial t}\right|_{\boldsymbol{R}=\text{const}} + \frac{\partial \boldsymbol{R}}{\partial t} \cdot \overset{\circ}{\nabla} \end{aligned} \tag{19}$$

The operator d°/dt is the total time derivative in the reference configuration. Then the rate of change of the quantity in the current configuration can be found by the chain rule:

$$\frac{d_r \tilde{\boldsymbol{f}}}{dt} \equiv \left.\frac{\partial \tilde{\boldsymbol{f}}(\boldsymbol{r},t)}{\partial t}\right|_{\boldsymbol{r}=\text{const}} + \frac{d^\circ \boldsymbol{r}}{dt} \cdot \nabla \tilde{f}. \tag{20}$$

The operator of the total time derivative in the current configuration, d_r/dt, is a generalization of $(18)_2$. After taking (19) into account, the operators (20) and $(18)_2$ can be expressed in the same manner:

$$\frac{d_r}{dt} \equiv \left.\frac{\partial}{\partial t}\right|_{\boldsymbol{r}=\text{const}} + \boldsymbol{v} \cdot \nabla. \tag{21}$$

According to Eq. (19) the velocity emerges as a function of the reference position vector $\boldsymbol{v} = \boldsymbol{v}_*(\boldsymbol{R},t)$. However, we may eliminate $\boldsymbol{R}$ by assuming that there exists an inverse of the single-valued function $\boldsymbol{r} = \boldsymbol{r}_*(\boldsymbol{R},t)$, so that it is possible to obtain the velocity as a function of spatial coordinates $\boldsymbol{v} = \tilde{\boldsymbol{v}}(\boldsymbol{r},t)$. In the first case the acceleration is

$$\boldsymbol{a}_*(\boldsymbol{R},t) = \frac{d^\circ \boldsymbol{v}_*(\boldsymbol{R},t)}{dt} = \lim_{\Delta t \to 0} \frac{\boldsymbol{v}_*(\boldsymbol{R}_*(\tilde{\boldsymbol{R}}, t+\Delta t), t+\Delta t) - \boldsymbol{v}_*(\boldsymbol{R}_*(\tilde{\boldsymbol{R}},t),t)}{\Delta t}, \tag{22}$$

whilst in the second

$$\tilde{\boldsymbol{a}} = \frac{d_r \tilde{\boldsymbol{v}}}{dt} = \lim_{\Delta t \to 0} \frac{\tilde{\boldsymbol{v}}(\boldsymbol{r}_*(\boldsymbol{R}_*(\tilde{\boldsymbol{R}}, t+\Delta t), t+\Delta t), t+\Delta t) - \tilde{\boldsymbol{v}}(\boldsymbol{r}_*(\boldsymbol{R}(\tilde{\boldsymbol{R}},t),t),t)}{\Delta t}. \tag{23}$$

With the rules of differentiation for a composite function it is easy to show that:

$$\frac{d^\circ \boldsymbol{v}_*(\boldsymbol{R},t)}{dt} = \frac{d_r \tilde{\boldsymbol{v}}(\boldsymbol{r},t)}{dt}. \tag{24}$$

This is valid for every physical quantity.

Thus, within the framework of a material description, the rate of change of a physical quantity of a material particle is determined by the total time derivative.

3.2 Equations of Balance

The equations of balance of continuum thermomechanics are mathematical statements of the conservation laws for mass, linear and angular momentum, and energy.

We take the mass balance as an example. Consider a material body occupying the region V_0 in the reference configuration. If a continuous medium of density $\rho_0(\boldsymbol{R})$ fills the region, the total mass in V_0 is:

$$m_0(\boldsymbol{R}^*) = \int_{V_0} \rho_0(\boldsymbol{R})\, dV_0, \tag{25}$$

where $\boldsymbol{R}^*$ is a position vector of a point within the region (e.g., the center of mass). Note that integration over the region does not imply independence of the result from a position vector in a case of inhomogeneous medium. This calls for further explanation: V_0 does not necessarily encompass all the mass there. Rather it may refer to a subvolume, e.g., one layer of a sandwich structure. And it is the position of this substructure we wish to identify by the label $\boldsymbol{R}^*$.

In the current configuration the body occupies the region $V(t)$ and its mass is:

$$\tilde{m}(\boldsymbol{r}^*, t) = \int_{V(t)} \tilde{\rho}(\boldsymbol{r}, t)\, dV, \quad \text{where} \qquad \boldsymbol{r}^* = \boldsymbol{r}(\boldsymbol{R}^*, t). \tag{26}$$

By taking into account the well-known expressions:

$$\frac{dV}{dV_0} = J_*(\boldsymbol{R}, t), \qquad J_*(\boldsymbol{R}, t) = \mathrm{Det}\left(\frac{\partial \boldsymbol{r}^*(\boldsymbol{R}, t)}{\partial \boldsymbol{R}}\right), \tag{27}$$

we may express the volume integral in the reference configuration:

$$\tilde{m}(\boldsymbol{r}^*, t) = m_*(\boldsymbol{r}^*, t) = \int_{V_0} \rho_*(\boldsymbol{R}, t)\, J_*(\boldsymbol{R}, t)\, dV_0. \tag{28}$$

The mass of the body is unchanged during the motion and therefore:

$$\begin{gathered}
\frac{d_*}{dt} \int_{V(t)} \tilde{\rho}(\boldsymbol{r}, t)\, dV = 0 \qquad \Leftrightarrow \qquad \frac{\overset{\circ}{d}_*}{dt} \int_{V_0} \rho_*(\boldsymbol{R}, t)\, J_*(\boldsymbol{R}, t)\, dV_0 = 0, \\
\frac{d_*}{dt} \equiv \left.\frac{\partial}{\partial t}\right|_{\boldsymbol{r}^*=\text{const}} + \frac{\overset{\circ}{d}_* \boldsymbol{r}^*}{dt} \cdot \nabla_*, \qquad \frac{\overset{\circ}{d}_*}{dt} \equiv \left.\frac{\partial}{\partial t}\right|_{\boldsymbol{R}^*=\text{const}} + \frac{\partial \boldsymbol{R}^*}{\partial t} \cdot \overset{\circ}{\nabla}_*, \\
\nabla_* = \frac{\partial}{\partial \boldsymbol{r}^*}, \quad \overset{\circ}{\nabla}_* = \frac{\partial}{\partial \boldsymbol{R}^*}.
\end{gathered} \tag{29}$$

Note that in (29)$_1$ the operators of differentiation and integration are not interchangeable. If $\boldsymbol{R} = \text{const}$ then $d/dt = \partial/\partial t$ and one may put differentiation in (29)$_2$ under the integral sign. Otherwise we have the following chain of equations:

$$\begin{aligned}\frac{d_*^\circ}{dt}\int_{V_0}\rho_*(\boldsymbol{R},t)\,J_*(\boldsymbol{R},t)\,dV_0 &= \frac{\partial}{\partial t}\int_{V_0}\rho_{*0}(\boldsymbol{R}_0,t)\,J_{*0}(\boldsymbol{R}_0,t)\,dV_0\\ &= \int_{V_0}\frac{\partial}{\partial t}\big[\rho_{*0}(\boldsymbol{R}_0,t)\,J_{*0}(\boldsymbol{R}_0,t)\big]dV_0\\ &= \int_{V_0}\frac{d^\circ}{dt}\big[\rho_*(\boldsymbol{R},t)\,J_*(\boldsymbol{R},t)\big]dV_0. \end{aligned}\tag{30}$$

After taking (30) into account and

$$J_*(\boldsymbol{R},t)=\tilde{J}(\boldsymbol{r},t)=\mathrm{Det}\left(\frac{\partial\tilde{\boldsymbol{R}}(\boldsymbol{r},t)}{\partial\boldsymbol{r}}\right)^{-1},\quad \nabla\cdot\tilde{\boldsymbol{v}}(\boldsymbol{r},t)=\tilde{J}^{-1}(\boldsymbol{r},t)\frac{d_r\tilde{J}(\boldsymbol{r},t)}{dt},\tag{31}$$

we can carry out the differentiation in $(29)_1$:

$$\begin{aligned}&\frac{d_*}{dt}\int_{V(t)}\tilde{\rho}(\boldsymbol{r},t)\,dV\\ &\quad=\frac{d_*^\circ}{dt}\int_{V_0}\rho_*(\boldsymbol{R},t)J_*(\boldsymbol{R},t)\,dV_0\\ &\quad=\int_{V_0}\frac{d^\circ}{dt}\big[\rho_*(\boldsymbol{R},t)J_*(\boldsymbol{R},t)\big]\,dV_0\\ &\quad=\int_{V(t)}\frac{d_r}{dt}\big[\tilde{\rho}(\boldsymbol{r},t)\tilde{J}(\boldsymbol{r},t)\big]\tilde{J}^{-1}(\boldsymbol{r},t)\,dV\\ &\quad=\int_{V(t)}\left[\frac{d_r\tilde{\rho}(\boldsymbol{r},t)}{dt}+\tilde{\rho}(\boldsymbol{r},t)\tilde{J}^{-1}(\boldsymbol{r},t)\frac{d_r\tilde{J}(\boldsymbol{r},t)}{dt}\right]dV\\ &\quad=\int_{V(t)}\left[\frac{d_r\tilde{\rho}(\boldsymbol{r},t)}{dt}+\tilde{\rho}(\boldsymbol{r},t)\nabla\cdot\tilde{\boldsymbol{v}}(\boldsymbol{r},t)\right]dV.\end{aligned}\tag{32}$$

By substituting this result into (29) we obtain the local conservation of mass:

$$\frac{d_r\tilde{\rho}(\boldsymbol{r},t)}{dt}+\tilde{\rho}(\boldsymbol{r},t)\nabla\cdot\tilde{\boldsymbol{v}}(\boldsymbol{r},t)=0.\tag{33}$$

Equation (33) often appears in the literature as:

$$\frac{\partial\tilde{\rho}(\boldsymbol{r},t)}{\partial t}+\nabla\cdot\big[\tilde{\rho}(\boldsymbol{r},t)\tilde{\boldsymbol{v}}(\boldsymbol{r},t)\big]=0.\tag{34}$$

This form is obtained after expanding the total derivative in (33).

In contrast to a partial derivative, the total time derivative is an objective operator, in the sense that it does not depend on the choice of coordinate system. That is why *it appears in balance equations in a natural way. A partial derivative can appear in balance equations only after substitution* (21).

We will now endeavor to define the total derivative even more stringently.

4 Definition of Total Derivative

Keeping mathematical rigor leads to many different notions of the same physical quality and symbols of the total derivative. In order to facilitate the notation without risking confusion, we shall introduce the general definition of the total time derivative below. However, each formula will be accompanied by verbal remarks, which seem in order, because physics is involved that goes way beyond mathematics. Let us proceed in this spirit.

All quantities in continuum mechanics are functions of spatial coordinates and time. The spatial coordinates may be constants or they may depend upon time. Note that the latter does not imply that we have a function with an argument (i.e., time). The moving coordinates have to depend on other variables that allow us to distinguish different substantial points. Therefore, in order to define a "total time derivative" we have to postulate which spatial coordinates are held constant. In other words, we have to choose a coordinate system with a distinctive feature. The frame of reference could be the one. At this point it is appropriate to introduce the notion "frame of reference" formally.

Imagine in a point O three rigidly connected, perpendicular pointers ("arrows"), $\boldsymbol{e}_1$, $\boldsymbol{e}_2$, and $\boldsymbol{e}_3$. The set $\{O,\ \boldsymbol{e}_1,\ \boldsymbol{e}_2,\ \boldsymbol{e}_3\}$ is called a "frame."

Definition 1 The body of reference is defined by a frame to which a set of points (in space) have been added, whereby a rigid body motion of all the points together with the frame is allowed. The position of the points are labeled relatively to the frame by establishing the reference coordinate system $x_1,\ x_2,\ x_3$ with origin O:

$$\boldsymbol{r}_* = x_1\boldsymbol{e}_1 + x_2\boldsymbol{e}_2 + x_3\boldsymbol{e}_3, \qquad -\infty < (x_1,\ x_2,\ x_3) < +\infty. \tag{35}$$

The frame and the reference coordinate system determine the reference body. They are "immutable." This is supposed to mean that once introduced they cannot be changed or this would lead to a different frame of reference (whose definition will come immediately). In order to describe quantitative characteristics of motion we must be able to measure distance *and* time. Hence a "clock" is needed as well:

Definition 2 The reference body with a "clock" is called the "Frame of Reference" (FoR).

Note that a frame of reference is *not* just a mathematical construct. Physics is involved due to the requirement of *measuring* distances in three independent directions and corresponding lengths as well as time.

It is impossible to say anything about the motion of the reference body, because it stands as such alone. However, it is possible to observe and quantify motions of other bodies with respect to the reference body. All physical qualities describing motion, such as velocity, for example, are measured with respect to the frame of reference and do not have any meaning without the reference frame.

In addition to the reference coordinate system one is free to choose any mathematical coordinate system in which the equations are specified. However, the reference coordinate system is a distinctive one since it determines the frame of reference. As an example consider a first coordinate transformation within an FoR, $x'_i = \hat{x}'_i(x_j),\ i, j \in (1, 2, 3)$. On top of that we now impose a second coordinate transformation $x''_i = \tilde{x}''_i(x'_j) = \tilde{x}''_i(\hat{x}'_j(x_k)) \equiv \hat{x}''_i(x_j),\ i, j, k \in (1, 2, 3)$. Note that if this operation is applied in context with the spatial dependence of a physical field quantity this would be a purely mathematical operation leading to no change of the meaning or value of that physical quantity. However, if we perform a change of the FoR this could result in a completely different story.

In this context it should be noted that many people do not distinguish between the concepts of frame of reference and coordinate system. Indeed, we read in Cornille (1993), p. 149:

> ... a distinction between mathematical sets of coordinates and physical frames of reference must be made. The ignorance of such distinction is the source of much confusion ...

or in Nerlich (1994), pp. 64–65:

> ... the idea of a reference frame is really quite different from that of a coordinate system. Frames differ just when they define different *spaces* (sets of *rest* points) or times (sets of simultaneous events). So the ideas of a space, a time, of rest and simultaneity, go inextricably together with that of frame. However, a mere shift of origin, or a purely spatial rotation of space coordinates results in a new coordinate system. So frames correspond at best to *classes* of coordinate systems. ...

In order to emphasize it once more: A change of the coordinate system is a purely mathematical operation, where an observer (i.e., the creator and user of the FoR) "sensing" vector quality is not needed. That is why in this case there is no difference how a vector is considered, as a directed segment or as a set of three components. Even more, we can completely exclude base vectors from our considerations and deal only with vector components. We use the notation employed with the coordinate transforms from above in an example. Suppose the coordinates of a vector in the reference coordinate system of the FoR are given by p_i. We would then obtain the corresponding coordinates w.r.t. the two other coordinate systems by $p'_j = \frac{\partial \hat{x}'_j}{\partial x_i} p_i$ and $p''_k = \frac{\partial \tilde{x}''_k}{\partial x'_j} p'_j = \frac{\partial \tilde{x}''_k}{\partial x'_j} \frac{\partial \hat{x}'_j}{\partial x_i} p_i = \frac{\partial \hat{x}''_k}{\partial x_i} p_i$.

Let $f(x_1, x_2, x_3, t)$ be a function of the reference coordinates and of time. The total time derivative of f is:

$$\frac{df(x_1, x_2, x_3, t)}{dt} = \lim_{\Delta t \to 0} \frac{f(x_1, x_2, x_3, t + \Delta t) - f(x_1, x_2, x_3, t)}{\Delta t}, \tag{36}$$

under the condition that the reference coordinates x_1, x_2, x_3 are held constant and there is an increment in the function only because of the increment in time.

Now let and $g(x(x_1, x_2, x_3, t), y(x_1, x_2, x_3, t), z(x_1, x_2, x_3, t), t)$ be a composite function of several variables, namely x, y, and z, which are functions like f. Then the total time derivative of g is:

$$\frac{dg}{dt} = \frac{\partial g}{\partial x}\frac{dx}{dt} + \frac{\partial g}{\partial y}\frac{dy}{dt} + \frac{\partial g}{\partial z}\frac{dz}{dt} + \frac{\partial g}{\partial t}. \tag{37}$$

Hence, we arrive at:

Definition 3 The total time derivative is the partial derivative with the reference coordinates held constant.

This definition allows us to drop the function arguments and keep the notation relative to different arguments. In other words we can simply write:

$$\boldsymbol{v} = \frac{d\boldsymbol{r}}{dt}, \qquad \boldsymbol{a} = \frac{d\boldsymbol{v}}{dt}, \qquad \frac{d\rho}{dt} + \rho\nabla\cdot\boldsymbol{v} = 0.$$

Note that in the case of partial derivatives the arguments of the function have to be present. Indeed:

$$\boldsymbol{a}(\boldsymbol{R}, t) = \frac{\partial \boldsymbol{v}_*(\boldsymbol{R}, t)}{\partial t}, \qquad \boldsymbol{a}(\boldsymbol{r}, t) \neq \frac{\partial \tilde{\boldsymbol{v}}(\boldsymbol{r}, t)}{\partial t},$$
$$\frac{\partial \tilde{\rho}(\boldsymbol{r}, t)}{\partial t} + \nabla\cdot\left[\tilde{\rho}(\boldsymbol{r}, t)\tilde{\boldsymbol{v}}(\boldsymbol{r}, t)\right] = 0, \qquad \frac{\partial \rho_*(\boldsymbol{R}, t)}{\partial t} + \nabla\cdot\left[\rho_*(\boldsymbol{R}, t)\boldsymbol{v}_*(\boldsymbol{R}, t)\right] \neq 0.$$

As we shall learn in the next chapter the distinction between various functions, identified by a hat and a tilde, will become obsolete if we turn to the spatial description, where the concepts of a reference and of a current configuration become obsolete and the motion and state of matter is described with respect to an independent grid in space.

5 Spatial Description

5.1 Body of General Type

The fundamental laws of mechanics are formulated for a body. Within the material description the body is a material volume. In the spatial description it is not so obvious which object should be considered as the body. In an attempt to make things clearer we start with some definitions.

Definition 4 Consider a closed surface undergoing deformation and motion. A set of material particles located at the present moment within the surface is called the "body." A set of material particles located outside the surface will be referred to as the "exterior of the body."[3]

Definition 5 The body is said to be closed if it exchanges no matter with its exterior, otherwise it is said to be open.

The material volume that we considered above is an example of a closed body. This sounds like a tautology at first glance, but, as it was mentioned before, the notion "material volume" is frequently claimed by the solids community. However, we also want to think in terms of a fixed ensemble of gas or fluid by the term "closed system." In the spatial description we deal with an open body as a set of particles within a certain volume in space. The specifics of how to formulate balance equations for an open body will now be demonstrated for the mass balance.

5.2 Balance Equations

Consider a closed, undeformed surface S whose position is fixed in space and which encloses a volume V. If $\rho(\boldsymbol{r}, t)$ is the density field at time t, the mass of matter enclosed by the surface at any moment is:

$$m(\boldsymbol{r}^*, t) = \int_V \rho(\boldsymbol{r}, t)\, dV, \tag{38}$$

where $\boldsymbol{r}^*$ is the position vector of a fixed point within the surface. Note that this point cannot be considered as the center of mass since the volume is undeformed and fixed in space while the density distribution within the volume changes during the evolution of the medium.

The rate of change of the total mass in the volume, after differentiation under the integral sign (remembering that the volume is fixed in space), is:

$$\frac{\partial m(\boldsymbol{r}^*, t)}{\partial t} = \lim_{\Delta t \to 0} \frac{m(\boldsymbol{r}^*,\ t + \Delta t) - m(\boldsymbol{r}^*,\ t)}{\Delta t} = \int_V \frac{\partial \rho(\boldsymbol{r}, t)}{\partial t}\, dV. \tag{39}$$

In the absence of a source of mass (an expression frequently used in fluid mechanics-oriented textbooks, cf., Batchelor (1970) or Pasipoularides (2009), but sometimes also in the more solid mechanics-based literature Malvern (1969), p. 451) inside V the mass change is equal to the mass flux through the surface:

$$\int_V \frac{\partial \rho(\boldsymbol{r}, t)}{\partial t}\, dV = -\int_S \boldsymbol{n}(\boldsymbol{r}) \cdot \boldsymbol{v}(\boldsymbol{r}, t) \rho(\boldsymbol{r}, t)\, dS = -\int_V \nabla \cdot (\boldsymbol{v}(\boldsymbol{r}, t) \rho(\boldsymbol{r}, t))\, dV, \tag{40}$$

[3]For simplicity it is assumed that there is no particle on the surface.

where $\boldsymbol{n}(\boldsymbol{r})$ is the unit outward normal to S. The last line follows from the divergence theorem. Since the relation (40) is valid for arbitrary choices of V we have a local form of the mass balance:

$$\frac{\partial\rho(\boldsymbol{r},t)}{\partial t}+\nabla\cdot\left[\rho(\boldsymbol{r},t)\boldsymbol{v}(\boldsymbol{r},t)\right]=0. \tag{41}$$

A different form of Eq. (41) is obtained by expanding the divergence term:

$$\frac{\delta_r\rho(\boldsymbol{r},t)}{\delta t}+\rho(\boldsymbol{r},t)\nabla\cdot\boldsymbol{v}(\boldsymbol{r},t)=0. \tag{42}$$

Here the following notation is introduced:[4]

$$\frac{\delta_r\rho(\boldsymbol{r},t)}{\delta t}\equiv\frac{\partial\rho(\boldsymbol{r},t)}{\partial t}+\boldsymbol{v}(\boldsymbol{r},t)\cdot\nabla\rho(\boldsymbol{r},t), \tag{43}$$

The operator

$$\frac{\delta_r}{\delta t}\equiv\left.\frac{\partial}{\partial t}\right|_{\boldsymbol{r}=\text{const}}+\boldsymbol{v}\cdot\nabla \tag{44}$$

is the *operator of the material derivative in spatial description*. The material derivative in form (44) is well known in hydrodynamics.

As long as the position vector $\boldsymbol{r}$ does not depend on time the total time derivative coincides with the partial derivative and Eq. (44) can be rewritten as:

$$\frac{\delta_r}{\delta t}=\frac{d}{dt}+\boldsymbol{v}\cdot\nabla. \tag{45}$$

This form is more convenient for comparison with the material derivative for the moving observation point that will be considered later.

5.3 Material Derivative

Consider a material point located at the observation point of position $\boldsymbol{r}$ at time t. In the small interval Δt it moves to the position $\boldsymbol{r}+\Delta\boldsymbol{s}$. Thus, the particle displacement is determined as $\Delta\boldsymbol{s}=\boldsymbol{v}(\boldsymbol{r},t)\Delta t$. In order to determine the change of a property $f(\boldsymbol{r},t)$ relevant to the given material point one has to find the material derivative.

Definition 6 The material derivative of $f(\boldsymbol{r},t)$ is:

[4] We will use symbol δ for the material derivative since the notation D introduced in Sect. 2 is often associated with the material description.

$$\frac{\delta_r f}{\delta t} = \lim_{\Delta t \to 0} \frac{f(\boldsymbol{r} + \Delta \boldsymbol{s}, t + \Delta t) - f(\boldsymbol{r}, t)}{\Delta t}. \tag{46}$$

The numerator on the right side of (46) describes the change of the property of the given material point in time Δt. Thus, the material derivative determines a rate of change of the property of the material point located at the observation point at time t.

We now show that the formulae (45), (44) are consistent with the definition of the material derivative (46). Indeed, the function $f(\boldsymbol{r} + \Delta \boldsymbol{s}, t + \Delta t)$ can be written as

$$f(\boldsymbol{r} + \Delta \boldsymbol{s}, t + \Delta t) = f(\boldsymbol{r}, t + \Delta t) + \Delta \boldsymbol{s} \cdot \nabla f(\boldsymbol{r}, t + \Delta t), \tag{47}$$

and then it follows from (46):

$$\begin{aligned} \frac{\delta_r f}{\delta t} &= \lim_{\Delta t \to 0} \frac{f(\boldsymbol{r}, t + \Delta t) - f(\boldsymbol{r}, t)}{\Delta t} + \lim_{\Delta t \to 0} \boldsymbol{v}(\boldsymbol{r}, t) \cdot \nabla f(\boldsymbol{r}, t + \Delta t) \\ &= \frac{df(\boldsymbol{r}, t)}{dt} + \boldsymbol{v}(\boldsymbol{r}, t) \cdot \nabla f(\boldsymbol{r}, t). \end{aligned} \tag{48}$$

It should be noted that even though the definition (46) looks like the definitions of the total and partial derivatives, there is a significant difference between them. The material derivative (46) is not a derivative of a function in the mathematical sense. Indeed, the displacement $\Delta \boldsymbol{s} = \boldsymbol{v}(\boldsymbol{r}, t)\Delta t$ on the right side of Eq. (46) cannot be expressed in terms of function arguments. This is due to a peculiarity of the spatial description in which the position vector $\boldsymbol{r}$ is *unrelated* to the evolution of matter and the velocity $\boldsymbol{v}(\boldsymbol{r}, t)$ is an *independent* characteristic. Since $\dfrac{d\boldsymbol{r}}{dt} = \boldsymbol{0}$ and $\nabla \boldsymbol{r} = \boldsymbol{I}$ ($\boldsymbol{I}$ is the unit tensor), the equation relating the position vector and the velocity,

$$\boldsymbol{v}(\boldsymbol{r}, t) \equiv \frac{\delta_r \boldsymbol{r}}{\delta t} = \frac{d\boldsymbol{r}}{dt} + \boldsymbol{v}(\boldsymbol{r}, t) \cdot \nabla \boldsymbol{r} \tag{49}$$

turns into an identity.

Thus, the velocity $\boldsymbol{v}(\boldsymbol{r}, t)$ is the primary quantity in the spatial description and all other quantities are expressed in terms of $\boldsymbol{v}(\boldsymbol{r}, t)$. For example, the acceleration of a material particle $\boldsymbol{a}(\boldsymbol{r}, t)$ is determined as the material derivative of the velocity:

$$\boldsymbol{a}(\boldsymbol{r}, t) \equiv \frac{\delta_r \boldsymbol{v}(\boldsymbol{r}, t)}{\delta t} = \frac{d\boldsymbol{v}(\boldsymbol{r}, t)}{dt} + \boldsymbol{v}(\boldsymbol{r}, t) \cdot \nabla \boldsymbol{v}(\boldsymbol{r}, t). \tag{50}$$

Note that the first term on the right side of (50) is the local rate of velocity change due to temporal changes at the observation point. It is *not* the acceleration of the material point at position $\boldsymbol{r}$ at time t, because the material point is located at that position only instantaneously.

The spatial description is used mostly in fluid and gas dynamics where the velocity, density, and the pressure are the main unknowns. Due to the complex motion of fluid and gas particles a monitoring of their motion, i.e., of their displacements is hardly feasible. As a result, the displacement vector is usually not considered in classical hydrodynamics. However, from a theoretical point of view, the introduction of this concept is an interesting task. There are different approaches to a formal introduction of the displacement vector. But all of them result in the following differential relation between the velocity $\boldsymbol{v}(\boldsymbol{r},\ t)$ and the displacement vector $\boldsymbol{u}(\boldsymbol{r},\ t)$:

$$\frac{\delta_r \boldsymbol{u}(\boldsymbol{r},\ t)}{\delta t} = \boldsymbol{v}(\boldsymbol{r},\ t). \tag{51}$$

Note that in spatial description this relation is used for determination of the displacement vector provided $\boldsymbol{v}$ is known. Then one can introduce the concept of the reference position vector in the same manner as in the case of the material description $\boldsymbol{R}(\boldsymbol{r},\ t) = \boldsymbol{r} - \boldsymbol{u}(\boldsymbol{r},\ t)$. In contrast to the material description, where the current position vector, $\boldsymbol{r}$, is a function of the reference position vector, $\boldsymbol{R}$, and time, t, the reference position vector, $\boldsymbol{R}$, within the spatial description is a function of the current position vector, $\boldsymbol{r}$, and time, t. This means that we have a different reference configuration for every moment of time. Since

$$\frac{\delta_r \boldsymbol{u}(\boldsymbol{r},\ t)}{\delta t} = \frac{\delta_r (\boldsymbol{R}(\boldsymbol{r},\ t) + \boldsymbol{r})}{\delta t} = \frac{\delta_r \boldsymbol{R}(\boldsymbol{r},\ t)}{\delta t} + \boldsymbol{v}(\boldsymbol{r},\ t) \tag{52}$$

it follows from (51) that

$$\frac{\delta_r \boldsymbol{R}(\boldsymbol{r},\ t)}{\delta t} = \frac{d\boldsymbol{R}}{dt} + \boldsymbol{v} \cdot \nabla \boldsymbol{R} = 0. \tag{53}$$

This differential equation determines the relation between the velocity of the material point, $\boldsymbol{v}$, and its reference position, $\boldsymbol{R}$.

5.4 Moving Observation Point

Now consider the closed surface S defined as the boundary of a volume that is no longer fixed in space but moves with a known velocity as a rigid body. The motion of points within the volume is expressed by the field of the position vector $\boldsymbol{r}(x_1, x_2, x_3, t)$, where x_1, x_2, x_3 is the reference coordinate system. The total mass in the volume is determined by Eq. (38). The vector $\boldsymbol{r}^*(t)$ is the position vector of a point fixed with respect to the volume but it moves with respect to the reference coordinate system. The rate of change of the total mass in the volume is the total time derivative of the mass:

$$\frac{dm(\boldsymbol{r}^*(t), t)}{dt} = \left.\frac{\partial m(\boldsymbol{r}^*, t)}{\partial t}\right|_{r^* = const} + \frac{d\boldsymbol{r}^*}{dt} \cdot \nabla_* m(\boldsymbol{r}^*, t), \qquad \nabla_* = \frac{\partial}{\partial \boldsymbol{r}^*}. \tag{54}$$

To clarify the meaning of Eq. (54) we note two special cases. The first of these concerns a volume fixed in space. Then $\boldsymbol{r}^*$ does not depend on time and the rate of change of the total mass is characterized only by the partial derivative. The second special case is relevant when the mass density is inhomogeneously distributed over space and this distribution does not change with time. In this case the first term on the right side of (54) is equal to zero and the change in mass is due to transport of the volume to a different position.

In order to pull the total derivative under the integral sign in (38) a change of variables is required:

$$\boldsymbol{r} = \boldsymbol{r}(\hat{\boldsymbol{r}}, t), \quad \rho(\boldsymbol{r}, t) = \hat{\rho}(\hat{\boldsymbol{r}}, t), \quad \boldsymbol{r}^* = \boldsymbol{r}^*(\hat{\boldsymbol{r}}^*, t), \quad m(\boldsymbol{r}^*, t) = \hat{m}(\hat{\boldsymbol{r}}^*, t), \tag{55}$$

where $\hat{\boldsymbol{r}}$ and $\hat{\boldsymbol{r}}^*$ are fixed in the reference system.

By doing so we can make the following transformations:

$$\frac{dm(\boldsymbol{r}^*, t)}{dt} = \frac{\partial \hat{m}(\hat{\boldsymbol{r}}^*, t)}{\partial t} = \frac{\partial}{\partial t} \int_V \hat{\rho}(\hat{\boldsymbol{r}}, t)\, dV = \int_V \frac{\partial \hat{\rho}(\hat{\boldsymbol{r}}, t)}{\partial t}\, dV = \int_V \frac{d\rho(\boldsymbol{r}, t)}{dt}\, dV, \tag{56}$$

where use has been made of the fact that the volume V is independent of time. Thus, in the case of a moving undeformed volume we obtain

$$\frac{d}{dt} \int_V \rho(\boldsymbol{r}, t)\, dV = \int_V \frac{d\rho(\boldsymbol{r}, t)}{dt}\, dV. \tag{57}$$

Here the total derivative of the mass density is:

$$\frac{d\rho(\boldsymbol{r}, t)}{dt} = \lim_{\Delta t \to 0} \frac{\rho(\boldsymbol{r}(t + \Delta t),\ t + \Delta t) - \rho(\boldsymbol{r}(t),\ t)}{\Delta t} = \frac{\partial \rho(\boldsymbol{r}, t)}{\partial t} + \frac{d\boldsymbol{r}}{dt} \cdot \nabla \rho(\boldsymbol{r}, t). \tag{58}$$

Equation (58) characterizes the rate of change of the mass density at the observation point that moves with velocity $\dfrac{d\boldsymbol{r}}{dt}$.

It should be emphasized that the meaning of the total derivative is the same in both descriptions. The total derivative determines the rate of change of a property related to the matter at the observation point. Within the material description the motion of the observation point coincides with the motion of the material point. This is why, in this particular case, the results of calculation of the material and total derivatives coincide.

The change of mass in the volume is equal to the mass flux through its surface. The rate of mass flow is determined by $\rho(\boldsymbol{r}, t)$ and by the relative velocity of the material points and the surface. Thus the mass balance reads:

$$\frac{d}{dt}\int_V \rho(\boldsymbol{r},t)\,dV = -\int_S \left[\boldsymbol{n}(\boldsymbol{r})\cdot\left(\boldsymbol{v}(\boldsymbol{r},t)-\frac{d\boldsymbol{r}}{dt}\right)\right]\rho(\boldsymbol{r},t)\,dS. \tag{59}$$

After transforming the integral on the right side by means of the divergence theorem and using (57), we arrive at the local mass balance:

$$\frac{d\rho(\boldsymbol{r},t)}{dt} + \nabla\cdot\left[\rho(\boldsymbol{r},t)\left(\boldsymbol{v}(\boldsymbol{r},t)-\frac{d\boldsymbol{r}}{dt}\right)\right] = 0. \tag{60}$$

By taking into the account the following relations:

$$\nabla\cdot\frac{d\boldsymbol{r}}{dt} = \nabla\cdot\frac{\partial\boldsymbol{r}}{\partial t} = \frac{\partial(\nabla\cdot\boldsymbol{r})}{\partial t} = 0, \tag{61}$$

Equation (60) is transformed as follows:

$$\frac{d\rho(\boldsymbol{r},t)}{dt} + \left(\boldsymbol{v}(\boldsymbol{r},t)-\frac{d\boldsymbol{r}}{dt}\right)\cdot\nabla\rho(\boldsymbol{r},t) + \rho(\boldsymbol{r},t)\nabla\cdot\boldsymbol{v}(\boldsymbol{r},t) = 0. \tag{62}$$

Upon introducing the notation

$$\frac{\delta\rho(\boldsymbol{r},t)}{\delta t} = \frac{d\rho(\boldsymbol{r},t)}{dt} + \left(\boldsymbol{v}(\boldsymbol{r},t)-\frac{d\boldsymbol{r}}{dt}\right)\cdot\nabla\rho(\boldsymbol{r},t) \tag{63}$$

the mass balance becomes:

$$\frac{\delta\rho(\boldsymbol{r},t)}{\delta t} + \rho(\boldsymbol{r},t)\nabla\cdot\boldsymbol{v}(\boldsymbol{r},t) = 0. \tag{64}$$

In order to obtain (64) we assume that the volume is not deformed (because of Eq. (57), which hold for an undeformed volume). Rejection of the assumption complicates the derivations but the final Eqs. (62)–(64) remain unchanged.

The operator

$$\frac{\delta}{\delta t} = \frac{d}{dt} + \left(\boldsymbol{v}-\frac{d\boldsymbol{r}}{dt}\right)\cdot\nabla \tag{65}$$

is a generalization of the material-derivative operator (45) for the moving observation point.

Definition 7 If the motion of the observation point $\boldsymbol{r}(t)$ is known then the material derivative of a material point property $f(\boldsymbol{r},t)$ is:

$$\frac{\delta f}{\delta t} = \lim_{\Delta t\to 0}\frac{f(\boldsymbol{r}(t+\Delta t)+\Delta\boldsymbol{s},t+\Delta t)-f(\boldsymbol{r},t)}{\Delta t}, \qquad \Delta\boldsymbol{s} = \left(\boldsymbol{v}-\frac{d\boldsymbol{r}}{dt}\right)\Delta t, \tag{66}$$

where $\Delta \boldsymbol{s}$ is the displacement with respect to the observation point of a material point that was in the observation point at time t.

The above definition has the same physical meaning as (46). The material derivative characterizes the rate of change a property of the material point that was in the observation point at time t.

It can be shown that Eq. (65) is in agreement with this definition. Since

$$f(\boldsymbol{r}(t+\Delta t)+\Delta \boldsymbol{s}, t+\Delta t) = f(\boldsymbol{r}(t+\Delta t), t+\Delta t) + \Delta \boldsymbol{s} \cdot \nabla f(\boldsymbol{r}(t+\Delta t), t+\Delta t), \tag{67}$$

Equation (66) yields:

$$\frac{\delta f}{\delta t} = \frac{df(\boldsymbol{r},t)}{dt} + \left(\boldsymbol{v}(\boldsymbol{r},t) - \frac{d\boldsymbol{r}}{dt}\right) \cdot \nabla f(\boldsymbol{r},t). \tag{68}$$

By taking into account

$$\frac{d}{dt} = \frac{\partial}{\partial t}\bigg|_{\boldsymbol{r}=\mathrm{const}} + \frac{d\boldsymbol{r}}{dt} \cdot \nabla, \tag{69}$$

we rewrite (65) in the form:

$$\frac{\delta}{\delta t} = \frac{\partial}{\partial t}\bigg|_{\boldsymbol{r}=\mathrm{const}} + \boldsymbol{v} \cdot \nabla. \tag{70}$$

It is easy to see that the expression for the material derivative (70) coincides with the expression for the material derivative with the fixed observation point (44). However, it is impossible to say from these expressions as to whether the observation point is fixed or not. Furthermore, the expression (70) looks similar to the total derivative in the current configuration within the material description (21). Such a coincidence is confusing and obscures the sense and meaning of the total and material derivatives. But from the expressions (65) and (69) the difference between the derivatives is obvious. The material derivative determines a rate of change of a property of the material point located at the observation point at time t, the total derivative determines a rate of change of the property at the observation point. It is true both in the spatial and the material descriptions. Within the material description the observation point is the material point, thus:

$$\boldsymbol{v} = \frac{d\boldsymbol{r}}{dt} \qquad \Rightarrow \qquad \frac{\delta}{\delta t} = \frac{d}{dt}, \tag{71}$$

and the material derivative coincides with the total derivative. Only in this particular case the statement “the total derivative, it is also the material derivative” can be made. In general, the observation point velocity $\dfrac{d\boldsymbol{r}}{dt}$ in Eq. (69) does not relate to a material point. If the observation point is fixed or moves independently of the motion of the medium, the total and material derivatives have different meanings and different values. If in a particular case their values coincide it does not mean that the physical meaning of a derivative changes. That is why the difference between the concepts of the total and material derivatives is important. This is particularly relevant when modeling a multicomponent medium, where all components have different velocities with respect to the common observation point.

In conclusion of this section note that the gradient operators have different properties in the material and spatial descriptions. This becomes important if one wants to investigate gradients of displacements, i.e., strains and their time derivatives, i.e., strain rates. Within the material description there are two gradient operators, $\overset{\circ}{\nabla}$ in the reference configuration, and ∇ in the current configuration. It is easy to show that:

$$\overset{\circ}{\nabla}\frac{d}{dt} = \frac{d}{dt}\overset{\circ}{\nabla}, \qquad \nabla\frac{d}{dt} \neq \frac{d}{dt}\nabla. \tag{72}$$

The spatial description deals with the gradient in the current configuration only. In the case of the fixed observation point we have

$$\nabla\frac{d}{dt} = \frac{d}{dt}\nabla, \qquad \nabla\frac{\delta_r}{\delta t} \neq \frac{\delta_r}{\delta t}\nabla. \tag{73}$$

Nevertheless, for a moving observation point the gradient operator is not interchangeable neither with the material nor with the total derivative.

6 Outlook and Conclusions

In Chap. 2 we started by presenting a rather detailed literature review of the various notions of time derivatives for the material and spatial description of continuum fields, which illustrated the confusing, almost desolate state of the subject. This made the need for a rigorous clarification apparent.

For this purpose the concept of material description was carefully analyzed in Chap. 3. The so-called total time derivative was introduced and analyzed for the reference and for the current configuration. Within the material description it may be interpreted as the rate of change of physical field quantities characterizing a material particle. The total time derivative was then examined in context with global balance equations, in particular, the mass balance. The property of the total time derivative being an objective operator independent of the choice of coordinate system was emphasized.

The latter property gave rise for a precise definition and further investigations of the total time derivative in combination with the concepts of Frames of Reference (FoR) and observers in Chap. 4. To this end an FoR was formally defined. The difference between an FoR, being a physics-based concept, and coordinates and transformations thereof, being purely mathematical operations, was pointed out.

Chapter 5 was dedicated to the description of continuum fields in spatial description. Here the considered matter is not necessarily a material volume any more. In order to point out the issue of a possible exchange of matter the notion of a body was introduced. The formulation of balance equations, specifically of the mass balance, was investigated and the operator of a material time derivative in spatial description for a nonmoving position vector, i.e., observation point was introduced. Moreover, an attempt was made to clarify the notion of displacement in spatial description. This culminated in a differential equation between the velocity of a material point and its reference configuration which, under these circumstances, must be viewed as continuously varying. The end of this chapter was devoted to the generalization of the material time derivative for a moving point of observation. It was shown that the material derivative characterizes the rate of change a property of the material point that was in the observation point at the certain moment of time, while the total derivative is the rate of change of property in an observation point. If this point coincides with a material particle (the material description) then (and only then) it is the rate of change of a quantity of the material point. In general, we may conclude that if the observation point is fixed or moves independently of the motion of the medium, the total and material derivatives have different meanings and different values.

Moreover, similarities regarding the mathematical form of the material derivative in spatial description with the total derivative in the current configuration within the material description are nothing else but *amis faux*.

Finally, in context with the mathematical description and the physical interpretation of time derivatives it became expedient to point out the difference between the mathematical concept of a coordinate system representation and the physics-based notion of an FoR. However, the question regarding the indifference of time derivatives w.r.t. changes of an FoR remains an open issue. In particular, an examination of the objectivity of time derivatives in context with the principle of material frame indifference will be presented in future work.

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