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Abstract

This paper consists of two main parts. In the first part, the fundamental equations of fluid dynamics are investigated and reformulated on the basis of the following main principles: (1) rigorous use of averaged quantities instead of local quantities (2) invariance of the balance equations' mathematical structure against averaging over arbitrary control volumes and invariance against multiple levels of averaging. The purpose of this approach is to establish balance equations that are particularly suited for flow fields with extreme fluctuations in density and velocity such as for turbulent multi-phase flow. In addition to the balance equations for mass and momentum new balance equations are introduced for the first moment of density and momentum distribution. These equations are discussed in comparison to micro-polar fluid theory. In the second part of the paper, an approximate closure of these balance equations is achieved using Taylor series expansion of the local fields up to order three. Boundary conditions are formulated consistent with this approximation. As an example, the complete set of equations is given for an incompressible fluid with significant variations in density and velocity.

Felder erster Momente für die Analyse turbulenter Mehrphasenströmung

Zusammenfassung

Diese Arbeit besteht aus zwei Hauptteilen. Zunächst werden die Grundgleichungen der Fluiddynamik untersucht und auf der Basis folgender Prinzipe neu formuliert: (1) Anstelle lokaler Größen werden grundsätzlich gemittelte Größen verwendet. (2) Die Invarianz der Gleichungsstruktur gegenüber beliebigen Kontrollvolumina und gegenüber mehrfacher Mittelung wird gefordert. Der Zweck dieses Vorgehens ist die Formulierung von Bilanzgleichungen, die speziell für Strömungsfelder mit erheblichen Schwankungen in der Dichte- und Geschwindigkeitsverteilung geeignet sind. Zusätzlich zu den Bilanzgleichungen für Dichte und Impuls werden Bilanzgleichungen für die ersten Momente dieser Größen eingeführt und im Vergleich zu der Theorie mikro-polarer Fluide diskutiert. Im zweiten Teil der Arbeit wird die näherungsweise Schließung des Gleichungssystems auf der Basis einer Taylor-Approximation dritter Ordnung vorgenommen. Randbedingungen, die mit dieser Approximation konsistent sind, werden aufgestellt. Als Beispiel wird der komplette Satz Gleichungen für eine inkompressible Strömung mit erheblichen Schwankungen in Dichte und Geschwindigkeit angegeben.

Contents

1 Introduction

Before we take a closer look at multi-phase flow, let us briefly summarize the basic equations of single-phase fluid dynamics.

Two different formulations of the basic fluid flow equation (for density and velocity) are normally in use: the local differential balance equations and their integral form.

A common formulation of the local differential form for the "local" mass balance in terms of the local density $\hat{\rho}$ and the local velocity $\hat{u}_i$ reads:

$$\frac{\partial \hat{\rho}}{\partial t} + \frac{\partial \hat{\rho}\hat{u}_n}{\partial \hat{x}_n} = 0 \tag{1}$$

Before we continue let us agree on the notation for co-ordinate subscripts in this paper. Any expression or equation containing subscripts $_{i,\ j,}$ or $_k$ represents three expressions or equations in which these subscripts $_{i,\ j,\ k}$ are replaced by the subscripts $_{1,\ 2,\ 3}$ and $_{2,\ 3,\ 1}$ and $_{3,\ 1,\ 2}$ respectively. If $_{i,\ j,}$ or $_k$ occur twice in an expression the expression still stands for a single expression (no summation convention applied). Any expression or equation containing subscripts $_n$ or $_m$ indicates that these may be replaced by $_1$ or $_2$ or $_3$ irrespective of the value of any other subscript in the expression. If $_n$ or $_m$ occur twice in a term the term stands for the sum of three terms in which $_n$ or $_m$ take the values $_{1,\ 2,\ 3}$ (summation convention applies).

Note, that we will use the hat indicator $\hat{}$ consistently to indicate "local" quantities.

The "local" momentum balance (which corresponds to the mass balance equation 1) in terms of the local density and the local velocity $\hat{u}_i$ reads:

$$\frac{\partial \hat{\rho}\hat{u}_i}{\partial t} + \frac{\partial \hat{\rho}\hat{u}_i\hat{u}_n}{\partial \hat{x}_n} = \hat{\rho}\hat{g}_i + \frac{\partial \hat{\tau}_{ni}}{\partial \hat{x}_n} \tag{2}$$

where $\hat{g}_i$ is the usual local specific body force and $\hat{\tau}_{ni}$ represents the usual local stress tensor. The sign convention for the stress is such that compressive stress would appear as a negative value.

Two integral formulations of the balance equations are common: either for a mass-conserving control volume (no flow across the boundary, Lagrangian formulation) or for a control volume that remains fixed in space and time (Eulerian formulation). For the mass-conserving control volume ($\mathbf{V}$) defined by

$$\frac{d}{dt}\int_{\mathbf{V}} \hat{\rho} d\hat{V} = 0 \tag{3}$$

the momentum balance is given by:

$$\frac{d}{dt}\int_{\mathbf{V}} \hat{\rho}\hat{u}_i d\hat{V} = \int_{\mathbf{V}} \hat{\rho}\hat{g} d\hat{V} + \int_{\mathbf{V}} \frac{\partial \hat{\tau}_{ni}}{\partial \hat{x}_n} d\hat{V} \tag{4}$$

Using the abbreviation

$$d\hat{V} = d\hat{x}_i d\hat{x}_j d\hat{x}_k \tag{5}$$

the mass balance for a control volume ($\mathbf{V}$) which remains constant in space and time reads:

$$\frac{\partial}{\partial t}\int_{\mathbf{V}} \hat{\rho} d\hat{V} + \int_{\mathbf{V}} \frac{\partial \hat{\rho}\hat{u}_n}{\partial \hat{x}_n} d\hat{V} = 0 \tag{6}$$

and the momentum balance for this control volume reads:

$$\frac{\partial}{\partial t}\int_{\mathbf{V}} \hat{\rho}\hat{u}_i d\hat{V} + \int_{\mathbf{V}} \frac{\partial \hat{\rho}\hat{u}_i\hat{u}_n}{\partial \hat{x}_n} d\hat{V} = \int_{\mathbf{V}} \hat{\rho}\hat{g}_i d\hat{V} + \int_{\mathbf{V}} \frac{\partial \hat{\tau}_{ni}}{\partial \hat{x}_n} d\hat{V} \tag{7}$$

The problem with the local formulation lies in the significant variation of these quantities over length scales that are smaller than those which we wish to (or can) resolve. The principal characteristic of the multi-phase flow concept is that we intend to abstract from those microscopic details. Turbulent flow is characterised by significant velocity fluctuations within scales that are smaller than we are able or willing to resolve by measurement or analysis. Hence, it appears that there is a basic contradiction between the term "local" on one side and the terms multi-phase or turbulent on the other.

The problem with the integral formulation is more subtle. The integration over some finite volume smooths all functions so that differentiation would not be a problem. There are, however, other problems, at least for turbulent flow. The concept of a mass-conserving control volume (equation 3 and equation 4) suffers from the fact that in turbulent flow the mass-conserving control volume will become mixed with its environment at its surface in any arbitrarily small amount of time. The surface will become blurred (fractal) in practically no time, so that we are unable to identify which portions of space are actually filled with material that constitutes a "mass-conserving body". With the concept of a fixed control volume the problem lies with the formulation of material flow across the boundary. As the local density and possibly also the velocity varies significantly over scales smaller than those we are able or willing to resolve we cannot perform the integration over the surface of the control volume with any degree of reliability.

Several different concepts are presently being used to overcome the problems of multi-phase flow analysis. One concept tries to resolve the details of the mixture by solving the respective balance equations in each phase separately, by tracking the motion of the interface, and by explicitly treating the interface condition. This approach appears to be suitable for problems where few large bubbles are embedded in a fluid.

Another concept treats bubbles or droplets as solid (mostly spherical) particles and solves the Lagrangian equation of motion of individual particles or for particles which are representative for larger clouds. This concept appears suitable for dust or mist embedded in a gaseous phase or for small bubbles embedded in a liquid.

Multi-fluid models appear to represent the most advanced methodology for dealing with multi-phase flow (see [1], e.g.). They use an entirely different approach. They describe ensemble averages or time averages over the various phases and introduce a coefficient $0 \leq \alpha \leq 1$ which characterises the mixture of both phases at any given point. The interaction of the phases is described by interfacial interaction terms. This approach appears to be suitable for mixtures that are not too close to either $\alpha = 0$ or $\alpha = 1$.

We will try to formulate a new approach that does not exhibit such limitations in applicability. This work is in some sense a continuation of the author's previous prior approach to the problem in [2].

2 Some important relationships for averaged quantities

Before we deal with the physically relevant quantities mass and momentum let us establish some general and useful mathematical relationships for averaged quantities. We first specify the characteristics of the functions and the control volumes that we plan to consider.

We will consider differentiable but otherwise arbitrary functions only. This may be surprising at first sight as we are aiming at multi-phase turbulent flow where one would normally expect that step changes of density and velocity at phase boundaries need to be accounted for. We argue, however, that such step changes are a mathematical abstraction of reality and a differentiable function (with an arbitrarily steep gradient) is just another and equally justified mathematical abstraction of reality. They both ignore the fact that

a field type description of the phenomena fails to do justice to reality when it comes to molecular sizes.

Regarding the control volume we allow arbitrary (not necessary contiguous) control volumes provided that they can be composed from arbitrarily large (but finite) numbers of small brick-type control volumes. A brick-type control volume is given by its extent in the three co-ordinate directions, by the (fixed) location of this shape relative to its reference point (x_i, x_j, x_k), and by the (variable) location of this reference point relative to the origin of the $(\hat{x}_i, \hat{x}_j, \hat{x}_k)$ co-ordinate system. We will subsequently often refer to two distinguished points which remain in constant orientation and location relative to such control volumes

$$\mathrm{V}(\mathrm{x}) = \mathrm{V}(x_i, x_j, x_k)$$

(in addition to their reference point): the volumetric centre (c_i, c_j, c_k) defined by

$$c_i = \int_{\mathrm{V}(\mathrm{x})} \hat{x}_i d\hat{V} \tag{8}$$

and the base point (y_i, y_j, y_k) which we will use to determine first moments of field distributions. With $\delta_{ni} = 0$ for $n \neq i$ and $\delta_{ni} = 1$ for $n = i$, this constant relative location may be expressed by:

$$\frac{\partial y_n}{\partial x_i} = \frac{\partial c_n}{\partial x_i} = \delta_{ni} \tag{9}$$

See figure 1 for an example of such a control volume with a simple shape. Figure 2 shows a control volume with a more complicated shape in two arbitrary positions.

2.1 The derivative of average quantities

The following well-known equation applies to arbitrary control volumes and arbitrary differentiable functions $\hat{\phi}(\hat{x}_i, \hat{x}_j, \hat{x}_k)$:

$$\frac{\partial}{\partial x_i} \int_{\mathrm{V}(\mathrm{x})} \hat{\phi} d\hat{V} = \int_{\mathrm{V}(\mathrm{x})} \frac{\partial \hat{\phi}}{\partial \hat{x}_i} d\hat{V} \tag{10}$$

2.2 The derivative of the first moment

Using equation 10, we find for an arbitrary differentiable function $\hat{\phi}(\hat{x}_i, \hat{x}_j, \hat{x}_k)$ the following relationship:

$$\frac{\partial}{\partial x_i} \int_{\mathrm{V}(\mathrm{x})} \hat{x}_n \hat{\phi} d\hat{V} = \delta_{ni} \int_{\mathrm{V}(\mathrm{x})} \hat{\phi} d\hat{V} + \int_{\mathrm{V}(\mathrm{x})} \hat{x}_n \frac{\partial \hat{\phi}}{\partial \hat{x}_i} d\hat{V} \tag{11}$$

Taking into account equation 9 some equivalent formulations are:

$$\begin{aligned}
& \frac{\partial}{\partial x_i} \int_{\mathrm{V}(\mathrm{x})} (\hat{x}_n - y_n) \hat{\phi} d\hat{V} \\
= & \int_{\mathrm{V}(\mathrm{x})} (\hat{x}_n - y_n) \frac{\partial \hat{\phi}}{\partial \hat{x}_i} d\hat{V} \\
= & \int_{\mathrm{V}(\mathrm{x})} \frac{\partial \hat{x}_n \hat{\phi}}{\partial \hat{x}_i} d\hat{V} - \int_{\mathrm{V}(\mathrm{x})} \frac{\partial y_n \hat{\phi}}{\partial \hat{x}_i} d\hat{V} - \delta_{ni} \int_{\mathrm{V}(\mathrm{x})} \hat{\phi} d\hat{V} \\
= & \oint_{\mathrm{S}(\mathrm{V}(\mathrm{x}))} (\hat{x}_n - y_n) \hat{\phi} d\hat{S}_i - \delta_{ni} \int_{\mathrm{V}(\mathrm{x})} \hat{\phi} d\hat{V}
\end{aligned} \tag{12}$$

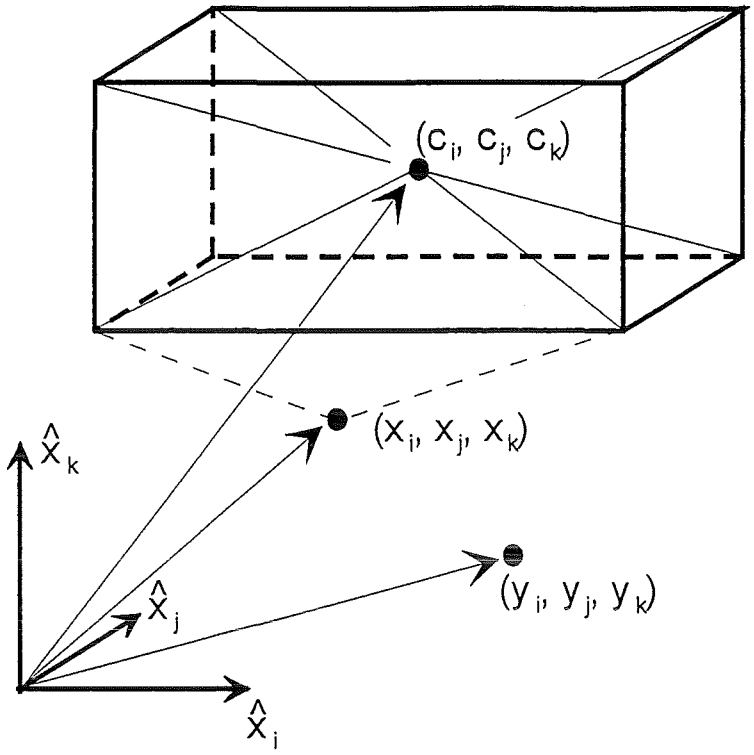

Figure 1: A brick-type control volume with its volumetric centre point $(c_i,\ c_j,\ c_k)$, its reference point $(x_i,\ x_j,\ x_k)$, and its base point $(y_i,\ y_j,\ y_k)$. The orientation and the position of the reference point, the base point, and the control volume (hence, also its centre point) will remain constant relative to each other as the reference point is swept through space.

where $\mathbf{S}(\mathbf{V}(\mathbf{x}))$ represents the surface of the control volume $\mathbf{V}(\mathbf{x})$ and $d\hat{S}_i$ is a surface element multiplied with the i-component of the outward directed normal direction vector.

2.3 The first moment in self-similar control volumes

Let us now introduce self-similar control volumes. Such control volumes are characterised by a reference point $\mathbf{x}$ and a length scale. We introduce the logarithm κ of such a length scale. Self-similar control volumes $\mathbf{V}(\kappa, \mathbf{x})$ are characterized by the fact that they are similar to each other with respect to their central point c_i which we also choose as base point y_i for determining the first moment of $\hat{\phi}$

$$y_i = c_i = \int_{\mathbf{V}(\kappa,\mathbf{x})} \hat{x}_i d\hat{V} \tag{13}$$

Corresponding points $\hat{x}_{iS}(\kappa, x_i)$ on their boundaries $S(\mathbf{V}(\kappa, \mathbf{x}))$ are defined by the co-ordinates

$$\hat{x}_{iS}(\kappa, x_i) = c_i + (\hat{x}_{iS}(0, x_i) - c_i) * e^{-\kappa} \tag{14}$$

For such control volumes one can show that the following relationship holds:

$$\frac{\partial}{\partial \kappa} \int_{\mathbf{V}(\kappa,\mathbf{x})} \hat{\phi} d\hat{V} = -\frac{\partial}{\partial x_n} \int_{\mathbf{V}(\kappa,\mathbf{x})} (\hat{x}_n - c_n)\hat{\phi} d\hat{V} \tag{15}$$

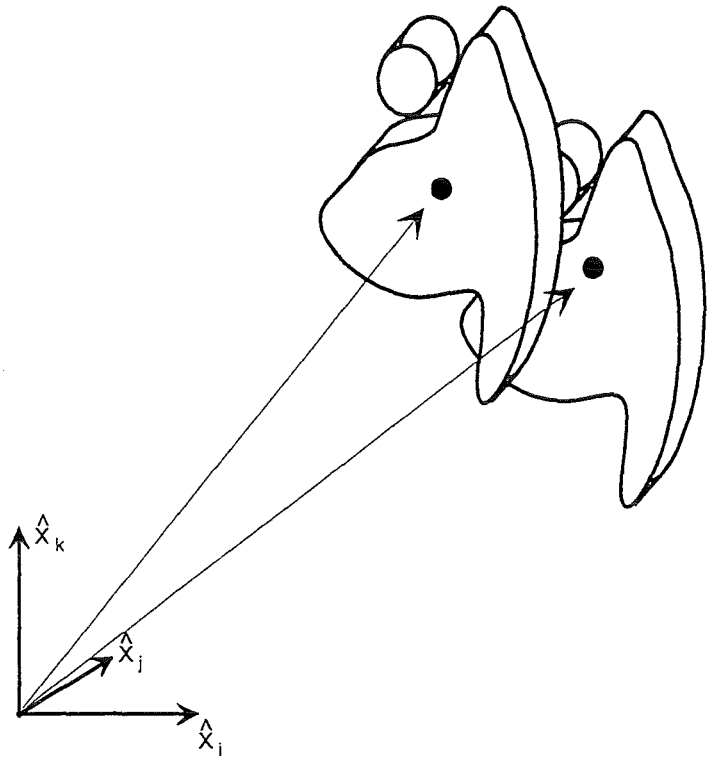

Figure 2: An arbitrary control volume in two different positions. Note that the positions of the control volume are continuously spred through space, not discretely arranged as is common for numerical discretisation of differential or integral equations.

For a proof see appendix 1.

Let us repeat this results as plain text: The divergence of the first moment of some local field with respect to the central point of the control volume is equal to the negative derivative of the average value of this field function (in the control volume) with respect to the (logarithmic) length scale of the control volume. This result shows an interesting property of the first moment and has added to the author's motivation to closer investigate the first moments of density (and momentum) field in the context of fluid dynamics.

3 The density pattern as an important multi-phase flow characteristic

Multi-phase flow is strongly influenced by the pattern of phase distribution in the multi-phase mixture. For technically relevant two-phase flow (in pipes, for instance) flow regime maps have been established which capture this kind of influence. For a general approach to three-dimensional flow a reference to these maps is of no help. Density patterns (this term is preferable to the usual term flow pattern) like bubble flow or droplet flow depend on the scale that is used to characterise them. For a certain size of control volume a two-phase mixture may appear as bubble flow. However, closer investigation may reveal that those bubbles are themselves filled with tiny droplets such that on a smaller scale one would conclude that droplet flow is the proper characterisation. The problem becomes worse if we wish to account for the fact that the density distribution may not be homogeneous (as in stratified flow or slug flow). What is needed in order to introduce the relevance

of density patterns into three-dimensional fluid dynamics is a mathematically rigorous characteristic for the density distribution *in some given control volume.* Special cases of this characteristic may then be interpreted as droplet flow or bubble flow, inhomogeneities in the distribution should also be captured. Let us give two illustrating examples: If such a mathematical characterisation of the density distribution allows us to determine that the density near the boundary of a control volume is very close to liquid density while the average density in the control volume is much less, then this indicates that the control volume should be considered as containing a bubble. If, however, the density on one side of the control volume is higher and on the other side it is lower than the volumetric average, then the control volume would have to be characterised as containing slug flow or stratified flow depending on whether the velocity vector is parallel or normal to those two sides. Obviously, such considerations are of no avail if we focus on "local" density.

We need to consider well-defined control volumes of finite size, characterised by a shape, a size, and a reference point (x_i, x_j, x_k) to which we assign any values evaluated for its associated control volume. As soon as we take this mental step seriously we are induced to borrow an important characterisation which has proven its usefulness in the mechanics of solid bodies: the centre of mass. We will determine the location of the centre of mass by evaluating the first moment of the density distribution. We call o_i the offset of the centre of gravity from some base point y_i of the control volume which we consider as rigidly connected with the control volume even though it may not be physically connected. Let us define the average density as

$$\rho = \frac{1}{V} \int_{\mathbf{V(x)}} \hat{\rho} d\hat{V} \tag{16}$$

and introduce for the first density moment

$$o_i = \frac{1}{\rho V} \int_{\mathbf{V(x)}} \hat{\rho}(\hat{x}_i - y_i) d\hat{V} \tag{17}$$

Below, we will show how this spatial moment can provide information about the density distribution at the control volume surface.

It is worth-while to remember that the centre of mass (characterized by the first moment of mass) together with the balance equation for the moment of momentum play an important role in solid body mechanics. Nobody would attempt to analyse the motion of solid bodies through space by limiting the applied equations to those of point mechanics (that is: using only the momentum equation). The balance equation for the first moment of momentum (the angular momentum) is essential for effectively describing rigid body mechanics. We expect that taking into account the first moment of mass and momentum will also be beneficial for the description of fluid mechanics.

The question may arise whether there is one especially preferred reference point x_i or preferred base point y_i for the control volumes. Intuitively, one might think that the reference point or the base point or both should be in the neighbourhood of the control volume and that perhaps the volumetric centre is such a preferred point. One could then assume $x_i = c_i$ or $y_i = c_i$ or even $x_i = c_i = y_i$. The analyses performed for this paper have given no indication that there is any preference as far as the formulation of balance equations is concerned. In this paper, the location of the reference point and the base point for determining first moments will generally be taken as arbitrary with respect to the control volume. Only in the context of self-similar control volumes (at which we have hinted in section 2.3 and to which we will return in section 3.4) and with respect to control volumes of spherical or brick-type shape (see sections 3.2 and 3.3) will we use special reference points and base points. Later in this paper (starting with section 6),

when we deal with the approximate closure of the set of balance equations and with the formulation of boundary conditions, we will restrict ourselves to specially shaped control volumes and will use $x_i = c_i = y_i$.

Note that the centre of mass does not qualify for such a preferred reference or base point as the centre of mass depends on the density distribution inside the control volume while we are looking for a point that depends only on the geometry of the control volume (not on the density distribution).

3.1 Arbitrary control volumes

According to section 2.2, in particular using equation 12 and using $\hat{\rho}$ instead of $\hat{\phi}$, and introducing the abbreviations

$$V = \int_{\mathbf{V(x)}} d\hat{V} \tag{18}$$

$$\rho = \frac{1}{V} \int_{\mathbf{V(x)}} \hat{\rho} d\hat{V} \tag{19}$$

$$\tilde{\rho} = \frac{1}{3V} \oint_{\mathbf{S(V(x))}} \hat{\rho}(\ \hat{x}_n - y_n) d\hat{S}_n \tag{20}$$

we find

$$\tilde{\rho} = \rho + \frac{1}{3} \frac{\partial \rho o_n}{\partial x_n} \tag{21}$$

This means that a distance-weighted average value of the density on the surface of the control volume ($\tilde{\rho}$) can be derived from the volume average value (ρ) and the divergence of the first moment of the density distribution.

3.2 Spherical control volumes

We now select a special control volume, a sphere with radius R, with a special base point, the centre of the sphere (hence $y_i = c_i$), and we denote the average quantities for this special case with the prefix $^{\odot}$. Equation 20 becomes

$$^{\odot}\tilde{\rho} = \frac{1}{3V} \oint_{\mathbf{S}(^{\odot}\mathbf{V(x)})} \hat{\rho}(\hat{x}_n - c_n) d\hat{S}_n = \frac{1}{4\pi R^2} \oint_{\mathbf{S}(^{\odot}\mathbf{V(x)})} \hat{\rho} d\hat{S} \tag{22}$$

and equation 21 may be written as

$$^{\odot}\tilde{\rho} = {}^{\odot}\rho + \frac{1}{3} \frac{\partial {}^{\odot}\rho {}^{\odot}o_n}{\partial x_n} \tag{23}$$

This is a very useful result. It means that for a spherical control volume with a reference point in its centre the average density on the control volume surface can be obtained by adding one third of the divergence of the first spatial density moment to the volume average density. Apparently, this result provides us with information about whether the spherical control volume under consideration is of bubble type or droplet type: we consider the control volume content as a "bubble" if the average density on the surface is larger than the volumetric average ($\tilde{\rho} > \rho$), and we consider it as a droplet if the average density on the surface is lower than the volumetric average ($\tilde{\rho} < \rho$).

3.3 Brick-shaped control volumes

We now deal with a control volume which is bounded by planar surfaces that are orthogonal to the Cartesian co-ordinate axes. We call such a control volume a "brick-type " control volume and indicate it by the symbol ${}^{\square}\mathbf{V}$ with the following domain:

$$ {}^{\square}\mathbf{V} = \begin{pmatrix} c_i - \frac{h_i}{2} & \leq \hat{x}_i \leq & c_i + \frac{h_i}{2} \\ c_j - \frac{h_j}{2} & \leq \hat{x}_j \leq & c_j + \frac{h_j}{2} \\ c_k - \frac{h_k}{2} & \leq \hat{x}_k \leq & c_k + \frac{h_k}{2} \end{pmatrix} \tag{24} $$

With $y_i = c_i$ and with

$$ {}^{\square}V = \int_{\square\mathbf{V}} d\hat{V} = h_i h_j h_k \tag{25} $$

we define the average density as

$$ {}^{\square}\rho = \frac{1}{{}^{\square}V} \int_{\square\mathbf{V}} \hat{\rho} d\hat{V} \tag{26} $$

The first moment of the density with respect to the central point of the control volume is defined as:

$$ {}^{\square}o_i = \frac{1}{{}^{\square}\rho {}^{\square}V} \int_{\square\mathbf{V}} (\hat{x}_i - c_i)\hat{\rho} d\hat{V} \tag{27} $$

If we define the average surface value of the density on the two opposing facing of the control volume normal to direction i as:

$$ {}^{\square}\rho^{S_i^+} = \frac{1}{h_j h_k} \int_{c_j - \frac{h_j}{2}}^{c_j + \frac{h_j}{2}} \int_{c_k - \frac{h_k}{2}}^{c_k + \frac{h_k}{2}} \hat{\rho}(c_i + \frac{h_i}{2}, \hat{x}_j, \hat{x}_k) d\hat{x}_j d\hat{x}_k \tag{28} $$

$$ {}^{\square}\rho^{S_i^-} = \frac{1}{h_j h_k} \int_{c_j - \frac{h_j}{2}}^{c_j + \frac{h_j}{2}} \int_{c_k - \frac{h_k}{2}}^{c_k + \frac{h_k}{2}} \hat{\rho}(c_i - \frac{h_i}{2}, \hat{x}_j, \hat{x}_k) d\hat{x}_j d\hat{x}_k \tag{29} $$

then we obtain for the mean value of the surface density on those two faces:

$$ {}^{\square}\rho_{mean}^{S_i} = \frac{1}{2}({}^{\square}\rho^{S_i^+} + {}^{\square}\rho^{S_i^-}) = {}^{\square}\rho + \frac{\partial^{\square}(\rho o_i)}{\partial x_i} \tag{30} $$

For a proof of these relationships see appendix 2. Apparently, if the derivative of ρo_i in direction i is large while the corresponding terms in directions j and k are small, then we have a layered density distribution. For a velocity vector parallel to direction i, slug flow is indicated. For a velocity vector normal to direction i, we have a stratified flow situation.

3.4 Self-similar control volumes

Replacing ϕ by ρ in the above section 2.3 on self-similar control volumes and with the definitions

$$ {}^{\kappa}\rho = \frac{1}{V} \int_{\mathbf{V}(\kappa,\mathbf{x})} \hat{\rho} d\hat{V} \tag{31} $$

and

$$ {}^{\kappa}o_i = \frac{1}{{}^{\kappa}\rho \ {}^{\kappa}V} \int_{\mathbf{V}(\kappa,\mathbf{x})} (\hat{x}_n - c_n)\hat{\rho} d\hat{V} \tag{32} $$

we obtain

$$ \frac{\partial \ {}^{\kappa}\rho}{\partial \kappa} = -\frac{\partial \ {}^{\kappa}\rho \ {}^{\kappa}o_n}{\partial x_n} \tag{33} $$

This is another result which emphasises the significance of the first moment of the density distribution: the divergence of the offset of the centre of mass (multiplied with density) from the volumetric centre of a control volume is a direct measure of the variation of the average density with the size of the control volume.

3.5 Some remarks on the velocity field

Similar results can of course be obtained for the velocity field by formally replacing $\hat{\rho}$ by $\hat{\rho}\hat{u}_i$ and corresponding replacements for the averaged quantities. We can expect that also for the velocity field (as well as for any other transported quantity) the information captured in the first moments is helpful to determine the difference between the volume averages of these quantities and some average value on the boundary of control volumes.

4 A new approach to balance equations for arbitrary volumes

We will now try to formulate balance equations for fluid flow in a way that does not depend either on the concept of local density or velocity nor on the concept of a transport velocity across a boundary. This new approach shall also provide information about the density pattern in an explicit form as described in the previous section. We will utilise mathematical relationships and avoid the introduction of constitutive relations as much as possible. The principles which govern our approach are:

Averaging principle: All balance equations shall be formulated in terms of average quantities of the field functions density and velocity and any other quantity for which balance equations are to be formulated. The only restriction is that the field functions need to be consistent: the same control volume shape, size, and placement relative to its reference point shall be used for all the different quantities combined in a consistent set of balance equations. The control volumes for averaging may be of arbitrary size (both arbitrarily large or small) and of arbitrary shape.

We do not wish to restrict ourselves to one averaging step, that is to the averages of the local quantities. We will consider the (first) averages of (local) quantities as equally representative of the flow situation as the underlying (local) fields and request that they may also be used as bases for another averaging step. Such repeated averaging may be performed any number of times, thus producing multiply averaged fields.

Averaging invariance: We require that the mathematical structure of the balance equations shall be identical independent of which control volume has been used to perform the averaging or how often an averaging process has been performed on the fields. In a somewhat different form this principle has been established by Germano [3]. Germano points out that the fluid dynamics equation are invariant with respect to arbitrary filtering functions applied. Here the filtering is restricted to volumetric

averaging over arbitrary control volumes, but it is extended to arbitrary repetitions of such averaging.

Principal validity of the conventional balance equations: No field function shall be preferred as "local" field function compared to averaged field functions. The term "local" field function shall merely express the fact that the control volume is so small that we do not care much about its size and shape. The conventional balance equations for mass and momentum (density and velocity) shall be considered as valid mathematical abstractions. However, the "local" density and the "local" velocity are considered as quantities that are inaccessible to measurement and unavailable to computational analysis. In other words, they may be used as mathematical foundation of differential equations but shall not be used themselves in any practical way.

4.1 The balance equation for averaged arbitrary quantities

4.1.1 A first approach

Let us assume the existence of a balance equation for an arbitrary (local) quantity $\hat{a}$ in the form:

$$\frac{\partial \hat{\rho}\hat{a}}{\partial t} + \frac{\partial \hat{\rho}\hat{a}\hat{u}_n}{\partial \hat{x}_n} = \widehat{rhs}[\hat{a}] \tag{34}$$

where $\widehat{rhs}[\hat{a}]$ stands for the right-hand side of the local balance equation. Integration over an arbitrary control volume results in

$$\frac{d}{dt}\int_{\mathbf{V(x)}} \hat{\rho}\hat{a}d\hat{V} \equiv \frac{\partial}{\partial t}\int_{\mathbf{V(x)}} \hat{\rho}\hat{a}d\hat{V} + \int_{\mathbf{V(x)}} \frac{\partial \hat{\rho}\hat{a}\hat{u}_n}{\partial \hat{x}_n} d\hat{V} = \int_{\mathbf{V(x)}} \widehat{rhs}[\hat{a}]d\hat{V} \tag{35}$$

We use previous definitions for V and ρ and introduce

$$u_i = \frac{1}{\rho V}\int_{\mathbf{V(x)}} \hat{\rho}\hat{u}_i d\hat{V} \tag{36}$$

$$a = \frac{1}{\rho V}\int_{\mathbf{V(x)}} \hat{\rho}\hat{a}d\hat{V} \tag{37}$$

As a point of clarification: u_i and a are not the averages of their local field functions; they are density weighted averages. In other words:

$$u_i \neq \frac{1}{V}\int_{\mathbf{V(x)}} \hat{u}_i d\hat{V} \tag{38}$$

$$a \neq \frac{1}{V}\int_{\mathbf{V(x)}} \hat{a}d\hat{V} \tag{39}$$

We also introduce

$$rhs[a] = \frac{1}{V}\int_{\mathbf{V(x)}} \widehat{rhs}[\hat{a}]d\hat{V} \tag{40}$$

$$F_n[a] = \frac{1}{\rho V}\int_{\mathbf{V(x)}} \hat{\rho}\hat{a}\hat{u}_n d\hat{V} - au_n \tag{41}$$

Thus, we can write 35 as

$$\frac{\partial \rho a}{\partial t} + \frac{\partial \rho a u_n}{\partial x_n} + \frac{\partial \rho F_n[a]}{\partial x_n} = rhs[a] \tag{42}$$

We will have to discuss this equation, but we delay this discussion until we have performed another averaging step.

4.1.2 The balance equation for averaged arbitrary quantities - revisited

This balance equation 42 has a similar mathematical structure as the initial equation 34, *similar but not identical.* A new term $\frac{\partial \rho F_n[a]}{\partial x_n}$ has appeared. In order to check whether our basic principles are viable we will now assume that this term is characteristic for all balance equations as they apply to finite control volumes. We, therefore, repeat the procedure of the previous section using equation 42 as a basis instead of equation 34.

For a new control volume $\bar{\mathrm{V}}$, defined in the x_i co-ordinates rather than in the $\hat{x}_i$ co-ordinates, we introduce the new quantities:

$$dV = dx_i dx_j dx_k \tag{43}$$

$$\bar{V} = \int_{\bar{\mathrm{V}}(\bar{\mathrm{x}})} dV \tag{44}$$

$$\bar{\rho} = \frac{1}{\bar{V}} \int_{\bar{\mathrm{V}}(\bar{\mathrm{x}})} \rho dV \tag{45}$$

$$\overline{u}_i = \frac{1}{\bar{\rho}\bar{V}} \int_{\bar{\mathrm{V}}(\bar{\mathrm{x}})} \rho u_i dV \tag{46}$$

$$\overline{a} = \frac{1}{\bar{\rho}\bar{V}} \int_{\bar{\mathrm{V}}(\bar{\mathrm{x}})} \rho a dV \tag{47}$$

As a point of clarification: $\overline{u}_i$ and $\overline{a}$ are not the averages of their local field functions; as for the averaging of the local balance equations, averaging applies always to the product of density and some other quantity. In other words:

$$\overline{u}_i \neq \frac{1}{\bar{V}} \int_{\bar{\mathrm{V}}(\bar{\mathrm{x}})} u_i dV \tag{48}$$

$$\overline{a} \neq \frac{1}{\bar{V}} \int_{\bar{\mathrm{V}}(\bar{\mathrm{x}})} a dV \tag{49}$$

We also introduce

$$\overline{rhs}[\bar{a}] = \frac{1}{\bar{V}} \int_{\bar{\mathrm{V}}(\bar{\mathrm{x}})} rhs[a] dV \tag{50}$$

$$\bar{F}_n[\bar{a}] = \frac{1}{\bar{\rho}\bar{V}} \int_{\bar{\mathrm{V}}(\bar{\mathrm{x}})} \rho a u_n dV + \frac{1}{\bar{\rho}\bar{V}} \int_{\bar{\mathrm{V}}(\bar{\mathrm{x}})} \rho F_n[a] dV - \bar{a}\bar{u}_n \tag{51}$$

In terms of these quantities, from an integration of equation 42, we obtain a balance equation with exactly the same mathematical structure as 42:

$$\frac{\partial \bar{\rho}\bar{a}}{\partial t} + \frac{\partial \bar{\rho}\bar{a}\bar{u}_n}{\partial \bar{x}_n} + \frac{\partial \bar{\rho}\bar{F}_n[\bar{a}]}{\partial \bar{x}_n} = \overline{rhs}[\bar{a}] \tag{52}$$

Apparently, we could perform another averaging step using equation 52 as the basis instead of equation 42. Equation 51, which is apparently a generalisation of equation 41 would have to be adapted by including the appropriate number of averaging steps.

Subsequently we will follow the general procedure outlined in this section.
Note that equation 51 may also be expressed in terms of the "local" quantities:

$$\bar{F}_n[\bar{a}] = \frac{1}{\bar{\rho}\bar{V}} \int_{\bar{\mathbf{V}}(\bar{\mathbf{x}})} \frac{1}{V} \left(\int_{\mathbf{V}(\mathbf{x})} \hat{a}\hat{u}_n\hat{\rho} d\hat{V} \right) dV - \bar{a}\bar{u}_n \tag{53}$$

But we will not use this formulation any further.

4.1.3 Some remarks on the "fluctuation flux" $F_n[a]$,the total derivative $\dot{a}$,and the"local" balance

Before we proceed, the term $\rho F_n[a]$ is to be discussed briefly. This quantity represents the difference of two fluxes of a quantity A (characterised by the local field $\hat{a}$):

- The average value of the total flux of quantity A in the control volume as determined from the exact "local" distribution of density, velocity, and the quantity under consideration, and
- the flux of this quantity as it would be determined from the averages of the individual quantities (on a per volume basis).

We will subsequently call this quantity $\rho F_n[a]$ the "fluctuation flux" of a. Such a term appears whenever some filtering or averaging is applied to the (non-linear) balance equations. In turbulence theory, the essential contribution to this term is from turbulent velocity fluctuations. Here, we have to account for variations in density and possibly other quantities as well.

It is common practice to use the notation $\dot{a}$ or $\frac{da}{dt}$ for the total derivative of some quantity a with the implicit understanding that

$$\dot{a} \equiv \frac{da}{dt} \equiv \frac{\partial a}{\partial t} + u_n \frac{\partial a}{\partial x_n}$$

The result which we just obtained indicates that this is an imprecise formulation. It applies only to the "local" fields. For any averaged quantities the proper formulation should be

$$\dot{a} \equiv \frac{da}{dt} \equiv \frac{\partial a}{\partial t} + u_n \frac{\partial a}{\partial x_n} + \frac{1}{\rho} \frac{\partial \rho F_n[a]}{\partial x_n}$$

As we have now found, with the inclusion of the fluctuation flux term, the balance equation has a form that is invariant not only for arbitrary control volumes but also for repeated averaging (see equations 42 and 52). The original "local" balance for $\hat{a}$ (equation 34), however, has a different form. One interpretation of this difference is to interpret the term "local" in the verbal sense that the quantities $\hat{a}$, $\hat{\rho}$, and $\hat{u}$ do not represent averages over small control volumes around each point but rather "at" a point. We prefer the interpretation that these local quantities represent nothing else but averages over control volumes that are most likely (but not necessarily) much smaller than those which are used for determining a, ρ, and u. With this interpretation we come to the conclusion that a more complete formulation of equation 34 would have to include a fluctuation flux term as well:

$$\frac{\partial \hat{\rho}\hat{a}}{\partial t} + \frac{\partial \hat{\rho}\hat{a}\hat{u}_n}{\partial \hat{x}_n} + \frac{\partial \hat{\rho}\hat{F}_n[\hat{a}]}{\partial \hat{x}_n} = \widehat{rhs}[\hat{a}] \tag{54}$$

The previous form of equation 34 is just a special case which applies whenever the fluctuation flux for $\hat{a}$ is negligible compared to the other terms in equation 54. Furthermore, by analogy with the expression for $\bar{F}_n[\bar{a}]$ (equation 51), the fluctuation flux term $F_n[a]$ (equation 41) should read more completely:

$$F_n[a] = \frac{1}{\rho V}\int_{V(x)} \hat{\rho}\hat{a}\hat{u}_n d\hat{V} + \frac{1}{\rho V}\int_{V(x)} \hat{\rho}\hat{F}_n[\hat{a}]d\hat{V} - au_n \tag{55}$$

4.2 The mass balance

4.2.1 The mass balance for finite control volumes

Starting from our principle of the validity of the conventional balance equations we repeat equation 1:

$$\frac{\partial \hat{\rho}}{\partial t} + \frac{\partial \hat{\rho}\hat{u}_n}{\partial \hat{x}_n} = 0 \tag{56}$$

Integration over some arbitrary control volume gives:

$$\frac{\partial}{\partial t}\int_{V(x)} \hat{\rho} d\hat{V} + \int_{V(x)} \frac{\partial \hat{\rho}\hat{u}_n}{\partial \hat{x}_n} d\hat{V} = 0 \tag{57}$$

Using previous definitions for V, ρ, and ρu_i we can write this as:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_n}{\partial x_n} = 0 \tag{58}$$

We note that this equation has exactly the same structure as the equation 56 from which we started.

4.2.2 The mass balance for finite control volumes - revisited

We will now check whether our invariance principle would also hold if we would use average density and velocity field of one control volume as the basis for determining the average density field of another control volume. Using previous definitions, repeating the procedure of the previous section is a trivial exercise and produces a result with exactly the same structure as before

$$\frac{\partial\, \bar{\rho}}{\partial t} + \frac{\partial\, \bar{\rho}\, \bar{u}_n}{\partial \bar{x}_n} = 0 \tag{59}$$

4.2.3 First interlude - on the mass balance

Before we continue to investigate other balance equations let us consider the meaning of the result just obtained.

We note that this balance equation for the average density has exactly the same structure as the equation 56 from which we started (this is not a new result but is common knowledge in continuum mechanics). A first reaction might be: So what's new here? This needs some discussion.

First of all, ρ and u_i are field functions in just the same way as the original $\hat{\rho}$ and $\hat{u}_i$. We should note, however, that they are defined in the x_i co-ordinates rather than in the $\hat{x}_i$ co-ordinates. It is important to recognise the distinction from the use of the averaging over control volumes as it is commonly performed for numerical solution of the balance equations in computer programs.. In the discretisation process performed for that purpose the average quantities are normally considered as being defined only for the discretised

numerical mesh (inside the mesh or sometimes on the mesh boundary). Here, we have derived a new *differential* equation which describes exactly the same flow situation as the original one albeit with some loss of detail information due to the averaging.

Next, since the balance equation for the average density has exactly the same structure and describes the same flow situation as the original one we can repeat the process we just performed using some other control volume in the next step. This next control volume is again arbitrary: it might be larger or smaller than the first one. This new averaging will again describe the same flow situation with further loss of detail. But this (admittedly less detailled) description is nevertheless exact provided that consistently averaged fields are used.

The structure of the mass balance equation is apparently very robust. It is invariant against averaging over arbitrary control volumes. Hence, if we are faced with a density field and a velocity field which satisfy the mass balance equation we have no way to find out whether these represent the real "local" values. The terms "local density" and "local velocity" become insignificant. The best definition is that they are determined for control volumes whose size is small enough to be of no concern. In particular, any notion of "particle velocity" has disappeared: velocity is *always* the momentum in a control volume divided by its mass! The notion of u_i being a "transport velocity" has disappeared.

In summary, the mass balance equation is in agreement with all the principles listed in section 4.

Finally, in order to describe a flow situation in a consistent way it is evidently a necessity to state explicitly what kind of control volume (shape, size, and placement relative to its reference point) has been used to determine the density and velocity fields. This requirement holds equally for experimentally and for computationally determined flow situations.

We conclude this interlude with the remark that while the equation which we have obtained for the balance of the average density is well familiar, its semantics has changed significantly compared to the common view.

4.3 The momentum balance

4.3.1 The momentum balance for finite control volumes

We start from our principle of the validity of the conventional balance equations and repeat equation 2:

$$\frac{\partial \hat{\rho}\hat{u}_i}{\partial t} + \frac{\partial \hat{\rho}\hat{u}_i\hat{u}_n}{\partial \hat{x}_n} = \hat{\rho}\hat{g}_i + \frac{\partial \hat{\tau}_{ni}}{\partial \hat{x}_n} \tag{60}$$

Integration over some arbitrary control volume gives:

$$\frac{\partial}{\partial t}\int_{\mathbf{V(x)}} \hat{\rho}\hat{u}_i d\hat{V} + \int_{\mathbf{V(x)}} \frac{\partial \hat{\rho}\hat{u}_i\hat{u}_n}{\partial \hat{x}_n} d\hat{V} = \int_{\mathbf{V(x)}} \hat{\rho}\hat{g}_i d\hat{V} + \int_{\mathbf{V(x)}} \frac{\partial \hat{\tau}_{ni}}{\partial \hat{x}_n} d\hat{V} \tag{61}$$

Using the previous definition for u_i together with the new definitions

$$g_i = \frac{1}{\rho V}\int_{\mathbf{V(x)}} \hat{\rho}\hat{g}_i d\hat{V} \tag{62}$$

$$\tau_{ni} = \frac{1}{V}\int_{\mathbf{V(x)}} \hat{\tau}_{ni} d\hat{V} \tag{63}$$

$$F_n[u_i] = e_{in} = e_{ni} = \frac{1}{\rho V}\int_{\mathbf{V(x)}} \hat{\rho}\hat{u}_i\hat{u}_n d\hat{V} - u_i u_n \tag{64}$$

and the rule for the integral of spatial derivatives (see equation 10) we obtain after some elementary algebraic manipulation:

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_n}{\partial x_n} + \frac{\partial \rho e_{in}}{\partial x_n} = \rho g_i + \frac{\partial \tau_{ni}}{\partial x_n} \tag{65}$$

4.3.2 The momentum balance - revisited

Comparing this equation with the original local momentum balance equation 60 we notice that the mathematical structure is *not* the same. A new term, the derivative of the fluctuation flux of momentum, has appeared. In order to apply our invariance principle we will now repeat the averaging procedure on the basis of this new formulation of the momentum balance equation. Integration over some arbitrary control volume gives:

$$\frac{\partial}{\partial t}\int_{\bar{\mathbf{V}}(\bar{\mathbf{x}})} \rho u_i dV + \int_{\bar{\mathbf{V}}(\bar{\mathbf{x}})} \frac{\partial \rho u_i u_n}{\partial x_n} dV + \int_{\bar{\mathbf{V}}(\bar{\mathbf{x}})} \frac{\partial \rho e_{in}}{\partial x_n} dV = \int_{\bar{\mathbf{V}}(\bar{\mathbf{x}})} \rho g_i dV + \int_{\bar{\mathbf{V}}(\bar{\mathbf{x}})} \frac{\partial \tau_{ni}}{\partial x_n} dV \tag{66}$$

Using previous definitions together with the new definitions

$$\bar{g}_i = \frac{1}{\bar{\rho}\bar{V}} \int_{\bar{\mathbf{V}}(\bar{\mathbf{x}})} \rho g_i dV \tag{67}$$

$$\bar{\tau}_{ni} = \frac{1}{\bar{V}} \int_{\bar{\mathbf{V}}(\bar{\mathbf{x}})} \tau_{ni} dV \tag{68}$$

$$\begin{aligned} \bar{F}_n[\bar{u}_i] \quad &= \bar{e}_{in} = \bar{e}_{ni} \\ &= \frac{1}{\bar{\rho}\bar{V}} \int_{\bar{\mathbf{V}}(\bar{\mathbf{x}})} \rho u_i u_n dV + \frac{1}{\bar{V}} \int_{\bar{\mathbf{V}}(\bar{\mathbf{x}})} \rho e_{in} dV - \bar{u}_i \bar{u}_n \end{aligned} \tag{69}$$

and the rule for the integral of spatial derivatives (see section 2.1) we obtain after some elementary algebraic manipulation:

$$\frac{\partial \bar{\rho}\bar{u}_i}{\partial t} + \frac{\partial \bar{\rho}\bar{u}_i\bar{u}_n}{\partial \bar{x}_n} + \frac{\partial \bar{\rho}\bar{e}_{in}}{\partial \bar{x}_n} = \bar{\rho}\bar{g}_i + \frac{\partial \bar{\tau}_{ni}}{\partial \bar{x}_n} \tag{70}$$

Comparing this equation with the momentum balance equation 64 we notice that the mathematical structure is now the same. All terms in this balance equations are based on definitions that correspond to the definitions of the respective terms in equation 64 - with one exception: The definition of the fluctuation flux $\bar{e}_{in}$ contains the average over e_{in}, while the definition of e_{in} does not contains a corresponding term. This difference needs to be eliminated in order to properly satisfy the principle of invariance of the balance equations wit respect to the averaging process. The next section is going to discuss this issue.

4.3.3 Second interlude - on the momentum balance

Let us consider the significance of the result obtained before we continue with our attempt to establish a new set of balance equations for multi-phase fluid flow.

While for the mass balance we had found that the mathematical structure of the "local" balance equation was identical to the one of the averaged balance equation this was initially not the case for the momentum balance. We have had to introduce the divergence of the fluctuation flux of momentum as an additional term in the momentum balance equation in order to satisfy our invariance principle. This term is not new. It is a term that is

commonly included in turbulent flow theory. However, our attitude towards this term is different. We do not consider it as an "additional term" which appears as result of the averaging process but rather as a term which ought to be included in the momentum balance equation to begin with. Only in special cases (laminar flow with minor density variations), this term may be insignificant compared to other terms in the momentum balance and may be ignored. But for the general case we come to the conclusion that this term ought to be present and that the conventional momentum balance equation 2 is just a special case of the more general formulation in equation 65. A more complete formulation of the local momentum balance should a local term $\hat{e}_{in}$ (corresponding to e_{in}) and would read:

$$\frac{\partial \hat{\rho}\hat{u}_i}{\partial t} + \frac{\partial \hat{\rho}\hat{u}_i\hat{u}_n}{\partial \hat{x}_n} + \frac{\partial \hat{\rho}\hat{e}_{in}}{\partial \hat{x}_n} = \hat{\rho}\hat{g}_i + \frac{\partial \hat{\tau}_{ni}}{\partial \hat{x}_n} \tag{71}$$

and the definition of the momentum fluctuation flux e_{in} in equation 64 should be extended:

$$e_{in} = e_{ni} = \frac{1}{\rho V}\int_{V(x)} \hat{\rho}\hat{e}_{in}d\hat{V} + \frac{1}{\rho V}\int_{V(x)} \hat{\rho}\hat{u}_i\hat{u}_n d\hat{V} - u_i u_n \tag{72}$$

With this change to the original definition of the fluctuation flux of momentum (equation 64) the invariance of the balance equation against arbitrary averaging has been achieved. The so-called "local" balance equation should, hence, be interpreted not as applying to a single point without spatial extent, but rather as applying to a finite, perhaps small, control volume for which the fluctuation flux is negligible compared to the other terms in the momentum balance equation. It is not necessary to take the word "local" verbally.

4.4 The balance equation for the first moment of mass

4.4.1 The balance equation for the first moment of mass for finite control volumes

Let us now analyse the balance equation for the first spatial moment of the density distribution in an arbitrary control volume. We obtain this balance equation by comparing two formulations for the total time derivative of the term $\int_{V(x)} \hat{x}_i\hat{\rho}d\hat{V}$. The first form reflects the general statement of mechanics that the time derivative of the first moment of mass is equal to the specific momentum of a body:

$$\frac{d}{dt}\int_{V(x)} \hat{\rho}\hat{x}_i d\hat{V} = \int_{V(x)} \frac{d\hat{x}_i}{dt}\hat{\rho}d\hat{V} = \int_{V(x)} \hat{\rho}\hat{u}_i d\hat{V} \tag{73}$$

Here we have integrated the local mass balance in the form of equation 1 and have substituted

$$\frac{d\hat{x}_i}{dt} = \hat{u}_i \tag{74}$$

The second formulation results from the general transport theorem applied to the first moment of mass:

$$\frac{d}{dt}\int_{V(x)} \hat{\rho}\hat{x}_i d\hat{V} = \frac{\partial}{\partial t}\int_{V(x)} \hat{\rho}\hat{x}_i d\hat{V} + \int_{V(x)} \frac{\partial \hat{\rho}\hat{x}_i\hat{u}_n}{\partial \hat{x}_n}d\hat{V} \tag{75}$$

These two formulations may be combined into:

$$\frac{\partial}{\partial t}\int_{\mathbf{V(x)}}\hat{\rho}\hat{x}_i d\hat{V} + \int_{\mathbf{V(x)}}\frac{\partial\hat{\rho}\hat{x}_i\hat{u}_n}{\partial\hat{x}_n}d\hat{V} = \int_{\mathbf{V(x)}}\hat{\rho}\hat{u}_i d\hat{V} \tag{76}$$

We introduce the definitions

$$z_i = \frac{1}{\rho V}\int_{\mathbf{V(x)}}\hat{\rho}\hat{x}_i d\hat{V} \tag{77}$$

$$F_n[z_i] = \frac{1}{\rho V}\int_{\mathbf{V(x)}}\hat{\rho}\hat{x}_i\hat{u}_n d\hat{V} - z_i u_n \tag{78}$$

Using previous definitions and the mass balance 58, the above balance equation 76 becomes

$$\frac{\partial\rho z_i}{\partial t} + \frac{\partial\rho z_i u_n}{\partial x_n} + \frac{\partial\rho F_n[z_i]}{\partial x_n} = \rho u_i \tag{79}$$

Actually, we prefer an alternative formulation which is based on two new definitions: (1) the definition of the "offset" o_i of the centre of mass relative to the control volume's base point (see figure 1):

$$o_i = z_i - y_i = \frac{1}{\rho V}\int_{\mathbf{V(x)}}\hat{\rho}\hat{x}_i d\hat{V} - y_i \tag{80}$$

and (2) the definition of the first spatial moment of the momentum distribution relative to the centre of mass:

$$\begin{aligned} s_{ni} = F_n[z_i] + o_i u_n = & \frac{1}{\rho V}\int_{\mathbf{V(x)}}\hat{\rho}(\hat{x}_i - y_i)\hat{u}_n d\hat{V} \\ = & \frac{1}{\rho V}\int_{\mathbf{V(x)}}\hat{\rho}\hat{x}_i\hat{u}_n d\hat{V} - y_i u_n \end{aligned} \tag{81}$$

Applying the mass balance 58 and the fact that

$$\frac{\partial y_i}{\partial t} = 0 \tag{82}$$

and

$$\frac{\partial\rho y_i u_n}{\partial x_n} = \delta_{in}\rho u_n + y_i\frac{\partial\rho u_n}{\partial x_n} = \rho u_i + y_i\frac{\partial\rho u_n}{\partial x_n} \tag{83}$$

we can then transform equation 79 into

$$\frac{\partial\rho o_i}{\partial t} + \frac{\partial\rho s_{ni}}{\partial x_n} = 0 \tag{84}$$

Comparing this balance equation with the balance equation for an arbitrary quantity (equation 42) and with the definition of $F_n[a]$ (equation 41) we conclude that

$$F_n[o_i] = \frac{1}{\rho V}\int_{\mathbf{V(x)}}\hat{\rho}(\hat{x}_i - y_i)\hat{u}_n d\hat{V} - o_i u_n \tag{85}$$

4.4.2 The balance equation for the first moment of mass - revisited

In order to apply our invariance principle we will repeat the averaging process using equation 79 as a basis. Integration over an arbitrary control volume produces:

$$\frac{\partial}{\partial t}\int_{\bar{\mathrm{V}}(\bar{\mathrm{x}})}\rho z_i dV + \int_{\bar{\mathrm{V}}(\bar{\mathrm{x}})}\frac{\partial \rho z_i u_n}{\partial x_n}dV + \int_{\bar{\mathrm{V}}(\bar{\mathrm{x}})}\frac{\partial \rho F_n[z_i]}{\partial x_n}dV = \int_{\bar{\mathrm{V}}(\bar{\mathrm{x}})}\rho u_i dV \tag{86}$$

If we now define

$$\bar{F}_n[\bar{z}_i] = \frac{1}{\bar{\rho}\bar{V}}\int_{\bar{\mathrm{V}}(\bar{\mathrm{x}})}\rho F_n[z_i]dV + \frac{1}{\bar{\rho}\bar{V}}\int_{\bar{\mathrm{V}}(\bar{\mathrm{x}})}\rho z_i u_n dV - \bar{z}_i\bar{u}_n \tag{87}$$

we obtain

$$\frac{\partial \rho\bar{z}_i}{\partial t} + \frac{\partial \rho\bar{z}_i\bar{u}_n}{\partial \bar{x}_n} + \frac{\partial \rho\bar{F}_n[\bar{z}_i]}{\partial \bar{x}_n} = \bar{\rho}\bar{u}_i \tag{88}$$

With

$$\bar{o}_i = \bar{z}_i - \bar{y}_i = \frac{1}{\bar{\rho}\bar{V}}\int_{\bar{\mathrm{V}}(\bar{\mathrm{x}})}\rho o_i dV + \frac{1}{\bar{\rho}\bar{V}}\int_{\bar{\mathrm{V}}(\bar{\mathrm{x}})}\rho y_i dV - \bar{y} \tag{89}$$

and

$$\bar{s}_{ni} = \bar{F}_n[\bar{z}_i] + \bar{o}_i\bar{u}_n \tag{90}$$

we obtain a formulation which corresponds to equation 84.

$$\frac{\partial \bar{\rho}\bar{o}_i}{\partial t} + \frac{\partial \bar{\rho}\bar{s}_{ni}}{\partial \bar{x}_n} = 0 \tag{91}$$

Comparing this balance equation with the balance equation for an averaged arbitrary quantity (equation 52) and with the definition of $\bar{F}_n[\bar{a}]$ (equation 51) we conclude that

$$\bar{F}_n[\bar{o}_i] = \frac{1}{\bar{\rho}\bar{V}}\int_{\bar{\mathrm{V}}(\bar{\mathrm{x}})}\rho o_i u_n dV + \frac{1}{\bar{\rho}\bar{V}}\int_{\bar{\mathrm{V}}(\bar{\mathrm{x}})}\rho F_n[o_i]dV - \bar{o}_i\bar{u}_n \tag{92}$$

4.4.3 Third interlude - on the balance for the first moment of mass

It is time again to lean back and consider the significance of the results just obtained for the balance of the first moment of mass. Remember that for the mass density the balance equation had the same appearance as in conventional fluid dynamics, but the semantics of the field quantities had drastically changed. For the momentum balance we had identified an "additional term". Now we have found a balance equation for a quantity which is not used in fluid mechanics so far: we call it the "offset" o_i because it is the offset of the centre of mass relative to the control volume's reference point.

What happens to the quantity o_i if we try to return to the concept of "local" quantities by reducing the size of the control volumes to zero. The intuitive answer is that the centre of mass co-ordinates z_i or $\bar{z}_i$ will then coincide with the co-ordinate $\hat{x}_i$ or x_i (except perhaps for some constant displacement). But this intuitive answer is not correct, at least not always! The result of the limit operation depends on the way how it is achieved. It is correct if we reduce the control volume to a single point while maintaining the function (whose average we determine) constant. But it is not correct if we reduce the control volume such that it takes the shape of a needle, or a plate, or several disjoint points. It is also not correct if we scale the function simultaneously with the reduction of the control

volume size in such a way that the function values remain constant on the control volume's boundary.

Another argument why we should concern ourselves seriously with the centre of mass as an important characteristic of fluid dynamics is the analogy to rigid body mechanics. As long as we consider rigid bodies as point masses the location of the (point) body and the location of the centre of mass are identical. However, for any finite size rigid bodies the location of the centre of mass relative to the geometry of the body is highly important.

We conclude that this new quantity characterising the centre of mass location and its governing balance equation should be included in the set of equations which we use to describe the dynamics of fluids with significantly varying density.

In section 3 we have found that the derivative of the first moment of the density distribution gives helpful information regarding the density pattern ("bubble pattern" or "droplet pattern"). We have now obtained a balance equation that allows to determine such information explicitly.

It is also possible to determine flow characteristics like "slug flow" or "stratified flow" by comparing the direction of the offset vector (o_i, o_j, o_k) with the direction of the velocity vector (u_i, u_j, u_k).

We conclude further that corresponding quantities $\hat{o}_i$ and $\hat{s}_{ni}$ could have been considered on the "local" level as well (as we interpret "local" as not referring to a point but rather to finite control volumes of a size that allows to neglect the difference between the volumetric centre and the centre of mass), with $\hat{o}_i$ being described by the balance equation:

$$\frac{\partial \hat{\rho}\hat{o}_i}{\partial t} + \frac{\partial \hat{\rho}\hat{s}_{ni}}{\partial \hat{x}_n} = 0 \tag{93}$$

Also, the definition of o_i in equation 80 should be completed to read:

$$o_i = \frac{1}{\rho V}\int_{\mathbf{V(x)}} \hat{\rho}\hat{x}_i d\hat{V} + \frac{1}{\rho V}\int_{\mathbf{V(x)}} \hat{\rho}\hat{o}_i d\hat{V} - y_i \tag{94}$$

4.5 The balance of the first moment of momentum

Up to now we have concentrated on motion of material in finite control volumes as far as it is characterised by the average motion. We will now deal with the first moment of motion which characterises the motion inside the control volume relative to the average motion. This quantity has already been introduced previously with equation 81.

4.5.1 The balance equation for the first moment of momentum - a first approach

Let us now analyse the balance equation for the first spatial moment of the momentum distribution in an arbitrary control volume. We obtain this balance equation by comparing two formulations for the total time derivative of the term $\int_{\mathbf{V(x)}} \hat{x}_i \hat{u}_m \hat{\rho} d\hat{V}$. The first form results from applying total differentiation to the integral:

$$\frac{d}{dt}\int_{\mathbf{V(x)}} \hat{x}_i \hat{u}_m \hat{\rho} d\hat{V} = \int_{\mathbf{V(x)}} \frac{d\hat{x}_i}{dt}\hat{u}_m \hat{\rho} d\hat{V} + \int_{\mathbf{V(x)}} \hat{x}_i \frac{d\hat{u}_m}{dt}\hat{\rho} d\hat{V} \tag{95}$$

We now formally substitute equation 74 and similarly

$$\hat{\rho}\frac{d\hat{u}_m}{dt} = \hat{\rho}\hat{g}_m + \frac{\partial \hat{\tau}_{nm}}{\partial \hat{x}_n} \tag{96}$$

Thus we obtain

$$
\begin{aligned}
&\frac{d}{dt}\int_{V(x)} \hat{\rho}\hat{x}_i\hat{u}_m d\hat{V} \\
&= \int_{V(x)} \hat{\rho}\hat{u}_i\hat{u}_m d\hat{V} + \int_{V(x)} \hat{\rho}\hat{x}_i\ \hat{g}_m d\hat{V} + \int_{V(x)} \hat{x}_i \frac{\hat{\tau}_{nm}}{\partial \hat{x}_n} d\hat{V} \\
&= \int_{V(x)} \hat{\rho}\hat{u}_i\hat{u}_m d\hat{V} + \int_{V(x)} \hat{\rho}\hat{x}_i\ \hat{g}_m d\hat{V} - \int_{V(x)} \hat{\tau}_{im} d\hat{V} + \int_{V(x)} \frac{\partial \hat{x}_i\hat{\tau}_{nm}}{\partial \hat{x}_n} d\hat{V}
\end{aligned}
\tag{97}
$$

The second formulation results from the general transport theorem applied to the moment of momentum:

$$
\frac{d}{dt}\int_{V(x)} \hat{\rho}\hat{x}_i\hat{u}_m d\hat{V} = \frac{\partial}{\partial t}\int_{V(x)} \hat{\rho}\hat{x}_i\hat{u}_m d\hat{V} + \int_{V(x)} \frac{\partial \hat{\rho}\hat{x}_i\hat{u}_m\hat{u}_n}{\partial \hat{x}_n} d\hat{V} \tag{98}
$$

Comparing these two formulations, we obtain:

$$
\begin{aligned}
&\frac{\partial}{\partial t}\int_{V(x)} \hat{\rho}\hat{x}_i\hat{u}_m d\hat{V} + \int_{V(x)} \frac{\partial \hat{\rho}\hat{x}_i\hat{u}_m\hat{u}_n}{\partial \hat{x}_n} d\hat{V} \\
&= \int_{V(x)} \hat{\rho}\hat{u}_i\hat{u}_m d\hat{V} + \int_{V(x)} \hat{\rho}\hat{x}_i\ \hat{g}_m d\hat{V} + \int_{V(x)} \hat{\tau}_{im} d\hat{V} + \int_{V(x)} \frac{\partial \hat{x}_i\hat{\tau}_{nm}}{\partial \hat{x}_n} d\hat{V}
\end{aligned}
\tag{99}
$$

With the definition of s_{ni} (equation 81) and of e_{in} (equation 64) and with the new definitions

$$
g_m = \frac{1}{\rho V}\int_{V(x)} \hat{\rho}\hat{g}_m d\hat{V} \tag{100}
$$

$$
\gamma_{mi} = \frac{1}{\rho V}\int_{V(x)} \hat{\rho}\hat{x}_i\hat{g}_m d\hat{V} - y_i g_m \tag{101}
$$

$$
\tau_{im} = \frac{1}{V}\int_{V(x)} \hat{\tau}_{im} d\hat{V} \tag{102}
$$

$$
\mu_{nmi} = \frac{1}{V}\int_{V(x)} \hat{x}_i\hat{\tau}_{nm} d\hat{V} - y_i\tau_{nm} \tag{103}
$$

we get

$$
\begin{aligned}
&\frac{\partial(\rho s_{mi} + \rho y_i u_m)}{\partial t} + \frac{1}{V}\int_{V(x)} \frac{\partial \hat{\rho}\hat{x}_i\hat{u}_m\ \hat{u}_n}{\partial \hat{x}_n} d\hat{V} \\
&= \rho e_{im} + \rho u_i u_m + y_i\rho g_m + \rho\gamma_{mi} + y_i\frac{\partial \tau_{nm}}{\partial x_n} + \frac{\partial \mu_{nmi}}{\partial x_n}
\end{aligned}
\tag{104}
$$

or with

$$
F_n[s_{mi} + y_i u_m] = \frac{1}{\rho V}\int_{V(x)} \hat{x}_i\hat{u}_m\hat{u}_n\hat{\rho} d\hat{V} - (s_{mi} + y_i u_m)u_n \tag{105}
$$

we get

$$
\begin{aligned}
&\frac{\partial(\rho s_{mi} + \rho y_i u_m)}{\partial t} + \frac{\partial(\rho s_{mi} + \rho y_i u_m)u_n}{\partial x_n} + \frac{\partial \rho F_n[s_{mi} + y_i u_m]}{\partial x_n} \\
&= \rho e_{im} + \rho u_i u_m + y_i\rho g_m + \rho\gamma_{mi} + y_i\frac{\partial \tau_{nm}}{\partial x_n} + \frac{\partial \mu_{nmi}}{\partial x_n}
\end{aligned}
\tag{106}
$$

Actually, we prefer a somewhat different formulation. We start from equation 104 and introduce the momentum balance equation 65 (multiplied by y_i in order to replace the term $\frac{\partial \rho y_i u_m}{\partial t}$) to obtain

$$\begin{aligned}&\frac{\partial \rho s_{mi}}{\partial t} + \rho y_i g_m + y_i \frac{\partial \tau_{nm}}{\partial x_n} - y_i \frac{\partial \rho u_m u_n}{\partial x_n} - y_i \frac{\partial \rho e_{mn}}{\partial x_n} + \frac{1}{V}\int_{V(x)} \frac{\partial \hat{\rho}\hat{x}_i \hat{u}_m\, \hat{u}_n}{\partial \hat{x}_n} d\hat{V} \\ &= \rho e_{im} + \rho u_i u_m + y_i \rho g_m + \rho \gamma_{mi} + y_i \frac{\partial \tau_{nm}}{\partial x_n} + \frac{\partial \mu_{nmi}}{\partial x_n}\end{aligned} \tag{107}$$

Using the definition equation for e_{mn} (equation 64) and introducing

$$F_n[s_{mi}] = \epsilon_{nmi} = \frac{1}{\rho V}\int_{V(x)} \hat{\rho}(\hat{x}_i - y_i)\hat{u}_m \hat{u}_n d\hat{V} - s_{mi}u_n \tag{108}$$

we obtain the balance equation for the first moment of momentum relative to the control volume reference point:

$$\frac{\partial \rho s_{mi}}{\partial t} + \frac{\partial \rho s_{mi} u_n}{\partial x_n} + \frac{\partial \rho \epsilon_{nmi}}{\partial x_n} = \rho \gamma_{mi} + \frac{\partial \mu_{nmi}}{\partial x_n} \tag{109}$$

4.5.2 The balance of the first moment of momentum - revisited

In order to apply our invariance principle we will perform an averaging process over control volume $\bar{V}$ using equation 106 as a basis.

$$\begin{aligned}&\frac{\partial}{\partial t}\frac{1}{\bar{V}}\int_{\bar{V}(\bar{x})}(\rho s_{mi} + \rho y_i u_m)dV \\ &+\frac{\partial}{\partial \bar{x}}\frac{1}{\bar{V}}\int_{\bar{V}(\bar{x})}(\rho s_{mi} + \rho y_i u_m)u_n dV + \frac{\partial}{\partial \bar{x}}\frac{1}{\bar{V}}\int_{\bar{V}(\bar{x})}\rho F_n[s_{mi} + y_i u_m]dV \\ &= \frac{1}{\bar{V}}\int_{\bar{V}(\bar{x})}(\rho e_{im} + \rho u_i u_m + \rho y_i g_m + \rho \gamma_{mi} + y_i \frac{\partial \tau_{nm}}{\partial x_n} + \frac{\partial \mu_{nmi}}{\partial x_n})dV\end{aligned} \tag{110}$$

Using the definitions for $\dot{F}_n[z_i]$ (equation 78) and s_{ni} (equation 81), $\bar{F}_n[\bar{z}_i]$ (equation 87) and $\bar{s}_{ni}$ (equation 90) we find

$$\begin{aligned}\frac{1}{\bar{\rho}\bar{V}}\int_{\bar{V}(\bar{x})}(\rho s_{mi} + \rho x_i u_m)dV &= \frac{1}{\bar{\rho}\bar{V}}\int_{\bar{V}(\bar{x})}(\rho F_m[z_i] + \rho z_i u_m)dV \\ &= \bar{F}_m[\bar{z}_i] + \bar{z}_i \bar{u}_m \\ &= \bar{s}_{mi} + \bar{y}_i \bar{u}_m\end{aligned} \tag{111}$$

We also use the definition of $\bar{e}_{in}$ (equation 69) and the new definitions

$$\bar{g}_m = \frac{1}{\bar{\rho}\bar{V}}\int_{\bar{V}(\bar{x})}\rho g_m dV \tag{112}$$

$$\bar{\gamma}_{mi} = \frac{1}{\bar{\rho}\bar{V}}\int_{\bar{V}(\bar{x})}\rho \gamma_{mi} dV + \frac{1}{\bar{\rho}\bar{V}}\int_{\bar{V}(\bar{x})}\rho y_i g_m dV - \bar{y}_i \bar{g}_m \tag{113}$$

$$\bar{\tau}_{nm} = \frac{1}{\bar{V}}\int_{\bar{V}(\bar{x})}\tau_{nm} dV \tag{114}$$

$$\bar{\mu}_{nmi} = \frac{1}{\bar{V}}\int_{\bar{V}(\bar{x})}\mu_{nmi} dV + \frac{1}{\bar{V}}\int_{\bar{V}(\bar{x})} y_i \tau_{nm} dV - \bar{y}_i \bar{\tau}_{nm} \tag{115}$$

$$\begin{aligned}\bar{F}_n[\bar{s}_{mi}+\bar{y}_i\bar{u}_m] = & \frac{1}{\bar{\rho}\bar{V}}\int_{\bar{V}}(\rho s_{mi}+\rho x_i u_m)u_n dV \\ & + \frac{1}{\bar{\rho}\bar{V}}\int_{\bar{\mathbf{V}}(\bar{\mathbf{x}})} F_n[s_{mi}+y_i u_m]dV - (\bar{s}_{mi}+\bar{y}_i\bar{u}_m)\bar{u}_n\end{aligned} \tag{116}$$

Thus we obtain

$$\begin{aligned}&\frac{\partial(\bar{\rho}\bar{s}_{mi}+\bar{\rho}\bar{y}_i\bar{u}_m)}{\partial t}+\frac{\partial(\bar{\rho}\bar{s}_{mi}+\bar{\rho}\bar{y}_i\bar{u}_m)\bar{u}_n}{\partial\bar{x}_n}+\frac{\partial\bar{\rho}\bar{F}_n[\bar{s}_{mi}+\bar{y}_i\bar{u}_m]}{\partial\bar{x}} \\ &\qquad = \bar{\rho}\bar{e}_{im}+\bar{\rho}\bar{u}_i\bar{u}_m+\bar{y}_i\bar{\rho}\bar{g}_m+\bar{\rho}\bar{\gamma}_{mi}+\bar{y}_i\frac{\partial\bar{\tau}_{nm}}{\partial\bar{x}_n}+\frac{\partial\bar{\mu}_{nmi}}{\partial\bar{x}_n}\end{aligned} \tag{117}$$

Actually, we prefer a different formulation, which we obtain from equation 117 by subtracting the momentum balance for $\bar{\mathbf{V}}$ (equation 70) after multiplying it with $\bar{y}_i$:

$$\bar{y}_i\frac{\partial\bar{\rho}\bar{u}_m}{\partial t}+\bar{y}_i\frac{\partial\bar{\rho}\bar{u}_m\bar{u}_n}{\partial\bar{x}_n}+\bar{y}_i\frac{\partial\bar{\rho}\bar{e}_{mn}}{\partial\bar{x}_n}=\bar{\rho}\bar{y}_i\bar{g}_m+\bar{y}_i\frac{\partial\bar{\tau}_{nm}}{\partial\bar{x}_n}$$

Combining this momentum balance with equation 117 we obtain

$$\frac{\partial\bar{\rho}\bar{s}_{mi}}{\partial t}+\frac{\partial\bar{\rho}\bar{s}_{mi}\bar{u}_n}{\partial\bar{x}_n}+\frac{\partial\bar{\rho}\bar{F}_n[\bar{s}_{mi}+\bar{y}_i\bar{u}_m]}{\partial\bar{x}_n}-\frac{\partial\bar{\rho}\bar{y}_i\bar{e}_{mn}}{\partial\bar{x}_n}=\bar{\rho}\bar{\gamma}_{mi}+\frac{\partial\bar{\mu}_{nmi}}{\partial\bar{x}_n} \tag{118}$$

We use the definition equation for $\bar{e}_{mn}$ (equation 69) and introduce

$$\begin{aligned}\bar{F}_n[\bar{s}_{mi}] &= \bar{\epsilon}_{nmi}=\bar{F}_n[\bar{s}_{mi}+\bar{y}_i\bar{u}_m]-\bar{y}_i\bar{e}_{mn} \\ &= \frac{1}{\bar{\rho}\bar{V}}\int_{\bar{\mathbf{V}}(\bar{\mathbf{x}})}\left(\frac{1}{V}\int_{\mathbf{V}(\mathbf{x})}\hat{\rho}(\hat{x}_i-\bar{y}_i)\hat{u}_m\hat{u}_n d\hat{V}\right)dV-\bar{s}_{mi}\bar{u}_n \\ &= \frac{1}{\bar{\rho}\bar{V}}\int_{\bar{\mathbf{V}}(\bar{\mathbf{x}})}\rho\epsilon_{nmi}dV+\frac{1}{\bar{\rho}\bar{V}}\int_{\bar{\mathbf{V}}(\bar{\mathbf{x}})}\rho s_{mi}u_n dV-\bar{s}_{mi}\bar{u}_n\end{aligned} \tag{119}$$

The last line relates this definition to the general formulation in equation 51. Thus, we obtain the balance equation for the first moment of momentum relative to the control volume reference point:

$$\frac{\partial\bar{\rho}\bar{s}_{mi}}{\partial t}+\frac{\partial\bar{\rho}\bar{s}_{mi}\bar{u}_n}{\partial\bar{x}_n}+\frac{\partial\bar{\rho}\bar{\epsilon}_{nmi}}{\partial\bar{x}_n}=\bar{\rho}\bar{\gamma}_{mi}+\frac{\partial\bar{\mu}_{nmi}}{\partial\bar{x}_n} \tag{120}$$

This equation has indeed the same mathematical structure as equation 109.

4.5.3 Fourth interlude - on the balance of the moment of momentum

Some remarks on γ_{mi} and μ_{nmi} The analysis of the moment of momentum has introduced not only a new balance equation but also three new quantities ϵ_{nmi}, γ_{mi}, and μ_{nmi}. ϵ_{nmi} is the fluctuation flux of the moment of momentum while γ_{mi} and μ_{nmi} are the first moments which correspond to the terms g_m and τ_{nm} in the momentum balance equation.

It is worthwhile to study the effect of γ_{ii} and μ_{nii} on s_{ii} (neglecting ϵ_{nmi} at this time). The definition of s_{ni} indicates that for $s_{ii}>0$ the material within the control volume is expanding, while for $s_{ii}<0$ we have compression. It is evident from the balance equation 109 that $\gamma_{ii}>0$ enhances expansion, while $\gamma_{ii}<0$ will tend to compress the material. Regarding μ_{nii} we recall the results of section 2.2 and can state:

$$\frac{\partial \mu_{nii}}{\partial x_n} = \frac{1}{V} \oint_{S(V(x))} (\hat{x}_n - y_n)\hat{\tau}_{ii} d\hat{S}_n - \tau_{ii}$$

As we have agreed to interpret positive values of τ_{ii} as tension, this result in connection with the balance equation indicates that expansive material motion is promoted whenever the (distance-weighted average) tension on the surface of a control volume is larger than its average value inside the control volume. This result is in agreement with our intuitive understanding.

We conclude further that also on the local level a local body force momentum $\hat{\gamma}_{mi}$, stress momentum $\hat{\mu}_{nmi}$, and fluctuation flux of the moment of momentum $\hat{\epsilon}_{nmi}$ could have been considered. $\hat{s}_{ni}$ should then have been described on the "local" level by the balance equation:

$$\frac{\partial \hat{\rho}\hat{s}_{mi}}{\partial t} + \frac{\partial \hat{\rho}\hat{s}_{mi}\hat{u}_n}{\partial \hat{x}_n} + \frac{\partial \hat{\rho}\hat{\epsilon}_{nmi}}{\partial \hat{x}_n} = \hat{\rho}\hat{\gamma}_{mi} + \frac{\partial \hat{\mu}_{nmi}}{\partial \hat{x}_n} \tag{121}$$

The definition of ϵ_{nmi} in equation 108, of γ_{mi} in equation 101 and of μ_{nmi} in equation 103 should then have been reformulated as:

$$\epsilon_{nmi} = \frac{1}{\rho V} \int_{V(x)} \hat{\rho}\hat{\epsilon}_{nmi} d\hat{V} + \frac{1}{\rho V} \int_{V(x)} \hat{\rho}\hat{s}_{mi}\hat{u}_n d\hat{V} - s_{mi}u_n \tag{122}$$

$$\gamma_{mi} = \frac{1}{\rho V} \int_{V(x)} \hat{\rho}\hat{\gamma}_{mi} dV + \frac{1}{\rho V} \int_{V(x)} \hat{\rho}\hat{y}_i\hat{g}_m dV - y_i g_m \tag{123}$$

and

$$\mu_{nmi} = \frac{1}{V} \int_{V(x)} \hat{\mu}_{nmi} d\hat{V} + \frac{1}{V} \int_{V(x)} \hat{x}_i\hat{\tau}_{nm} d\hat{V} - y_i\tau_{nm} \tag{124}$$

Comparison with the moment of momentum balance in micro-fluid theory
A balance equation for the first moment of momentum also appears in the theory of micro-polar continua (see, e.g., [4]). In micro-polar continuum theory it is assumed that every "material particle" carries not only mass and momentum but also a first moment of momentum and an inertia tensor. The concept is a significantly different from our approach where we associate the additional quantities not with "material particles" but with arbitrary finite control volumes. Nevertheless there is a striking similarity in the resulting balance equations. We use [5] as a reference and first quote the balance equation for the moment of momentum as given in the reference with slight renaming of the co-ordinate subscripts and adapted to the Cartesian co-ordinates used in this paper, also renaming Eringen's s_{kl} into t^*_{kl} in order to avoid confusion with our definition of s_{ni}:

$$\rho\dot{\sigma}_{mi} = \rho l_{mi} + t_{im} - t^*_{im} + \frac{\partial \lambda_{nmi}}{\partial x_n} \tag{125}$$

The symbols (as far as they are different from the ones used in this paper) mean:
σ_{mi} = first moment of momentum per unit mass
t_{im} = stress tensor
$t^*_{im} = t^*_{mi}$ = micro-stress average
λ_{nmi} = first stress moment
l_{mi} = first body moment per unit mass
Using the notation of this paper, using the usually accepted definition for the dot operator

$$\dot{a} \equiv \frac{da}{dt} \equiv \frac{\partial a}{\partial t} + u_n \frac{\partial a}{\partial x_n}$$

and also taking into account the mass balance equation, equation 125 would read

$$\frac{\partial \rho \sigma_{mi}}{\partial t} + \frac{\rho \partial \sigma_{mi} u_n}{\partial x_n} = \rho l_{mi} + t_{im} - t^*_{im} + \frac{\partial \lambda_{nmi}}{\partial x_n} \tag{126}$$

We have to recall that the equations for the micro-polar continua have a background that is entirely different from ours. They intend to describe local quantities in a continuum whose material particles carry a local (microscopic) moment of momentum, while ours represent averages over arbitrarily large control volumes. Nevertheless, both representations would match if

- Eringen's σ_{mi} corresponds to our s_{mi}
- Eringen's l_{mi} corresponds to our γ_{mi}
- Eringen's λ_{nmi} corresponds to our μ_{nmi}.
- Eringen's stress tensor t_{im} and the micro-stress average t^*_{im} cancel each other in the micro-fluid model
- The fluctuation flux of the moment of momentum (in our balance equation) is negligible.

4.6 The balance of the first moment of an arbitrary quantity

The balance equation for the first moment of an arbitrary quantity can be derived in the same way as the balance equation for the first moment of momentum. We will not repeat the process here but just give the result.

We define the first moment α_i of the arbitrary quantity a which is associated with mass as

$$\alpha_i = \frac{1}{\rho V} \int_{\mathbf{V(x)}} \hat{x}_n \hat{\rho} \hat{a} \, d\hat{V} - y_n a \tag{127}$$

If we follow the procedure used for the first moment of momentum we obtain:

$$\frac{\partial \rho \alpha_i}{\partial t} + \frac{\partial \rho \alpha_i u_n}{\partial x_n} + \frac{\partial \rho F_n[\alpha_i]}{\partial x_n} = \frac{1}{V} \int_{\mathbf{V(x)}} \hat{x}_i \widehat{rhs}[\hat{a}] d\hat{V} - y_i rhs[a] \tag{128}$$

Similarly, for a second averaging step with

$$\overline{\alpha}_i = \frac{1}{\overline{\rho} \overline{V}} \int_{\overline{\mathbf{V}}(\overline{\mathbf{x}})} x_i \rho a d\hat{V} - \overline{y}_i \overline{a} \tag{129}$$

we obtain:

$$\frac{\partial \overline{\rho} \overline{\alpha}_i}{\partial t} + \frac{\partial \overline{\rho} \overline{\alpha}_i \overline{u}_n}{\partial \overline{x}_n} + \frac{\partial \overline{\rho} \bar{F}_n[\overline{\alpha}_i]}{\partial \overline{x}_n} = \frac{1}{\overline{V}} \int_{\overline{\mathbf{V}}(\overline{x}_i)} \frac{1}{V} \int_{\mathbf{V(x)}} \hat{x}_i \widehat{rhs}[\hat{a}] d\hat{V} dV - \overline{y}_i \overline{rhs}[\overline{a}] \tag{130}$$

We do not deal further with the right-hand sides of these equations as they depend entirely on the physical quantity under consideration.

5 Summary of equations

Let us now collect all balance equations derived in the previous sections:

Mass balance

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_n}{\partial x_n} = 0 \tag{131}$$

Balance of the centre of mass offset

$$\frac{\partial \rho o_i}{\partial t} + \frac{\partial \rho s_{in}}{\partial x_n} = 0 \tag{132}$$

Momentum balance

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_n}{\partial x_n} + \frac{\partial \rho e_{in}}{\partial x_n} = \rho g_i + \frac{\partial \tau_{ni}}{\partial x_n} \tag{133}$$

Balance of the moment of momentum

$$\frac{\partial \rho s_{mi}}{\partial t} + \frac{\partial \rho s_{mi} u_n}{\partial x_n} + \frac{\partial \rho \epsilon_{nmi}}{\partial x_n} = \rho \gamma_{mi} + \frac{\partial \mu_{nmi}}{\partial x_n} \tag{134}$$

In addition to these equations we also need to consider balance equations for arbitrary quantities and their first moments if such quantities are relevant for the flow field under consideration.

$$\frac{\partial \rho a}{\partial t} + \frac{\partial \rho a u_n}{\partial x_n} + \frac{\partial \rho F_n[a]}{\partial x_n} = rhs[a] \tag{135}$$

$$\frac{\partial \rho \alpha_i}{\partial t} + \frac{\partial \rho \alpha_i u_n}{\partial x_n} + \frac{\partial \rho F_n[\alpha_i]}{\partial x_n} = \frac{1}{V} \int_{\mathbf{V(x)}} \hat{x}_i \widehat{rhs}[\hat{a}] d\hat{V} - y_i rhs[a] \tag{136}$$

However, for the most important quantities of fluid dynamics, mass and momentum, which are governed by equations 131 through 134 we note that balance equations for the four physical quantities ρ, ρo_i, ρu_i, and ρs_{mi} (corresponding to 16 scalar balance equations) have been established instead of the conventional two balance equations (four scalar ones).

We also repeat the definitions of those terms for which no balance equation is given and which are new compared to conventional fluid dynamics:

The fluctuation flux of momentum

$$e_{in} = e_{ni} = \frac{1}{\rho V} \int_{\mathbf{V(x)}} \hat{\rho} \hat{e}_{in} dV + \frac{1}{\rho V} \int_{\mathbf{V(x)}} \hat{\rho} \hat{u}_i \hat{u}_n d\hat{V} - u_i u_n \tag{137}$$

The fluctuation flux of the first moment of momentum

$$\epsilon_{nmi} = \frac{1}{\rho V} \int_{\mathbf{V(x)}} \hat{\rho} \hat{\epsilon}_{nmi} d\hat{V} + \frac{1}{\rho V} \int_{\mathbf{V(x)}} \hat{\rho} \hat{s}_{mi} \hat{u}_n d\hat{V} - s_{mi} u_n \tag{138}$$

The first body force moment

$$\gamma_{mi} = \frac{1}{\rho V} \int_{\mathbf{V(x)}} \hat{\rho} \hat{\gamma}_{mi} dV + \frac{1}{\rho V} \int_{\mathbf{V(x)}} \hat{\rho} \hat{y}_i \hat{g}_m dV - y_i g_m \tag{139}$$

The first stress moment

$$\mu_{nmi} = \frac{1}{V} \int_{\mathbf{V(x)}} \hat{\mu}_{nmi} d\hat{V} + \frac{1}{V} \int_{\mathbf{V(x)}} \hat{x}_i \hat{\tau}_{nm} d\hat{V} - y_i \tau_{nm} \tag{140}$$

6 Approximate closure of the balance equations

6.1 The closure problem

The closure problem we have to discuss has two aspects:

- the closure problem introduced by averaging
- the closure problem introduced by the consideration of the first spatial moment

The first aspect is well known in fluid mechanics. Different approaches to solve the closure problem have been pursued with much success in turbulence theory (see e.g. [6]). Additional balance equations and algebraic approximations are used to close the set of equations. In this paper, we will develop algebraic approximations of the fluctuation flux terms. These approximations will be established on the basis of Taylor series expansions of the local quantities and by applying physical reasoning where the Taylor series approach leaves us with a choice among equally valid expressions.

The second aspect refers to the first body force moment γ_{mi} and the first stress moment μ_{nmi}. These are quantities for which new constitutive relations are required. Some work has been done in the field of micro-polar fluid theory (see [5], [4] or [7]) in order to establish the constraints (equipresence, well-posedness, objectivity, compatibility with an entropy principle) which ought to govern such new constitutive relations (see [8]).

6.2 Basis for the approximations

We will attempt to formulate approximate algebraic expressions for the fluctuation flux terms and will then try to show that these approximations are accurate up to a certain degree provided that the control volume size and the behaviour of the underlying "local" density and velocity fields satisfy certain conditions. This is admittedly a significant step away from our previous attitude which was to allow arbitrary functions and arbitrarily large control volumes. But we will maintain the finiteness of the control volume size and we will not discard any of the first moments and the fluctuation flux terms using the argument that they would become arbitrarily small and finally vanish if we approach (but never reach) zero control volume size.

We will, however, introduce significant restrictions to the control volumes as compared to the previous chapters:

		previous chapters	now used for approximation
1	control volume shape	arbitrary	cube with side length h_0 and edges parallel to the co-ordinate axes
2	control volume size	arbitrary	small
3	control volume reference point	arbitrary relative to control volume	volumetric centre
4	base point for determining first moments	arbitrary relative to reference point	volumetric centre

The expression "small" in row 2 means: small enough to justify ignoring any fluctuation flux term $\frac{1}{\rho \hat{V}} \int_{\mathrm{V}(\mathbf{x})} \hat{\rho} \hat{F}_n[\hat{a}] d\hat{V}$ and 4^{th} order terms in Taylor expansions (see below)

Furthermore, we assume that all our "local" field functions can be expanded into Taylor series. The question is up to which order we need to account for this expansion. Since this paper concentrates on the use of average quantities rather than local quantities, we

need to carry out a Taylor series expansion far enough so that the difference between an average value in a control volume and the local value at its reference does not vanish. It is easily shown that a first-order approximation is insufficient as first-order terms will vanish during integration over a control volume which has the shape of a cube and is centered about its reference point. Hence, the minimum order to be taken into account is two. However, since the approximate expressions which we are to derive involve derivatives of average quantities we have to carry the expansion one order further, that is up to order three. All higher-order terms will be neglected. More explicitly, any terms involving the product of four or more of the following factors will be ignored:

a co-ordinate value	$\hat{x}_n$
a reference point co-ordinate	x_n
the size of the control volume	h_0

In fact, if an approximate expression is correct up to order three then it is also correct up to order four as all even-order terms will cancel due to the integration over a control volume that is symmetrically arranged relative to the reference point. This statement holds also if derivatives are involved.

6.3 Taylor series expansion and approximation of the fluctuation flux

The analysis of the approximations has been done for fully three-dimensional fields. Before we determine the approximate expression for the fluctuation flux term it is worth-while to investigate certain approximate expressions. Using

$$\Theta = \frac{1}{V}\int_V (\hat{x}_i - x_i)^2 d\hat{V} = \frac{h^2}{12}$$

we find, for instance, for the average density:

$$\rho = \hat{\rho} + \Theta\frac{\partial^2\hat{\rho}}{\partial\hat{x}_n^2}$$

For the (density weighted) average value of an arbitrary quantity we find

$$a = \hat{a} + \frac{\partial\hat{a}}{\partial\hat{x}_n}\Theta\frac{\partial\hat{\rho}}{\hat{\rho}\partial\hat{x}_n} + \Theta\frac{\partial^2\hat{a}}{\partial\hat{x}_n^2}$$

Always taking into account third-order approximation, this may be rewritten as

$$a = \hat{a}|_{x_i+o_i} + \Theta\frac{\partial^2\hat{a}}{\partial\hat{x}_n^2}$$

which is an expression that looks much the same as for the average density. However, the local value used for comparison with the average value ought to be taken at the centre of mass of the control volume instead of the volumetric centre.

For the expressions concerning the first moments we find first for the density:

$$o_i = \Theta\frac{\partial\hat{\rho}}{\hat{\rho}\partial\hat{x}_i}$$

and for arbitrary quantities:

$$\alpha_i = \Theta\frac{\partial\hat{a}}{\partial\hat{x}_i} + \hat{a}\Theta\frac{\partial\hat{\rho}}{\hat{\rho}\partial\hat{x}_i} = \Theta\frac{\partial\hat{a}}{\partial\hat{x}_i} + \hat{a}o_i$$

These approximations were proven with the Maple V program listed in 3.

We now wish to approximate the fluctuation flux term. In equation 55 we have formulated the fluctuation flux term. We ignore the local fluctuation flux $\frac{1}{\rho V}\int_{\mathbf{V(x)}}\hat{\rho}\hat{F}_n[\hat{a}]d\hat{V}$ and find:

$$F_n[a] = \frac{1}{\rho V}\int_{\mathbf{V(x)}}\hat{\rho}\hat{a}\hat{u}_n d\hat{V} - au_n \tag{141}$$

This expression may be approximated up to order three by the following approximation (see appendix 4, $O(l^4)$ represents all terms that contain the product of at least four factors which are either co-ordinates, such as $\hat{x}_i$ or the size of the control volume h_0):

$$F_n[a] = \frac{1}{2}\left((s_{nm} - o_m u_n)\frac{\partial a}{\partial x_m} + (\alpha_m - o_m a)\frac{\partial u_n}{\partial x_m}\right) + O(l^4) \tag{142}$$

A physical interpretation is easily associated with the terms in this approximate formulation. $(s_{mi} - o_m u_i)$ is the first moment of the velocity distribution relative to the centre of mass in the control volume (we recall that s_{mi} represents the first moment of the local velocity u_m relative to the volumetric centre). Similarly, $(\alpha_i - o_i a)$ is the first moment of the $\hat{a}$ field relative to the centre of mass.

Let us now deal with the fluctuation flux terms for first moments: $F_n[\alpha_i]$ in general and $F_n[s_{im}]$ in the special case of the first moment of the momentum field. For consistency with our approximation approach we neglect all terms that are of higher degree than three in linear dimensions. The result is that we obtain

$$F_n[\alpha_i] = O(l^4) \tag{143}$$

for the general case and

$$F_n[s_{mi}] = O(l^4) \tag{144}$$

for the first moment of momentum.

Let us now summarize the balance equations formulated before using this approximation approach.

Mass balance

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_n}{\partial x_n} = 0 \tag{145}$$

Balance of the centre of mass offset balance

$$\frac{\partial \rho o_i}{\partial t} + \frac{\partial \rho s_{ni}}{\partial x_n} = 0 \tag{146}$$

Momentum balance

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_n}{\partial x_n} + \frac{\partial}{\partial x_n}\left(\rho(s_{nm} - o_m u_n)\frac{\partial u_i}{\partial x_m}\right) = \rho g_i + \frac{\partial \tau_{ni}}{\partial x_n} \tag{147}$$

Balance of the moment of momentum

$$\frac{\partial \rho s_{mi}}{\partial t} + \frac{\partial \rho s_{mi} u_n}{\partial x_n} = \rho\gamma_{mi} + \frac{\partial \mu_{nmi}}{\partial x_n} \tag{148}$$

Balance of an arbitrary quantity

$$\frac{\partial \rho a}{\partial t} + \frac{\partial \rho a u_n}{\partial x_n} + \frac{\partial}{2\partial x_n}\left(\rho(s_{nm} - o_m u_n)\frac{\partial a}{\partial x_m}\right) + \frac{\partial}{2\partial x_n}\left(\rho(\alpha_m - o_m a)\frac{\partial u_n}{\partial x_m}\right) = rhs[a] \tag{149}$$

Balance of the first moment of an arbitrary quantity

$$\frac{\partial \rho \alpha_i}{\partial t} + \frac{\partial \rho \alpha_i u_n}{\partial x_n} = rhs[\alpha_i] \tag{150}$$

The first two equations are unmodified as they are exact. No fluctuation flux term appears in the balance equation of the first moment of momentum (equation 148) as this term would involve approximation terms that are of higher order than three. The momentum balance equation, when compared with the classical local momentum balance, shows a term that is of diffusive type. We note that this approximate representation of the fluctuation flux of momentum has a formal similarity to a viscosity term. It is tempting to interpret the 3 by 3 tensor expression (using the double braces $\{\{..\}\}$ to indicate a tensor built from the enclosed components)

$$S_{nm} = \{\{s_{nm} - o_m u_n\}\}$$

as the representation of a turbulent viscosity tensor. Note that this tensor is not necessarily symmetric. Not only the momentum balance but also the balance equation for an arbitrary quantity contains terms that represent the effect of the first moments of the field distributions.

6.4 More physical interpretation

Let us represent the first moment of the velocity distribution (S_{nm}) by three new quantities to which we apply names that hint at their physical interpretation (all names starting with "s"):

The split value

$$s_0 = s_{nn} - o_n u_n \tag{151}$$

This quantity (which we propose to call split value) is the trace of S_{nm} and characterizes the local volumetric expansion or contraction of the fluid away from its local centre of mass.

The skew-symmetric part of S_{nm} is

$$\frac{1}{2}\{\{s_{nm} - o_m u_n\}\} - \frac{1}{2}\{\{s_{mn} - o_n u_m\}\}$$

and may be represented as a vector with components

$$\frac{1}{2}\begin{Bmatrix} s_{23} - o_3 u_2 - s_{32} + o_2 u_3 \\ s_{31} - o_1 u_3 - s_{13} + o_3 u_1 \\ s_{12} - o_2 u_1 - s_{21} + o_1 u_2 \end{Bmatrix} \tag{152}$$

This quantity (which we propose to call spin vector) characterizes the local rotation of the fluid about its local centre of mass.

The deviator of S_{nm} is the following tensor

$$\frac{1}{2}\begin{Bmatrix} 2\left(s_{11} - o_1 u_1 - \frac{1}{3}s_0\right) & s_{12} + o_2 u_1 + s_{21} + o_1 u_2 & s_{31} + o_1 u_3 + s_{13} + o_3 u_1 \\ s_{12} + o_2 u_1 + s_{21} + o_1 u_2 & 2\left(s_{22} - o_2 u_2 - \frac{1}{3}s_0\right) & s_{23} + o_3 u_2 + s_{32} + o_2 u_3 \\ s_{31} + o_1 u_3 + s_{13} + o_3 u_1 & s_{23} + o_3 u_2 + s_{32} + o_2 u_3 & 2\left(s_{33} - o_3 u_3 - \frac{1}{3}s_0\right) \end{Bmatrix} \tag{153}$$

This quantity (which we propose to call shear tensor) characterizes the local shear deformation of the fluid.

6.5 Incompressibility contstraint and boundary conditions

The following conditions have been formulated in close analogy to the boundary conditions usually applied in computational fluid dynamics. No detailled analysis has been performed so far on the effect of the boundary conditions on the solution of the balance equation developed in this paper.

6.5.1 Internal constraint for incompressible flow

For incompressible fluids we are used to apply the following restriction to the local mass balance

$$\left.\frac{\partial \hat{\rho}}{\partial t}\right|_{incompressible} + \hat{u}_n \left.\frac{\partial \hat{\rho}}{\partial \hat{x}_n}\right|_{incompressible} = 0$$

which (taking into account the local mass conservation) is equivalent to the well-known restriction on the local velocity field of incompressible fluids:

$$\left.\frac{\partial \hat{u}_n}{\partial \hat{x}_n}\right|_{incompressible} = 0 \tag{154}$$

Since we consider fields of average quantities rather than local quantities we need to reconsider the effect of incompressibility. Apparently, for *constant density* flow ($\hat{\rho} = const$ in both space and time), the continuity equation 58 degenerates into

$$\left.\frac{\partial u_n}{\partial x_n}\right|_{\text{constant density}} = 0$$

and the definition equation for the first moment of mass (see equation 80 with $y_i = c_i$) degenerates into

$$o_i|_{\text{constant density}} = 0$$

But for an incompressible fluid with spatially varying density the situation is different. The constraint 154 on the local velocity field is identically satisfied if we assume that the local velocity is equal to the rotation of a vector field $\hat{\Psi}$. Thus we write for incompressible flow

$$\hat{u}_i|_{incompressible} = \frac{\partial \hat{\Psi}_j}{\partial \hat{x}_k} - \frac{\partial \hat{\Psi}_k}{\partial \hat{x}_j}$$

If we now determine the split value s_0 for such a local velocity field and arbitrary density using the approximation assumptions specified above we obtain:

$$s_0|_{incompressible} = (s_{nn} - o_n u_n)|_{incompressible} = \Theta \frac{\partial \hat{u}_n}{\partial \hat{x}_n} + O(l^4) = 0 + O(l^4) \tag{155}$$

This relation has been derived in appendix 5.

6.5.2 Boundaries which are crossed by the flowing fluid

The boundary conditions which may be formulated on boundaries across which fluids flows into or out of the domain under consideration depend very much on the character of the set of differential equations (elliptic, hyperbolic). This character is influenced by the constitutive equations. Since we do not deal with constitutive equations in this paper we cannot discuss such boundary conditions in more detail.

6.5.3 Wall type boundaries

For wall type boundaries we are faced with a principal problem. The averaged fields are defined only as far as the control volumes are fully embedded in the fluid or just barely touch the boundary. On the other hand, in order to solve the set of differential equations average values or their derivatives on the boundary need to be specified. This will require some kind of extrapolation of the local fields in order to make the volume averages meaningful. We have to find ways to resolve this conflict.

Before we propose a solution to this dilemma let us ask ourselves what kind of boundary conditions would be physically meaningful at wall type boundaries. In computational fluid dynamics based on the local field equations for density and momentum no wall boundary condition is required for density. The velocity component normal to the wall is usually prescribed (most often 0 for a fixed rigid wall), the velocity components parallel to the wall are prescribed (most often 0 for no-slip walls) or requested to have vanishing derivative normal to the wall (for free-slip walls). For multi-phase flow we might wish to state that the wall in non-wetting (density equal to the density of the gaseous phase) or wetting (density equal to the density of the liquid phase). We also might wish to prescribe the velocity. Strictly speaking we do not mean the density and velocity *on* the wall but rather *within the fluid directly adjacent to the wall.* Furthermore, we do not wish to prescribe volume average quantity but rather quantities that are averaged over the face which is adjacent to the wall. This interest in face average values reminds us of the discussion in section 3.3. Assuming that direction i is normal to the wall and directed into the fluid domain while directions j and k are parallel to the wall we repeat equation 30 here (omitting the prefix which indicated the brick type):

$$\rho^{S_i}_{mean} = \frac{1}{2}(\rho^{S_i^+} + \rho^{S_i^-}) = \rho + \frac{\partial(\rho o_i)}{\partial x_i} \tag{156}$$

and equations 28 and 29 (considering $h_i = h_j = h_k = h_0$ which we assume in our approximation):

$$\rho^{S_i^\pm} = \frac{1}{h_0^2}\int_{c_j-\frac{h_0}{2}}^{c_j+\frac{h_0}{2}}\int_{c_k-\frac{h_0}{2}}^{c_k+\frac{h_0}{2}} \hat{\rho}(c_i \pm \frac{h_0}{2}, \hat{x}_j, \hat{x}_k)d\hat{x}_j d\hat{x}_k \tag{157}$$

If we now consider a control volume centered on the wall then one of the face S_i^+ is located at a distance $\frac{h_0}{2}$ from the wall inside the fluid domain while the face S_i^- is located at a distance $\frac{h_0}{2}$ from the wall outside the fluid domain. If we select an extrapolation of the local fields in a symmetric way beyond the wall boundary then

$$\rho^{S_i^+} = \rho^{S_i^-}$$

and consequently the boundary condition for prescribing the value of $\rho^{S_i^+}$:

$$\frac{\partial(\rho o_i)}{\partial x_i} = \rho|_{prescribed} - \rho \tag{158}$$

plus (due to the symmetry assumption):

$$\frac{\partial \rho}{\partial x_i} = 0$$

By analogy, replacing the local mass density $\hat{\rho}$ in our arguments by the momentum density $\hat{\rho}u_n$, we can also prescribe the velocity at (or better: close to) the wall:

$$\frac{\partial \rho s_{ni}}{\partial x_i} = \rho u_n|_{prescribed} - \rho u_n \tag{159}$$

and:

$$\frac{\partial \rho u_n}{\partial x_i} = 0 \tag{160}$$

7 A complete example using the constitutive equation for an incompressible fluid

The above set of equations still contains quantities which describe forces acting on the fluid. These quantities need to be defined by constitutive relations. They depend on the fluid and on the force fields which we wish to take into account. We will give here an example for constitutive relations which are typical for an inviscid mixture of liquids with different density.

We assume that the body force field represents gravity. This is a smooth field and, hence, its first moment γ_{im} becomes

$$\gamma_{im} = \frac{1}{\rho V}\int_{V(x)} \hat{\rho}\hat{x}_m \hat{g}_i dV - x_m g_i = \frac{g_i}{\rho V}\int_{V(x)} \hat{\rho}(\hat{x}_m - x_m)dV = g_i o_m \tag{161}$$

We also assume that the stress tensor contains only one component: the pressure p which we consider as smoothly varying over the dimensions of our small cubic control volumes. The first moment of the stress field μ_{nmi} vanishes for this assumption.

Thus we obtain the following set of equations

Mass balance

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_n}{\partial x_n} = 0 \tag{162}$$

Balance of the centre of mass offset balance

$$\frac{\partial \rho o_i}{\partial t} + \frac{\partial \rho s_{in}}{\partial x_n} = 0 \tag{163}$$

Momentum balance

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_n}{\partial x_n} + \frac{\partial}{\partial x_n}\left(\rho(s_{nm} - o_m u_n)\frac{\partial u_i}{\partial x_m}\right) = \rho g_i + \frac{\partial p}{\partial x_i} \tag{164}$$

Balance of the moment of momentum

$$\frac{\partial \rho s_{mi}}{\partial t} + \frac{\partial \rho s_{mi} u_n}{\partial x_n} = \rho o_m g_i \tag{165}$$

The pressure field has to be determined such that the constraint on the local velocity field (equation 155) is satisfied:

$$s_{nn} + o_n u_n = 0$$

Appropriate boundary conditions as formulated in section 6.5 have to be added.

Assuming sufficient knowledge about the initial local density and velocity field $\hat{\rho}$ and $\hat{\rho}\hat{u}_i$, the initial conditions can be determined as follows:

- determine an appropriate side length h_0 of the cubic control volume.
- determine the fields of the average quantities ρ and ρu_i
- determine the fields of face-average values

$$\rho^{S_i^{\pm}} = \frac{1}{(h_0)^2} \int_{x_j - \frac{h_0}{2}}^{x_j + \frac{h_0}{2}} \int_{x_k - \frac{h_0}{2}}^{x_k + \frac{h_0}{2}} \hat{\rho}(x_i \pm h_0, \hat{x}_j, \hat{x}_k) d\hat{x}_j d\hat{x}_k$$

- determine the derivative of the first moment of the mass distribution according to

$$\frac{\partial(\rho o_i)}{\partial x_i} = \frac{1}{2}(\rho^{S_i^+} + \rho^{S_i^-}) - \rho$$

- solve this differential equation taking into account the appropriate boundary conditions in order to determine the initial field of ρo_i
- determine the fields of face-average values

$$(\rho u_n)^{S_i^{\pm}} = \frac{1}{(h_0)^2} \int_{x_j - \frac{h_0}{2}}^{x_j + \frac{h_0}{2}} \int_{x_k - \frac{h_0}{2}}^{x_k + \frac{h_0}{2}} \hat{\rho}(x_i \pm h_0, \hat{x}_j, \hat{x}_k) \hat{u}_n(x_i \pm h_0, \hat{x}_j, \hat{x}_k) d\hat{x}_j d\hat{x}_k$$

- determine the derivative of the first moment of the momentum distribution according to

$$\frac{\partial(\rho s_{in})}{\partial x_i} = \frac{1}{2}((\rho u_n)^{S_i^+} + (\rho u_n)^{S_i^-}) - \rho u_n$$

- solve this differential equation taking into account the appropriate boundary conditions in order to determine the initial field of ρs_{in}

This complete set of equations should provide us with the basis for determining the flow field for an incompressible inviscid fluid with strong variations in the local density and velocity distribution up to third order accuracy in the local quantities.

8 Concluding remarks

What did we gain, what did we lose due to our approach? The advantages are of different categories:

- Advantages of conceptual nature

  We have found a set of equations that satisfies the principles that we had originally established (see section 4).

  1. The set of equations is based on average quantities rather than local quantities;
  2. it is independent of the control volume for which the averaging is performed;
  3. it is valid even if the fields over which averaging is performed contain extreme variations, even discontinuities, provided that the control volume is large enough or the number of averaging operations is sufficient to smooth those fields;

4. The conventional "local" balance equations are still valid - in some sense: our mass balance equation is identical to the conventional formulation; the conventional momentum balance equation can be interpreted as a special case of our formulation; the two additional balance equations for the first moments of density and velocity degenerate if there are only negligible variations inside the control volumes under consideration;
5. as a side effect, our approach discarded interpretations of velocity that do not fit into the concept of velocity as "momentum per unit mass". Concepts like "particle velocity" or "material transport velocity across a boundary" could be eliminated.

- Advantage for formulating constitutive relationships

  Constitutive relationships need experimental determination. The quantities which are not governed by balance equations (see section 6.1) are all based on volume integrals. Experiments to determine these relationships need not to concentrate on microscopic phenomena. Any arbitrarily large control volumes can be used for such investigations. This appears to be a significant benefit in comparison to approaches which require the study of detail interactions at a bubble interface as would be required in some other approaches to multi-phase flow modeling.

- Advantages for computational fluid dynamics

  We have careful avoided any discussion of numerical computation so far. The intent was not to formulate averages over the meshes of a computational grid or over finite elements. But it appears that also for numerical applications our set of averaged balance equations will be useful. In particular, the balance equation for the first moments will give more information about field characteristics inside such meshes or finite elements. Since these balance equations are exact rather than approximate, we expect better results from explicitly treating the additional balance equations (on first moments) than from refining the computational grid.

We certainly have to pay a price for these advantages. Most important, the pragmatic validation of our new set of equations is as yet missing. A theory may be correct but nonetheless may not be useful because it lacks the necessary data (in this case, the constitutive relations) for practical application. Or else, results may not be improved compared to other approaches (such as waiting for a further increase of computer power in order to utilise finer computational grids). The next required step is the application of the new set of equations to specific flow problems and to solve them using the available techniques of computational fluid dynamics. If the new approach reproduces otherwise known results (hopefully better or faster) then this could be taken as a confirmation of the approach proposed in this paper. This confirmation is yet to be undertaken.

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1 Appendix: Proof of equations for self-similar control volumes

We intend to prove that for an arbitrary function $\hat{\phi}(\hat{x}_i, \hat{x}_j, \hat{x}_k)$ in self-similar control volumes characterised by a boundary of the type

$$\hat{x}_{iS}(\kappa, x_i) = c_i + (\hat{x}_{iS}(0, x_i) - c_i) * e^{-\kappa} \tag{166}$$

the following relationship is valid:

$$\frac{\partial}{\partial x_n} \int_{\mathbf{V}(\kappa,\mathbf{x})} (\hat{x}_n - c_n)\, \hat{\phi} d\hat{V} = -\frac{\partial}{\partial \kappa} \int_{\mathbf{V}(\kappa,\mathbf{x})} \hat{\phi} d\hat{V} \tag{167}$$

We will prove this relationship in three steps:

1. Prove equation 167 for brick-shaped control volumes.
2. Prove equation 167 for the union of two arbitrary non-overlapping control volumes.
3. Finally we conclude that since any arbitrary control volume can be constructed to any desired degree of accuracy from smaller brick-shaped control volumes, equation 167 will hold for arbitrary control volumes.

1.1 The proof for brick-type control volumes

The first step of this proof is performed by the following MAPLE V program [9]:

```
> with(student,Tripleint):with(student,value):
> domain:='xh[1]=lb[1]..ub[1],xh[2]=lb[2]..ub[2 ],xh[3]=lb[3]..ub[3]':
> for l from 1 to 3 do
> lb[l]:=x[l]+m[l]-h[l]/2*exp(-kappa):
> ub[l]:=x[l]+m[l]+h[l]/2*exp(-kappa):od:
> V:=expand(value(Tripleint(1,domain)));
```

$$V := \frac{h_1\, h_2\, h_3}{(e^{\kappa})^3}$$

```
> for l from 1 to 3 do c[l]:=
> simplify(value(Tripleint(xh[l],domain)/V));od;
```

$$c_1 := x_1 + m_1$$

$$c_2 := x_2 + m_2$$

$$c_3 := x_3 + m_3$$

```
> Phi:=Tripleint(phih(xh[1],xh[2],xh[3]),domain ):
> phi:=Phi/V:
> dphi_dkappa:=diff(phi,kappa):
> for l from 1 to 3 do xphi[l]:=
> Tripleint((xh[l]-c[l])*phih(xh[1],xh[2],xh[3]),domain)/V;od:
> dxphi_dx:=diff(xphi[1],x[1])+diff(xphi[2],x[2 ])+diff(xphi[3],x[3]):
> expand(dphi_dkappa+dxphi_dx);
```

$$0$$

1.2 The proof for a union of two non-overlapping control volumes

The second step of this proof assumes the validity of equation 167 for two control volumes $\mathbf{A}\kappa$ and $\mathbf{B}\kappa$. With

$$c_{Ai} = \int_{\mathbf{A}\kappa} \hat{x}_i d\hat{V} \tag{168}$$

$$c_{Bi} = \int_{\mathbf{B}\kappa} \hat{x}_i d\hat{V} \tag{169}$$

the equations for the separate control volumes read

$$\frac{\partial}{\partial x_n} \int_{\mathbf{A}\kappa} (\,\hat{x}_n - c_{An})\,\hat{\phi} d\hat{V} = -\frac{\partial}{\partial \kappa} \int_{\mathbf{A}\kappa} \hat{\phi} d\hat{V} \tag{170}$$

$$\frac{\partial}{\partial x_n} \int_{\mathbf{A}\kappa} (\,\hat{x}_n - c_{An})\,\hat{\phi} d\hat{V} = -\frac{\partial}{\partial \kappa} \int_{\mathbf{A}\kappa} \hat{\phi} d\hat{V} \tag{171}$$

Summation of these equations gives:

$$\frac{\partial}{\partial x_n}\int_{(A\cup B)\kappa}(\hat{x}_n - c_{(A\cup B)n}(\kappa))\,\hat{\phi}d\hat{V} = -\frac{\partial}{\partial \kappa}\int_{(A\cup B)\kappa}\hat{\phi}d\hat{V} \tag{172}$$

with

$$c_{(A\cup B)i}(\kappa) = \int_{(A\cup B)\kappa}\hat{x}_i d\hat{V} \tag{173}$$

1.3 The proof for arbitrary control volumes

Since any arbitrary control volume can be constructed from smaller control volumes up to any desired accuracy we conclude that equation 167 holds for arbitrary control volumes.

2 Appendix: Average density on two opposing faces of a brick-type control volume

This is to prove equation 30. The proof is performed for co-ordinates $x_i = x_1$ by the following MAPLE V program [9]:

```
> V:=h[1]*h[2]*h[3]:
> Face[1]:=h[2]*h[3]:
> domain[1]:='xh[1]=x[1]-h[1]/2..x[1]+h[1]/2':
> domain[2]:='xh[2]=x[2]-h[2]/2..x[2]+h[2]/2':
> domain[3]:='xh[3]=x[3]-h[3]/2..x[3]+h[3]/2':
> box_rho_Face_plus[1]:=int(int(rhoh(x[1]+h[1]/ 2,xh[2],xh[3])
> ,domain[3]),domain[2])/Face[1]:
> box_rho_Face_minus[1]:=int(int(rhoh(x[1]-h[1] /2,xh[2],xh[3])
> ,domain[3]),domain[2])/Face[1]:
> box_rho_Face_mean[1]:=
> (box_rho_Face_plus[1]+box_rho_Face_minus[1])/2:
> rho:=int(int(int(rhoh(xh[1],xh[2],xh[3])
> ,domain[3]),domain[2]),domain[1])/V:
> box_rho_o[1]:=int(int(int((xh[1]-x[1])*rhoh(x h[1],xh[2],xh[3])
> ,domain[3]),domain[2]),domain[1])/V:
> simplify(box_rho_Face_mean[1]-(diff(box_rho_o [1],x[1])+rho));
                                0
```

Cyclic exchange of the co-ordinate subscripts $1, 2, 3$ completes the proof for convex control volumes.

3 Appendix: Proof of approximate representation of average and first moment quantities

We intend to prove that with $\Theta = \int_V (\hat{x}_i - x_i)^2 d\hat{V} = \frac{h^2}{12}$ the approximations

$$\rho = \hat{\rho} + \Theta \frac{\partial^2 \hat{\rho}}{\partial \hat{x}_n^2}$$

$$a = \hat{a} + \frac{\partial \hat{a}}{\partial \hat{x}_n} \Theta \frac{\partial \hat{\rho}}{\hat{\rho} \partial \hat{x}_{ni}} + \Theta \frac{\partial^2 \hat{a}}{\partial \hat{x}_n^2}$$

Always taking into account third-order approximation, his may be rewritten as

$$a = \hat{a}|_{x_i + o_i} + \Theta \frac{\partial^2 \hat{a}}{\partial \hat{x}_n^2}$$

$$o_i = \Theta \frac{\partial \hat{\rho}}{\hat{\rho} \partial \hat{x}_i}$$

$$\alpha_i = \Theta \frac{\partial \hat{a}}{\partial \hat{x}_i} + \hat{a} \Theta \frac{\partial \hat{\rho}}{\hat{\rho} \partial \hat{x}_{ni}} = \Theta \frac{\partial \hat{a}}{\partial \hat{x}_i} + \hat{a} o_i$$

are accurate up to third order Taylor series approximation. This proof is performed by the following Maple [9] program.

```
> with(student,powsubs):with(student,Tripleint) :
> with(student,value):
> Theta[0]:=T:Theta[1]:=Theta[0]:Theta[2]:=Thet a[0]:Theta[3]:=Theta[0]:
```

vspec computes the approximation of rho/rc[0,0,0] up to order 3
using 1/(1+eps)=1-eps+eps**2-eps**3

```
> vspec:=proc(z) local y,eps,ep2,ep3;
> eps:=expand((subs(
> x[1]=y[1],x[2]=y[2],x[3]=y[3],rho)-rc[0,0,0])/rc[0,0,0]):
> ep2:=approximate_product(eps,eps,y);
> ep3:=approximate_product(ep2,eps,y);
> expand(subs(y=z,(1-eps+ep2-ep3))/rc[0,0,0]);
> end:
```

approximate product computes the product of two polynomials up to order 3

```
> approximate_product:=proc(f1,f2,z)
> local ll,l,n,n1,n2,n3,f,noTheta,someTheta,terms,
> oneterm,oforder,interim,z_only,z_2,z_3,result;
> # preconditions:
> # f[1] are polynomials with at least two terms in x[i]
> # up to order 3; Theta[1] counts as order 2
```

```
> f[1]:=expand(f1);f[2]:=expand(f2);
> if f[1]=z[1] or f[1]=z[2] or f[1]=z[3] then ll:=2;
> else ll:=1; fi;
> for l from ll to 2 do
> noTheta[l]:=powsubs(Theta[1]=0,Theta[2]=0,Theta[3]=0,f[l]);
> someTheta[l]:=f[l]-noTheta[l];od:
> for l from ll to 2 do
> terms:=nops(someTheta[l]);
> oforder[2,l]:=0;
> for n from 1 to terms do oneterm:=op(n,someTheta[l]);
> for n1 from 1 to 3 do oneterm:=subs(z[n1]=0,oneterm); od;
> oforder[2,l]:=oforder[2,l]+oneterm;
> od;
> oforder[3,l]:=someTheta[l]-oforder[2,l];
> od:
> for l from ll to 2 do
> oforder[0,l]:=powsubs(z[1]=0,z[2]=0,z[3]=0,noTheta[l]);
> noTheta[l]:=noTheta[l]-oforder[0,l]; od:
> for l from ll to 2 do
> noTheta[l]:=expand(noTheta[l]);terms:=nops(noTheta[l]);
> interim:=0;
> for n from 1 to terms do
> oneterm:=op(n,noTheta[l]);
> for n1 from 1 to 3 do for n2 from 1 to 3 do
> oneterm:=powsubs(z[n1]*z[n2]=0,oneterm); od; od;
> interim:=interim+oneterm;
> od;
> oforder[1,l]:=interim;
> noTheta[l]:=expand(noTheta[l]-interim);
> od:  #now orders 0 and 1 are ok, 2 and 3 contain Theta only
> for l from ll to 2 do
> z_only:=powsubs(z[2]=0,z[3]=0,noTheta[l]):
> z_2:=expand(z[1]^2*powsubs(z[1]=0,expand(z_only/z[1]^2))):
> z_3:=z_only-z_2:
> oforder[2,l]:=oforder[2,l]+z_2:oforder[3,l]:=oforder[3,l]+z_3;
> noTheta[l]:=noTheta[l]-z_only:
> z_only:=powsubs(z[3]=0,z[1]=0,noTheta[l]):
```

```
> z_2:=expand(z[2]^2*powsubs(z[2]=0,expand(z_only/z[2]^2))):
> z_3:=z_only-z_2:
> oforder[2,1]:=oforder[2,1]+z_2:oforder[3,1]:=oforder[3,1]+z_3;
> noTheta[1]:=noTheta[1]-z_only:
> z_only:=powsubs(z[1]=0,z[2]=0,noTheta[1]):
> z_2:=expand(z[3]^2*powsubs(z[3]=0,expand(z_only/z[3]^2))):
> z_3:=z_only-z_2:
> oforder[2,1]:=oforder[2,1]+z_2:oforder[3,1]:=oforder[3,1]+z_3;
> noTheta[1]:=noTheta[1]-z_only:
> z_only:=subs( z[1]=0,noTheta[1] ):
> z_2:=powsubs(z[2]=0,z[3]=0,expand(z_only/(z[3]*z[2])))*z[2]*z[3]:
> z_3:=z_only-z_2:
> oforder[2,1]:=oforder[2,1]+z_2:oforder[3,1]:=oforder[3,1]+z_3;
> noTheta[1]:=noTheta[1]-z_only:
> z_only:=subs( z[2]=0,noTheta[1] ):
> z_2:=powsubs(z[3]=0,z[1]=0,expand(z_only/(z[1]*z[3])))*z[3]*z[1]:
> z_3:=z_only-z_2:
> oforder[2,1]:=oforder[2,1]+z_2:oforder[3,1]:=oforder[3,1]+z_3;
> noTheta[1]:=noTheta[1]-z_only:
> z_only:=subs( z[3]=0,noTheta[1] ):
> z_2:=powsubs(z[1]=0,z[2]=0,expand(z_only/(z[2]*z[1])))*z[1]*z[2]:
> z_3:=z_only-z_2:
> oforder[2,1]:=oforder[2,1]+z_2:oforder[3,1]:=oforder[3,1]+z_3;
> noTheta[1]:=noTheta[1]-z_only:
> oforder[3,1]:=oforder[3,1]+noTheta[1];
> od:
> if ll=1 then
> result:=oforder[0,1]*
> (oforder[0,2]+oforder[1,2]+oforder[2,2]+oforder[3,2]);
> result:=result+oforder[1,1]*
> (oforder[0,2]+oforder[1,2]+oforder[2,2]);
> result:=result+oforder[2,1]*(oforder[0,2]+oforder[1,2]);
> result:=expand(result+oforder[3,1]*oforder[0,2]);
> else
> result:=f[1]*(oforder[0,2]+oforder[1,2]+oforder[2,2]);
> result:=expand(result);
> fi;
```

```
> end:
> for l from 1 to 3 do h[l]:=sqrt(12*Theta[l]):  od:
> rhoh:=0:  ah:=0:  for l from 1 to 3 do uh[l]:=0;od:
> for n1 from 0 to 3 do for n2 from 0 to (3-n1) do
> for n3 from 0 to (3-n1-n2) do rhoh:=
> rhoh+rc[n1,n2,n3]*xh[1]^n1*xh[2]^n2*xh[3]^n3/(n1!*n2!*n3!)
> od;od;od;
> for n1 from 0 to 3 do for n2 from 0 to (3-n1) do
> for n3 from 0 to (3-n1-n2) do ah:=
> ah+ac[n1,n2,n3]*xh[1]^n1*xh[2]^n2*xh[3]^n3/(n1!*n2!*n3!)
> od;od;od;
> for l from 1 to 3 do lb[l]:=x[l]-h[l]/2:  od:
> for l from 1 to 3 do ub[l]:=x[l]+h[l]/2; od:
> domain:='xh[1]=lb[1]..ub[1],xh[2]=lb[2]..ub[2 ],xh[3]=lb[3]..ub[3]':
> V:=expand(value(Tripleint(1,domain))):
> for l from 1 to 3 do c[l]:=
> simplify(value(Tripleint(xh[l],domain))/V); od;
```

$$c_1 := x_1$$

$$c_2 := x_2$$

$$c_3 := x_3$$

```
> rho:=simplify(value(Tripleint(rhoh,domain))/V ):
> for l from 1 to 3 do
> term1:=simplify(int(int(int(approximate_product(xh[l],rhoh,xh),
> xh[1]=lb[1]..ub[1]),xh[2]=lb[2]..ub[2]),xh[3]=lb[3]..ub[3])/V):
> term2:=approximate_product(x[l],rho,x):
> rhoo[l]:=term1-term2:
> od:
> v:=vspec(x):
> proof:=approximate_product(v,rho,x);
```

$$proof := 1$$

```
> for n from 1 to 3 do o[n]:= approximate_product(v,rhoo[n],x):od:
> rhohah:=approximate_product(rhoh,ah,xh):
> rhoa:=simplify(value(Tripleint(rhohah,domain) )/V):
> a:=approximate_product(v,rhoa,x):
> rhoh_ah:=approximate_product(rhoh,ah,xh):
> for n from 1 to 3 do
> term1:=simplify(int(int(int(approximate_product(xh[n],rhoh_ah,xh),
> xh[1]=lb[1]..ub[1]),xh[2]=lb[2]..ub[2]),xh[3]=lb[3]..ub[3])/V):
> term2:=approximate_product(x[n],rhoa,x):
> rho_alpha[n]:=term1-term2:
> alpha[n]:=approximate_product(v,rho_alpha[n],x);
> od:
```

Proof of approximation for average density

```
> expand(rho-subs(xh=x,rhoh+1/2*Theta[0]*(diff( rhoh,xh[1],xh[1])
> +diff(rhoh,xh[2],xh[2])+diff(rhoh,xh[3],xh[3])));
```

$$0$$

Proof of approximation for offset

```
> for l from 1 to 3 do error[l]:=expand(o[l]- subs(xh=x,approximate_product(subs(T=
approximate_product(Theta[0],diff(rhoh,xh[l]),xh),xh)));od;
```

$$error_1 := 0$$

$$error_2 := 0$$

$$error_3 := 0$$

Proof of approximation for the average of an arbitrary quantity

```
> for l from 1 to 3 do
> Theta_diff_rhoh[l]:=Theta[0]*diff(rhoh,xh[l]):od:
> for l from 1 to 3 do
> for n1 from 1 to 3 do for n2 from 1 to 3 do
> Theta_diff_rhoh[l]:=powsubs(Theta[0]*xh[n1]*xh[n2]=0,
> expand(Theta_diff_rhoh[l]));od;od;od;
> approximate_difference:=0:
> for l from 1 to 3 do
> approximate_difference:=approximate_difference+
> approximate_product(subs(T=0,x=xh,v),
> approximate_product(Theta_diff_rhoh[l],diff(ah,xh[l]),xh),xh)
> +1/2*Theta[0]*diff(ah,xh[l],xh[l]):od:
> expand(a-subs(xh[1]=x[1],xh[2]=x[2],xh[3]=x[3 ]
```

```
> ,ah+approximate_difference));
```

$$0$$

Proof of approximation for the first moment of an arbitrary quantity

```
> for n from 1 to 3 do error[n]:=expand(alpha[n]-
> subs(xh=x,approximate_product(Theta[0],diff(a h,xh[n]),xh))
> -approximate_product(o[n],subs(xh=x,ah),x) );od;
```

$$error_1 := 0$$

$$error_2 := 0$$

$$error_3 := 0$$

4 Appendix: Proof of approximate representation of the fluctuation flux

We intend to prove that the approximations

$$F_n[a] = \frac{1}{2}((s_{nm} - o_m u_n)\frac{\partial a}{\partial x_m} + (\alpha_m - o_m a)\frac{\partial u_n}{\partial x_m}) + O(l^4) \tag{174}$$

or by

$$F_n[a] = \frac{1}{2}(s_{nm}\frac{\partial a}{\partial x_m} + \alpha_m \frac{\partial u_n}{\partial x_m} - o_m \frac{\partial a u_n}{\partial x_m}) + O(l^4) \tag{175}$$

are accurate up to third order Taylor series approximation. This proof is performed by the following Maple [9] program.

```
> with(student,powsubs):with(student,Tripleint) :
> with(student,value):
```

vspec computes the approximation of rho/rc[0,0,0] up to order 3
using 1/(1+eps)=1-eps+eps**2-eps**3

```
> vspec:=proc(z) local y,eps,ep2,ep3;
> eps:=expand((subs(
> x[1]=y[1],x[2]=y[2],x[3]=y[3],rho)-rc[0,0,0])/rc[0,0,0]):
> ep2:=approximate_product(eps,eps,y);
> ep3:=approximate_product(ep2,eps,y);
> expand(subs(y=z,(1-eps+ep2-ep3))/rc[0,0,0]);
> end:
```

approximate product computes the product of two polynomials up to order 3

```
> approximate_product:=proc(f1,f2,z)
> local ll,l,n,n1,n2,n3,f,noTheta,someTheta,terms,
> oneterm,oforder,interim,z_only,z_2,z_3,result;
> # preconditions:
```

```
> # f[1] are polynomials with at least two terms in x[i]
> # up to order 3; Theta[1] counts as order 2
> f[1]:=expand(f1);f[2]:=expand(f2);
> if f[1]=z[1] or f[1]=z[2] or f[1]=z[3] then ll:=2;
> else ll:=1; fi;
> for l from ll to 2 do
> noTheta[l]:=powsubs(Theta[1]=0,Theta[2]=0,Theta[3]=0,f[l]);
> someTheta[l]:=f[l]-noTheta[l];od:
> for l from ll to 2 do
> terms:=nops(someTheta[l]);
> oforder[2,l]:=0;
> for n from 1 to terms do oneterm:=op(n,someTheta[l]);
> for n1 from 1 to 3 do oneterm:=subs(z[n1]=0,oneterm); od;
> oforder[2,l]:=oforder[2,l]+oneterm;
> od;
> oforder[3,l]:=someTheta[l]-oforder[2,l];
> od:
> for l from ll to 2 do
> oforder[0,l]:=powsubs(z[1]=0,z[2]=0,z[3]=0,noTheta[l]);
> noTheta[l]:=noTheta[l]-oforder[0,l]; od:
> for l from ll to 2 do
> noTheta[l]:=expand(noTheta[l]);terms:=nops(noTheta[l]);
> interim:=0;
> for n from 1 to terms do
> oneterm:=op(n,noTheta[l]);
> for n1 from 1 to 3 do for n2 from 1 to 3 do
> oneterm:=powsubs(z[n1]*z[n2]=0,oneterm); od; od;
> interim:=interim+oneterm;
> od;
> oforder[1,l]:=interim;
> noTheta[l]:=expand(noTheta[l]-interim);
> od:  #now orders 0 and 1 are ok, 2 and 3 contain Theta only
> for l from ll to 2 do
> z_only:=powsubs(z[2]=0,z[3]=0,noTheta[l]):
> z_2:=expand(z[1]^2*powsubs(z[1]=0,expand(z_only/z[1]^2))):
> z_3:=z_only-z_2:
> oforder[2,l]:=oforder[2,l]+z_2:oforder[3,l]:=oforder[3,l]+z_3;
```

```
> noTheta[1]:=noTheta[1]-z_only:
> z_only:=powsubs(z[3]=0,z[1]=0,noTheta[1]):
> z_2:=expand(z[2]^2*powsubs(z[2]=0,expand(z_only/z[2]^2))):
> z_3:=z_only-z_2:
> oforder[2,1]:=oforder[2,1]+z_2:oforder[3,1]:=oforder[3,1]+z_3;
> noTheta[1]:=noTheta[1]-z_only:
> z_only:=powsubs(z[1]=0,z[2]=0,noTheta[1]):
> z_2:=expand(z[3]^2*powsubs(z[3]=0,expand(z_only/z[3]^2))):
> z_3:=z_only-z_2:
> oforder[2,1]:=oforder[2,1]+z_2:oforder[3,1]:=oforder[3,1]+z_3;
> noTheta[1]:=noTheta[1]-z_only:
> z_only:=subs( z[1]=0,noTheta[1] ):
> z_2:=powsubs(z[2]=0,z[3]=0,expand(z_only/(z[3]*z[2])))*z[2]*z[3]:
> z_3:=z_only-z_2:
> oforder[2,1]:=oforder[2,1]+z_2:oforder[3,1]:=oforder[3,1]+z_3;
> noTheta[1]:=noTheta[1]-z_only:
> z_only:=subs( z[2]=0,noTheta[1] ):
> z_2:=powsubs(z[3]=0,z[1]=0,expand(z_only/(z[1]*z[3])))*z[3]*z[1]:
> z_3:=z_only-z_2:
> oforder[2,1]:=oforder[2,1]+z_2:oforder[3,1]:=oforder[3,1]+z_3;
> noTheta[1]:=noTheta[1]-z_only:
> z_only:=subs( z[3]=0,noTheta[1] ):
> z_2:=powsubs(z[1]=0,z[2]=0,expand(z_only/(z[2]*z[1])))*z[1]*z[2]:
> z_3:=z_only-z_2:
> oforder[2,1]:=oforder[2,1]+z_2:oforder[3,1]:=oforder[3,1]+z_3;
> noTheta[1]:=noTheta[1]-z_only:
> oforder[3,1]:=oforder[3,1]+noTheta[1];
> od:
> if ll=1 then
> result:=oforder[0,1]*
> (oforder[0,2]+oforder[1,2]+oforder[2,2]+oforder[3,2]);
> result:=result+oforder[1,1]*
> (oforder[0,2]+oforder[1,2]+oforder[2,2]);
> result:=result+oforder[2,1]*(oforder[0,2]+oforder[1,2]);
> result:=expand(result+oforder[3,1]*oforder[0,2]);
> else
> result:=f[1]*(oforder[0,2]+oforder[1,2]+oforder[2,2]);
```

```
> result:=expand(result);
> fi;
> end:
> for l from 1 to 3 do h[l]:=sqrt(12*Theta[l]):  od:
> rhoh:=0:  ah:=0:  for l from 1 to 3 do uh[l]:=0;od:
> for n1 from 0 to 3 do for n2 from 0 to (3-n1) do
> for n3 from 0 to (3-n1-n2) do rhoh:=
> rhoh+rc[n1,n2,n3]*xh[1]^n1*xh[2]^n2*xh[3]^n3/(n1!*n2!*n3!)
> od;od;od;
> for n1 from 0 to 3 do for n2 from 0 to (3-n1) do
> for n3 from 0 to (3-n1-n2) do ah:=
> ah+ac[n1,n2,n3]*xh[1]^n1*xh[2]^n2*xh[3]^n3/(n1!*n2!*n3!)
> od;od;od;
> for l from 1 to 3 do for n1 from 0 to 3 do
> for n2 from 0 to (3-n1) do for n3 from 0 to (3-n1-n2) do uh[l]:=
> uh[l]+uc[l,n1,n2,n3]*xh[1]^n1*xh[2]^n2*xh[3]^n3/(n1!*n2!*n3!)
> od;od;od;od;
> for l from 1 to 3 do lb[l]:=x[l]-h[l]/2:  od:
> for l from 1 to 3 do ub[l]:=x[l]+h[l]/2; od:
> domain:='xh[1]=lb[1]..ub[1],xh[2]=lb[2]..ub[2 ],xh[3]=lb[3]..ub[3]':
> V:=expand(value(Tripleint(1,domain))):
> for l from 1 to 3 do c[l]:=
> simplify(value(Tripleint(xh[l],domain))/V); od;
```

$$c_1 := x_1$$

$$c_2 := x_2$$

$$c_3 := x_3$$

```
> rho:=simplify(value(Tripleint(rhoh,domain))/V ):
> v:=vspec(x):
> proof:=approximate_product(v,rho,x);
```

$$proof := 1$$

```
> rhohah:=approximate_product(rhoh,ah,xh):
> rhoa:=simplify(value(Tripleint(rhohah,domain) )/V):
> a:=approximate_product(v,rhoa,x):
> for l from 1 to 3 do
> rhohuh[l]:=approximate_product(rhoh,uh[l],xh);
> rhou[l]:=simplify(value(Tripleint(rhohuh[l],domain))/V):
> u[l]:=approximate_product(v,rhou[l],x):
> od:
> for l from 1 to 3 do
> interim:=approximate_product(rhoh,ah,xh):
> rhoF_a[l]:=simplify(value(Tripleint(
> approximate_product(interim,uh[l],xh),domain))/V)
> -approximate_product(rhoa,u[l],x):
> for m from 1 to 3 do
> term1:=simplify(value(Tripleint(
> approximate_product(xh[l],rhohuh[m],xh),domai n))/V):
> term2:=approximate_product(x[l],rhou[m],x):
> rhos[l,m]:=term1-term2:
> od:
> term1:=simplify(value(Tripleint(
> approximate_product(xh[l],rhohah,xh),domain))/V):
> term2:=approximate_product(x[l],rhoa,x):
> rhoalpha[l]:=term1-term2:
> od:
> for l from 1 to 3 do
> term1:=simplify(value(Tripleint(
> approximate_product(xh[l],rhoh,xh),domain))/V):
> term2:=approximate_product(x[l],rho,x):
> rhoo[l]:=term1-term2:
> od:
```

Proof of approximation

```
> for l from 1 to 3 do rsminrhoouda[l]:=
> sum('approximate_product(rhos[m,l]
> -approximate_product(u[l],rhoo[m],x),
> diff(a,x[m]),x)','m'=1..3):od:
> for l from 1 to 3 do raminrhoadu[l]:=
```

```
> sum('approximate_product(rhoalpha[m]
> -approximate_product(a,rhoo[m],x),
> diff(u[l],x[m]),x)','m'=1..3):od:
> for l from 1 to 3 do error[l]:=
> rhoF_a[l]-(rsminrhoouda[l]+raminrhoadu[l])/2:od:
> print(error);
```

$$\text{table}([\ 3 = 0,\ 1 = 0,\ 2 = 0\ ])$$

5 Appendix: Proof of approximate incompressibility constraint

We intend to prove that for an incompressible (not necessarily isochoric) fluid the following constraint holds up to third order accuracy:

$$(s_{nn} - o_n u_n)|_{incompressible} = O(l^4)$$

```
> with(student,powsubs):
```

vspec computes the approximation of rho/rc[0,0,0] up to order 3
using 1/(1+eps)=1-eps+eps**2-eps**3

```
> vspec:=proc(z) local y,eps,ep2,ep3;
> eps:=
> expand((subs(x[1]=y[1],x[2]=y[2],x[3]=y[3],rho) -rc[0,0,0]) /rc[0,0,0]):
> ep2:=approximate_product(eps,eps,y);
> ep3:=approximate_product(ep2,eps,y);
> expand(subs(y=z,(1-eps+ep2-ep3))/rc[0,0,0]);
> end:
```

approximate product computes the product of two polynomials up to order 3

```
> approximate_product:=proc(f1,f2,z)
> local ll,l,n,n1,n2,n3,f,noTheta,someTheta,terms,
> oneterm,oforder,interim,z_only,z_2,z_3,result;
> # preconditions:
> # f[l] are polynomials with at least two terms in x[i] up to order 3;
> # Theta0 counts as order 2
> f[1]:=expand(f1);f[2]:=expand(f2);
> if f[1]=z[1] or f[1]=z[2] or f[1]=z[3] then ll:=2; else ll:=1; fi;
```

```
> for l from ll to 2 do
> noTheta[l]:=powsubs(Theta0=0,f[l]);
> someTheta[l]:=f[l]-noTheta[l];od:
> for l from ll to 2 do
> terms:=nops(someTheta[l]);
> oforder[2,l]:=0;
> for n from 1 to terms do oneterm:=op(n,someTheta[l]);
> for n1 from 1 to 3 do oneterm:=subs(z[n1]=0,oneterm); od;
> oforder[2,l]:=oforder[2,l]+oneterm;
> od;
> oforder[3,l]:=someTheta[l]-oforder[2,l];
> od:
> for l from ll to 2 do
> oforder[0,l]:=powsubs(z[1]=0,z[2]=0,z[3]=0,noTheta[l]);
> noTheta[l]:=noTheta[l]-oforder[0,l]; od:
> for l from ll to 2 do
> noTheta[l]:=expand(noTheta[l]);terms:=nops(noTheta[l]);interim:=0;
> for n from 1 to terms do
> oneterm:=op(n,noTheta[l]);
> for n1 from 1 to 3 do for n2 from 1 to 3 do
> oneterm:=powsubs(z[n1]*z[n2]=0,oneterm); od; od;
> interim:=interim+oneterm;
> od;
> oforder[1,l]:=interim;
> noTheta[l]:=expand(noTheta[l]-interim);
> od:  #now orders 0 and 1 are ok, 2 and 3 contain Theta only
> for l from ll to 2 do
> z_only:=powsubs(z[2]=0,z[3]=0,noTheta[l]):
> z_2:=expand(z[1]^2*powsubs(z[1]=0,expand(z_only/z[1]^2))):
> z_3:=z_only-z_2:
> oforder[2,l]:=oforder[2,l]+z_2:oforder[3,l]:=oforder[3,l]+z_3;
> noTheta[l]:=noTheta[l]-z_only:
> z_only:=powsubs(z[3]=0,z[1]=0,noTheta[l]):
> z_2:=expand(z[2]^2*powsubs(z[2]=0,expand(z_only/z[2]^2))):
> z_3:=z_only-z_2:
> oforder[2,l]:=oforder[2,l]+z_2:oforder[3,l]:=oforder[3,l]+z_3;
> noTheta[l]:=noTheta[l]-z_only:
```

```
> z_only:=powsubs(z[1]=0,z[2]=0,noTheta[l]):
> z_2:=expand(z[3]^2*powsubs(z[3]=0,expand(z_only/z[3]^2))):
> z_3:=z_only-z_2:
> oforder[2,l]:=oforder[2,l]+z_2:oforder[3,l]:=oforder[3,l]+z_3;
> noTheta[l]:=noTheta[l]-z_only:
> z_only:=subs( z[1]=0,noTheta[l] ):
> z_2:=powsubs(z[2]=0,z[3]=0,expand( z_only /(z[3]*z[2]) ))*z[2]*z[3]:
> z_3:=z_only-z_2:
> oforder[2,l]:=oforder[2,l]+z_2:oforder[3,l]:=oforder[3,l]+z_3;
> noTheta[l]:=noTheta[l]-z_only:
> z_only:=subs( z[2]=0,noTheta[l] ):
> z_2:=powsubs(z[3]=0,z[1]=0,expand( z_only /(z[1]*z[3]) ))*z[3]*z[1]:
> z_3:=z_only-z_2:
> oforder[2,l]:=oforder[2,l]+z_2:oforder[3,l]:=oforder[3,l]+z_3;
> noTheta[l]:=noTheta[l]-z_only:
> z_only:=subs( z[3]=0,noTheta[l] ):
> z_2:=powsubs(z[1]=0,z[2]=0,expand( z_only /(z[2]*z[1]) ))*z[1]*z[2]:
> z_3:=z_only-z_2:
> oforder[2,l]:=oforder[2,l]+z_2:oforder[3,l]:=oforder[3,l]+z_3;
> noTheta[l]:=noTheta[l]-z_only:
> oforder[3,l]:=oforder[3,l]+noTheta[l];
> od:
> if ll=1 then
> result:=oforder[0,1]*
> (oforder[0,2]+oforder[1,2]+oforder[2,2]+oforder[3,2]);
> result:=result+oforder[1,1]*(oforder[0,2]+oforder[1,2]+oforder[2,2]);
> result:=result+oforder[2,1]*(oforder[0,2]+oforder[1,2]);
> result:=expand(result+oforder[3,1]*oforder[0,2]);
> else
> result:=f[1]*(oforder[0,2]+oforder[1,2]+oforder[2,2]);
> result:=expand(result);
> fi;
> end:
> for l from 1 to 3 do h[l]:=sqrt(12*Theta0):  od:
> rhoh:=0:ah:=0:for l from 1 to 3 do Psih[l]:=0;od:
> for l from 1 to 3 do uh[l]:=0;od:
> for n1 from 0 to 3 do for n2 from 0 to (3-n1) do
```

```
> for n3 from 0 to (3-n1-n2) do rhoh:=rhoh+
> rc[n1,n2,n3]*xh[1]^n1*xh[2]^n2*xh[3]^n3/(n1!*n2!*n3!)  od;od;od;
> for n1 from 0 to 3 do for n2 from 0 to (3-n1) do
> for n3 from 0 to (3-n1-n2) do ah:=ah+
> ac[n1,n2,n3]*xh[1]^n1*xh[2]^n2*xh[3]^n3/(n1!*n2!*n3!)  od;od;od;
> for l from 1 to 3 do for n1 from 0 to 4 do
> for n2 from 0 to (4-n1) do for n3 from 0 to (4-n1-n2) do
> Psih[l]:=Psih[l]+
> Psic[l,n1,n2,n3]*xh[1]^n1*xh[2]^n2*xh[3]^n3/(n1!*n2!*n3!)
> od;od;od;od;
> uh[1]:=diff(Psih[2],xh[3])-diff(Psih[3],xh[2] ):
> uh[2]:=diff(Psih[3],xh[1])-diff(Psih[1],xh[3] ):
> uh[3]:=diff(Psih[1],xh[2])-diff(Psih[2],xh[1] ):
> divuh:=0:for l from 1 to 3 do divuh:=divuh+diff(uh[l],xh[l]);od:
> for l from 1 to 3 do lb[l]:=x[l]+h[l]/2:  od:
> for l from 1 to 3 do ub[l]:=x[l]-h[l]/2; od:
> V:=expand(int(int(int(1,xh1=lb[1]..ub[1]),
> xh2=lb[2]..ub[2]),xh3=lb[3]..ub[3])):
> rho:=simplify(int(int(int(rhoh,
> xh[1]=lb[1]..ub[1]),xh[2]=lb[2]..ub[2]),xh[3]=lb[3]..ub[3])/V):
> v:=vspec(x):
> for l from 1 to 3 do
> rhohuh[l]:=approximate_product(rhoh,uh[l],xh);
> rhou[l]:=simplify(int(int(int(rhohuh[l],
> xh[1]=lb[1]..ub[1]),xh[2]=lb[2]..ub[2]),xh[3]=lb[3]..ub[3])/V):
> u[l]:=approximate_product(v,rhou[l],x):
> od:
> for l from 1 to 3 do
> term1:=simplify(int(int(int(approximate_product(xh[l],rhohuh[l],xh),
> xh[1]=lb[1]..ub[1]),xh[2]=lb[2]..ub[2]),xh[3]=lb[3]..ub[3])/V):
> term2:=approximate_product(x[l],rhou[l],x):
> rhos[l,l]:=term1-term2:
> od:
> for l from 1 to 3 do
> term1:=simplify(int(int(int(approximate_product(xh[l],rhoh,xh),
> xh[1]=lb[1]..ub[1]),xh[2]=lb[2]..ub[2]),xh[3]=lb[3]..ub[3])/V):
> term2:=approximate_product(x[l],rho,x):
```

```
> rhoo[l]:=term1-term2:
> od:
```

Incompressibility condition

```
> s0:=0:
> for l from 1 to 3 do
> s0 := s0 + subs(rhos[l,l]-approximate_product(rhoo[l],u[l],x)):
> od:
> s0;
```

$$0$$

6 Appendix: List of symbols

Some symbols are used only locally and are explained at the point of their use. The following symbols are used consistently throughout this paper. The following indicators in connection with a (or another field) modify the meaning of the symbol a:

- Indicators which modify the meaning of a symbol (other than x_n)

a (no indicator)	average value
$\hat{a}$	local value of a
$\bar{a}$	average of the average value of a
$\tilde{a}$	average value on a control volume surface, weighted by the distance from the reference point
$^{\odot}a$	prefix; indicating a spherical control volume
$^{\square}a$	prefix, indicating a box-type control volume

- Latin symbols

a	an arbitrary quantity
c_i	displacement of the volumetric centre of a control volume from the reference point
dS_n	surface differential normal to direction n
e_{ni}	momentum fluctuation flux per unit mass
$F_n[a]$	fluctuation flux of a
g_n	body force per unit mass
h_i	width of a brick-type control volume relative to the
i_{in}	inertia of a control volume per unit mass reference point
i, j, k	subscripts i, j, k indicate Cartesian co-ordinates; summation convention does not apply
n, m	subscripts n and m indicate Cartesian co-ordinates; summation convention does apply
o_n	offset of the centre of mass from the reference point of a control volume
$rsh[a]$	right-hand side of balance equation for a
s_{ni}	moment of momentum (in direction i about the n direction in the reference point of a control volume) per unit mass
$\mathbf{S(V(x))}$	surface of a control volume
t	time
u_n	velocity equivalent to momentum per unit mass
$\mathbf{V}$	control volume in which local fields are defined
$\bar{\mathbf{V}}$	control volume in which averaged fields are defined
V	the volume of control volume $\mathbf{V}$
$\hat{x}_n$	co-ordinate for local fields
x_n	location of the reference point of a control volume on the $\hat{x}_n$ co-ordinate axis; also co-ordinate for fields of average values
$\bar{x}_n$	location of the reference point of a control volume on the x_n co-ordinate axis; also co-ordinate for fields of averaged average values
z_i	location of the centre of mass of a control volume

- Greek symbols

α_i	the first moment of an arbitrary quantity
γ_{mi}	moment of the body force (in direction m) per unit mass relative to the reference point of a control volume
δ_{ni}	Cronecker Delta; 1 for $n = i$, 0 otherwise
ϵ_{nmi}	fluctuation flux of the moment of momentum s_{mi} per unit mass (in the n direction in the reference point of a control volume)
κ	Logarithm of the length scale for self-similar control volumes
μ_{nmi}	moment of the stress τ_{nm} per unit volume relative to the reference point of a control volume
ρ	density
τ_{ni}	stress (in direction i on face normal to direction n)