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MECHANICS

SHORT COMMUNICATION

# Comments on mesoscopic continuum physics: evolution equation for the distribution function and open questions

Heiko Herrmann* and Jüri Engelbrecht

Centre for Nonlinear Studies, Institute of Cybernetics at Tallinn University of Technology, Akadeemia tee 21, 12618 Tallinn, Estonia; je@ioc.ee

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**Abstract.** In mesoscopic continuum physics it is common to introduce a mesoscopic distribution function. Often also an evolution equation is derived for this distribution function. The mesoscopic balance equations for mass and the evolution equation for the distribution function, however, are not independent. We discuss different usage cases of mesoscopic balances in connection with the evolution equation. Furthermore, the problem of virtual boundaries is discovered, referring to cases where the domain in the mesoscopic description becomes non-contiguous despite the macroscopic domain being contiguous.

**Key words:** mesoscopic continuum physics, virtual boundaries, evolution equation, balance equations.

## 1. INTRODUCTION

The goal of this short note is to describe the usage scenarios for the evolution equation contra balance equations and draw attention to a potentially serious gap in the theory of mesoscopic continuum physics. In particular, it is possible to create configurations in which the high-dimensional mesoscopic domain is non-contiguous (non-connected), whereas the 3-dimensional domain is connected. This leads to "virtual boundaries", for which additional boundary conditions need to be formulated. The treatment of these conditions is an unanswered question.

## 2. MESOSCOPIC CONTINUUM PHYSICS

Mesoscopic continuum physics enlarges the space by use of independent degrees of freedom of the material under consideration. The space $\mathbf{x}$ generalizes to $\mathbf{x} \to (\mathbf{x}, \mathbf{n}) = \tilde{\mathbf{x}}$, where $\mathbf{n}$ is, e.g., the orientation (angles) of particles, the velocity is given by $\mathbf{v} \to (\mathbf{v}, \mathbf{u}) = (\tilde{\mathbf{v}}_{\mathbf{x}}, \tilde{\mathbf{v}}_{\mathbf{n}}) = \tilde{\mathbf{v}}$, and the mass density is generalized to $\rho(\mathbf{x}) \to \tilde{\rho}(\tilde{\mathbf{x}})$ (see, e.g., [1–3]).

Balance equations for the mesoscopic quantities are motivated analogously to the macroscopic case. Constitutive functions must be introduced into the mesoscopic balances, like in the macroscopic theory. Here the choice is only indirectly restricted by the Second Law of thermodynamics, which is not directly applicable to the mesoscopic description, but of course is valid for the averaged macroscopic quantities, because the macroscopic quantities are constructed from the mesoscopic ones by averaging [4,5]:

$$\rho(\mathbf{x},t) = \oint_{S^2} \tilde{\rho}(\tilde{\mathbf{x}},t)\, d^2n. \tag{1}$$

## 3. MESOSCOPIC BALANCES

The general procedure for obtaining local balances on the mesoscopic space follows the same principles as in the macroscopic theory. First global balance equations are motivated, then, using an extended version of the Reynolds transport theorem, the local balance equations are derived from the global ones.

Here one has to note that the balance of mesoscopic velocity has five independent component equations.

* Corresponding author, hh@cens.ioc.ee

Three of them refer to the linear momentum and the others to the spin (internal angular momentum) [3].

As an example the mesoscopic balance of mass and for comparison also the macroscopic balance of mass are presented.

**Mesoscopic mass:**

$$\frac{\partial}{\partial t}\tilde{\rho}(\tilde{\mathbf{x}},t)+\nabla_{\tilde{\mathbf{x}}}\cdot(\tilde{\mathbf{v}}(\tilde{\mathbf{x}},t)\tilde{\rho}(\tilde{\mathbf{x}},t)) = 0. \quad (2)$$

**Macroscopic mass:**

$$\frac{\partial}{\partial t}\rho(\mathbf{x},t)+\nabla_{x}\cdot(\mathbf{v}(\mathbf{x},t)\rho(\mathbf{x},t)) = 0. \quad (3)$$

Although similar at first glance, Eq. (2) and Eq. (3) differ by the domain on which the quantities are defined. The mesoscopic balance of mass also contains the orientation change velocity as components of $\tilde{\mathbf{v}}$. Both equations will be used in the next section (Sec. 4).

## 4. DERIVATION OF THE EVOLUTION EQUATION FOR THE DISTRIBUTION FUNCTION

In mesoscopic continuum physics it is common to introduce a distribution function (e.g. orientation distribution function for liquid crystals)

$$f(\tilde{\mathbf{x}},t) := \frac{\tilde{\rho}(\tilde{\mathbf{x}},t)}{\rho(\mathbf{x},t)} \quad (4)$$

and to derive an evolution equation for the distribution function. This can be done by using the macroscopic balance of mass and the mesoscopic balance of mass. The steps are as follows:

1. multiply the macroscopic balance of mass by $\frac{\tilde{\rho}}{\rho^2}$,
2. multiply the mesoscopic balance of mass by $\frac{\rho}{\rho^2}$,
3. subtract the new mesoscopic balance of mass from the new macroscopic balance of mass,
4. compare with $\frac{\partial f}{\partial t}+\nabla\cdot(\mathbf{v}f) = \sigma$ and look for missing/additional terms in the divergence part.

The resulting evolution equation is

$$\frac{\partial f}{\partial t}+\nabla_{\tilde{\mathbf{x}}}\cdot(\tilde{\mathbf{v}}f)-f\nabla_{\mathbf{x}}\cdot\mathbf{v}_{\mathbf{x}} = 0 \quad (5)$$

or, with the divergence split into spatial and rotational parts,

$$\frac{\partial f}{\partial t}+\nabla_{\mathbf{x}}\cdot(\mathbf{v}_{\mathbf{x}}f)+\nabla_{\mathbf{n}}\cdot(\mathbf{v}_{\mathbf{n}}f)-f\nabla_{\mathbf{x}}\cdot\mathbf{v}_{\mathbf{x}} = 0. \quad (6)$$

## 5. EVOLUTION EQUATION CONTRA BALANCE EQUATIONS: USAGE SCENARIOS

The evolution equation introduced above is, however, not independent of the mesoscopic balance of mass. Up to now it has not been discussed in literature under which circumstances it is preferable to use the evolution equation for the distribution function instead of the balance equation. An initial analysis has shown that at least three different scenarios are possible.

- Use of the distribution function, no use of the balance of mass.

  This is useful if the macroscopic density does not change; microcracks serve as an example for this case. Microcracks do not heal (disappear), they are not produced and do not flow with respect to the surrounding material.The information content of the *length distribution function* and the mesoscopic balance of mass are identical, because the only changes are within the mesoscopic domain.
- Use of the distribution function and use of the *macroscopic* balance of mass.

  The distribution function is normalized, therefore it describes only the percentage of particles/mass with a special property (orientation, length, ...) and not the absolute number. If the macroscopic density changes, some information is missing if only the evolution equation for the distribution function is used; this information is contained in the macroscopic balance of mass.
- Use of the *mesoscopic* balance of mass, no use of the distribution function.

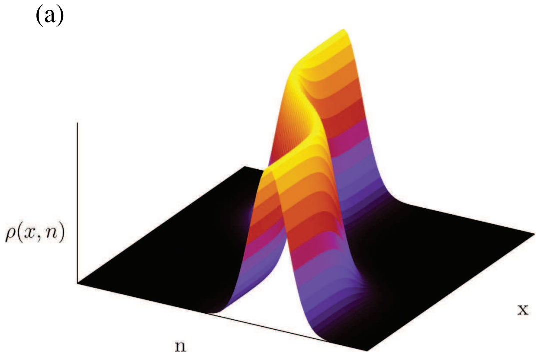
  The mesoscopic balance of mass contains the same information as the distribution function and the macroscopic balance of mass together. It is therefore an alternative description to the previous case.

In cases where the macroscopic density does not change it is preferable to use the evolution equation for the distribution function, because in this description the changes are more visible and calculations are easier. The other two choices are equivalent and have to be used when the macroscopic density changes as well. If an integrated point of view is preferred, the mesoscopic balance of mass will be used. If it is preferred to differentiate between macroscopic changes and "internal" changes that affect only the mesoscopic variables, the macroscopic balance of mass together with the evolution equation will be used.

## 6. OPEN QUESTION: VIRTUAL BOUNDARIES

Furthermore, we discovered that it is possible to create configurations in the mesoscopic space where the material seems to be non-contiguous (see Fig. 1b), despite the macroscopic material being contiguous. These, sort of "pathological" configurations have been noticed when formulating the constitutive equation for the mesoscopic stress tensor for calculations for twist-waves in liquid crystals [1]. After this discovery we thought about other fields, configurations, and phenomena that would create a similar "effect".

(a)




(b)

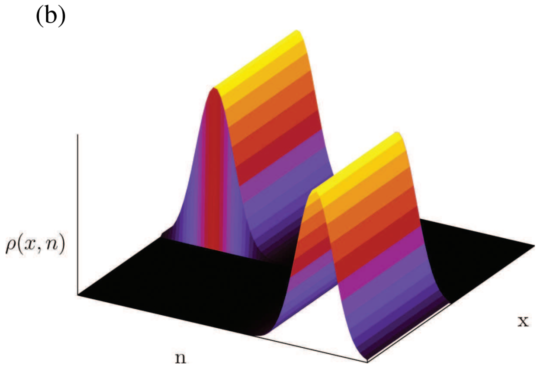



**Fig. 1.** Possible artificial splitting of the computational domain. Although in macroscopic description the domain (material) is connected, mesoscopic configurations are possible so that the domain is non-connected. (a) A connected mesoscopic domain containing a rapid change in material properties. (b) A non-connected mesoscopic domain containing a rapid change in material properties. Of course fluxes (e.g. heat flux) should pass from one part to the other, therefore specific boundary conditions have to be invented.

Examples for such fields are liquid crystals with different orientations in different areas, layered sandstone with different grain sizes for different layers, and Weiss' domains, with the direction of the magnetization as the mesoscopic variable. These three examples are described in more detail below.

**Liquid crystals:** In one part ($\mathbb{R}^3_-$) of the domain only orientations, say, between 25° and 40° and in the other part ($\mathbb{R}^3_+$) only orientations between 45° and 60° are present. The areas of the mesoscopic space with non-zero density would be $\mathbb{R}^3_- \times [25,40]$ for the first part and $\mathbb{R}^3_+ \times [45,60]$ for the second part. Or, joined as $\mathbb{R}^3 \times ([25,40] \cup [45,60])$, these parts represent two disjunct areas. In a macroscopic description the density is non-zero in $\mathbb{R}^3$ and the area is contiguous.

**Sandstone:** The grain diameter is used as the mesoscopic variable. In this case we assume a layer with grain size between 0.02 and 0.08 mm and the next layer with grain size between 0.06 and 0.12 mm. Figure 1a shows a mesoscopic material with a rapid change in the mesoscopic variable.

The step in the mesoscopic variable gives a vivid idea about why reflections of acoustic waves occur at layer interfaces, e.g. in geology. This idea is easy to grasp though not quite correct, because intuitively in Fig. 1b one would assume that total reflection will occur and nothing is transmitted to the second domain. In Fig. 1b the transmission of the wave *seems* only impossible due to the discontiguous domain, therefore appropriate (artificial) boundary conditions have to be introduced.

**Weiss' domains:** Near-discontinuities appear in the case of Weiss' domains, with the direction of the magnetization as the mesoscopic variable. Although the change in magnetization is continuous, the thickness of the Bloch wall is about 30 nm, which is below the resolution for simulations on a macroscopic length scale and can therefore be considered a discontinuity.

Another possibility is that particles with distinct properties exist in the same three-dimensional volume element, e.g. particles with orientations within 25–40° and particles with orientations between 45° and 60°, or the above-mentioned sand could be a mixture of grains with sizes between 0.02 and 0.08 mm and between 0.12 and 0.2 mm. This would lead to obvious schematic plots like Fig. 2 in terms of n.

For all the above cases the macroscopic material consists of one contiguous piece. In the mesoscopic description, however, the material becomes non-contiguous. These cases need not be static but may disappear or appear during the process or calculation. In these cases "virtual" boundaries appear and boundary conditions have to be introduced with care, because the fluxes can flow from one part to the other.

The discontinuity in the mesoscopic variable is more serious than just a discontinuity of a function (e.g. temperature or density) on the space. A macroscopic analogy of the discontinuity in a mesoscopic variable would be water-splashes (drops separating from the water body), or cracks.

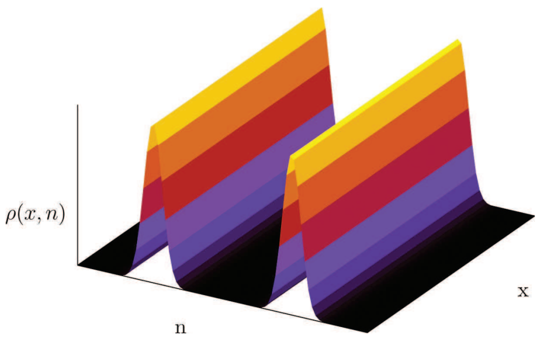



**Fig. 2.** Mesoscopic distribution of a mixture of two components with distinct properties (e.g. grain sizes).

The problem of virtual boundaries has not been discussed in literature up to now and needs further investigation. Potentially there is a serious gap in the theory.

Figures 1b and 2 clearly show that a non-local stress tensor is necessary, because the material in the two mesoscopically non-connected domains is macroscopically connected. One possibility is to postulate a stress tensor with the following dependence:

$$\tilde{\mathbf{t}}((\mathbf{x},\mathbf{n}),t) = \tilde{\mathbf{t}}\left(\left(\int_{\mathbf{x}-\delta\mathbf{x}}^{\mathbf{x}+\delta\mathbf{x}} \oint \alpha(|\eta-\mathbf{n}|,|\xi-\mathbf{x}|)\rho((\xi,\eta),t)\,d\eta\, d\xi\right),t\right),$$

because, e.g., for liquid crystals the particles close to the virtual boundary affect each other, even if they are in different domains.

## 7. CONCLUSIONS AND OUTLOOK

Different scenarios of the usage of the distribution function with its evolution equation together with different versions of the balance of mass were described. Although these usages may seem obvious, they have not been mentioned in the literature before.

(Virtually) disconnected mesoscopic domains were discussed. The problem that continuous three-dimensional domains may become discontinuous when using the mesoscopic space is not inherent to the strict high-dimensional formulation employed here, but just more visible. It also appears in the "traditional formulation" used by other authors (e.g. [2]).

Under certain circumstances, i.e., when the mesoscopic domain becomes non-connected, mesoscopic continuum physics requires a strongly non-local formulation of constitutive functions. A weakly non-local formulation containing gradients is not sufficient any more.

It is important to answer these open questions as continuum methods are desirable also at micro- and nanoscale, although the assumption of a continuum breaks down at atomistic scales, because they are often computationally more efficient and can lead to physically illuminating analytical solutions [6]. The authors currently investigate if numerical methods like the ones discussed in [6] are suitable for determining the virtual boundary conditions.

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# Selgitusi mesoskoopilise pideva keskkonna füüsika juurde: jaotusfunktsiooni evolutsioonivõrrand ja lahtised küsimused

Heiko Herrmann ja Jüri Engelbrecht

On selgitatud mesoskoopilise massijäävuse seaduse ja massi jaotusfunktsiooni seoseid. On näidatud jaotusfunktsiooni evolutsioonivõrrandi tuletamise võimalusi ja analüüsitud vastavaid stsenaariume. Uudse momendina selgub, et makroskoopilisest pidevusest hoolimata on mesoskoopilises skaalas võimalik pidevuse kadu. Taolised "virtuaalsed" piirid vajavad aga täiendavaid rajatingimusi. See tähendab, et mesoskoopiline pideva keskkonna teooria nõuab olekuvõrrandite tugevat mittelokaalsust, mis väärib süvendatud analüüsi koos füüsikaliste parameetrite määramisega.