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Reviewing the roots of continuum formulations in molecular systems. Part III: Stresses, couple stresses, heat fluxes — Source link

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Reviewing the roots of continuum formulations in molecular systems. Part III: Stresses, couple stresses, heat fluxes

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Abstract
This contribution is the third part in a series devoted to the fundamental link between discrete particle systems and continuum descriptions. The basis for such a link is the postulation of the primary continuum fields such as density and kinetic energy in terms of atomistic quantities using space and probability averaging.

In this part, solutions to the flux quantities (stress, couple stress, and heat flux), which arise in the balance laws of linear and angular momentum, and energy are discussed based on the Noll's lemma. We show especially that the expression for the stress is not unique. Integrals of all the fluxes over space are derived. It is shown that the integral of both the microscopic Noll–Murdoch and Hardy couple stresses (more precisely their potential part) equates to zero. Space integrals of the Hardy and the Noll–Murdoch Cauchy stress are equal and symmetric even though the local Noll–Murdoch Cauchy stress is not symmetric. Integral expression for the linear momentum flux and the explicit heat flux are compared to the virial pressure and the Green–Kubo expression for the heat flux, respectively.

It is proven that in the case when the Dirac delta distribution is used as kernel for spatial averaging, the Hardy and the Noll–Murdoch solution for all fluxes coincide.

The heat fluxes resulting from both the so-called explicit and implicit approaches are obtained and compared for the localized case. We demonstrate that the spatial averaging of the localized heat flux obtained from the implicit approach does not equate to the expression obtained using a general averaging kernel. In contrast this happens to be true for the linear momentum flux, i.e. the Cauchy stress.

Keywords
Molecular mechanics, continuum mechanics, statistical mechanics, balance equations, averaging

1. Introduction

This contribution is the third part in a series devoted to the fundamental link between discrete and continuum descriptions. The foundation of this approach was laid down by works of Irving and Kirkwood [1] and Noll [2]. In an attempt to clarify several open questions (e.g. the non-uniqueness of stress measure, central force decomposition and others) as well as to unify two different approaches of deriving the balance of energy from the discrete system, we re-obtained the continuum balance laws of mass, linear and angular momentum, and energy in parts I and II [3, 4] based on particle mechanics and statistical physics. Thereby the resulting fluxes (the stress, the couple stress and the heat flux) are given implicitly in terms of their divergences.

The roots of the atomistic-to-continuum correspondence could be traced back to the beginning of modern thermodynamics. The most acknowledged contribution was that of Boltzmann leading to establish statistical

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thermodynamics and in the attempt to provide a strict derivation of Clausius's second principle [5]. Through the collision integral of Boltzmann it is possible to derive the Navier–Stokes equations of fluids [6]. Considering the harmonic potential and the long wavelength approximation the macroscopic elasticity tensor corresponding to the Wigner–Seitz cell of periodic crystal could be obtained [7]. Relationships between atomistic and continuum worlds have been also considered in the context of thermal properties of matter [8–11] as well as dissipation effects in solids [12]. Note that some processes, such as electron–phonon interaction, can not be explained within the molecular mechanics formulation and require the quantum-mechanical approach.

The link between the atomistic and continuum worlds is of technological interest to new, rapidly growing, fields of engineering such as porous materials, nano-composites and microstructured continuous media [13–17].

In the present part of the series we obtain the corresponding fluxes from their divergences based on Noll's lemma. There are at least two different possible solutions for each flux in terms of atomistic quantities (such as inter-particle forces, position vectors, masses, etc.). The two solutions will be denoted in the sequel as either of the Hardy [18] or the Noll–Murdoch [2, 19] type.

By applying Noll's lemma to obtain the linear momentum flux we show that the Cauchy stress obtained by space-probability averaging is not unique. That is similar to the case when space-temporal averaging is used to derive the corresponding fluxes [18, 19].

Since molecular dynamics (MD) simulations are often used to describe the macroscopic response of a representative volume element (RVE) [20, 21], integrals of the flux quantities over space are desired and thus are developed in this contribution. As a result we show that macroscopically both the Hardy and the Noll–Murdoch stresses coincide in spite of the Noll–Murdoch stress being non-symmetric microscopically, whereas the Hardy stress is always symmetric. A similar comparison is made of the other fluxes (the microscopic couple stress and the heat flux) appearing in the balance laws. It is shown that macroscopically the non-diffusive part of the Hardy and Noll–Murdoch couple stresses equates to zero.

In order to make more parallels between the Hardy and the Noll–Murdoch-type solutions, we look at the case when the Dirac delta distribution is used as a spatial averaging kernel. It then follows that the resulting fluxes are equal not only macroscopically but also microscopically.

The balance of energy is generally derived either in the explicit or the implicit form [4]. Localized expressions for heat fluxes obtained for the two approaches are compared.

The paper is organized as follows. Equations that define all the fluxes considered here are briefly reviewed in Section 2. In Section 3, Noll's lemma is given, localized generator functions are compared and some important properties of the averaging kernel are discussed. In Sections 4 and 5, the fluxes occurring in the balance laws of linear and angular momentum as well as their integral are obtained. Sections 6 and 7 are devoted to the fluxes obtained from the implicit and explicit approaches to the balance of energy, respectively. At last, the discussion and conclusions are presented in Section 8.

2. Fluxes in space-probability averaging

In this section we briefly recall some definitions and results obtained in the first two parts of this series [3, 4].

Generally, the δ-distribution of any extensive (additive) property g^α is defined as

$$g_\delta(\mathsf{z}, \boldsymbol{\xi}) = \sum_\alpha g_\delta^\alpha(\mathsf{z}, \boldsymbol{\xi}) := \sum_\alpha g^\alpha(\mathsf{z})\delta(\mathsf{x}^\alpha - \boldsymbol{\xi}). \tag{1}$$

Here z, $\boldsymbol{\xi}$, x^α denote the phase space coordinates, the microscopic spatial variable and the current position of a particle α, respectively.

By postulating the continuum density $\varrho(\boldsymbol{x}, \tau)$, the continuum velocity $\boldsymbol{v}$ is then obtained from the balance of mass as

$$\boldsymbol{v}(\boldsymbol{x}, \tau) := \frac{\boldsymbol{p}(\boldsymbol{x}, \tau)}{\varrho(\boldsymbol{x}, \tau)} = \frac{\langle\langle \mathsf{p}_\delta(\mathsf{z}, \boldsymbol{\xi})\rangle_{\mathcal{P}}\rangle_{\mathcal{S}}}{\langle\langle \mathsf{m}_\delta(\mathsf{z}, \boldsymbol{\xi})\rangle_{\mathcal{P}}\rangle_{\mathcal{S}}} = \frac{\sum_\alpha \int_{\mathcal{P}} \mathsf{p}^\alpha w(\mathsf{x}^\alpha - \boldsymbol{x})\mathsf{W}(\mathsf{z}, \tau)d\mathsf{z}}{\sum_\alpha \int_{\mathcal{P}} \mathsf{m}^\alpha w(\mathsf{x}^\alpha - \boldsymbol{x})\mathsf{W}(\mathsf{z}, \tau)d\mathsf{z}}, \tag{2}$$

where p^α and m^α are the linear momentum and mass of the particle α respectively, and $\boldsymbol{x}$ is the macroscopic spatial variable. $W(\mathsf{z}, \tau)$ is the probability density function and $w(\boldsymbol{\xi} - \boldsymbol{x})$ with $\int_{\mathcal{S}} \delta(\mathsf{x}^\alpha - \boldsymbol{\xi})w(\boldsymbol{\xi} - \boldsymbol{x}) = w(\mathsf{x}^\alpha - \boldsymbol{x})$ is the spatial averaging kernel, $\boldsymbol{p}(\boldsymbol{x}, \tau)$ is the continuum linear momentum.

For each particle α the fluctuation of the particle velocity field is then defined as

$$\widetilde{\mathsf{v}}^\alpha(\boldsymbol{x}, \tau) := \mathsf{v}^\alpha - \boldsymbol{v}(\boldsymbol{x}, \tau). \tag{3}$$

Furthermore the microscopic diffusive momentum flux $\widetilde{\mathbf{s}}^{\alpha}$ is introduced as

$$\widetilde{\mathbf{s}}^{\alpha} = \frac{1}{2}\mathbf{p}^{\alpha} \otimes \widetilde{\mathbf{v}}^{\alpha}(\boldsymbol{x}, \tau), \tag{4}$$

whereby its trace is denoted by $\widetilde{s}^{\alpha} = \mathrm{tr}(\widetilde{\mathbf{s}}^{\alpha})$.

We then define the macroscopic diffusive momentum flux $\widetilde{\boldsymbol{s}}$ via

$$\widetilde{\boldsymbol{s}} = \langle\langle \widetilde{\mathbf{s}}_{\delta}(\mathbf{z}, \boldsymbol{\xi}; \boldsymbol{x}, \tau)\rangle_{\mathcal{P}}\rangle_{\mathcal{S}}. \tag{5}$$

The distance between each particle position and the considered continuum point is called the microscopic distance

$$\bar{\mathbf{r}}^{\alpha}(\boldsymbol{x}) = \mathbf{x}^{\alpha} - \boldsymbol{x}. \tag{6}$$

Next, the particle microscopic angular momentum flux $\bar{\mathbf{n}}^{\alpha}$ and the particle diffusive microscopic angular momentum flux $\widetilde{\mathbf{m}}^{\alpha}$ are defined as

$$\bar{\mathbf{n}}^{\alpha} = \frac{1}{2}\bar{\mathbf{l}}^{\alpha} \otimes \mathbf{v}^{\alpha} \quad \text{and} \quad \widetilde{\mathbf{m}}^{\alpha} = \frac{1}{2}\bar{\mathbf{l}}^{\alpha} \otimes \widetilde{\mathbf{v}}^{\alpha}(\boldsymbol{x}, \tau), \tag{7}$$

where $\bar{\mathbf{l}}^{\alpha} = \bar{\mathbf{r}}^{\alpha}(\boldsymbol{x}) \times \mathbf{p}^{\alpha}(\tau)$ denotes particle microscopic angular momentum w.r.t. the continuum coordinate $\boldsymbol{x}$.

The corresponding continuum microscopic angular momentum flux $\bar{\boldsymbol{\nu}}$ and continuum diffusive microscopic angular momentum flux $\widetilde{\boldsymbol{m}}$ read accordingly:

$$\bar{\boldsymbol{\nu}} = \frac{1}{2}\bar{\boldsymbol{l}}(\boldsymbol{x}, \tau) \otimes \boldsymbol{v}(\boldsymbol{x}, \tau) \quad \text{and} \quad \widetilde{\boldsymbol{m}} = \langle\langle \widetilde{\mathbf{m}}_{\delta}(\mathbf{z}, \boldsymbol{\xi}; \boldsymbol{x}, \tau)\rangle_{\mathcal{P}}\rangle_{\mathcal{S}}, \tag{8}$$

where $\bar{\boldsymbol{l}} = \langle\langle \mathbf{l}_{\delta}(\mathbf{z}, \boldsymbol{\xi}; \boldsymbol{x}, \tau)\rangle_{\mathcal{P}}\rangle_{\mathcal{S}}$ is the continuum angular momentum density w.r.t. $\boldsymbol{x}$.

The following flux quantities appear in the balance of energy, linear and angular momentum:

- Cauchy stress $\boldsymbol{s}$

$$\boldsymbol{s} = \widehat{\boldsymbol{s}} - 2\widetilde{\boldsymbol{s}}, \tag{9}$$

where $\widehat{\boldsymbol{s}}$ is to be obtained from

$$\mathrm{div}\,\widehat{\boldsymbol{s}} := \mathrm{div}(\boldsymbol{s} + 2\widetilde{\boldsymbol{s}}) = \sum_{\alpha\beta} \langle \mathbf{f}^{\alpha\beta}(\tau) w(\mathbf{x}^{\alpha} - \boldsymbol{x})\rangle_{\mathcal{P}}. \tag{10}$$

- Couple stresses[1] $\overline{\boldsymbol{m}}$

$$\overline{\boldsymbol{m}} = \widehat{\boldsymbol{m}} - 2\widetilde{\boldsymbol{m}}. \tag{11}$$

The unknown second order tensor $\widehat{\boldsymbol{m}}$ is given by

$$\mathrm{div}\,\widehat{\boldsymbol{m}} := \mathrm{div}(\overline{\boldsymbol{m}} + 2\widetilde{\boldsymbol{m}}) = \sum_{\alpha\beta} \langle \bar{\mathbf{r}}^{\alpha}(\boldsymbol{x}) \times \mathbf{f}^{\alpha\beta}(\tau) w(\boldsymbol{x}^{\alpha} - \boldsymbol{x})\rangle_{\mathcal{P}}. \tag{12}$$

- Diffusive energy flux

$$\widetilde{\boldsymbol{q}} := -\frac{1}{2}\sum_{\alpha} \left\langle \widetilde{\mathbf{s}}^{\alpha}(\tau) \widetilde{\mathbf{v}}^{\alpha}(\boldsymbol{x}, \tau) w(\boldsymbol{x}^{\alpha} - \boldsymbol{x})\right\rangle_{\mathcal{P}}. \tag{13}$$

- Heat flux for the implicit approach

$$\boldsymbol{q}^{\mathrm{i}} = \widehat{\boldsymbol{q}}^{\mathrm{i}} - 2\widetilde{\boldsymbol{q}}, \tag{14}$$

where $\widehat{\boldsymbol{q}}^{\mathrm{i}}$ and q are defined by

$$\mathrm{div}\widehat{\boldsymbol{q}}^{\mathrm{i}} + q(\boldsymbol{x}, \tau) := -\langle \sum_{\alpha} \widetilde{\mathbf{v}}^{\alpha} \cdot \sum_{\beta} \mathbf{f}^{\alpha\beta} w(\mathbf{x}^{\alpha} - \boldsymbol{x})\rangle_{\mathcal{P}} \tag{15}$$

Here q denotes the local self-heating density [22]. In contrast to previous definitions of fluxes (e.g. equations (10) and (12)) the RHS of equation (15), as it will be shown later, can not be expressed only as a divergence of $\widehat{\boldsymbol{q}}^{\mathrm{i}}$; therefore, a scalar term q has to be introduced. Note that in this approach the internal potential energy is introduced implicitly (thus the name for this formulation) via

$$v_{,\tau} + \operatorname{div}(v\boldsymbol{v}) := \operatorname{grad}\boldsymbol{v}(\boldsymbol{x},\tau) : \widehat{\boldsymbol{s}}(\boldsymbol{x},\tau) + q(\boldsymbol{x},\tau). \tag{16}$$

In contrast to the explicit approach (see below), the implicit approach avoids the need to localize the potential energy to a single particle. That would then allow introducing the density of potential energy via equation (1). Since potential energy is attributed to a group of particles (two and more), this localization is not unique. Moreover it becomes cumbersome in case of three- and more point potentials. Thus in the sequel we consider the explicit approach only for two-point potentials. An advantage of this approach is that the energy density is readily available, as opposed to the necessity to integrate equation (16) in case of the implicit approach. For more discussion we refer to Part II [4].

- Heat flux for the explicit approach (applied to two-point interactions)

$$\boldsymbol{q}^e = \widehat{\boldsymbol{q}}^e - 2\widetilde{\boldsymbol{q}}. \tag{17}$$

The unknown part of the flux $\widehat{\boldsymbol{q}}^e$ is to be determined from

$$\begin{aligned} -\Big\langle \sum_{\alpha\beta} \mathbf{f}^{\alpha\beta}(\tau)\cdot \frac{[\mathbf{v}^\alpha + \mathbf{v}^\beta]}{2} w(\mathbf{x}^\alpha - \boldsymbol{x})\Big\rangle_{\mathcal{P}} &= \operatorname{div}(\widehat{\boldsymbol{q}}^e - \boldsymbol{q}_T - \boldsymbol{v}\cdot\widehat{\boldsymbol{s}}) \\ &=: \operatorname{div}\widehat{\boldsymbol{q}}^e + q^* =: -\operatorname{div}\widehat{\boldsymbol{q}}^*, \end{aligned} \tag{18}$$

where the transport energy flux $\boldsymbol{q}_T$ is expressed in terms of the localized particle potential energy v^α as

$$\boldsymbol{q}_T := \Big\langle \sum_{\alpha} \mathsf{v}^\alpha(\tau)\widetilde{\mathbf{v}}^\alpha(\boldsymbol{x},\tau) w(\mathbf{x}^\alpha - \boldsymbol{x})\Big\rangle_{\mathcal{P}}. \tag{19}$$

For the two point interaction case, the potential energy attributed to each particle v^α can be introduced as

$$\mathsf{v}^\alpha = \frac{1}{2!}\sum_{\beta} \mathsf{v}^{\alpha\beta}(\mathbf{x}^{\alpha\beta}), \tag{20}$$

where $\mathsf{v}^{\alpha\beta}$ is a potential energy of interaction between particles α and β. In other words, the potential energy is equally distributed among interacting particles.

In equation (19) we also introduced $q^* = -\operatorname{div}(\boldsymbol{q}_T + \boldsymbol{v}\cdot\widehat{\boldsymbol{s}})$ to make it look consistent with the implicit approach (equation (15)). Note, that the interpretation of q^* and q are different. In the implicit approach q enters the definition of potential energy (equation (16)), whereas in the explicit approach q^* can be represented as a divergence of a vector quantity which affects the non-diffusive part of a heat flux, i.e. $\widehat{\boldsymbol{q}}^e = \boldsymbol{q}_T + \boldsymbol{v}\cdot\widehat{\boldsymbol{s}} - \widehat{\boldsymbol{q}}^*$.

3. Noll's lemma

In this section we briefly recall the lemma, introduced by Noll [2].

Let $\boldsymbol{g}(\boldsymbol{x},\boldsymbol{y})$ be a C^1 tensor-valued function of vector variables $\boldsymbol{x},\boldsymbol{y}$ such that

- $\boldsymbol{g}(\boldsymbol{x},\boldsymbol{y})$ is defined $\forall \boldsymbol{x},\boldsymbol{y}$ and continuously differentiable.
- $\exists\,\delta > 0 : \boldsymbol{g}(\boldsymbol{x},\boldsymbol{y})|\boldsymbol{x}|^{3+\delta}|\boldsymbol{y}|^{3+\delta}$ and its gradients are bounded.
- $\boldsymbol{g}(\boldsymbol{x},\boldsymbol{y}) = -\boldsymbol{g}(\boldsymbol{y},\boldsymbol{x})$ is antisymmetric.

For such a case, the following holds[2]

$$\boxed{\int_{\mathcal{S}} \boldsymbol{g}(\boldsymbol{x},\boldsymbol{y})d\boldsymbol{y} = -\frac{1}{2}\operatorname{div}\int_{\mathcal{S}}\int_0^1 \boldsymbol{g}\big(\boldsymbol{x}+a\mathbf{z}, \boldsymbol{x}-[1-a]\mathbf{z}\big)da\otimes\mathbf{z}d\mathbf{z}.} \tag{21}$$

In other words, it provides one possible solution

$$\boldsymbol{G}(\boldsymbol{x}) = -\frac{1}{2}\int_{\mathcal{S}}\int_0^1 \boldsymbol{g}\big(\boldsymbol{x} + a\mathbf{z}, \boldsymbol{x} - [1-a]\mathbf{z}\big)da \otimes \mathbf{z}d\mathbf{z} \tag{22}$$

to

$$\int_{\mathcal{S}} \boldsymbol{g}(\boldsymbol{x},\boldsymbol{y})d\boldsymbol{y} = \operatorname{div}\boldsymbol{G}(\boldsymbol{x}). \tag{23}$$

The function $\boldsymbol{g}$ is called a generator. As we will see later, different generator functions give different flux candidates. At least two different types of solutions are possible:

- Hardy-type [18], based on the δ-distribution. In such a case, the generator function is given by

$$\boldsymbol{g}_H(\boldsymbol{x},\boldsymbol{y}) = \sum_{\alpha\beta}\big\langle \mathbf{A}^{\alpha\beta} w(\mathbf{x}^\alpha - \boldsymbol{x})\delta([\mathbf{x}^\beta - \boldsymbol{y}] - [\mathbf{x}^\alpha - \boldsymbol{x}])\big\rangle_{\mathcal{P}}, \tag{24}$$

  where $\mathbf{A}^{\alpha\beta}$ is a tensor of an arbitrary order expressed in terms of the atomistic quantities related to the particles α and β. (However here we only need to consider scalar and vector-valued $\mathbf{A}^{\alpha\beta}$.)
- Noll–Murdoch-type [2, 23], based on a general averaging kernel. The generator function has the following format

$$\boldsymbol{g}_N(\boldsymbol{x},\boldsymbol{y}) = \sum_{\alpha\beta}\big\langle \mathbf{A}^{\alpha\beta} w(\mathbf{x}^\alpha - \boldsymbol{x}) w(\mathbf{x}^\beta - \boldsymbol{y})\big\rangle_{\mathcal{P}}. \tag{25}$$

Recall the normalization condition for the spatial averaging kernel:

$$\int_{\mathcal{S}} w(\boldsymbol{y})d\boldsymbol{y} = 1. \tag{26}$$

Thus it is clear that

$$\int_{\mathcal{S}} \boldsymbol{g}_N(\boldsymbol{x},\boldsymbol{y})d\boldsymbol{y} = \int_{\mathcal{S}} \boldsymbol{g}_H(\boldsymbol{x},\boldsymbol{y})d\boldsymbol{y} = \sum_{\alpha\beta}\big\langle \mathbf{A}^{\alpha\beta} w(\mathbf{x}^\alpha - \boldsymbol{x})\big\rangle_{\mathcal{P}}. \tag{27}$$

These two options coexist and are valid for all the unknown fluxes in the balance equations. Apart from these two options, for each flux quantity we consider the case, when the δ-distribution is used for space-probability averaging. Such solutions are called "localized" in our terms. It is easy to see that the localized versions of the two generator functions are actually equal, i.e.

$$\boldsymbol{g}_{H\delta}(\boldsymbol{x},\boldsymbol{y}) = \sum_{\alpha\beta}\big\langle \mathbf{A}^{\alpha\beta}\delta(\mathbf{x}^\alpha - \boldsymbol{x})\delta([\mathbf{x}^\beta - \boldsymbol{y}] - [\mathbf{x}^\alpha - \boldsymbol{x}])\big\rangle_{\mathcal{P}} = \sum_{\alpha\beta}\big\langle \mathbf{A}^{\alpha\beta}\delta(\mathbf{x}^\alpha - \boldsymbol{x})\delta([\mathbf{x}^\beta - \boldsymbol{y}])\big\rangle_{\mathcal{P}}, \tag{28}$$

$$\boldsymbol{g}_{N\delta}(\boldsymbol{x},\boldsymbol{y}) = \sum_{\alpha\beta}\big\langle \mathbf{A}^{\alpha\beta}\delta(\mathbf{x}^\alpha - \boldsymbol{x})\delta(\mathbf{x}^\beta - \boldsymbol{y})\big\rangle_{\mathcal{P}}. \tag{29}$$

Therefore flux quantities obtained from the Hardy and Noll–Murdoch localized generator functions are always equal. Therefore, we will not consider the localized case separately for each flux quantity, but only note that the corresponding expression can be easily obtained by substituting the general averaging kernel w in the Hardy-type solutions by the delta distribution. Alternatively the general averaging kernel w in the Noll–Murdoch-type solutions could be replaced by the delta distribution δ. That does, of course, lead to exactly the same results.

Lastly, let us say some words about the averaging kernel w. We consider w to be a function of the invariant of its argument, i.e.

$$w(\boldsymbol{y}) = w(|\boldsymbol{y}|). \tag{30}$$

Note that this is actually a requirement for the resulting fields to be independent of change of observer. Otherwise an artificial anisotropy of the resulting fields is introduced.

It is obvious that w is an even function

$$w(\boldsymbol{y}) = w(-\boldsymbol{y}), \tag{31}$$

and therefore the first moment of the weighting function equals zero

$$\int_{\mathcal{S}} w(\boldsymbol{y})\boldsymbol{y}d\boldsymbol{y} = \boldsymbol{0}. \tag{32}$$

This holds since the product of an even function and an odd function is an odd function, and the integral of an odd function over space is zero if it is evaluated by limits that are symmetric w.r.t. the origin.

Let us quickly prove the above for a one-dimensional case for an odd function $f(y)$:

$$\int_{-a}^{0} f(y)dy \Rightarrow \left[\begin{array}{c} x := -y \\ dx = -dy \end{array} \right] \Rightarrow -\int_{a}^{0} f(-x)dx = \int_{0}^{a} f(-x)dx = -\int_{0}^{a} f(x)dx \tag{33}$$

and therefore

$$\int_{-a}^{a} f(y)dy = 0. \tag{34}$$

Note that the second moment $\int_{\mathcal{S}} w(\boldsymbol{y})\boldsymbol{y} \otimes \boldsymbol{y}d\boldsymbol{y}$ (an integral of an even function) is not necessarily zero.[3]

4. Stresses

We start with the solution for the part of the Cauchy stress due to the interaction forces

$$\operatorname{div} \widehat{\boldsymbol{s}}(\boldsymbol{x}, \tau) = \sum_{\alpha\beta} \left\langle \mathbf{f}^{\alpha\beta}(\tau) w(\mathbf{x}^{\alpha} - \boldsymbol{x}) \right\rangle_{\mathcal{P}} \doteq \int_{\mathcal{S}} \boldsymbol{g}^{s}(\boldsymbol{x}, \boldsymbol{y}, \tau)d\boldsymbol{y}. \tag{35}$$

The total Cauchy stress is given by equation (9). Different choices for the stress generator $\boldsymbol{g}^{s}$, which satisfy equation (35), are possible.

4.1. Hardy-type stress generator

The Hardy-type generator function reads

$$\boldsymbol{g}_{H}^{s}(\boldsymbol{x},\boldsymbol{y},\tau) = \sum_{\alpha\beta} \left\langle \mathbf{f}^{\alpha\beta}(\tau) w(\mathbf{x}^{\alpha} - \boldsymbol{x})\delta([\mathbf{x}^{\beta} - \boldsymbol{y}] - [\mathbf{x}^{\alpha} - \boldsymbol{x}]) \right\rangle_{\mathcal{P}} = -\boldsymbol{g}_{H}^{s}(\boldsymbol{y},\boldsymbol{x},\tau) \tag{36}$$

Note that on the evaluation of $\boldsymbol{g}\big(\boldsymbol{x} + a\boldsymbol{z}, \boldsymbol{x} - [1 - a]\boldsymbol{z}\big)$ in equation (22), the argument of the δ-distribution simplifies to $\boldsymbol{z} - \mathbf{x}^{\alpha\beta}$, giving the resulting expression for the Hardy-type stress as

$$\widehat{\boldsymbol{s}}_{H}(\boldsymbol{x}, \tau) = -\frac{1}{2} \sum_{\alpha\beta} \left\langle \mathbf{f}^{\alpha\beta}(\tau) \otimes \widehat{\mathbf{x}}_{H}^{\alpha\beta}(\boldsymbol{x}, \mathbf{x}^{\alpha}, \mathbf{x}^{\beta}) \right\rangle_{\mathcal{P}}, \tag{37}$$

$$\widehat{\mathbf{x}}_{H}^{\alpha\beta}(\boldsymbol{x}, \mathbf{x}^{\alpha}, \mathbf{x}^{\beta}) = \widehat{w}_{H}^{\alpha\beta}\mathbf{x}^{\alpha\beta}, \tag{38}$$

$$\widehat{w}_{H}^{\alpha\beta}(\boldsymbol{x}, \mathbf{x}^{\alpha}, \mathbf{x}^{\beta}) = \int_{0}^{1} w\big(\mathbf{x}^{\alpha} - \boldsymbol{x} - a\mathbf{x}^{\alpha\beta}\big)da. \tag{39}$$

Since $\mathbf{f}^{\alpha\beta} \times \mathbf{x}^{\alpha\beta} = 0$ for any interaction potential in the system of constant point-mass particles [3], we conclude that $\widehat{\boldsymbol{s}}$ and thus $\boldsymbol{s}$ are symmetric.

Using equation (31) and equation (26), we can show that

$$\begin{aligned}
\int_{\mathcal{S}} \widehat{\mathbf{x}}_{H}^{\alpha\beta}(\boldsymbol{x}, \mathbf{x}^{\alpha}, \mathbf{x}^{\beta})d\boldsymbol{x} &= \mathbf{x}^{\alpha\beta} \int_{0}^{1} \left[\int_{\mathcal{S}} w\big(\mathbf{x}^{\alpha} - \boldsymbol{x} - a\mathbf{x}^{\alpha\beta}\big)d\boldsymbol{x} \right] da \\
&\Rightarrow \left[\begin{array}{c} \mathbf{x}^{\alpha} - \boldsymbol{x} - a\mathbf{x}^{\alpha\beta} =: -\boldsymbol{y} \\ \boldsymbol{x} = \mathbf{x}^{\alpha} + \boldsymbol{y} - a\mathbf{x}^{\alpha\beta} \\ d\boldsymbol{x} = d\boldsymbol{y} \end{array} \right] \Rightarrow \mathbf{x}^{\alpha\beta} \int_{0}^{1} \left[\int_{\mathcal{S}} w\big(-\boldsymbol{y}\big)d\boldsymbol{y} \right] da \\
&= \mathbf{x}^{\alpha\beta} \int_{0}^{1} da = \mathbf{x}^{\alpha\beta}.
\end{aligned} \tag{40}$$

Thus the space integral of the Cauchy stress, i.e. the macroscopic (averaged) stress, results in

$$\int_{\mathcal{S}} \widehat{\boldsymbol{s}}_H(\boldsymbol{x},\tau)d\boldsymbol{x} = -\frac{1}{2}\sum_{\alpha\beta}\left\langle \mathbf{f}^{\alpha\beta}(\tau)\otimes \mathbf{x}^{\alpha\beta}\right\rangle_{\mathcal{P}}. \tag{41}$$

Note that the resulting expression does not depend on the choice of w, as expected.

4.2. Noll–Murdoch-type stress generator

The Noll–Murdoch-type generator function for stresses reads

$$\boldsymbol{g}_N^s(\boldsymbol{x},\boldsymbol{y},\tau) = \sum_{\alpha\beta}\left\langle \mathbf{f}^{\alpha\beta}(\tau)w(\mathbf{x}^\alpha - \boldsymbol{x})w(\mathbf{x}^\beta - \boldsymbol{y})\right\rangle_{\mathcal{P}} = -\boldsymbol{g}_N^s(\boldsymbol{y},\boldsymbol{x},\tau). \tag{42}$$

Its substitution to equation (22) gives the Noll–Murdoch-type stress candidate

$$\widehat{\boldsymbol{s}}_N(\boldsymbol{x},\tau) = -\frac{1}{2}\sum_{\alpha\beta}\left\langle \mathbf{f}^{\alpha\beta}(\tau)\otimes \widehat{\mathbf{x}}_N^{\alpha\beta}(\boldsymbol{x},\mathbf{x}^\alpha,\mathbf{x}^\beta)\right\rangle_{\mathcal{P}}, \tag{43}$$

$$\widehat{\mathbf{x}}_N^{\alpha\beta}(\boldsymbol{x},\mathbf{x}^\alpha,\mathbf{x}^\beta) = \int_{\mathcal{S}} \widehat{w}_N^{\alpha\beta}\boldsymbol{z}d\boldsymbol{z}, \tag{44}$$

$$\widehat{w}_N^{\alpha\beta}(\boldsymbol{x},\mathbf{x}^\alpha,\mathbf{x}^\beta,\boldsymbol{z}) = \int_0^1 w\big(\mathbf{x}^\alpha - \boldsymbol{x} - a\boldsymbol{z}\big)w\big(\mathbf{x}^\beta - \boldsymbol{x} + [1-a]\boldsymbol{z}\big)da. \tag{45}$$

Neither $\widehat{\boldsymbol{s}}_N(\boldsymbol{x},\tau)$ nor $\boldsymbol{s}_N(\boldsymbol{x},\tau)$ are symmetric in such a case.

Using equations (31), (26) and (32), we can prove the following:

$$\begin{aligned}
\int_{\mathcal{S}} \widehat{\mathbf{x}}_N^{\alpha\beta}d\boldsymbol{x} &= \int_0^1\int_{\mathcal{S}}\left[\int_{\mathcal{S}} w\big(\mathbf{x}^\alpha - \boldsymbol{x} - a\boldsymbol{z}\big)w\big(\mathbf{x}^\beta - \boldsymbol{x} + [1-a]\boldsymbol{z}\big)d\boldsymbol{x}\right]\boldsymbol{z}d\boldsymbol{z}da \\
&\Rightarrow \begin{bmatrix} \mathbf{x}^\alpha - \boldsymbol{x} - a\boldsymbol{z} =: -\boldsymbol{y} \\ \boldsymbol{x} = \mathbf{x}^\alpha - a\boldsymbol{z} + \boldsymbol{y} \\ d\boldsymbol{x} = d\boldsymbol{y} \end{bmatrix} \Rightarrow \int_0^1\int_{\mathcal{S}} w(-\boldsymbol{y})\left[\int_{\mathcal{S}} w\big(\boldsymbol{z} - \boldsymbol{y} - \mathbf{x}^{\alpha\beta}\big)\boldsymbol{z}d\boldsymbol{z}\right]d\boldsymbol{y}da \\
&\Rightarrow \begin{bmatrix} -\boldsymbol{y} + \boldsymbol{z} - \mathbf{x}^{\alpha\beta} =: \boldsymbol{y}' \\ \boldsymbol{z} = \boldsymbol{y}' + \boldsymbol{y} + \mathbf{x}^{\alpha\beta} \\ d\boldsymbol{z} = d\boldsymbol{y}' \end{bmatrix} \Rightarrow \int_0^1\int_{\mathcal{S}} w(-\boldsymbol{y})\int_{\mathcal{S}} w\big(\boldsymbol{y}'\big)[\boldsymbol{y}' + \boldsymbol{y} + \mathbf{x}^{\alpha\beta}]d\boldsymbol{y}'\,d\boldsymbol{y}da \\
&= \int_0^1\int_{\mathcal{S}} w(-\boldsymbol{y})[\boldsymbol{y} + \mathbf{x}^{\alpha\beta}]d\boldsymbol{y}da = \int_0^1 \mathbf{x}^{\alpha\beta}da \\
&= \mathbf{x}^{\alpha\beta}.
\end{aligned} \tag{46}$$

It then follows that

$$\int_{\mathcal{S}} \widehat{\boldsymbol{s}}_N(\boldsymbol{x},\tau)d\boldsymbol{x} = -\frac{1}{2}\sum_{\alpha\beta}\left\langle \mathbf{f}^{\alpha\beta}(\tau)\otimes \mathbf{x}^{\alpha\beta}\right\rangle_{\mathcal{P}} \tag{47}$$

which is equal to equation (41). Therefore, the space integrals of the Hardy and Noll–Murdoch stresses are equal and symmetric. Note that this result holds despite the microscopic Noll–Murdoch-type Cauchy stress being not symmetric.

5. Couple stresses

We are looking for the solutions of the unknown part of the microscopic angular momentum flux due to the interaction forces in the following form:

$$\operatorname{div}\widehat{\boldsymbol{m}}(\boldsymbol{x},\tau) = \sum_{\alpha\beta}\left\langle \overline{\mathbf{r}}^\alpha(\boldsymbol{x})\times \mathbf{f}^{\alpha\beta}(\tau)w(\mathbf{x}^\alpha - \boldsymbol{x})\right\rangle_{\mathcal{P}} \doteq \int_{\mathcal{S}} \boldsymbol{g}^m(\boldsymbol{x},\boldsymbol{y},\tau)d\boldsymbol{y}. \tag{48}$$

The total couple stress is given by equation (11). Different choices for the stress generator $\widehat{\boldsymbol{m}}$, which satisfy equation (48), are possible.

5.1. Hardy-type couple stress generator

The Hardy-type generator function reads

$$\boldsymbol{g}_H^m(\boldsymbol{x},\boldsymbol{y},\tau) = \frac{1}{2}\sum_{\alpha\beta}\big\langle[\bar{\mathbf{r}}^\alpha(\boldsymbol{x}) + \bar{\mathbf{r}}^\beta(\boldsymbol{y})] \times \mathbf{f}^{\alpha\beta}(\tau)w(\mathbf{x}^\alpha - \boldsymbol{x})\delta([\mathbf{x}^\alpha - \boldsymbol{x}] - [\mathbf{x}^\beta - \boldsymbol{y}])\big\rangle_{\mathcal{P}}. \tag{49}$$

Note that the following holds

$$\frac{1}{2}[\bar{\mathbf{r}}^\alpha(\boldsymbol{x}) + \bar{\mathbf{r}}^\beta(\boldsymbol{y})]\delta(\bar{\mathbf{r}}^\alpha(\boldsymbol{x}) - \bar{\mathbf{r}}^\beta(\boldsymbol{y})) = \bar{\mathbf{r}}^\alpha(\boldsymbol{x})\delta(\bar{\mathbf{r}}^\alpha(\boldsymbol{x}) - \bar{\mathbf{r}}^\beta(\boldsymbol{y})) = \bar{\mathbf{r}}^\beta(\boldsymbol{y})\delta(\bar{\mathbf{r}}^\alpha(\boldsymbol{x}) - \bar{\mathbf{r}}^\beta(\boldsymbol{y})), \tag{50}$$

and therefore equation (48) is satisfied. The Hardy-type couple stress follows as

$$\widehat{\boldsymbol{m}}_H(\boldsymbol{x},\tau) = \frac{1}{2}\sum_{\alpha\beta}\big\langle \mathbf{f}^{\alpha\beta}(\tau) \times \widehat{\mathbf{r}}_H^{\alpha\beta}(\boldsymbol{x},\mathbf{x}^\alpha,\mathbf{x}^\beta)\big\rangle_{\mathcal{P}}, \tag{51}$$

$$\widehat{\mathbf{r}}_H^{\alpha\beta}(\boldsymbol{x},\mathbf{x}^\alpha,\mathbf{x}^\beta) = \int_0^1 [\mathbf{x}^\alpha - \boldsymbol{x} - a\mathbf{x}^{\alpha\beta}]w\big(\mathbf{x}^\alpha - \boldsymbol{x} - a\mathbf{x}^{\alpha\beta}\big)da \otimes \mathbf{x}^{\alpha\beta}. \tag{52}$$

Note that we deliberately changed the order of $\mathbf{f}^{\alpha\beta}(\tau)$ and $\widehat{\mathbf{r}}_H^{\alpha\beta}$ so that it is consistent with the expressions for the Cauchy stress derived in Section 5.

Using equation (32) it immediately follows that

$$\int_{\mathcal{S}} \widehat{\mathbf{r}}_H^{\alpha\beta}(\boldsymbol{x},\mathbf{x}^\alpha,\mathbf{x}^\beta)d\boldsymbol{x} = \mathbf{0}, \tag{53}$$

thus

$$\int_{\mathcal{S}} \widehat{\boldsymbol{m}}_H(\boldsymbol{x},\tau)d\boldsymbol{x} = \mathbf{0}. \tag{54}$$

Therefore, the macroscopic non-diffusive part of the Hardy-type couple stress is always zero.

5.2. Noll–Murdoch-type couple stress generator

A Noll–Murdoch-type generator function is postulated as

$$\boldsymbol{g}_N^m(\boldsymbol{x},\boldsymbol{y},\tau) = \sum_{\alpha\beta}\big\langle[\bar{\mathbf{r}}^\alpha(\boldsymbol{x}) + \bar{\mathbf{r}}^\beta(\boldsymbol{y})] \times \mathbf{f}^{\alpha\beta}(\tau)w(\mathbf{x}^\alpha - \boldsymbol{x})w(\mathbf{x}^\beta - \boldsymbol{y})\big\rangle_{\mathcal{P}}. \tag{55}$$

Due to equation (32) the following holds

$$\int_{\mathcal{S}} \bar{\mathbf{r}}^\beta(\boldsymbol{y})w(\mathbf{x}^\beta - \boldsymbol{y})d\boldsymbol{y} = 0, \tag{56}$$

thus equation (48) is satisfied.

The non-diffusive part of the Noll–Murdoch-type microscopic angular momentum flux (i.e. the couple stress) then follows as

$$\widehat{\boldsymbol{m}}_N(\boldsymbol{x},\tau) = \frac{1}{2}\sum_{\alpha\beta}\big\langle \mathbf{f}^{\alpha\beta}(\tau) \times \widehat{\mathbf{r}}_N^{\alpha\beta}(\boldsymbol{x},\mathbf{x}^\alpha,\mathbf{x}^\beta)\big\rangle_{\mathcal{P}}, \tag{57}$$

$$\widehat{\mathbf{r}}_N^{\alpha\beta} = \int_{\mathcal{S}}\int_0^1 \Big[[\bar{\mathbf{r}}^\alpha(\boldsymbol{x}) - a\boldsymbol{z}] + [\bar{\mathbf{r}}^\beta(\boldsymbol{x}) + [1-a]\boldsymbol{z}]\Big]\, w\big(\bar{\mathbf{r}}^\alpha(\boldsymbol{x}) - a\boldsymbol{z}\big)w\big(\bar{\mathbf{r}}^\beta(\boldsymbol{x}) + [1-a]\boldsymbol{z}\big)da\boldsymbol{z}d\boldsymbol{z}.$$

Again, note the changed order of $\mathbf{f}^{\alpha\beta}(\tau)$ and $\widehat{\mathbf{r}}_H^{\alpha\beta}$.

Using equations (31), (26) and (32), we can prove the following:

$$\begin{aligned}
&\int_{\mathcal{S}} \widehat{\mathbf{r}}_N^{\alpha\beta}(\boldsymbol{x}, \mathbf{x}^\alpha, \mathbf{x}^\beta) d\boldsymbol{x} = \\
&\int_0^1 \int_{\mathcal{S}} \left[\int_{\mathcal{S}} [\mathbf{x}^\alpha - 2\boldsymbol{x} - 2a\boldsymbol{z} + \mathbf{x}^\beta + \boldsymbol{z}] w\big(\mathbf{x}^\alpha - \boldsymbol{x} - a\boldsymbol{z}\big) w\big(\mathbf{x}^\beta - \boldsymbol{x} + [1-a]\boldsymbol{z}\big) d\boldsymbol{x} \right] da \otimes \boldsymbol{z} d\boldsymbol{z} \\
&\Rightarrow \begin{bmatrix} \mathbf{x}^\alpha - \boldsymbol{x} - a\boldsymbol{z} =: -\boldsymbol{y} \\ \boldsymbol{x} = \mathbf{x}^\alpha - a\boldsymbol{z} + \boldsymbol{y} \\ d\boldsymbol{x} = d\boldsymbol{y} \end{bmatrix} \Rightarrow \int_0^1 \int_{\mathcal{S}} w(-\boldsymbol{y}) \left[\int_{\mathcal{S}} [\boldsymbol{z} - 2\boldsymbol{y} - \mathbf{x}^{\alpha\beta}] w\big(\boldsymbol{z} - \boldsymbol{y} - \mathbf{x}^{\alpha\beta}\big) \otimes \boldsymbol{z} d\boldsymbol{z} \right] d\boldsymbol{y} da \\
&\Rightarrow \begin{bmatrix} \boldsymbol{z} - \boldsymbol{y} - \mathbf{x}^{\alpha\beta} =: \boldsymbol{y}' \\ \boldsymbol{z} = \boldsymbol{y}' + \boldsymbol{y} + \mathbf{x}^{\alpha\beta} \\ d\boldsymbol{z} = d\boldsymbol{y}' \end{bmatrix} \Rightarrow \int_{\mathcal{S}} \int_{\mathcal{S}} [\boldsymbol{y}' - \boldsymbol{y}] \otimes [\boldsymbol{y}' + \boldsymbol{y} + \mathbf{x}^{\alpha\beta}] w(-\boldsymbol{y}) w\big(\boldsymbol{y}'\big) d\boldsymbol{y}' d\boldsymbol{y} \\
&= \int_{\mathcal{S}} \boldsymbol{y}' \otimes \boldsymbol{y}' w(\boldsymbol{y}') d\boldsymbol{y}' - \int_{\mathcal{S}} \boldsymbol{y} \otimes \boldsymbol{y}\, w(-\boldsymbol{y}) d\boldsymbol{y} = \mathbf{0}.
\end{aligned} \tag{58}$$

Thus, the integral of the non-diffusive part of the microscopic Noll–Murdoch couple stress is zero, i.e.

$$\int_{\mathcal{S}} \widehat{\boldsymbol{m}}_N(\boldsymbol{x}, \tau) d\boldsymbol{x} = \mathbf{0}. \tag{59}$$

This agrees with the macroscopic Noll–Murdoch stress being symmetric (equation (47)).

6. Heat fluxes from the implicit approach

In the implicit approach the total heat flux $\widehat{\boldsymbol{q}}^i$ and the source term q due to interaction forces are determined via

$$\operatorname{div}\widehat{\boldsymbol{q}}^i(\boldsymbol{x}, \tau) + q(\boldsymbol{x}, \tau) = -\sum_{\alpha\beta} \left\langle \widetilde{\mathbf{v}}^\alpha(\boldsymbol{x}, \tau) \cdot \mathbf{f}^{\alpha\beta}(\tau) w(\mathbf{x}^\alpha - \boldsymbol{x}) \right\rangle_{\mathcal{P}} \doteq \int_{\mathcal{S}} g(\boldsymbol{x}, \boldsymbol{y}, \tau) d\boldsymbol{y}. \tag{60}$$

Both $\widehat{\boldsymbol{q}}^i$ and q depend on the particular choice of the generator function. Following [23], we divide g into skewsymmetric and symmetric parts

$$g = g^{\text{skw}} + g_{\text{sym}}, \tag{61}$$

such that

$$\int_{\mathcal{S}} g^{\text{skw}}(\boldsymbol{x}, \boldsymbol{y}, \tau) d\boldsymbol{y} = \operatorname{div}\widehat{\boldsymbol{q}}^i(\boldsymbol{x}, \tau) \tag{62}$$

and

$$\int_{\mathcal{S}} g_{\text{sym}}(\boldsymbol{x}, \boldsymbol{y}, \tau) d\boldsymbol{y} = q(\boldsymbol{x}, \tau) \tag{63}$$

hold.

6.1. Hardy-type heat flux generator

The Hardy-type generator function can be chosen as

$$g_{\text{sym}}^{\text{skw}}(\boldsymbol{x}, \boldsymbol{y}, \tau) = -\frac{1}{2} \sum_{\alpha\beta} \left\langle [\widetilde{\mathbf{v}}^\alpha(\boldsymbol{x}, \tau) \pm \widetilde{\mathbf{v}}^\beta(\boldsymbol{y}, \tau)] \cdot \mathbf{f}^{\alpha\beta}(\tau) w(\mathbf{x}^\alpha - \boldsymbol{x}) \delta([\mathbf{x}^\alpha - \boldsymbol{x}] - [\mathbf{x}^\beta - \boldsymbol{y}]) \right\rangle_{\mathcal{P}}. \tag{64}$$

It is easy to see that

$$\int_{\mathcal{S}}[g^{\text{skw}}(\boldsymbol{x},\boldsymbol{y},\tau)+g_{\text{sym}}(\boldsymbol{x},\boldsymbol{y},\tau)]d\boldsymbol{y}=$$
$$-\int_{\mathcal{S}}\sum_{\alpha\beta}\big\langle\widetilde{\mathbf{v}}^{\alpha}(\boldsymbol{x},\tau)\cdot\mathbf{f}^{\alpha\beta}(\tau)w(\mathbf{x}^{\alpha}-\boldsymbol{x})\delta(\mathbf{x}^{\alpha\beta}-\boldsymbol{x}+\boldsymbol{y})\big\rangle_{\mathcal{P}}d\boldsymbol{y}=$$
$$-\sum_{\alpha\beta}\big\langle\widetilde{\mathbf{v}}^{\alpha}(\boldsymbol{x},\tau)\cdot\mathbf{f}^{\alpha\beta}(\tau)w(\mathbf{x}^{\alpha}-\boldsymbol{x})\big\rangle_{\mathcal{P}}.$$

Since $g^{\text{skw}}_{\text{sym}}$ includes $\delta(\mathbf{x}^{\alpha\beta}-\boldsymbol{x}+\boldsymbol{y})$, it follows that $\mathbf{x}^{\alpha}-\boldsymbol{x}=\mathbf{x}^{\beta}-\boldsymbol{y}$, thus

$$\begin{aligned}
g^{\text{skw}}(\boldsymbol{x},\boldsymbol{y},\tau)&=-\frac{1}{2}\sum_{\alpha\beta}\big\langle[\widetilde{\mathbf{v}}^{\alpha}(\boldsymbol{x},\tau)+\widetilde{\mathbf{v}}^{\beta}(\boldsymbol{y},\tau)]\cdot\mathbf{f}^{\alpha\beta}(\tau)w(\mathbf{x}^{\alpha}-\boldsymbol{x})\delta(\mathbf{x}^{\alpha\beta}-\boldsymbol{x}+\boldsymbol{y})\big\rangle_{\mathcal{P}}\\
&=-\frac{1}{2}\sum_{\alpha\beta}\big\langle[\widetilde{\mathbf{v}}^{\alpha}(\boldsymbol{x},\tau)+\widetilde{\mathbf{v}}^{\beta}(\boldsymbol{y},\tau)]\cdot\mathbf{f}^{\alpha\beta}(\tau)w(\mathbf{x}^{\beta}-\boldsymbol{y})\delta(\mathbf{x}^{\beta\alpha}-\boldsymbol{y}+\boldsymbol{x})\big\rangle_{\mathcal{P}}\\
&=\frac{1}{2}\sum_{\alpha\beta}\big\langle[\widetilde{\mathbf{v}}^{\beta}(\boldsymbol{y},\tau)+\widetilde{\mathbf{v}}^{\alpha}(\boldsymbol{x},\tau)]\cdot\mathbf{f}^{\beta\alpha}(\tau)w(\mathbf{x}^{\beta}-\boldsymbol{y})\delta(\mathbf{x}^{\beta\alpha}-\boldsymbol{y}+\boldsymbol{x})\big\rangle_{\mathcal{P}}\\
&=-g^{\text{skw}}(\boldsymbol{y},\boldsymbol{x},\tau).
\end{aligned}\tag{65}$$

Using g^{skw} in equation (22), the Hardy-type heat flux follows as

$$\widehat{\boldsymbol{q}}^{i}_{H}(\boldsymbol{x},\tau)=\frac{1}{4}\sum_{\alpha\beta}\big\langle\mathbf{f}^{\alpha\beta}(\tau)\cdot\widehat{\mathbf{w}}^{\alpha\beta}_{H}(\boldsymbol{x},\mathbf{x}^{\alpha},\mathbf{x}^{\beta},\tau)\,\mathbf{x}^{\alpha\beta}\big\rangle_{\mathcal{P}},\tag{66}$$

$$\widehat{\mathbf{w}}^{\alpha\beta}_{H}(\boldsymbol{x},\mathbf{x}^{\alpha},\mathbf{x}^{\beta},\tau)=\int_0^1\widehat{\mathbf{v}}^{\alpha\beta}_{H}(\boldsymbol{x},\mathbf{x}^{\alpha},\mathbf{x}^{\beta},\tau;a)w\big(\mathbf{x}^{\alpha}-\boldsymbol{x}-a\mathbf{x}^{\alpha\beta}\big)da,\tag{67}$$

$$\widehat{\mathbf{v}}^{\alpha\beta}_{H}(\boldsymbol{x},\mathbf{x}^{\alpha},\mathbf{x}^{\beta},\tau;a)=\widetilde{\mathbf{v}}^{\alpha}(\boldsymbol{x}+a\mathbf{x}^{\alpha\beta},\tau)+\widetilde{\mathbf{v}}^{\beta}(\boldsymbol{x}-[1-a]\mathbf{x}^{\alpha\beta},\tau).\tag{68}$$

The expression for $q(\boldsymbol{x},\tau)$ is then obtained from equation (63) as

$$\begin{aligned}
q_H(\boldsymbol{x},\tau)&=\int_{\mathcal{S}}g_{\text{sym}}(\boldsymbol{x},\boldsymbol{y},\tau)d\boldsymbol{y}\\
&=-\frac{1}{2}\sum_{\alpha\beta}\big\langle\widetilde{\mathbf{v}}^{\alpha}(\boldsymbol{x},\tau)\cdot\mathbf{f}^{\alpha\beta}(\tau)w(\mathbf{x}^{\alpha}-\boldsymbol{x})\big\rangle_{\mathcal{P}}\\
&\quad+\int_{\mathcal{S}}\frac{1}{2}\sum_{\alpha\beta}\big\langle\widetilde{\mathbf{v}}^{\beta}(\boldsymbol{y},\tau)\cdot\mathbf{f}^{\alpha\beta}(\tau)w(\mathbf{x}^{\alpha}-\boldsymbol{x})\delta(\mathbf{x}^{\alpha\beta}-\boldsymbol{x}+\boldsymbol{y})\big\rangle_{\mathcal{P}}d\boldsymbol{y}\\
&=-\frac{1}{2}\sum_{\alpha\beta}\big\langle[\widetilde{\mathbf{v}}^{\alpha}(\boldsymbol{x},\tau)-\widetilde{\mathbf{v}}^{\beta}(\boldsymbol{x}-\mathbf{x}^{\alpha\beta},\tau)]\cdot\mathbf{f}^{\alpha\beta}(\tau)w(\mathbf{x}^{\alpha}-\boldsymbol{x})\big\rangle_{\mathcal{P}}.
\end{aligned}\tag{69}$$

Since the resulting expression (equation (66)) for the heat flux in the implicit approach contains an integral which includes the continuum velocity in $\widetilde{\mathbf{v}}^{\alpha}=\mathbf{v}^{\alpha}-\boldsymbol{v}$ and $\widetilde{\mathbf{v}}^{\beta}=\mathbf{v}^{\beta}-\boldsymbol{v}$ (equations (67) and (68)), the straightforward application of such an approach would require evaluation of the continuum velocity at each quadrature point in that integral. Obviously, this is computationally inefficient. A mathematical development of the integral quantities is not possible either.

One of the possible ways to circumvent this is to assume that the continuum velocity $\boldsymbol{v}(\boldsymbol{x})$ is constant on the length-scale of inter-particle distance $\mathbf{x}^{\alpha\beta}$. In other words, we assume the following

$$\widehat{\mathbf{v}}^{\alpha\beta}_{H}(\boldsymbol{x},\mathbf{x}^{\alpha},\mathbf{x}^{\beta},\tau)\approx\widetilde{\mathbf{v}}^{\alpha}(\boldsymbol{x},\tau)+\widetilde{\mathbf{v}}^{\beta}(\boldsymbol{x},\tau).\tag{70}$$

Therefore $\widehat{\mathbf{v}}_H^{\alpha\beta}$ can be taken out of the integral in equation (67). This leads to the following expression for the heat flux

$$\widehat{\boldsymbol{q}}_H^i(\boldsymbol{x},\tau) \approx \frac{1}{2}\sum_{\alpha\beta}\big\langle \mathbf{f}^{\alpha\beta}(\tau)\cdot\frac{[\widetilde{\mathbf{v}}^{\alpha}(\boldsymbol{x},\tau)+\widetilde{\mathbf{v}}^{\beta}(\boldsymbol{x},\tau)]}{2}\widehat{\mathbf{x}}_H^{\alpha\beta}(\boldsymbol{x},\mathbf{x}^{\alpha},\mathbf{x}^{\beta})\big\rangle_{\mathcal{P}}, \tag{71}$$

where $\widehat{\mathbf{x}}_H^{\alpha\beta}$ is given by equation (38).

An alternative approach, as advocated in [24], is to consider the delta-distribution instead of the general averaging kernel w in equation (67). In such a case it is obvious that $\boldsymbol{x}+a\mathbf{x}^{\alpha\beta}=\mathbf{x}^{\alpha}$, and therefore the expression for $\widehat{\mathbf{v}}_H^{\alpha\beta}$ reads

$$\widehat{\mathbf{v}}_\delta^{\alpha\beta}(\mathbf{x}^{\alpha},\mathbf{x}^{\beta},\tau)=\widetilde{\mathbf{v}}^{\alpha}(\mathbf{x}^{\alpha},\tau)+\widetilde{\mathbf{v}}^{\beta}(\mathbf{x}^{\beta},\tau). \tag{72}$$

Substituting this to equation (67) results in a form similar to equation (71), however, with the delta distribution used as an averaging kernel:

$$\widehat{\boldsymbol{q}}_\delta^i(\boldsymbol{x},\tau)=\frac{1}{4}\sum_{\alpha\beta}\big\langle \mathbf{f}^{\alpha\beta}(\tau)\cdot\widehat{\mathbf{v}}_\delta^{\alpha\beta}(\mathbf{x}^{\alpha},\mathbf{x}^{\beta},\tau)\,\widehat{\mathbf{x}}_\delta^{\alpha\beta}(\boldsymbol{x},\mathbf{x}^{\alpha},\mathbf{x}^{\beta})\big\rangle_{\mathcal{P}} \tag{73}$$

where

$$\widehat{\mathbf{x}}_\delta^{\alpha\beta}(\boldsymbol{x},\mathbf{x}^{\alpha},\mathbf{x}^{\beta})=\widehat{w}_\delta^{\alpha\beta}\mathbf{x}^{\alpha\beta}, \tag{74}$$

$$\widehat{w}_\delta^{\alpha\beta}(\boldsymbol{x},\mathbf{x}^{\alpha},\mathbf{x}^{\beta})=\int_0^1\delta\big(\mathbf{x}^{\alpha}-\boldsymbol{x}-a\mathbf{x}^{\alpha\beta}\big)da. \tag{75}$$

The "localized" version of $q_H(\boldsymbol{x},\tau)$ reads accordingly

$$q_\delta(\boldsymbol{x},\tau)=-\frac{1}{2}\sum_{\alpha\beta}\big\langle[\widetilde{\mathbf{v}}^{\alpha}(\mathbf{x}^{\alpha},\tau)-\widetilde{\mathbf{v}}^{\beta}(\mathbf{x}^{\beta},\tau)]\cdot\mathbf{f}^{\alpha\beta}(\tau)\delta(\mathbf{x}^{\alpha}-\boldsymbol{x})\big\rangle_{\mathcal{P}}, \tag{76}$$

which is consistent with results obtained in Admal and Tadmor [24].

Since the only term in equation (73) which depends on $\boldsymbol{x}$ is $\widehat{\mathbf{x}}_\delta^{\alpha\beta}$, using equation (40) the space integral of this quantity follows as

$$\int_{\mathcal{S}}\widehat{\boldsymbol{q}}_\delta^i(\boldsymbol{x},\tau)d\boldsymbol{x}=\frac{1}{4}\sum_{\alpha\beta}\big\langle \mathbf{f}^{\alpha\beta}(\tau)\cdot\widehat{\mathbf{v}}_\delta^{\alpha\beta}(\mathbf{x}^{\alpha},\mathbf{x}^{\beta},\tau)\,\mathbf{x}^{\alpha\beta}\big\rangle_{\mathcal{P}}. \tag{77}$$

Furthermore it is obvious that

$$\int_{\mathcal{S}}q_\delta(\boldsymbol{x},\tau)d\boldsymbol{x}=-\frac{1}{2}\sum_{\alpha\beta}\big\langle[\widetilde{\mathbf{v}}^{\alpha}(\mathbf{x}^{\alpha},\tau)-\widetilde{\mathbf{v}}^{\beta}(\mathbf{x}^{\beta},\tau)]\cdot\mathbf{f}^{\alpha\beta}(\tau)\big\rangle_{\mathcal{P}}. \tag{78}$$

6.2. Noll–Murdoch-type heat flux generator

The Noll–Murdoch-type generator function is introduced as

$$g_{\mathrm{sym}}^{\mathrm{skw}}(\boldsymbol{x},\boldsymbol{y},\tau)=-\frac{1}{2}\sum_{\alpha\beta}\big\langle[\widetilde{\mathbf{v}}^{\alpha}(\boldsymbol{x},\tau)\pm\widetilde{\mathbf{v}}^{\beta}(\boldsymbol{y},\tau)]\cdot\mathbf{f}^{\alpha\beta}(\tau)w(\mathbf{x}^{\alpha}-\boldsymbol{x})w(\mathbf{x}^{\beta}-\boldsymbol{y})\big\rangle_{\mathcal{P}}. \tag{79}$$

Changing α and β, it is obvious that $g^{\mathrm{skw}}(\boldsymbol{x},\boldsymbol{y},\tau)=-g^{\mathrm{skw}}(\boldsymbol{y},\boldsymbol{x},\tau)$; therefore, Noll's lemma can be applied to obtain the following heat flux:

$$\begin{aligned}\widehat{\boldsymbol{q}}_N^i(\boldsymbol{x},\tau)&=-\frac{1}{2}\int_{\mathcal{S}}\int_0^1 g^{\mathrm{skw}}\big(\boldsymbol{x}+a\boldsymbol{z},\boldsymbol{x}-[1-a]\boldsymbol{z}\big)da\otimes\boldsymbol{z}d\boldsymbol{z}\\&=\frac{1}{4}\sum_{\alpha\beta}\big\langle \mathbf{f}^{\alpha\beta}(\tau)\cdot\widehat{\mathbf{w}}_N^{\alpha\beta}(\boldsymbol{x},\mathbf{x}^{\alpha},\mathbf{x}^{\beta})\big\rangle_{\mathcal{P}},\end{aligned} \tag{80}$$

with

$$\widehat{\mathbf{w}}_N^{\alpha\beta}(\boldsymbol{x},\mathbf{x}^\alpha,\mathbf{x}^\beta,\tau)=\int_{\mathcal{S}}\int_0^1\widehat{\mathbf{v}}_N^{\alpha\beta}w\big(\mathbf{x}^\alpha-\boldsymbol{x}-a\boldsymbol{z}\big)w\big(\mathbf{x}^\beta-\boldsymbol{x}+[1-a]\boldsymbol{z}\big)da\otimes\boldsymbol{z}d\boldsymbol{z}, \tag{81}$$

and

$$\widehat{\mathbf{v}}_N^{\alpha\beta}(\boldsymbol{x},\mathbf{x}^\alpha,\mathbf{x}^\beta,\tau,\boldsymbol{z},a)=\widetilde{\mathbf{v}}^\alpha(\boldsymbol{x}+a\boldsymbol{z},\tau)+\widetilde{\mathbf{v}}^\beta(\boldsymbol{x}-[1-a]\boldsymbol{z},\tau). \tag{82}$$

Substitution of g_{sym} into equation (63) leads to

$$\begin{aligned}q_N(\boldsymbol{x},\tau)&=\int_{\mathcal{S}}g_{\text{sym}}(\boldsymbol{x},\boldsymbol{y},\tau)d\boldsymbol{y}\\&=-\frac{1}{2}\sum_{\alpha\beta}\big\langle\widetilde{\mathbf{v}}^\alpha(\boldsymbol{x},\tau)\cdot\mathbf{f}^{\alpha\beta}(\tau)w(\mathbf{x}^\alpha-\boldsymbol{x})\big\rangle_{\mathcal{P}}\\&\quad+\int_{\mathcal{S}}\frac{1}{2}\sum_{\alpha\beta}\big\langle\widetilde{\mathbf{v}}^\beta(\boldsymbol{y},\tau)\cdot\mathbf{f}^{\alpha\beta}(\tau)w(\mathbf{x}^\alpha-\boldsymbol{x})w(\mathbf{x}^\beta-\boldsymbol{y})\big\rangle_{\mathcal{P}}d\boldsymbol{y}.\end{aligned} \tag{83}$$

Note the difference from the Hardy solution (equation (69)), where it was possible to evaluate the integral due to the presence of the delta-distribution.

Any further simplifications of either equation (83) or equation (80) are possible only when assuming the localized version of the generator function. In such a case, as discussed in Section 3, the solution is fully equivalent to the localized Hardy solution for the heat flux, which was presented in the previous section.

7. Heat fluxes from the explicit approach

The generator function for the unknown part of the heat flux $\widehat{\boldsymbol{q}}^*$ must satisfy

$$\text{div}\widehat{\boldsymbol{q}}^*(\boldsymbol{x},\tau)=\sum_{\alpha\beta}\Big\langle\mathbf{f}^{\alpha\beta}(\tau)\cdot\frac{[\mathbf{v}^\alpha+\mathbf{v}^\beta]}{2}w(\mathbf{x}^\alpha-\boldsymbol{x})\Big\rangle_{\mathcal{P}}\doteq\int_{\mathcal{S}}\boldsymbol{g}^e(\boldsymbol{x},\boldsymbol{y},\tau)d\boldsymbol{y}. \tag{84}$$

7.1. Hardy-type heat flux generator

The Hardy-type generator function

$$\boldsymbol{g}_H^e(\boldsymbol{x},\boldsymbol{y},\tau)=\sum_{\alpha\beta}\Big\langle\mathbf{f}^{\alpha\beta}(\tau)\cdot\frac{[\mathbf{v}^\alpha+\mathbf{v}^\beta]}{2}w(\mathbf{x}^\alpha-\boldsymbol{x})\delta([\mathbf{x}^\alpha-\boldsymbol{x}]-[\mathbf{x}^\beta-\boldsymbol{y}])\Big\rangle_{\mathcal{P}}=-\boldsymbol{g}_H^e(\boldsymbol{y},\boldsymbol{x},\tau) \tag{85}$$

gives rise to the following heat flux

$$\widehat{\boldsymbol{q}}_H^*(\boldsymbol{x},\tau)=-\frac{1}{2}\sum_{\alpha\beta}\Big\langle\mathbf{f}^{\alpha\beta}(\tau)\cdot\frac{[\mathbf{v}^\alpha+\mathbf{v}^\beta]}{2}\otimes\widehat{\mathbf{x}}_H^{\alpha\beta}(\boldsymbol{x},\mathbf{x}^\alpha,\mathbf{x}^\beta)\Big\rangle_{\mathcal{P}}. \tag{86}$$

Using equation (40) it follows that the space integral of $\widehat{\boldsymbol{q}}_H^*$ results in

$$\int_{\mathcal{S}}\widehat{\boldsymbol{q}}_H^*(\boldsymbol{x},\tau)d\boldsymbol{x}=-\frac{1}{2}\sum_{\alpha\beta}\Big\langle\mathbf{f}^{\alpha\beta}(\tau)\cdot\frac{\mathbf{v}^\alpha+\mathbf{v}^\beta}{2}\otimes\mathbf{x}^{\alpha\beta}\Big\rangle_{\mathcal{P}}. \tag{87}$$

7.2. Noll–Murdoch-type heat flux generator

The Noll–Murdoch-type generator function

$$\boldsymbol{g}_N^e(\boldsymbol{x},\boldsymbol{y},\tau)=\sum_{\alpha\beta}\Big\langle\mathbf{f}^{\alpha\beta}(\tau)\cdot\frac{[\mathbf{v}^\alpha+\mathbf{v}^\beta]}{2}w(\mathbf{x}^\alpha-\boldsymbol{x})w(\mathbf{x}^\beta-\boldsymbol{y})\Big\rangle_{\mathcal{P}}=-\boldsymbol{g}_N^e(\boldsymbol{y},\boldsymbol{x},\tau) \tag{88}$$

leads to the unknown part of the heat flux $\widehat{\boldsymbol{q}}_N^*$ as

$$\widehat{\boldsymbol{q}}_N^*(\boldsymbol{x},\tau) = -\frac{1}{2}\sum_{\alpha\beta}\left\langle \mathbf{f}^{\alpha\beta}(\tau)\cdot\frac{[\mathbf{v}^\alpha+\mathbf{v}^\beta]}{2}\widehat{\mathbf{x}}_N^{\alpha\beta}(\boldsymbol{x},\mathbf{x}^\alpha,\mathbf{x}^\beta)\right\rangle_{\mathcal{P}}. \tag{89}$$

Using equation (46) the space integral of this quantity follows as

$$\int_{\mathcal{S}}\widehat{\boldsymbol{q}}_N^*(\boldsymbol{x},\tau)d\boldsymbol{x} = -\frac{1}{2}\sum_{\alpha\beta}\left\langle \mathbf{f}^{\alpha\beta}(\tau)\cdot\frac{[\mathbf{v}^\alpha+\mathbf{v}^\beta]}{2}\otimes\mathbf{x}^{\alpha\beta}\right\rangle_{\mathcal{P}}, \tag{90}$$

which equals the space integral of the Hardy-type heat flux equation (87).

7.3. Total heat flux and its comparison to the implicit approach

In contrast to fluxes in Sections 4, 5 and 6, the results obtained in the above expression for $\widehat{\boldsymbol{q}}^*$ do not represent the total flux, but only a part of it.

Given the Hardy-type (the Noll–Murdoch) solutions $\widehat{\boldsymbol{s}}_H$ ($\widehat{\boldsymbol{s}}_N$) and $\widehat{\boldsymbol{q}}_H^*$ ($\widehat{\boldsymbol{q}}_N^*$), we can evaluate $\widehat{\boldsymbol{q}}^e$ in the explicit approach for the system with two-point potentials (see equation (19)):

$$\begin{aligned}\boldsymbol{q}_P(\boldsymbol{x}) := \widehat{\boldsymbol{q}}^e(\boldsymbol{x}) - \boldsymbol{q}_T(\boldsymbol{x}) &= \boldsymbol{v}(\boldsymbol{x})\cdot\widehat{\boldsymbol{s}}(\boldsymbol{x}) - \widehat{\boldsymbol{q}}^*(\boldsymbol{x})\\ &= \frac{1}{2}\sum_{\alpha\beta}\left\langle \mathbf{f}^{\alpha\beta}\cdot\frac{[\mathbf{v}^\alpha+\mathbf{v}^\beta]}{2}\widehat{\mathbf{x}}^{\alpha\beta}(\boldsymbol{x})\right\rangle_{\mathcal{P}} - \boldsymbol{v}(\boldsymbol{x})\cdot\frac{1}{2}\sum_{\alpha\beta}\left\langle \mathbf{f}^{\alpha\beta}\otimes\widehat{\mathbf{x}}^{\alpha\beta}(\boldsymbol{x})\right\rangle_{\mathcal{P}}\\ &= \frac{1}{2}\sum_{\alpha\beta}\left\langle \mathbf{f}^{\alpha\beta}\cdot\frac{[\widetilde{\mathbf{v}}^\alpha(\boldsymbol{x})+\widetilde{\mathbf{v}}^\beta(\boldsymbol{x})]}{2}\widehat{\mathbf{x}}^{\alpha\beta}(\boldsymbol{x})\right\rangle_{\mathcal{P}}.\end{aligned} \tag{91}$$

Note that in the above we deliberately dropped subscripts N and H in $\widehat{\mathbf{x}}^{\alpha\beta}$, since it holds for both cases if and only if flux candidates of the same type are used.

The total heat flux for the explicit approach is thus given by

$$\boldsymbol{q}^e(\boldsymbol{x}) = \boldsymbol{q}_P(\boldsymbol{x}) + \boldsymbol{q}_T(\boldsymbol{x}) - 2\widetilde{\boldsymbol{q}}(\boldsymbol{x}). \tag{92}$$

By comparing equation (91) to the approximate implicit Hardy-type total heat flux equation (71) it is clear that

$$\boldsymbol{q}_P(\boldsymbol{x}) = \widehat{\boldsymbol{q}}_H^e(\boldsymbol{x}) - \boldsymbol{q}_T(\boldsymbol{x}) = \widehat{\boldsymbol{q}}_H^i(\boldsymbol{x}). \tag{93}$$

Remark 1 *From the continuum perspective, the energy balance equation has to be closed by the constitutive relationship, e.g. a Fourier law for $\boldsymbol{q} = \boldsymbol{q}(T)$. Since both $\boldsymbol{q}$ and T can be calculated from the atomistic simulations, the validity of different constitutive relationships could be verified.*

At last, we compare the heat flux obtained from the explicit approach to the implicit one for the localized version

$$\boldsymbol{q}_\delta^e(\boldsymbol{x}) - \boldsymbol{q}_\delta^i(\boldsymbol{x}) = \widehat{\boldsymbol{q}}_\delta^e(\boldsymbol{x}) - \widehat{\boldsymbol{q}}_\delta^i(\boldsymbol{x}) = \boldsymbol{q}_T + \left\langle\sum_{\alpha\beta}\mathbf{f}^{\alpha\beta}\cdot\frac{[\boldsymbol{v}(\mathbf{x}^\alpha)-\boldsymbol{v}(\boldsymbol{x})+\boldsymbol{v}(\mathbf{x}^\beta)-\boldsymbol{v}(\boldsymbol{x})]}{2}\widehat{\mathbf{x}}_\delta^{\alpha\beta}(\boldsymbol{x})\right\rangle_{\mathcal{P}} \tag{94}$$

and the approximate solutions

$$\boldsymbol{q}_H^e(\boldsymbol{x}) - \boldsymbol{q}_H^i(\boldsymbol{x}) = \widehat{\boldsymbol{q}}_H^e(\boldsymbol{x}) - \widehat{\boldsymbol{q}}_H^i(\boldsymbol{x}) = \boldsymbol{q}_T \tag{95}$$

respectively.

Thus we can conclude that the two approaches differ mainly by the diffusive potential energy term $\boldsymbol{q}_T$ introduced in the explicit case.

8. Discussion and conclusions

Molecular dynamics simulations are usually conducted under periodic boundary conditions. In such a case, the volume V of the particle system is uniquely[4] defined. Recall the following equation proven in Part I [3]:

$$\widetilde{\boldsymbol{s}}(\boldsymbol{x}) = \Big\langle \sum_{\alpha} \frac{1}{2} \mathsf{m}^{\alpha} \mathbf{v}^{\alpha} \otimes \mathbf{v}^{\alpha}\, w(\mathbf{x}^{\alpha} - \boldsymbol{x}) \Big\rangle_{\mathcal{P}} - \frac{1}{2} \boldsymbol{p}(\boldsymbol{x}) \otimes \boldsymbol{v}(\boldsymbol{x}). \tag{96}$$

The space average over the RVE reads

$$\frac{1}{V} \int_{\mathcal{S}} \widetilde{\boldsymbol{s}}(\boldsymbol{x}) d\boldsymbol{x} = \frac{1}{V} \Big\langle \sum_{\alpha} \frac{1}{2} \mathsf{m}^{\alpha} \mathbf{v}^{\alpha} \otimes \mathbf{v}^{\alpha} \Big\rangle_{\mathcal{P}} - \frac{1}{2V} \int_{\mathcal{S}} \boldsymbol{p}(\boldsymbol{x}) \otimes \boldsymbol{v}(\boldsymbol{x}) d\boldsymbol{x}, \tag{97}$$

where the second term on the right hand side can be assumed to be zero if there is no macroscopic motion of the RVE.

Using this, the macroscopic Cauchy stress follows from equations (9), (41) and (47) as

$$\frac{1}{V} \int_{\mathcal{S}} \boldsymbol{s} d\boldsymbol{x} = \frac{1}{V} \int_{\mathcal{S}} [\, \widehat{\boldsymbol{s}} - 2\widetilde{\boldsymbol{s}}\,] d\boldsymbol{x} = \frac{1}{V} \Big\langle -\frac{1}{2} \sum_{\alpha\beta} \mathbf{f}^{\alpha\beta} \otimes \mathbf{x}^{\alpha\beta} - \sum_{\alpha} \mathsf{m}^{\alpha} \mathbf{v}^{\alpha} \otimes \mathbf{v}^{\alpha} \Big\rangle_{\mathcal{P}}. \tag{98}$$

Thus, we arrive at the well known expression called the virial stress, which is often used as a measure of the macroscopic stresses in a particle system. In other words, the virial stress can be considered as space integral of either Hardy or Noll–Murdoch Cauchy stress over the RVE. Note that this conclusion is different from Admal and Tadmor [25], where the authors prove that the Hardy solution of the Cauchy stress equals the virial only in the case of a constant averaging kernel $w = 1/V$.

In a similar manner, the macroscopic heat flux in the explicit approach can be developed for the localized solution

$$\begin{aligned} \frac{1}{V} \int_{\mathcal{S}} \boldsymbol{q}^{e}_{\delta} d\boldsymbol{x} = \frac{1}{V} \Big\langle & \sum_{\alpha} \frac{1}{2} \mathsf{m}^{\alpha} \mathbf{v}^{\alpha} \cdot [\mathbf{v}^{\alpha} - \boldsymbol{v}(\mathbf{x}^{\alpha})]\, [\mathbf{v}^{\alpha} - \boldsymbol{v}(\mathbf{x}^{\alpha})] \\ & + \sum_{\alpha} \mathbf{v}^{\alpha} [\mathbf{v}^{\alpha} - \boldsymbol{v}(\mathbf{x}^{\alpha})] \\ & + \frac{1}{2} \sum_{\alpha\beta} \mathbf{f}^{\alpha\beta} \cdot \left[\frac{[\mathbf{v}^{\alpha} + \mathbf{v}^{\beta}]}{2} - \int_0^1 \boldsymbol{v}(\mathbf{x}^{\alpha} - a\mathbf{x}^{\alpha\beta}) da \right] \mathbf{x}^{\alpha\beta} \Big\rangle_{\mathcal{P}}. \end{aligned} \tag{99}$$

On assuming the continuum velocity $\boldsymbol{v}$ to be zero, we obtain

$$\frac{1}{V} \int_{\mathcal{S}} \boldsymbol{q}^{e}_{\delta} d\boldsymbol{x} = \frac{1}{V} \Big\langle \sum_{\alpha} \frac{1}{2} \mathsf{m}^{\alpha} \mathbf{v}^{\alpha} \cdot \mathbf{v}^{\alpha}\, \mathbf{v}^{\alpha} + \sum_{\alpha} \mathbf{v}^{\alpha} \mathbf{v}^{\alpha} + \frac{1}{2} \sum_{\alpha\beta} \mathbf{f}^{\alpha\beta} \cdot \frac{[\mathbf{v}^{\alpha} + \mathbf{v}^{\beta}]}{2} \mathbf{x}^{\alpha\beta} \Big\rangle_{\mathcal{P}}, \tag{100}$$

which is fully consistent with the heat flux used in the Green–Kubo approach [26, 27] to evaluate the thermal conductivity from MD simulations. Therefore we showed that the integral Hardy-type quantities of fluxes are consistent with those commonly used in atomistic simulations.

From equation (94) it follows that the space integral of the heat flux for the implicit approach in a quasi-static case ($\boldsymbol{v}(\boldsymbol{x}) = \boldsymbol{0}$) is different from the explicit one

$$\frac{1}{V} \int_{\mathcal{S}} [\boldsymbol{q}^{e}_{\delta} - \boldsymbol{q}^{i}_{\delta}] d\boldsymbol{x} = \frac{1}{V} \Big\langle \sum_{\alpha} \mathbf{v}^{\alpha} \mathbf{v}^{\alpha} \Big\rangle_{\mathcal{P}}. \tag{101}$$

A result of this work that distinguishes it from Admal and Tadmor [25] is a strict proof that both the Hardy and the Noll–Murdoch solutions are possible for the space-probability averaging approach. Thus, both the space-probability and the space-temporal averaging approaches have the same source of the non-uniqueness of the linear momentum flux. It was concluded by Admal and Tadmor [25] that the space-probability averaging approach is preferable over the space-temporal averaging approach due to the absence of the non-uniqueness of a generator function. The reason for this is that the authors first derived the balance equations for space-probability averaging with the δ-distribution, and then applied the spatial averaging to the resulting fields. By doing so, the generator-function for the stress-fluxes is of "localized" type in our terms; thus there seemed to be no non-uniqueness in choosing it. As we have shown, however, space-probability averaging has the same non-uniqueness related to the choice of the generator function as the space-temporal averaging used by Murdoch. Thus, the preferable approach is to introduce both space and probability averaged continuum fields at the onset and then develop the balance equations. The same procedure is also preferable for the space-temporal averaging approach.

By comparing the resulting quantities for the total heat flux, we conclude that the explicit approach (used by Noll [2] and Hardy [18] among others) naturally leads to easy-to-implement expressions (equation (86)). Moreover, both the Cauchy stress and the heat flux are written in terms of the same $\widehat{w}^{\alpha\beta}$, therefore the evaluation of the linear momentum and energy fluxes, as well as the internal energy requires less computational resources. The explicit approach, however, can be applied directly only to two-point potentials.

By contrast, the expressions arising from the implicit approach are much harder to evaluate in general, since they require integration of the continuum velocity field over the segment $\mathsf{x}^{\alpha\beta}$. This can be circumvented via an approximate solution (equation (71)).

An alternative approach is first to consider the localized solution (i.e. the delta-distribution instead of the general averaging kernel w) to obtain $\boldsymbol{q}_\delta$ (equation (73)). The expression to be applied to the results of real MD simulation is then obtained from an additional spatial averaging

$$\boldsymbol{q} = \langle \boldsymbol{q}_\delta \rangle_{\mathcal{S}}. \tag{102}$$

The numerical study of this approach was performed in Admal and Tadmor [24].

Here, we would rather draw the attention to the following. In this approach it is assumed that $\boldsymbol{q}$ obtained using equation (102) does indeed correspond to primary continuum fields introduced during the derivation using the general averaging kernel w (that is continuum density ρ and the kinetic energy density k introduced in Parts I and II [3, 4] respectively). This, however, is not the case for the heat flux. In other words,

$$\widehat{\boldsymbol{q}}^i_H(\boldsymbol{x}) \neq \langle \widehat{\boldsymbol{q}}_\delta \rangle_{\mathcal{S}}. \tag{103}$$

It is interesting to note in contrast that for the non-diffusive part of the linear momentum flux it holds that

$$\widehat{\boldsymbol{s}}_H(\boldsymbol{x}) \equiv \langle \widehat{\boldsymbol{s}}_\delta \rangle_{\mathcal{S}}, \tag{104}$$

due to the dependence of $\widehat{\boldsymbol{s}}_\delta$ on $\boldsymbol{x}$ being concentrated solely in $\widehat{w}^{\alpha\beta}_\delta(\boldsymbol{x}, \mathsf{x}^\alpha, \mathsf{x}^\beta)$.

Let us quickly prove equations (104) and (103). First of all, note that

$$\begin{aligned} \int_{\mathcal{S}} \widehat{w}^{\alpha\beta}_\delta(\boldsymbol{y}, \mathsf{x}^\alpha, \mathsf{x}^\beta) w(\boldsymbol{x}-\boldsymbol{y}) d\boldsymbol{y} &= \int_{\mathcal{S}} \left[\int_0^1 \delta\big(\mathsf{x}^\alpha - \boldsymbol{y} - a\mathsf{x}^{\alpha\beta}\big) da \right] w(\boldsymbol{x}-\boldsymbol{y}) d\boldsymbol{y} \\ &= \int_0^1 \left[\int_{\mathcal{S}} \delta\big(\mathsf{x}^\alpha - \boldsymbol{y} - a\mathsf{x}^{\alpha\beta}\big) w(\boldsymbol{x}-\boldsymbol{y}) d\boldsymbol{y} \right] da \\ &= \int_0^1 w\big(\mathsf{x}^\alpha - \boldsymbol{x} - a\mathsf{x}^{\alpha\beta}\big) da \\ &= \widehat{w}^{\alpha\beta}_H(\boldsymbol{x}, \mathsf{x}^\alpha, \mathsf{x}^\beta). \end{aligned} \tag{105}$$

Using equation (105) and keeping in mind the expression for $\widehat{\boldsymbol{s}}_H(\boldsymbol{x})$ (equation (37)), it is easy to see that

$$\begin{aligned} \int_{\mathcal{S}} \widehat{\boldsymbol{s}}_\delta(\boldsymbol{y}) w(\boldsymbol{x}-\boldsymbol{y}) d\boldsymbol{y} &= -\frac{1}{2} \int_{\mathcal{S}} \big\langle \mathsf{f}^{\alpha\beta} \otimes \mathsf{x}^{\alpha\beta} \widehat{w}^{\alpha\beta}_\delta(\boldsymbol{y}, \mathsf{x}^\alpha, \mathsf{x}^\beta) \big\rangle_{\mathcal{P}} w(\boldsymbol{x}-\boldsymbol{y}) d\boldsymbol{y} \\ &= -\frac{1}{2} \big\langle \mathsf{f}^{\alpha\beta} \otimes \mathsf{x}^{\alpha\beta} \widehat{w}^{\alpha\beta}_H(\boldsymbol{y}, \mathsf{x}^\alpha, \mathsf{x}^\beta) \big\rangle_{\mathcal{P}} = \widehat{\boldsymbol{s}}_H(\boldsymbol{x}). \end{aligned} \tag{106}$$

In a similar manner we can develop the spatially smoothed version of a localized implicit heat flux as

$$\int_{\mathcal{S}} \widehat{\boldsymbol{q}}_{\delta}(\boldsymbol{y}) w(\boldsymbol{x}-\boldsymbol{y}) d\boldsymbol{y} \tag{107}$$

$$= \frac{1}{4} \sum_{\alpha\beta} \Big\langle \mathbf{f}^{\alpha\beta}(\tau) \cdot \left[\widetilde{\mathbf{v}}^{\alpha}(\mathbf{x}^{\alpha}) + \widetilde{\mathbf{v}}^{\beta}(\mathbf{x}^{\beta}) \right] \mathbf{x}^{\alpha\beta} \int_{\mathcal{S}} \widehat{w}_{\delta}^{\alpha\beta}(\boldsymbol{y}, \mathbf{x}^{\alpha}, \mathbf{x}^{\beta}) w(\boldsymbol{x}-\boldsymbol{y}) d\boldsymbol{y} \Big\rangle_{\mathcal{P}}$$

$$= \frac{1}{4} \sum_{\alpha\beta} \Big\langle \mathbf{f}^{\alpha\beta}(\tau) \cdot \left[\widetilde{\mathbf{v}}^{\alpha}(\mathbf{x}^{\alpha}) + \widetilde{\mathbf{v}}^{\beta}(\mathbf{x}^{\beta}) \right] \mathbf{x}^{\alpha\beta} \widehat{w}_{H}^{\alpha\beta}(\boldsymbol{x}, \mathbf{x}^{\alpha}, \mathbf{x}^{\beta}) \Big\rangle_{\mathcal{P}}. \tag{108}$$

This, however, is not the same as the general expression for the Hardy-type implicit heat flux $\widehat{\boldsymbol{q}}_{H}^{i}(\boldsymbol{x})$ given in equation (66).

Consequently, we might say that the application of the localized implicit approach somewhat lacks the consistency with the introduced primary kinematic fields. That difference, however, becomes small if one assumes slowly varying local velocity fields at both the length scale of the averaging kernel w and the length-scale of inter-particle distance (compare equations (70) and (72)). It is worth noting that the localized solution (or rather its integral over the finite volume) was successfully used to couple continuum mechanics and atomistic simulations of liquids [28].

In the present part of this series, we reviewed some of the possible solutions for all the fluxes arising in the balance equations previously obtained in Parts I and II [3, 4]. We have shown that the localized solutions of Hardy and Noll–Murdoch types are equal. In addition, the integral quantities of all the fluxes were developed. These can be trivially linked to the average over the RVE in case of MD simulations with periodic boundary conditions, thereby providing the mathematical background to the homogenization of particle systems. In addition, we proved that for the spatial kernel dependent only on the norm of its argument, both Hardy and Noll's couple stresses are zero macroscopically (if the diffusive contributions to the fluxes $\widetilde{\boldsymbol{s}}$ and $\widetilde{\boldsymbol{m}}$ are also zero macroscopically). This is consistent with the macroscopic Cauchy stresses resulting from the two approaches being symmetric, which corresponds to standard (as opposed to generalized) continuum mechanics.

At last, we reviewed and compared results from the explicit and implicit approaches to the balance of energy. It was shown that the two are different by the diffusive potential energy flux introduced in the explicit approach. Additionally, the consistency of the localized implicit heat flux to the introduced kinematic fields was discussed. An approximate solution to the Hardy-type implicit heat flux was proposed (equation (71)). Note, that in both cases we arrived at the equations containing the first gradient only, as opposed to the higher gradient theories, which, for example, could be obtained during the homogenization of pantographic-type structures [29].

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Conflict of interest

None declared.

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Notes

1. It appears in the balance of microscopic angular momentum [4].
2. For a proof we refer the reader to Noll [2] and Lehoucq and Lilienfeld-Toal [30].
3. As an example, consider the Gaussian distribution with zero mean (it satisfies both equation (30) and equation (26)). The second moment is not zero and equals σ^2.

4. Note that in general the volume of the particle system can not be uniquely defined. Often it is introduced for homogeneous states with the known constant-in-space density.

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