On consistent definitions of momentum and energy fluxes for molecular dynamics models with multi-body interatomic potentials

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Abstract
Results from molecular dynamics simulations often need to be further processed to understand the physics on a larger scale. This paper considers the definitions of momentum and energy fluxes obtained from a control-volume approach. To assess the validity of these defined quantities, two consistency criteria are proposed. As examples, the embedded atom potential and the Tersoff potential are considered. The consistency is verified using analytical and numerical methods.

Keywords: energy flux, momentum, Tersoff potential

1. Introduction
Molecular dynamics (MD) plays a unique role in the modeling and simulation of modern material science problems [1, 2]. In principle, at this level, it is convenient to introduce lattice structures and material defects and then study their implications for the overall mechanical and thermal properties. Examples include crack propagation, dislocation dynamics, energy conduction, etc. An important step in MD-based simulations is the calculation of quantities of interest based on particle trajectories. In particular, this method provides a connection between molecular trajectories and processes on macro- and mesoscopic scales.

The main purpose of this paper is to discuss consistent definitions of momentum and energy fluxes, both of which are essential components of continuum thermoelasticity models [3] and micro-polar models [4]. Computation of mechanical quantities from a molecular-level...
description is by no means a new concept. Perhaps the earliest works date back to Clausius and Maxwell [5–7] in 1870. Thanks to recent papers [8–14], many interesting issues have been brought to light. The current paper does not attempt to review these important contributions. Instead, we choose to address the issue of consistency to a greater extent. More specifically, we consider consistency on two levels. First, these definitions should be consistent with fundamental conservation laws. Such consistency can be ensured by following the Irving–Kirkwood approach [15], an example of which is Hardy’s derivation [16, 17]. Hardy’s approach has been implemented and improved upon in various different ways by several groups [18–24]. In this paper, however, we follow the control-volume approach [25], which is typically the starting point for deriving a continuum mechanics model. As a result, we obtain expressions for the momentum flux—the traction and the energy flux for the interfaces between the control volumes, which can be viewed as a finite-volume representation of the fundamental conservation laws.

Meanwhile, it is well known that even when the fundamental conservation laws are obeyed, there are still ambiguities in defining these continuum quantities [26]. More specifically, the expressions depend on how the interatomic forces and energy are partitioned among the atoms. This is clearly an alarming issue, and has motivated us to postulate a second level of consistency: i.e. consistency with the continuum limit. For crystalline solids, the continuum limit exists in the form of elastic wave equations, augmented with the Cauchy–Born rule [27–29]. The Cauchy–Born rule does not in principle depend on how the force and energy are decomposed. As a result, it provides an alternative guideline for the consistency check. In this paper, we formulate this criterion and examine the consistency both analytically and numerically.

For MD models with pairwise interaction, the calculation of elastic stress, or traction (the projection of the stress to a specific interface) is relatively easy. For multi-body interactions, however, the issue is much more complicated [18, 26, 30, 31]. On one hand, the formulas that are directly generalized from pair potentials may not satisfy the consistency criteria postulated here. On the other hand, although in principle one can write the interatomic potential as the sum of pairwise, three-body and four-body interactions, etc., and derive the stress and energy flux following conservation laws, many models, such as the embedded atoms model (EAM) [32] and the Tersoff potential [33], are not written in this form. Therefore, more explicit formulas pertinent to these particular function forms are needed. Finally, even though several formulas have been derived based on conservation laws [18, 26, 31], the second consistency criterion has not been evaluated.

To address the issues of consistency with sufficient specificity, we consider two concrete examples: EAM [32] and the Tersoff potential [33], which are among the most popular empirical potentials in modern molecular simulations. For each of these two models, we discuss how to compute the traction and energy flux within the molecular simulation. The consistency at both levels is carefully assessed. In particular, for the EAM potential, consistency with the Cauchy–Born rule is theoretically verified for any arbitrary deformation gradient. For the Tersoff potential, consistency is verified via numerical tests. Furthermore, for the Tersoff potential, we provide a pseudo-code for the calculation of the traction and energy flux to help interested readers to implement the formulas.

The paper is organized as follows. First, we introduce the general framework for the control-volume approach and demonstrate how the traction and energy flux arise under this framework. Then, we focus on the explicit expressions for the traction and energy flux for the EAM and Tersoff potentials. The consistency criteria are discussed in sections 2.3 and 3. In the appendix, we provide the pseudo-code for the Tersoff potential.
2. Derivation of the traction and energy flux

As is customary, our definition of all the quantities is based on the coordinates and velocities of the atoms, denoted here as $x_i(t)$ and $v_i(t) = \dot{x}_i(t)$. The trajectory of the atoms is determined from the molecular dynamics (MD) model,

$$m_i \ddot{x}_i = f_i, \quad f_i = -\frac{\partial V}{\partial x_i}.$$  

(1)

Here, $V$ is an empirical potential.

The main ingredient in deriving molecular expressions for the stress and energy fluxes is to follow fundamental conservation laws, which are the mathematical foundation of many continuum mechanics models. The general framework was put forward by Irving and Kirkwood [15] and by Hardy [16]. We refer readers to [18, 21, 22, 26, 30, 31, 34] for a thorough introduction, as well as recent progress and applications. In the present approach, however, we follow a control-volume approach, which is a discrete representation of the conservation laws [35]. More specifically, we divide the system into separate cells, each denoted by $\Omega_{\alpha}$, as illustrated in figure 1. Defining these cells will provide us with a means to extract average physical quantities.

In the finite volume formulation, which was first proposed in [25] for MD models, we can define the total momentum in the cell $\Omega_{\alpha}$,

$$p_{\alpha}(t) = \sum_{i \in \Omega_{\alpha}} m_i v_i(t).$$  

(2)

Here, we follow the reference (Lagrangian) coordinate. Namely, the notation $i \in \Omega_{\alpha}$ indicates that the reference position of the $i$th atom is in the cell $\Omega_{\alpha}$. Our choice is the same as the material frame used in [22], while most other derivations are based on current (Eulerian) coordinates. In particular, the Hardy formalism would yield the Piola–Kirchhoff stress, and the connection to the Cauchy stress has been examined in [22].

Similarly, the local energy is defined as

$$E_{\alpha}(t) = V_{\alpha} + \sum_{i \in \Omega_{\alpha}} \frac{p_i^2}{2m_i},$$  

(3)

where $V_{\alpha}$ is the potential energy in the domain $\Omega_{\alpha}$, whose definition will later be made more precise.
With the local momentum and energy selected based on the position and velocity of the atoms, we now seek to define a momentum flux (traction) and energy flux between the cell \( \Omega_\alpha \) and a neighboring cell \( \Omega_\beta \). We denote the traction and energy flux from the cell \( \Omega_\alpha \) to the cell \( \Omega_\beta \) as \( t_{\alpha,\beta} \) and \( q_{\alpha,\beta} \), respectively. Similar to most previous works, we emphasize the compatibility of these molecular expressions with the MD model. In addition, the fundamental conservation laws are

\[
\frac{d}{dt} p_\alpha(t) = \sum_{\beta} t_{\alpha,\beta}, \quad \frac{d}{dt} E_\alpha(t) = \sum_{\beta} q_{\alpha,\beta},
\]

together with the properties \( t_{\alpha,\beta} = -t_{\beta,\alpha} \) and \( q_{\alpha,\beta} = -q_{\beta,\alpha} \). Finally, for an empirical potential with short-range interactions, \( t_{\alpha,\beta} \) and \( q_{\alpha,\beta} \) should only depend on the atoms near the interface between \( \Omega_\alpha \) and \( \Omega_\beta \) so that they can be associated with the flux across the interface.

In general, for the momentum balance, the key ingredient to achieve these properties is a decomposition of the force,

\[
f_i = \sum_j f_{ij},
\]

with the property that \( f_{ij} = -f_{ji} \). This, however, does not imply that the interatomic interaction is pairwise. In fact, the force \( f_{ij} \) may depend on other atoms.

Combining (2) and (4), we find that

\[
\frac{d}{dt} p_\alpha(t) = \sum_{i \in \Omega_\alpha} \sum_j f_{ij}.
\]

Note that due to the asymmetry of \( f_{ij} \), we have \( \sum_{i \in \Omega_\alpha} \sum_{j \in \Omega_\alpha} f_{ij} = 0 \). As a result, we can restrict \( j \) to outside of \( \Omega_\alpha \),

\[
\frac{d}{dt} p_\alpha(t) = \sum_{i \in \Omega_\alpha} \sum_{j \not\in \Omega_\alpha} f_{ij},
\]

which naturally leads to a definition of the traction,

\[
t_{\alpha,\beta} = \sum_{i \in \Omega_\alpha} \sum_{j \in \Omega_\beta} f_{ij}.
\]

This molecular expression for the traction is consistent with Cauchy’s direct intuition that traction acting on an internal surface stems from the bonding forces across the interface, which was later extended to dynamics problems [8].

The traction defined this way clearly satisfies the conditions listed above. Meanwhile, for the energy balance, the difficulty lies in dividing the potential energy among the atoms. We need to define energy \( V_i \), such that

\[
V = \sum_i V_i.
\]

Once we have this energy partition at hand, we define

\[
V_\alpha = \sum_{i \in \Omega_\alpha} V_i.
\]

Another important issue, as raised by Admal and Tadmor [31], is that the force/energy decomposition is generally not unique. We will defer this discussion to section 3 where we discuss the second-level consistency. In the next two subsections, we will discuss the derivations for two specific empirical potentials.
2.1. The embedded atom potential

The first model to be considered is EAM [32]:

\[
V_{\text{EAM}} = \frac{1}{2} \sum_{1 \leq i \leq N} \sum_{1 \leq j \leq N, j \neq i} \varphi(r_{ij}) + \sum_{1 \leq l \leq N} E(\rho_l), \quad \rho_l = \sum_{1 \leq j \leq N, j \neq l} \rho(r_{lj}).
\] (9)

Here, we have adopted the usual notation in molecular simulations: \( r_{ij} = r_i - r_j \) and \( r_{ij} = |r_{ij}| \). The function \( \rho \) represents the influence of local electron density and because of the nonlinearity of the function \( E \), the interaction has a multi-body nature.

2.1.1. The definition of the traction.

For the EAM potential (9), the force on atom \( i \) can be obtained with direct calculations, and is given by

\[
f_i = \sum_{j \neq i} \left\{ \varphi'(r_{ij}) + \rho'(r_{ij}) \left[ E'(\rho_i) + E'(\rho_j) \right] \right\} \frac{r_{ij}}{r_{ij}},
\] (10)

where \( \varphi' \), \( \rho' \) and \( E' \) indicate derivatives of \( \varphi \), \( \rho \) and \( E \), respectively. The most commonly used (and perhaps most natural) force decomposition is as follows:

\[
f_{ij} = -\left\{ \varphi'(r_{ij}) + \rho'(r_{ij}) \left[ E'(\rho_i) + E'(\rho_j) \right] \right\} \frac{r_{ij}}{r_{ij}}.
\] (11)

This clearly satisfies the two conditions in (4) and leads to the definition of the traction:

\[
t_{\alpha, \beta} = \sum_{i \in \Omega_{\alpha}} \sum_{j \in \Omega_{\beta}} -\left\{ \varphi'(r_{ij}) + \rho'(r_{ij}) \left[ E'(\rho_i) + E'(\rho_j) \right] \right\} \frac{r_{ij}}{r_{ij}}.
\] (12)

2.1.2. The definition of the energy flux.

To obtain the energy flux, we first choose

\[
V_i = \frac{1}{2} \sum_{j \neq i} \varphi(r_{ij}) + E(\rho_i).
\] (13)

For the pair interaction \( \varphi(r_{ij}) \), we split the energy among the two atoms equally. The second part comes from the embedded energy, and these energy terms clearly add up to the total potential energy \( V \), i.e. equation (7) is satisfied.

To continue, we start with (3) and calculate the time derivatives of the kinetic and potential energy as follows:

\[
\frac{d}{dt} \sum_{i \in \Omega} \frac{1}{2} m_i v_i^2 = \sum_{i \in \Omega} f_i \cdot v_i
\]

\[
= -\sum_{i \in \Omega} \sum_{j \neq i} \left[ E'(\rho_i) + E'(\rho_j) \right] \rho'(r_{ij}) \frac{r_{ij}}{r_{ij}} \frac{v_i}{r_{ij}} - \sum_{i \in \Omega} \sum_{j \neq i} \varphi'(r_{ij}) \frac{r_{ij}}{r_{ij}} \frac{v_i - v_j}{r_{ij}}.
\]

and,

\[
\frac{d}{dt} \sum_{i \in \Omega} V_i = \sum_{i \in \Omega} E'(\rho_i) \sum_{j \neq i} \rho'(r_{ij}) \frac{r_{ij}}{r_{ij}} \frac{v_i}{r_{ij}} - \sum_{i \in \Omega} E'(\rho_i) \sum_{j \neq i} \rho'(r_{ij}) \frac{r_{ij}}{r_{ij}} \frac{v_j}{r_{ij}}
\]

\[
+ \frac{1}{2} \sum_{i \in \Omega} \sum_{j \neq i} \varphi'(r_{ij}) \frac{r_{ij}}{r_{ij}} \frac{v_i}{r_{ij}} - \frac{1}{2} \sum_{i \in \Omega} \sum_{j \neq i} \varphi'(r_{ij}) \frac{r_{ij}}{r_{ij}} \frac{v_j}{r_{ij}}.
\]
Combining terms, we obtain
\[
\frac{d}{dt} \sum_{i \in \Omega_\alpha} \left( E_i + \frac{1}{2} m_i v_i^2 \right) = - \frac{1}{2} \sum_{i \in \Omega_\alpha} \sum_{j \neq i} \phi'(r_{ij}) \frac{r_{ij} \cdot (v_i + v_j)}{r_{ij}} \\
- \sum_{i \in \Omega_\alpha} \sum_{j \neq i} \left[ E'(\rho_j) \rho_j' r_{ij} \frac{r_{ij} \cdot v_i}{r_{ij}} + E'(\rho_i) \rho_i' r_{ij} \frac{r_{ij} \cdot v_j}{r_{ij}} \right].
\]

Now we can easily see that within the summation terms on the right-hand side, each term changes sign when the indices \( i \) and \( j \) are exchanged. Hence, we can restrict \( j \) to outside \( \Omega_\alpha \), and the energy flux can be defined as
\[
q_{\alpha,\beta} = \frac{1}{2} \sum_{i \in \Omega_\alpha} \sum_{j \in \Omega_\beta} \phi'(r_{ij}) \frac{r_{ij} \cdot (v_i + v_j)}{r_{ij}} - \sum_{i \in \Omega_\alpha} \sum_{j \in \Omega_\beta} \left[ (E'(\rho_i) v_j + E'(\rho_j) v_i) \cdot \frac{r_{ij}}{r_{ij}} \right].
\]

It can be directly verified that this energy flux satisfies all of the requirements listed in the previous section.

**Remark 1.** In the case when \( E \equiv 0 \), i.e. the EAM potential is reduced to a pair potential, the energy flux can be written in compact form
\[
q_{\alpha,\beta} = \frac{1}{2} \sum_{i \in \Omega_\alpha} \sum_{j \in \Omega_\beta} f_{ij} \cdot (v_i + v_j).
\]

Unfortunately, for multi-body interactions, this formula is no longer correct and should not be used in practice. This can be seen from (14).

### 2.2. The Tersoff potential

Another important empirical potential is the Tersoff potential \([33, 36]\), consisting of a pairwise interaction and a multi-body interaction:
\[
E = \sum_{i \neq j} \left[ \frac{1}{2} f_{RC}(r_{ij}) + V_{ij} \right].
\]

Since the pair potential \( f_{RC}(r) \) is much easier to work with, we will only focus on the second part.

This model may seem to be a three-body interaction, but the interaction is actually among more neighboring atoms. Therefore, the total energy cannot be written as
\[
V = \sum_{i,j,k} V(r_i, r_j, r_k).
\]

Due to the complexity of the function forms, we will derive the formulas in several steps. The calculation is a bit lengthy, but we choose to show all the steps for the purpose of mathematical clarity. We are not aware of any simpler derivations.

Following \([33, 36]\), we express the multi-body term as follows:
\[
V_{ij} = \frac{1}{2} f_{AC}(r_{ij}) B(\xi_{ij}), \quad \xi_{ij} = \sum_{k \neq i,j} V_3(r_{ij}, r_{ik}),
\]

where we have defined
\[
V_3(u, v) = f_C(v) g(c(u, v)), \quad c(u, v) = \frac{u \cdot v}{uv}.
\]
We can compute the interatomic forces due to \( V_{ij} \) as follows:

\[
\frac{\partial V_{ij}}{\partial r_i} = \frac{1}{2} f_A'(r_{ij}) B(\zeta_{ij}) \frac{r_{ij}}{r_{ij}} + \frac{1}{2} f_A(r_{ij}) B'(\zeta_{ij}) \sum_{k \neq i, j} \left[ \frac{\partial V_3(r_{ij}, r_{ik})}{\partial r_{ij}} + \frac{\partial V_3(r_{ij}, r_{ik})}{\partial r_{ik}} \right],
\]

\[
\frac{\partial V_{ij}}{\partial r_j} = -\frac{1}{2} f_A(r_{ij}) B(\zeta_{ij}) \frac{r_{ij}}{r_{ij}} - \frac{1}{2} f_A(r_{ij}) B'(\zeta_{ij}) \sum_{k \neq i, j} \frac{\partial V_3(r_{ij}, r_{ik})}{\partial r_{ij}},
\]

\[
\frac{\partial V_{ij}}{\partial r_k} = -\frac{1}{2} f_A(r_{ij}) B'(\zeta_{ij}) \frac{\partial V_3(r_{ij}, r_{ik})}{\partial r_{ik}}, \quad \text{for any } k \neq i, j.
\]

One can easily check that

\[
\frac{\partial V_3(u, v)}{\partial u} = -\frac{f_C(v) g'(c) c}{u v} u + \frac{f_C(v) g'(c)}{v^2} v
def \overset{\text{def}}{=} s_{11}(u, v) u + s_{12}(u, v) v,
\]

\[
\frac{\partial V_3(u, v)}{\partial v} = \frac{f_C(v) g'(c) c}{u v} u + \left[ \frac{f_C(v) g'(c)}{v^2} - \frac{f_C(v) g'(c) c}{v^2} \right] v
def \overset{\text{def}}{=} s_{21}(u, v) u + s_{22}(u, v) v.
\]

(20)

Note that \( s_{12} = s_{21} \).

To arrive at an appropriate force decomposition of the form (4), we first make the observation that by properly reorganizing terms using (20), the equation (19) can be written as

\[
-\frac{\partial V_{ij}}{\partial r_i} = f_{ij,ij} + \sum_{k \neq i, k \neq j} f_{ij,ik},
\]

\[
-\frac{\partial V_{ij}}{\partial r_j} = f_{ij,ji} + \sum_{k \neq i, k \neq j} f_{ij,jk},
\]

\[
-\frac{\partial V_{ij}}{\partial r_k} = f_{ij,ki} + f_{ij,kj}, \quad \text{for } k \neq i, k \neq j,
\]

where

\[
f_{ij,ij} = -\frac{1}{2} f_A'(r_{ij}) B(\zeta_{ij}) \frac{r_{ij}}{r_{ij}} - \frac{1}{2} f_A(r_{ij}) B'(\zeta_{ij}) \sum_{k \neq i, j} (s_{11} + s_{12}) r_{ij},
\]

\[
f_{ij,ik} = -\frac{1}{2} f_A(r_{ij}) B'(\zeta_{ij}) (s_{12} + s_{22}) r_{ik},
\]

\[
f_{ij,ji} = -\frac{1}{2} f_A'(r_{ij}) B(\zeta_{ij}) \frac{r_{ij}}{r_{ij}} - \frac{1}{2} f_A(r_{ij}) B'(\zeta_{ij}) \sum_{k \neq i, j} (s_{11} + s_{12}) r_{ji},
\]

\[
f_{ij,jk} = \frac{1}{2} f_A(r_{ij}) B'(\zeta_{ij}) s_{12} r_{jk},
\]

\[
f_{ij,ki} = -\frac{1}{2} f_A(r_{ij}) B'(\zeta_{ij}) (s_{12} + s_{22}) r_{ki},
\]

\[
f_{ij,kj} = \frac{1}{2} f_A(r_{ij}) B'(\zeta_{ij}) s_{12} r_{kj}.
\]

These force components are defined in such a way as to ensure that (a) they are anti-symmetry, e.g. \( f_{ij,ik} = -f_{ij,ki} \), and (b) they are central forces, e.g. \( f_{ij,jk} \parallel r_{jk} \).
As a result, to obtain a force decomposition of the general form (4), the force on atom $i$ is written as follows:

$$f_i = \sum_{j \neq i} [f_{ij,ij} + f_{ji,ij}] + \sum_{j \in \Omega_a} \sum_{k \neq i, k \neq j} [f_{ij,ik} + f_{ji,ik}] + \frac{1}{2} \sum_{k \neq i, k \neq j} [f_{ik,ik} + f_{ki,ik} + f_{ik,lk} + f_{lk,ik}].$$

The first term is viewed as the direct interaction between atoms $i$ and $j$. The second term includes forces pointing to other atoms. The last term contains the forces due to other pairs of atoms that do not involve atom $i$. Note that the first two terms can be combined. However, we will keep them separate to make the following calculations more transparent. In addition, the factor $\frac{1}{2}$ takes into account double counting. It is also written this way to make later calculations easier.

### 2.2.1. Definition of the traction

We first derive the traction following (2). From (23), we start with the first sum,

$$\sum_{i \in \Omega_a} \sum_{j \neq i} [f_{ij,ij} + f_{ji,ij}] = \sum_{i \in \Omega_a} \sum_{j \in \Omega_a} [f_{ij,ij} + f_{ji,ij}].$$

So we define

$$t_{ij,\alpha}^{(2)} = \sum_{i \in \Omega_a} \sum_{j \neq i} [f_{ij,ij} + f_{ji,ij}].$$

(24)

The remaining terms in the force (23) will be combined as follows:

$$\sum_{i \in \Omega_a} \sum_{j \neq i, k \neq i, j \neq k} [f_{ij,ik} + f_{ji,ik} + f_{jk,ik} + f_{kj,ik}].$$

Note that for the third term in (23), we changed the index $\ell$ to $j$.

Let us use the fact that the summation over the following range is zero:

$$\sum_{i \in \Omega_a} \sum_{j \in \Omega_a} \sum_{k \in \Omega_a} = 0.$$

This can be verified by changing the indices $(i, j, k)$ to $(j, k, i)$ for the first term, and $(i, j, k)$ to $(k, j, i)$ for the second term. Thus, we can split the triple sum into three:

$$\sum_{i \in \Omega_a} \sum_{j \neq i, k \neq i, j \neq k} = \sum_{i \in \Omega_a} \sum_{j \in \Omega_a} \sum_{k \in \Omega_a} + \sum_{i \in \Omega_a} \sum_{j \in \Omega_a} \sum_{i \in \Omega_a} + \sum_{i \in \Omega_a} \sum_{j \in \Omega_a} \sum_{k \in \Omega_a}.$$

We collect the first two terms in the first sum and the last two terms in the third sum. We define

$$t_{ij,\alpha}^{(3)} = \sum_{i \in \Omega_a} \sum_{j \in \Omega_a} \sum_{k \in \Omega_a} [f_{ij,ik} + f_{ji,ik}] - \sum_{i \in \Omega_a} \sum_{j \in \Omega_a} \sum_{k \in \Omega_a} [f_{jk,ij} + f_{kj,ik}].$$

(25)

Meanwhile, the second sum can be simplified to

$$\sum_{i \in \Omega_a} \sum_{j \in \Omega_a} \sum_{k \in \Omega_a} [f_{ij,ik} + f_{jk,ik}].$$

The second and fourth terms cancel if we change the indices $(i, j, k)$ to $(k, j, i)$ in the second term. Therefore, all of the remaining terms can be written as

$$t_{ij,\alpha}^{(4)} = \sum_{i \in \Omega_a} \sum_{j \in \Omega_a} \sum_{k \in \Omega_a} [f_{jk,ij} + f_{kj,ik}] + \sum_{i \in \Omega_a} \sum_{j \in \Omega_a} \sum_{k \in \Omega_a} [f_{ij,ik} + f_{jk,ik}]$$

$$+ \sum_{i \in \Omega_a} \sum_{j \in \Omega_a} \sum_{k \in \Omega_a} [f_{ij,ik} + f_{ji,ik}].$$
Next, we define local energy as follows:

\[ V_i = \frac{1}{2} \sum_{j \neq i} [V_{ij} + V_{ji}] \]  

\[ (27) \]

The energy flux will be reflected in the rate of energy change. In particular, we will compute \( \frac{d}{dt} E_u(t) \). It is clear that the derivative of the kinetic energy is as follows:

\[ \frac{d}{dt} \sum_{i \in \Omega_u} \frac{p_i^2}{2m_i} = \sum_{i \in \Omega_u} \mathbf{f}_i \cdot \mathbf{v}_i = \sum_{j \neq i} [f_{ij,ij} + f_{ji,ij}] \cdot \mathbf{v}_i + \sum_{j \neq i} \sum_{k \neq i} [f_{ij,ik} + f_{ji,ik}] \cdot \mathbf{v}_i + \frac{1}{2} \sum_{k \neq i} [f_{ij,ik} + f_{ji,ik}] \cdot \mathbf{v}_i. \]  

\[ (28) \]

To calculate the change of the potential energy, we begin with

\[ \frac{1}{2} \frac{d}{dt} (V_{ij} + V_{ji}) = - \frac{1}{2} [f_{ij,ij} + f_{ji,ij}] \cdot \mathbf{v}_i - \frac{1}{2} \sum_{k \neq i, k \neq j} [f_{ij,ik} + f_{ji,ik}] \cdot \mathbf{v}_i - \frac{1}{2} [f_{ij,ji} + f_{ji,ji}] \cdot \mathbf{v}_j - \frac{1}{2} \sum_{k \neq i, k \neq j} [f_{ij,ki} + f_{ji,ki} + f_{ij,kj} + f_{ji,kj}] \cdot \mathbf{v}_k. \]  

\[ (29) \]

We now combine (29) and (28). We start by collecting similar terms. First, we have

\[ \sum_{i \in \Omega_u} \sum_{j \neq i} [f_{ij,ij} + f_{ji,ij}] \cdot \mathbf{v}_i - \frac{1}{2} [f_{ij,ij} + f_{ji,ij}] \cdot \mathbf{v}_i - \frac{1}{2} [f_{ij,ji} + f_{ji,ji}] \cdot \mathbf{v}_j \]

\[ = \sum_{i \in \Omega_u} \sum_{j \neq i} \frac{1}{2} \left( [f_{ij,ij} + f_{ji,ij}] \cdot \mathbf{v}_i - [f_{ij,ji} + f_{ji,ji}] \cdot \mathbf{v}_j \right) \]

\[ = \sum_{i \in \Omega_u} \sum_{j \neq i} \frac{1}{2} \left( [f_{ij,ij} + f_{ji,ij}] \cdot \mathbf{v}_i - [f_{ij,ji} + f_{ji,ji}] \cdot \mathbf{v}_j \right). \]

This expression can be further simplified to

\[ \sum_{i \in \Omega_u} \sum_{j \neq i} \frac{1}{2} [f_{ij,ij} + f_{ji,ij}] \cdot \mathbf{v}_i + \mathbf{v}_j. \]  

\[ (30) \]

However, this formula only holds for this part of the flux.
Here, we have used the fact that when $j \in \Omega_\alpha$, the terms in the bracket $(\cdot)$ would cancel. As a result, this flux is only dependent on atoms near the boundary of $\Omega_\alpha$. For two neighboring cells, we define $\Omega_\alpha$ and $\Omega_\beta$, 

$$
q_{\alpha,\beta}^j = \frac{1}{2} \sum_{i \in \Omega_\alpha} \sum_{j \in \Omega_\beta} \left\{ \left[ f_{i,j,i} + f_{j,i,j} \right] \cdot v_i - \left[ f_{i,j,i} + f_{j,i,j} \right] \cdot v_j \right\}. \tag{31}
$$

We proceed with the following terms:

$$
\sum_{i \in \Omega_\alpha} \sum_{j \not\in \Omega_\alpha} \sum_{k \neq i, k \neq j} \left\{ \left[ f_{i,j,i} + f_{j,i,k} \right] \cdot v_i - \frac{1}{2} \left[ f_{i,j,i} + f_{j,i,k} \right] \cdot v_i - \frac{1}{2} \left[ f_{i,j,k} + f_{j,i,k} \right] \cdot v_j \right\}
$$

$$
= \frac{1}{2} \sum_{i \in \Omega_\alpha} \sum_{j \not\in \Omega_\alpha} \sum_{k \neq i, k \neq j} \left\{ \left[ f_{i,j,i} + f_{j,i,k} \right] \cdot v_i - \left[ f_{i,j,k} + f_{j,i,k} \right] \cdot v_j \right\}
$$

$$
= \frac{1}{2} \sum_{i \in \Omega_\alpha} \sum_{j \not\in \Omega_\alpha} \sum_{k \neq i, k \neq j} \left\{ \left[ f_{i,j,i} + f_{j,i,k} \right] \cdot v_i - \left[ f_{i,j,k} + f_{j,i,k} \right] \cdot v_j \right\}. \tag{32}
$$

Again, we have used the same trick to eliminate the terms for which $j \in \Omega_\alpha$. Let us define the flux as

$$
q_{\alpha,\beta}^{ij} = \frac{1}{2} \sum_{i \in \Omega_\alpha} \sum_{j \in \Omega_\beta} \sum_{k \neq i, k \neq j} \left\{ \left[ f_{i,j,i} + f_{j,i,k} \right] \cdot v_i - \left[ f_{i,j,k} + f_{j,i,k} \right] \cdot v_j \right\}. \tag{33}
$$

The intuition is that these forces represent the interaction of the pair $(i, j)$ with a third atom in a neighboring cell.

We now collect the remaining terms. In the equation (28), we change the dummy index $\ell$ to $j$ and the remaining terms are

$$
\frac{1}{2} \sum_{i \in \Omega_\alpha} \sum_{j \not\in \Omega_\alpha} \sum_{k \neq i, k \neq j} \left\{ \left[ f_{i,j,k} + f_{j,i,k} + f_{k,j,i} + f_{k,j,j} \right] \cdot v_i - \left[ f_{i,j,k} + f_{j,i,k} + f_{j,i,k} + f_{j,i,j} \right] \cdot v_j \right\}
$$

We exchange the order of summation over $j$ and $k$,

$$
\frac{1}{2} \sum_{i \in \Omega_\alpha} \sum_{k \neq i} \sum_{j \neq k} \left\{ \left[ f_{i,j,k} + f_{j,i,k} + f_{k,j,i} + f_{k,j,j} \right] \cdot v_i - \left[ f_{i,j,k} + f_{j,i,k} + f_{j,i,k} + f_{j,i,j} \right] \cdot v_j \right\}
$$

$$
= \frac{1}{2} \sum_{i \in \Omega_\alpha} \sum_{k \neq i} \sum_{j \neq k} \left\{ \left[ f_{i,j,k} + f_{j,i,k} + f_{k,j,i} + f_{k,j,j} \right] \cdot v_i - \left[ f_{i,j,k} + f_{j,i,k} + f_{j,i,k} + f_{j,i,j} \right] \cdot v_j \right\}.
$$

As a result, the flux only involves atoms near the boundary. To this end, we consider the following:

$$
\frac{1}{2} \sum_{i \in \Omega_\alpha} \sum_{k \in \Omega_\beta} \sum_{j \neq k, j \neq k} \left\{ \left[ f_{i,j,k} + f_{j,i,k} + f_{k,j,i} + f_{k,j,j} \right] \cdot v_i - \left[ f_{i,j,k} + f_{j,i,k} + f_{j,i,k} + f_{j,i,j} \right] \cdot v_j \right\}. \tag{33}
$$
To incorporate these formulas into the algorithm, we split the summation into
\[
\frac{1}{2} \sum_{i \in \Omega_\alpha} \sum_{k \in \Omega_\beta} \sum_{j \in \Omega_\beta, j \neq i} \left[ f_{kj,ik} + f_{jk,ik} + f_{kj,ij} + f_{jk,ij} \right] \cdot v_i
\]
\[+ \frac{1}{2} \sum_{i \in \Omega_\alpha} \sum_{k \in \Omega_\beta} \sum_{j \in \Omega_\beta} \left[ f_{kj,ik} + f_{jk,ik} + f_{kj,ij} + f_{jk,ij} \right] \cdot v_i
\]
\[- \frac{1}{2} \sum_{i \in \Omega_\alpha} \sum_{k \in \Omega_\beta} \sum_{j \in \Omega_\beta} \left[ f_{ij,ki} + f_{ji,ki} + f_{ij,kj} + f_{ji,kj} \right] \cdot v_k
\]
\[- \frac{1}{2} \sum_{i \in \Omega_\alpha} \sum_{k \in \Omega_\beta} \sum_{j \in \Omega_\beta, j \neq k} \left[ f_{ij,ki} + f_{ji,ki} + f_{ij,kj} + f_{ji,kj} \right] \cdot v_k.
\] (34)

For the second and third terms, we define
\[
q_{III}^{\alpha,\beta} = \frac{1}{2} \sum_{i \in \Omega_\alpha} \sum_{k \in \Omega_\beta} \sum_{j \in \Omega_\beta, j \neq k} \left[ f_{kj,ik} + f_{jk,ik} + f_{kj,ij} + f_{jk,ij} \right] \cdot v_i
\]
\[- \frac{1}{2} \sum_{i,j \in \Omega_\alpha, j \neq i} \sum_{k \in \Omega_\beta} \left[ f_{ij,ki} + f_{ji,ki} + f_{ij,kj} + f_{ji,kj} \right] \cdot v_k
\] (35)

In addition, for the first sum, we can change \( j \to i, k \to j \) and \( i \to k \), and combine it with the fourth term:
\[
q_{IV}^{\alpha,\beta} = \frac{1}{2} \sum_{i \in \Omega_\alpha} \sum_{j \in \Omega_\beta} \sum_{k \in \Omega_\alpha} \left[ f_{ij,ik} + f_{ji,ik} + f_{ij,kj} + f_{ji,kj} \right] \cdot v_k
\]
\[- \frac{1}{2} \sum_{i \in \Omega_\alpha} \sum_{j \in \Omega_\beta} \sum_{k \in \Omega_\beta, j \neq k} \left[ f_{ij,ik} + f_{ji,ik} + f_{ij,kj} + f_{ji,kj} \right] \cdot v_k.
\] (36)

As the last step, we combine (32) and (36):
\[
q_{II}^{\alpha,\beta} + q_{IV}^{\alpha,\beta} = \frac{1}{2} \sum_{i \in \Omega_\alpha} \sum_{j \in \Omega_\beta} \sum_{k \in \Omega_\alpha} \left[ f_{ij,ik} + f_{ji,ik} \right] \cdot (v_i - v_k)
\]
\[- \frac{1}{2} \sum_{i,j \in \Omega_\alpha} \sum_{k \in \Omega_\beta} \left[ f_{ij,ji} \right] \cdot (v_j + v_k)
\]
\[+ \frac{1}{2} \sum_{i \in \Omega_\alpha} \sum_{j \in \Omega_\beta} \sum_{k \in \Omega_\beta} \left[ f_{ij,ik} + f_{ji,ik} \right] \cdot (v_i + v_k)
\]
\[- \frac{1}{2} \sum_{i \in \Omega_\alpha} \sum_{j \in \Omega_\beta} \sum_{k \in \Omega_\beta, j \neq k} \left[ f_{ij,ik} + f_{ji,ik} \right] \cdot (v_j - v_k).
\] (37)

The total flux is defined by combining equations (31), (35) and (37). These formulas might appear to be complicated, but the implementation is quite straightforward. In the appendix, we provide a pseudo-code for this algorithm.

2.3. Numerical tests

In this section, we will show numerical tests to verify the consistency of our definitions of the traction and energy flux with the conservation laws for the Tersoff potential.

In the computer experiments, we consider a system of silicon atoms with diamond structure. The lattice spacing is given by \( a_0 = 5.43183 \text{ Å} \) at zero temperature. The system
contains 24000 atoms with periodic boundary condition in all directions. The bulk is equally divided into 7 blocks in the horizontal direction. Following an MD simulation, we calculate the total momentum and energy in each block, along with the traction and energy flux across the interfaces of the blocks.

We choose a random initial velocity by setting the temperature of the system to be 30 K. Verlet’s algorithm [2] is used to generate the trajectory of the atoms. The time step $\Delta t$ is $5.395 \times 10^{-5}$ fs, which is much smaller than the time step typically used in molecular dynamics so that the numerical error plays no role. We examine the consistency by checking the following equations:

$$
t_{\alpha+\frac{1}{2}}(\tau) - t_{\alpha-\frac{1}{2}}(\tau) = \lim_{\Delta t \to 0} \frac{p_{\alpha}(\tau + \frac{1}{2} \Delta t) - p_{\alpha}(\tau - \frac{1}{2} \Delta t)}{\Delta t}
$$

$$
q_{\alpha+\frac{1}{2}}(\tau) - q_{\alpha-\frac{1}{2}}(\tau) = \lim_{\Delta t \to 0} \frac{E_{\alpha}(\tau + \frac{1}{2} \Delta t) - E_{\alpha}(\tau - \frac{1}{2} \Delta t)}{\Delta t},
$$

where $t_{\alpha+\frac{1}{2}} = t_{\alpha,\alpha+1}$ and $q_{\alpha+\frac{1}{2}} = q_{\alpha,\alpha+1}$ are the traction and energy flux between the $\alpha$th and $(\alpha + 1)$th cells.

The results, as summarized in figure 2, demonstrate the consistency with (38).

3. The consistency with continuum mechanics models

Having discussed consistency with the conservation laws, we now show another criterion for consistency. For a crystalline system with smooth displacement, it has been proven [28, 29] that
the corresponding continuum limit is the elasticity model with a constitutive relation provided by the Cauchy–Born rule [27, 37, 38].

As a result, the Cauchy–Born rule provides a crucial bridge between atomistic and continuum models. In addition, it is also an important part of some coarse-graining methods [39–42]. For the validity of the Cauchy–Born rule, the work of E and Ming established sharp criteria for both simple and complex lattices [29, 43]. Examples where the Cauchy–Born approximation may fail can be found in the work of Friesecke and Theil [38]. Finally, Cauchy–Born seems to have little success beyond crystalline materials.

A simple description of the Cauchy–Born rule is as follows: given the deformation gradient $A$, one can follow the uniform deformation gradient and define an affine displacement field from which the energy density $W_{CB}(A)$ is defined. $W_{CB}(A)$ is the potential energy per unit volume. Furthermore, the elastic stress is given by

$$P = \frac{\partial W_{CB}}{\partial A}.$$ (39)

This is known as the Piola–Kirchhoff stress. For any interface, the total traction per unit area would be given by $t_{CB} = \mathbf{P} \cdot \mathbf{n}$, with $\mathbf{n}$ being the unit normal. An important observation is that this definition, in its original form, requires no force or energy decomposition. Therefore, it provides a unique reference for comparison.

In order to demonstrate the comparison procedure with Cauchy–Born elasticity, let us consider the (1 0 0) plane in a bcc lattice. The projected atoms to the plane (0 0 1) are shown in figure 3. To keep our demonstration brief, we assume that the interaction is among nearest and second nearest neighbors. We compare the traction (per unit area) from the Cauchy–Born model with our definition for a system with a uniform but arbitrary deformation gradient. Fortunately, explicit expressions are available for the EAM model.

Due to the uniform deformation gradient $A$, the traction corresponding to the Cauchy–Born rule can be written as

$$P = \frac{1}{v_0} \sum_i f_{i0} \otimes \mathbf{X}_i,$$ (40)
and
\[ t_{CB} = \frac{1}{\nu_0} \sum_i f_{0i} X_i \cdot n, \]  
(41)

where \( \nu_0 \) is the volume per atom and \( X_i \) represents the reference (undeformed) position of the \( i \)th atom. The matrix \( a \otimes b \) is defined as \( (a \otimes b)_{ij} = a_i b_j \). Several comments need to be made to clarify this formula. First, the expression of the stress is derived from \( P = \frac{\partial}{\partial A} W_{CB} \), and it is equivalent to the virial stress. Second, the force component \( f_{0i} \) comes from the force decomposition (4). However, in principle, this decomposition is not needed. In its original form, the elasticity energy density is defined as
\[ W_{CB}(A) = \lim_{|\Omega| \to +\infty} \frac{V(A X_1, A X_2, \ldots, A X_N)}{|\Omega|}, \]  
(42)

where \( |\Omega| \) is the region occupied by the \( N \) atoms. This part is clearly independent of the energy or force decomposition. Upon taking the derivatives with respect to the deformation gradient, we obtain
\[ \frac{\partial}{\partial A} V(A X_1, A X_2, \ldots, A X_N) = -\sum_i f_i \otimes X_i, \]
which, with any force decomposition (4), becomes
\[ \frac{1}{2} \sum_i \sum_j f_{ij} \otimes X_{ij}, \]

where \( X_{ij} = X_i - X_j \).

This is where the force components can be introduced, and the formula is the better known expression of the Cauchy stress. At this point, any force decomposition would give the same result. However, if we further assume that for the uniformly deformed state, the decomposed force \( f_{ij} \) only depends on the relative positions of the \( i \)th and \( j \)th atoms, then it is sufficient to consider the atoms around the zeroth atom and simplify the expression to the form in (40).

For the EAM potential, the force decomposition (11) does exhibit this translational invariance, since for the uniformly deformed state the electron density is constant throughout the system.

Now let us return to the bcc lattice, shown in figure 3. The left panel illustrates the neighboring atoms around the zeroth atom. Using inversion symmetry, it is only necessary to consider the atoms with labels 0 ∼ 4. Furthermore, we used the open circles (0, 2 and 4) to indicate the atoms on the plane, and the filled circles are the atoms above or below the planes with distance \( a_0/2 \). In the latter case, we label the atoms as 1, \( \bar{1} \), 3, \( \bar{3} \), etc. From (40), the stress from the Cauchy–Born rule is given by
\[ P = \frac{2}{a_0^2} \left[ f_{00} \otimes X_{00} + f_{01} \otimes X_{01} + f_{01} \otimes X_{01} + f_{02} \otimes X_{02} + f_{03} \otimes X_{03} + f_{03} \otimes X_{03} \right. \]
\[ \left. + f_{04} \otimes X_{04} \right]. \]  
(43)

The projection to the interface with normal vector \( n = (1, 0, 0) \) is given by
\[ t_{CB} = \frac{1}{a_0^2} \left[ f_{01} + f_{01} + 2 f_{02} + f_{03} + f_{03} \right]. \]  
(44)

Meanwhile, the traction we defined in (12) can be calculated based on the right panel of figure 3. More specifically, we have the traction per unit area,
\[ t = \frac{1}{a_0^2} \left( f_{51} + f_{01} + f_{01} + f_{02} + f_{01} + f_{01} \right). \]  
(45)
Figure 4. Traction determined from the Cauchy–Born elasticity and our definition (left panel). The actual difference (right panel).

We chose these pairs since other pairs are replicas of these bonds. Again, due to the translational symmetry, we have $f_{51} = f_{10}$, and the consistency of the two formulas are confirmed. It appears that this argument also applies to other potentials, and the only requirement is that the force decomposition satisfy translation symmetry for a uniformly deformed state.

For complex lattices, the Cauchy–Born rule needs to be formulated with care. For clarity, we consider the case where there are two atoms in each primitive cell. In the Cauchy–Born rule, the first atom in each unit cell would follow the uniform deformation gradient $A$, while the displacement of the second atom in each cell will be donated by $p$ as an internal degree of freedom. The energy density in this case is written as $W(A, p)$. The continuum elastic energy is then obtained by a minimization step,

$$W_{CB}(A) = \min_{p} W(A, p).$$  (46)

Now, we consider the diamond structure of silicon modeled by the Tersoff potential. In this case, it would be a tedious procedure to verify the consistency by hand. Instead, we rely on a numerical test. For (46), we minimize $W(A, p)$ using the BFGS method [44]. Two tests, one with a uniform stretch (up to 5%) and the other with a uniform shear (up to 5%), are conducted and the results are shown in figure 4. Clearly, the agreement is on the order of machine precision.

To summarize briefly, we have shown that our definitions of traction for both the EAM and the Tersoff potential are consistent with the continuum mechanics models. In general, our consistency criterion at this level is stated as follows: for any uniform deformation gradient $A$ and any rational planes, the traction per unit area is the same as $Pn$, with $P$ being the stress derived from the Cauchy–Born rule.
Remark 2. The current approach does not rule out other definitions of the traction or stress. In fact, in [31], an elegant idea was presented to construct other force decompositions. Our calculations based on figure 3 suggest an additional constraint on the force decomposition, at least for simple lattices. That is, for a uniformly deformed system, $f_{ij}$ should exhibit translational invariance. For instance, the idea in [31] relies on a fictitious term that does not change the total energy, but gives different force decompositions. Suppose that this additional term is introduced uniformly along the interface, then the resulting traction would still be consistent. However, if it is only introduced to some of the atoms, then the traction may not be consistent according to our criterion.

Remark 3. Thus far, we have only discussed the consistency of the traction. For the energy flux and in the absence of heat conduction, we expect, as suggested by continuum mechanics models, that the energy flux only contains the convection part: $q = v^T P n$, where $v$ is the macroscopic velocity. In this case, our consistency criterion is stated as follows: for a system with any uniform deformation gradient $A$ and any uniform velocity $v$, the energy flux per unit area is the same as $v^T P n$, with $P$ being the stress derived from the Cauchy–Born rule. If the traction is consistent, then it is easy to see that the energy flux that we defined is also consistent in this sense since the velocity can be factored out from the energy flux (14). The same holds for the Tersoff potential as well. Further comparison would be in the context of heat conduction. Such effort has been undertaken in the works of [45, 46]. This issue, however, is generally very complicated and will not be addressed in the current paper.

4. A non-homogeneous example

Unlike the homogenous case, the definition of traction and energy flux for non-homogenous systems is difficult to validate. However, physically, when a system is at mechanical equilibrium, the traction should be zero across the whole sample. For the following example, we try to validate the definition of the traction in this particular setting: we consider a silicon system of dimension $20a_0 \times 20a_0 \times 20a_0$ with a void at the center. The radius of the void is $5a_0$. The system is equally divided into 23 blocks along the horizontal axis. Since each unit cell contains eight atoms, the block size has been chosen to be less than $a_0$. We initialize the system from a perfect diamond lattice and create the void by removing the atoms in the middle. The atomistic model is the Tersoff potential [36], and we minimize the system to an equilibrium state using the BFGS method [44]. The atoms at the boundary are left free. Figure 5 shows that the tractions are initially non-uniform along the $x$ axis. However, all the tractions settle to zero after the minimization steps. Therefore, they are consistent with the mechanical equilibrium state.

5. Summary and discussion

In this paper, we discussed the procedure for extracting average quantities based on the data from molecular dynamics simulations. In particular, we presented a control-volume representation of the fundamental conservation laws, from which the tractions and energy fluxes along the cell edges can be identified. Compared to formulations that are based on the continuous form of the conservation laws [11, 12, 16, 18–22, 26, 31, 41, 47], which usually lead to the divergence of the stress and energy flux, the control-volume approach directly yields the traction and energy flux along a plane. In this case, these formulas will be helpful in a multiscale method where the molecular dynamics model is directly coupled to a finite volume
The traction before and after minimization.

Figure 5. Numerical test for a non-homogeneous system. The traction before and after minimization.

approximation of the continuum model [41, 42, 48], or coarse-grained models where the coarse-grain variables are local averages of the momentum and energy [49]. Admal and Tadmor [31] also noted that, in general, the traction defined based on the sum of forces (e.g. (12)) is not equivalent to the stress (projected to the cell interface) derived from Hardy’s procedure unless the support of the weight function \( \phi_\varepsilon \) is set to zero (\( \varepsilon \to 0 \)).

We chose to work with the EAM and Tersoff models because of their practical importance. The formulas that we have derived may not be new. In particular, it is unclear if they coincide with the formulas derived by Admal and Tadmor [26, 31], since no explicit formulas were provided there for the Tersoff potential. Chen [18] already provided formulas based on the conservation of momentum and energy, but the Tersoff potential was mistreated as a three-body interaction. Further emphasis, however, is placed on whether these formulas are properly defined. This has become an issue, particularly when the non-uniqueness of the force decomposition was demonstrated in [26, 31]. In this paper, we proposed a two-level criteria to check the consistency of these defined quantities. We first require that the conservation laws be exactly satisfied. This procedure has to be repeated if a new interatomic potential is introduced to the MD model. More specifically, although the formulas (12) and (14) are valid for all EAM potentials, they may not hold for modified EAM potentials with different functional forms, such as those in [50, 51]. The second postulated condition is consistency with the continuum model, with the constitutive relation given by the Cauchy–Born rule. To our knowledge, this additional criterion has not been carefully examined in the literature. In this paper, we have verified that the expressions that we have derived are consistent with the Cauchy–Born rule. For simple lattices, our direct analysis revealed a checkable condition: the force decomposition \( f_{ij} \) is consistent with the Cauchy–Born rule if under uniform deformation it only depends on the relative position of the two atoms.

It is possible, however, that for every empirical potential, the natural force and energy decomposition, and the traction and energy fluxes defined based on such decomposition, satisfy both of the criteria listed here. However, at least by verifying the two conditions, one can use these formulas with confidence.

Finally, we have included in the appendix a pseudo-code for the Tersoff potential with the hope that MD practitioners might be interested in implementing the formulas developed in this paper.
Appendix

Pseudo-code for computing the traction (Tersoff Potential)

1: \( t_{\alpha,\beta} = 0; \)
2: \( t_{\beta,\alpha} = 0; \)
3: for \( i \neq j \) do
4:  \( \text{if } i \in \Omega_\alpha \text{ and } j \in \Omega_\beta \text{ and } \Omega_\alpha \cap \Omega_\beta \neq \emptyset \text{ then} \)
5:  \( t_{\alpha,\beta} \leftarrow t_{\alpha,\beta} + f_{ij,ij}; \)
6:  \( t_{\beta,\alpha} \leftarrow t_{\beta,\alpha} - f_{ij,ij}; \)
7:  \( \triangleright \text{From 1st and 2nd terms eq (24)} \)
8: end if
9: for \( k = 1, 2, \ldots, N \) do
10:  \( \text{if } k \in \Omega_\alpha \text{ and } k \neq i \text{ then} \)
11:  \( t_{\alpha,\beta} \leftarrow t_{\alpha,\beta} + f_{ij,ik} \cdot (v_j - v_k); \)
12:  \( t_{\beta,\alpha} \leftarrow t_{\beta,\alpha} - f_{ij,ik} \cdot (v_j - v_k); \)
13:  \( \triangleright \text{From the 1st and 2nd terms in eq (25)} \)
14: end if
15: end for
16: end for
17: if \( i \in \Omega_\alpha \text{ and } j \in \Omega_\alpha \) then
18: for \( k = 1, 2, \ldots, N \) do
19:  \( \text{if } k \in \Omega_\beta \text{ and } k \neq j \text{ then} \)
20:  \( t_{\alpha,\beta} \leftarrow t_{\alpha,\beta} + f_{ij,ik} \cdot (v_i + v_k); \)
21:  \( t_{\beta,\alpha} \leftarrow t_{\beta,\alpha} - f_{ij,ik} \cdot (v_i + v_k); \)
22:  \( \triangleright \text{From equations (31)} \)
23: end if
24: end for
25: end if
26: end for

Pseudo-code for computing the energy flux (Tersoff Potential)

1: \( q_{\alpha,\beta} = 0; \)
2: \( q_{\beta,\alpha} = 0; \)
3: for \( i \neq j \) do
4:  \( \text{if } i \in \Omega_\alpha \text{ and } j \in \Omega_\beta \text{ and } \Omega_\alpha \cap \Omega_\beta \neq \emptyset \text{ then} \)
5:  \( q_{\alpha,\beta} \leftarrow q_{\alpha,\beta} + f_{ij,ij} \cdot (v_i + v_j); \)
6:  \( q_{\beta,\alpha} \leftarrow q_{\beta,\alpha} - f_{ij,ij} \cdot (v_i + v_j); \)
7:  \( \triangleright \text{From equations (31)} \)
8: end if
9: for \( k = 1, 2, \ldots, N \) do
10:  \( \text{if } k \in \Omega_\alpha \text{ and } k \neq i \text{ then} \)
11:  \( q_{\alpha,\beta} \leftarrow q_{\alpha,\beta} + f_{ij,ik} \cdot (v_j - v_k); \)
12:  \( q_{\beta,\alpha} \leftarrow q_{\beta,\alpha} - f_{ij,ik} \cdot (v_j - v_k); \)
13:  \( \triangleright \text{From the 1st and 2nd terms in eq (37)} \)
14: end if
15: \( \text{if } k \in \Omega_\beta \text{ and } k \neq j \text{ then} \)
16:  \( q_{\alpha,\beta} \leftarrow q_{\alpha,\beta} + f_{ij,ik} \cdot (v_i + v_k); \)
17:  \( q_{\beta,\alpha} \leftarrow q_{\beta,\alpha} - f_{ij,ik} \cdot (v_i + v_k); \)
18:  \( \triangleright \text{From the 3rd and 4th terms in eq (37)} \)
19: end if
20: end for
end if
end for

if \( i \in \Omega_\alpha \) and \( j \in \Omega_\alpha \) then
for \( k = 1, 2, \ldots, N \) do
if \( k \in \Omega_\beta \) and \( k \neq j \) then
\[
q_{\alpha,\beta} \leftarrow q_{\alpha,\beta} + 2 \left[ f_{ij,ik} + f_{ij,jk} \right] \cdot v_k; \quad \text{From the 2nd term in (35)}
\]
\[
q_{\beta,\alpha} \leftarrow q_{\beta,\alpha} - 2 \left[ f_{ij,jk} + f_{ij,jk} \right] \cdot v_k; \quad \text{From the 1st term in (35)}
\]
end if
end for
end if
end for

\[
q_{\alpha,\beta} \leftarrow q_{\alpha,\beta}/2.
\]

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