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Heat flux expressions that satisfy the conservation laws in atomistic system involving multibody potentials

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ABSTRACT

Heat flux expressions are derived for multibody potential systems by extending the original Hardy's methodology and modifying Admal & Tadmor's formulas. The continuum thermomechanical quantities obtained from these two approaches are easy to compute from molecular dynamics (MD) results, and have been tested for a constant heat flux model in two distinctive systems: crystalline iron and polyethylene (PE) polymer. The convergence criteria and affecting parameters, i.e. spatial and temporal window size, and specific forms of localization function are found to be different between the two systems. The conservation of mass, momentum, and energy are discussed and validated within this atomistic–continuum bridging.

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1. Introduction

The success of continuum mechanics on predicting material response and failure in the macroscopic length scale is undeniable. Accompanied with the development of new techniques of reducing feature size, the applicability of continuum mechanics to fine scale phenomena attracts increasing attention. There is a growing need to interpret continuum concepts and laws in terms of atomistic/molecular behaviors to extend the concepts of continuum mechanics such as stress and strain to nano-scale. Classical molecular dynamics (MD) simulations have been widely used to capture the microscopic behaviors with atomistic resolution. Even though classical MD cannot resolve the electronic degrees of freedom, which is critical for understanding chemical reactions, bond breaking, and some of other fundamental aspects of atomic interactions, it can address the interaction of up to millions of atoms with satisfying accuracy thus being well suited to investigate nano-scale phenomena [1–3]. In MD simulations, the trajectories of interacting atoms are computed based on Newton's laws of motion, where the force on each atom is obtained from the spatial derivative of the interatomic potential energy.

The atomistic variables retrieved from MD simulations have been attempted to interpret the continuum quantities, in order to enable the multiscale linkage between microscopic and macroscopic scales in either hierarchical or concurrent modeling [4–12]. Virial stress by Clausius [13] and Maxwell [14,15] is probably the first attempt to derive microscopic definitions of stress tensor through the so-called virial theorem. Virial stress has been widely used in atomistic simulations due to its simple form and ease of computation. Irving and Kirkwood [16] developed point-wise stress tensor and heat flux vector as a statistical average of atomistic variables in their classical paper on the equations of hydrodynamics. However,

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the definitions of stress and heat flux are difficult to implement in atomistic simulations because the formulation involves a series expansion of the Dirac delta function and the probability density distribution function of the dynamic ensemble which is usually not known *a prior*. In order to obtain the stress and heat flux fields from MD simulations of non-equilibrium systems, Hardy [17,18] established conservation laws in which continuum thermomechanical fields are defined in terms of atomistic quantities through a localization function. The so-called Hardy stress has arbitrary spatial resolution and is often used in atomistic simulations [19–22]. However, Hardy's formulation has been explicitly based on the assumption of pair interatomic potential. Zimmerman et al. [21,22] examined the conditions under which the formulas could be valid and extended Hardy's work to include embedded atom method (EAM) potentials. Chen [23] further attempted formulating the stress and heat flux expressions in Hardy's framework to include three-body potentials of the Tersoff type [24,25] and the Stillinger–Weber type [26]. Multibody potentials have been considered by Delph [27], who discussed the applicability of Hardy's approach in more general context. However, the ambiguity on how to distribute the total potential energy among the atoms still remains one of the difficulties to extend Hardy's formulation to general multibody potential systems.

Murdoch [28–32] developed stress and heat flux expressions in a similar manner with Hardy by directly taking spatial average of the atomistic equation of motion with a normalized weighting function. Note that, in this work, Murdoch also considered temporal averaging besides spatial averaging to identify the computed quantities with experimentally measured values that are local averages of molecular behaviors in both space and time. In contrast to Hardy's approach, Murdoch's approach does not explicitly restrict the type of interatomic potentials for the systems under study. However, the disadvantage is the multiple integration involved in the resulting expressions, which makes it comparably more computationally expensive to implement for MD simulations. Admal and Tadmor [33] adopted Murdoch's methodology to avoid the ambiguities of energy decomposition among the atoms. By conducting combined ensemble and spatial averaging, Admal and Tadmor developed stress and heat flux expressions suitable for atomistic modeling.

Due to the lack of consensus on the definitions of continuum thermomechanical quantities in terms of atomistic variables that satisfy the conservation equations, in this study, we will discuss and compare the thermomechanical expressions developed by different approaches, with special focus on the heat flux definitions from Hardy and Admal & Tadmor. In Section 2, we briefly recall Hardy's formalism and extend it to multibody potential systems in the similar manner as Delph [27]. The validity of the conservation of mass, momentum, and energy are examined in detail. In Section 3, the potential part of heat flux expression is proposed the same as Hardy's original formulae and that in Admal & Tadmor's work. The energy density expression can be derived from the conservation of energy and involves integration over time. In Section 4, constant heat flux MD models are established for a crystalline iron described by the EAM potential and a coarse-grained (CG) model of amorphous polyethylene (PE) polymer system which involves up to four-body potentials. The expressions from Hardy's and Admal & Tadmor's methodologies are employed to compute the heat flux vectors in the two systems. Balance of energy is also investigated numerically in Hardy's and Admal & Tadmor's frameworks.

2. Expressions of the thermomechanical quantities involving multibody potentials using Hardy's approach

Hardy's original work can be found in Refs. [17,18]. Here we apply a similar procedure to obtain the stress and heat flux expressions for multibody potential systems. The essence of Hardy's approach is to link the continuum and atomistic scales through a localization function, $\psi(\mathbf{x},t)$, which assigns weights to the atoms that contribute to the interested continuum quantities at the spatial point $\mathbf{x}$ and time t. Hardy defines mass density, $\rho(\mathbf{x},t)$, momentum density, $\mathbf{p}(\mathbf{x},t)$, and energy density, $e^h(\mathbf{x},t)$, as follows:

$$\rho(\mathbf{x},t) := \sum_i m^i \psi\left(\mathbf{r}^i - \mathbf{x}\right) \tag{2.1a}$$

$$\mathbf{p}(\mathbf{x},t) := \sum_i m^i \mathbf{v}^i \psi\left(\mathbf{r}^i - \mathbf{x}\right) \tag{2.1b}$$

$$\rho e^h(\mathbf{x},t) := \sum_i \left(\frac{1}{2} m^i \left(\mathbf{v}^i\right)^2 + \phi^i\right) \psi\left(\mathbf{r}^i - \mathbf{x}\right) \tag{2.1c}$$

where m^i, $\mathbf{v}^i$, $\mathbf{r}^i$, and ϕ^i are the mass, velocity, position, and potential energy of atom i. Superscript 'h' represents the thermomechanical expressions of Hardy's approach. The total potential energy of the system $\Phi = \sum_i \phi^i$. The continuum velocity, $\mathbf{v}(\mathbf{x},t)$, is given by

$$\mathbf{v}(\mathbf{x},t) := \rho(\mathbf{x},t)^{-1} \mathbf{p}(\mathbf{x},t) \tag{2.2}$$

The localization function, $\psi(\mathbf{x})$, has the dimension of inverse volume that satisfies $\int_{\mathbb{R}^3} \psi(\mathbf{x}) \mathrm{d}\mathbf{x} = 1$. It can also be proved that

$$\psi\left(\mathbf{r}^i - \mathbf{x}\right) - \psi\left(\mathbf{r}^j - \mathbf{x}\right) = -\mathbf{r}^{ij} \cdot \nabla B\left(\mathbf{x}; \mathbf{r}^i, \mathbf{r}^j\right) \tag{2.3}$$

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