Atomic-level stress calculation

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Summary

An atomistic level stress tensor is cast with physical clarity, based on the SPH method. The formulation is easier to implement compared to other stress tensors that has been widely used in atomistic analysis, and is validated by numerical examples. The present formulation is very robust and accuracy.

Introduction

Atomic-level stress calculation plays a very important role in comparisons of continuum predictions with atomistic simulations. It bridges the atomistic mechanics and the continuum mechanics. There are different ways to calculate stress in atomistic simulations. Pioneering work has been done in this filed by Born and Huang [1] who proposed the Cauchy-Born rule for homogeneous deformation. The widely used stress measure at the atomic scale is the virial stress [2], BDT stress or atomic stress [3], Lutsko stress [4, 5], and mechanical stress [6]. As pointed in [7], the virial, BDT, Lutsko and mechanical stresses, are not the Cauchy stresses or any other form of mechanical stresses. However, if the kinematics term in their expressions is thrown off, they are Cauchy stress with physical meaning. In this paper, we will not include the kinematics term in BDT and Lutsko stresses. BDT stress is put forward by Basinski, Duesbery, and Taylor [3], and is based on a volumetric partition of the homogeneous deformed bulk. BDT stress is defined as:

$$\sigma^{BDT}(\mathbf{r}) = \frac{1}{2\Omega^i}\sum_{j\neq i}\mathbf{r}_{ij}\otimes\mathbf{f}_{ij} \tag{1}$$

where Ω^i is the a small volume around an atom i, $\mathbf{r}_{ij}$ and $\mathbf{f}_{ij}$ are radial and force vectors from atom i to j, respectively. Theoretically, the above definitions are valid only for homogeneous system. We have proved that the BDT stress in eq. (1) is equivalent to the Cauchy-Born rule for homogeneous deformation [8].

The local stress proposed by Lutsko [4] and extended by Cormier et al. [5] is based on the local stress tensor of statistical mechanics. The Lutsko stress can be expressed as

$$\sigma^{Lutsko}(\mathbf{r}) = \frac{1}{2\Omega^{Avg}}\sum_{i}\sum_{j\neq i}\mathbf{r}_{ij}\otimes\mathbf{f}_{ij}l_{ij} \tag{2}$$

where Ω^{Avg} is the averaging volume, l_{ij} $(0 \leq l_{ij} \leq 1)$ denotes the fraction of the length of the $i-j$ bond lying inside the same averaging volume. For a homogeneously deformed

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system, σ^{Lutsko} approaches σ^{BDT} for large averaging volumes. Lutsko stress has been used to evaluate local elastic properties of grain boundaries in metals. Lutsko stress assumes that the stress state is homogenous in the averaging volume.

In this paper, a new atomistic stress is proposed, which is appropriate for both homogeneously and inhomogeneously deformations. The results are compared with the BDT atomic stress and the Lutsko stress.

The definition of the stress tensor

As we discussed in the previous section, there are lots of atomistic stress tensors. Here, we will give an atomistic tensor with physical clarity.

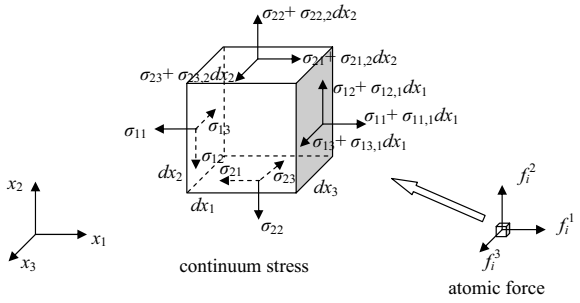

Figure 1: The definition of the stress tensor

Consider a discrete atomic system, the interatomic force on atom i is $\mathbf{f}_i$. As well known, the concept of stress is a continuum concept. Hence, to derive the atomistic stress, at first, we should make the discrete atomic system to be an equivalent continuum system. The same idea as the SPH method [9] will be employed here. SPH is very popular in astrophysics, where the real physical system is discrete. In order to avoid singularity, a local continuous field is generated by introducing a localized kernel function, which can serve as a smoothing interpolation field. If one wishes to interpret the physical meaning of the kernel function as the probability of a particle's position, one is dealing with a probabilistic method. Otherwise, it is only a smoothing technique. In this paper, we will smooth the discrete atomic force. In this case, the force per volume, i.e. the force density $\mathbf{g}(\mathbf{r})$, can be

written as

$$\mathbf{g}(\mathbf{r}) = \sum_i \mathbf{f}_i w(\mathbf{r} - \mathbf{r}_i, h) \tag{3}$$

where w is the smooth kernel function, the summation is over all the particles. Notice we do not have to divide by volume because the kernel is normalized to unite volume (w has the units of inverse volume), so the division by volume is effectively incorporate into w. A common choice for a kernel is a Gaussian, namely

$$w(\mathbf{x}, h) = \frac{1}{\left(\sqrt{\pi}h\right)^d} \exp\left(-\frac{\mathbf{x}^2}{h^2}\right) \tag{4}$$

where d is the number of spatial dimensions in the problem, and h is the smoothing length. We normalize the kernel such that its integral is unity. In general, the kernel function has to be a compact-supported positive function and its integral is unity. Moreover, as $h \to 0$, the kernel function should approach to $\delta(\mathbf{x})$. Other commonly used kernel functions include the cubic spline and the quartic spline. It is important to realize that although the summations are formally over all the particles, only a small number actually contribute because w can be chosen so that it falls off rapidly for appropriate h.

Now, in the equivalent continuum system, we consider an infinitesimal parallelepiped at point $\mathbf{r}$ with surfaces parallel to the coordinate planes (as shown in Fig. 1). In the infinitesimal volume, the volume of the infinitesimal parallelepiped is $dv = dx_1 dx_2 dx_3$, and the Cauchy stress at point $\mathbf{r}$ is σ, then, the resultant forces at point $\mathbf{r}$ in x_i direction are: $\sigma_{ji,j} dv$. As discussed before, the resultant forces at point $\mathbf{r}$ should be equal to $\mathbf{g}(r)dv$. Thus, we have

$$\frac{\partial}{\partial \mathbf{r}} \sigma(\mathbf{r})\, dv = \mathbf{g}(\mathbf{r})\, dv \tag{5}$$

Then, we have

$$\frac{\partial \sigma(\mathbf{r})}{\partial \mathbf{r}} = \sum_i \mathbf{f}_i w(\mathbf{r} - \mathbf{r}_i, h) \tag{6}$$

By using the Fourier transformation, equation (6) can be written as

$$\begin{aligned} i\mathbf{s} \cdot \hat{\sigma}(\mathbf{s}) &= -\sum_i \mathbf{f}_i \hat{w}(\mathbf{s}) e^{i\mathbf{s}\cdot\mathbf{r}_i} = -\sum_i \sum_{j \neq i} \mathbf{f}_{ij} e^{i\mathbf{s}\cdot\mathbf{r}_i} \hat{w}(\mathbf{s}) \\ &= -\tfrac{1}{2} \sum_i \sum_{j \neq i} \left[\mathbf{f}_{ij} e^{i\mathbf{s}\cdot\mathbf{r}_i} + \mathbf{f}_{ji} e^{i\mathbf{s}\cdot\mathbf{r}_j}\right] \hat{w}(\mathbf{s}) \\ &= i\mathbf{s} \cdot \tfrac{1}{2} \sum_i \sum_{j \neq i} \mathbf{r}_{ij} \otimes \mathbf{f}_{ij} \frac{e^{i\mathbf{s}\cdot\mathbf{r}_i} - e^{i\mathbf{s}\cdot\mathbf{r}_j}}{i\mathbf{s}\cdot\mathbf{r}_{ji}} \hat{w}(\mathbf{s}) \end{aligned} \tag{7}$$

Noting that

$$\frac{e^{i\mathbf{s}\cdot\mathbf{r}_i} - e^{i\mathbf{s}\cdot\mathbf{r}_j}}{i\mathbf{s}\cdot\mathbf{r}_{ji}} = e^{i\mathbf{s}\cdot\mathbf{r}_j}\int_0^1 e^{(i\mathbf{s}\cdot\mathbf{r}_{ji})c}dc \tag{8}$$

By carrying out the inverse transform of equation (7), the Cauchy stress of the atomic level can be obtained as

$$\begin{aligned}\sigma(\mathbf{r}) &= \tfrac{1}{2}\sum_i\sum_{j\neq i}\mathbf{r}_{ij}\otimes\mathbf{f}_{ij}\left\{\tfrac{1}{(2\pi)^3}\int_{V^s} e^{i\mathbf{s}\cdot\mathbf{r}_j}\int_0^1 e^{(i\mathbf{s}\cdot\mathbf{r}_{ji})c}dc\hat{w}(\mathbf{s})e^{-i\mathbf{s}\cdot\mathbf{r}}dV^s\right\}\\ &= \tfrac{1}{2}\sum_i\sum_{j\neq i}\mathbf{r}_{ij}\otimes\mathbf{f}_{ij}\left\{\int_0^1\left[\tfrac{1}{(2\pi)^3}\int_{V^s}\hat{w}(\mathbf{s})e^{i\mathbf{s}\cdot(\mathbf{r}_{ji}c+\mathbf{r}_j-\mathbf{r})}dV^s\right]dc\right\}\\ &= \tfrac{1}{2}\sum_i\sum_{j\neq i}\mathbf{r}_{ij}\otimes\mathbf{f}_{ij}\int_0^1 w[\mathbf{r}-(\mathbf{r}_{ji}c+\mathbf{r}_j)]dc\end{aligned} \tag{9}$$

As $h\to 0$, the kernel function $w(\mathbf{x})$ should approach to $\delta(\mathbf{x})$, and equation (9) will be reduced to

$$\sigma(\mathbf{r}) = \frac{1}{2}\sum_i\sum_{j\neq i}\mathbf{r}_{ij}\otimes\mathbf{f}_{ij}\delta[\mathbf{r}-(\mathbf{r}_{ji}k+\mathbf{r}_j)] \tag{10}$$

where $0\le k\le 1$. This singular expression can be used to obtain the average stress over any region of an atomistic ensemble, i.e. the Lutsko stress. For a region with volume Ω^{Avg}, by integrating equation (10), and divided by Ω^{Avg}, equation (2) is derived. The calculation of the Cauchy stress in equation (9) does not involve ad hoc specification of a relevant volume. The evaluation of the BDT stress (or the Cauchy-Born rule) for any set of atoms requires the identification of a proper volume whose extent is not always obvious.

Numerical examples

We now apply the new stress (9) to the case of a homogeneously deformed cubic, crystalline solid. The results for the inhomogeneously deformation are given in [8]. We consider a collection of 2048 atoms, initially on the sites of a fcc lattice and confined to a periodic cubic simulation cell at temperature T=0. A modified Lennard-Jones potential [10], which have energy and length parameters ε and σ, respectively, and the cut-off radius r=2.5 σ. The perfect fcc crystal has a lattice parameter of $a_0 = 1.5505\sigma$ and the corresponding energy per atom 7.45ε. We consider the simple case of uniform applied deformations, with corresponding strain tensor components $\varepsilon_{11} = \varepsilon_{22} = \varepsilon_{33} = 0.002$, the remain components are 0. In this case, the BDT stress (or the Cauchy-Born rule) is equal to the bulk stress. Fig. 2 show the magnitude of the stress σ_{11} at a observation point versus the radius $r_w$of the spherical averaging volume Ω^{Avg} (for the present stress, $h = 0.4r_w$). Fig. 3 shows the normalized stress σ_{11} at different observation points along the closed-packed [110] direction. In this case, we take the radius $r_w = 1.5a_0$. In these figures, the results of the present formulation are almost overlap with the bulk stress, and the Lutsko stress is

vibrated around the bulk stress. From these figures, we can find that the present stress is very robust and accuracy, while the Lutsko stress depends on the radius of the spherical averaging volume and the position. Moreover, for inhomogeneously deformation, the present stress can still get very better result than the other stress, that is given in [8]. The atomistic stress tensor derived in this paper will play an important role in the multiscale simulation and molecular dynamics.

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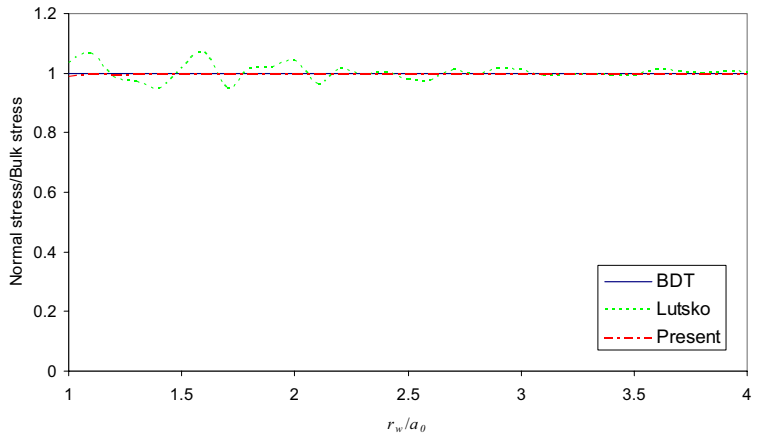

Figure 2: The effect of the radius of the averaging volume on stress for uniform deformation.

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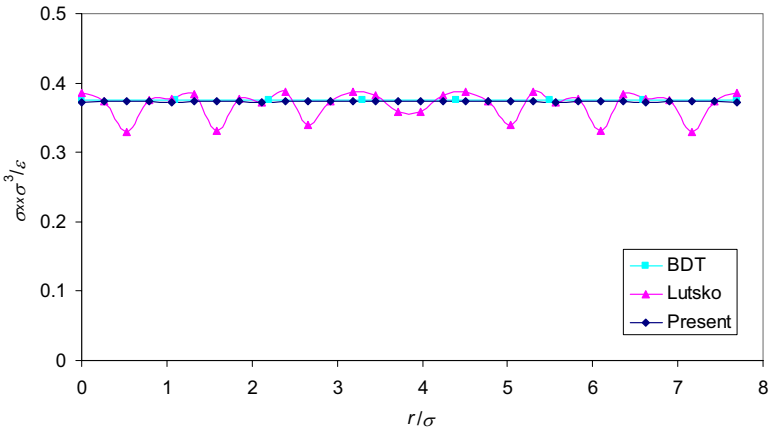

Figure 3: The stress at different point along [110] direction.

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