

## 0.1 notation

|              |   |   |
|--------------|---|---|
| position     | $\mathbf{x}$                                  | $= (x, y, z) = (x^x, x^y, x^z)$   |
| vector       | $\mathbf{r}_i$                                | $= (r_i^x, r_i^y, r_i^z), \mathbf{F} = (F^x, F^y, F^z)$   |
| basis vector | $\mathbf{e}^x$                                | $= (1, 0, 0), \mathbf{e}^y = (0, 1, 0), \mathbf{e}^z = (0, 0, 1)$   |
| tensor       | $(\mathbf{A} \circ \mathbf{B})^{\alpha\beta}$ | $= A^\alpha B^\beta$  |
|              | $\mathbf{A} \circ \mathbf{B}$                 | $= \sum_{\alpha, \beta=x, y, z} A^\alpha B^\beta \mathbf{e}^\alpha \circ \mathbf{e}^\beta$  |
|              | $\mathbf{P}$                                  | $= \sum_{\alpha, \beta=x, y, z} P^{\alpha\beta} \mathbf{e}^\alpha \circ \mathbf{e}^\beta, P^{\alpha\beta} = \mathbf{e}^\alpha \cdot \mathbf{P} \cdot \mathbf{e}^\beta.$ |

## 0.2 How to install it

Our implementation of the pressure profile is based on the lammmps-22Mar13. Therefore, from <http://lammmps.sandia.gov/tars/>, download appropriately older version than 22Mar13. Then, download our files from [9], and put all files and directories in "modified\_22Mar13" directory into "src" directory. Note that every files in CLASS2, MOLECULE, USER-CG-CMM, and USER-MISC directory have to be replaced from the original directories to those in modified\_22Mar13. To update the files for pair, bond, angle, etc in src directory, type

```
make yes-molecule yes-class2 yes-user-cg-cmm yes-user-misc
```

. After updating, you can make lammmps as usual. Then you can use the command "compute stress/spatial".

## 0.3 Syntax:

**compute ID all stress/spatial group-ID keyword values...**

- ID, group-ID are documented in compute command
- stress/spatial = style name of this compute command
- keyword = *sphere, plane, field*

*sphere* args = bin ( coord x y z *additional* )  
 bin = width bin (distance units)  
 x,y,z = center of spherical coordinate ( distance units )

*plane* args = dim bin (origin *additional* )  
 dim= x or y or z = axis along the slice.  
 origin= upper, lower, center, coord value  
 value=position of the origin (distance units )

*field* args = nx ny nz: number of bin along x,y,z axis respectively

## 0.4 Examples:

```
compute 99 all stress/spatial oil sphere 1.0
compute 88 all stress/spatial all sphere 1.0 coord 0.0 0.0 0.0
compute 77 all stress/spatial all field 40 40 80
compute 66 all stress/spatial oil plane 1.0 z
compute 55 all stress/spatial all plane 1.0 z origin 0.0
```

## 0.5 Description

From the microscopically defined local stress tensor  $\Sigma^{\alpha\beta}(\mathbf{x})$  defined in the appendix, we define the volume-averaged stress tensor given as

$$\Sigma^{\alpha\beta}(\mathcal{V}_i) = \frac{1}{|\mathcal{V}_i|} \int_{\mathcal{V}_i} d\mathbf{x} \Sigma^{\alpha\beta}(\mathbf{x}). \quad (1)$$

Depending on the shape of the volume, we can choose the three style *sphere*, *plane*, and *field*. The size of volumes are given  $4\pi[i^3 - (i-1)^3]*\text{bin}*\text{bin}*\text{bin}/3$ ,  $(\text{lx}*\text{ly}*\text{bin})$ , and  $\text{vol}/(\text{nx}*\text{ny}*\text{nz})$  respectively. Here  $\text{vol}$  is volume of the system and  $\text{lx}, \text{ly}, \text{lz}$  are box lengths in  $x, y, z$  axis respectively (See `thermo_style`).

For the *sphere* style, averaging-volume is given as  $\mathcal{V}_i = \{\mathbf{x} \mid (i-1)\text{bin} < |\mathbf{x} - \mathbf{o}| < i\text{bin}\}$  for  $i = 1, 2, 3, \dots, \text{nbin}$ . The maximum bin size "nbin" is determined as  $\text{nbin} = \text{MIN}(\text{lx}/2, \text{ly}/2, \text{lz}/2)/(\text{bin})$ . Here,  $\mathbf{o}$  represent the origin we choose. If we choose group-ID "all" without specifying "coord", then  $\mathbf{o} = \mathbf{0}$  is chosen. If we choose group-ID "all" and specify "coord x y z", then the origin will be specified as  $o^x=x, o^y=y$ , and  $o^z=z$ . If we specify some group-ID, then  $\mathbf{o}$  is chosen as a center of mass of the group. The normal and tangential stresses along the radial direction  $\Sigma^N$  and  $\Sigma^T$  are calculated. Then the center of bin  $((i-0.5)\text{bin})$ ,  $\Sigma^N, \Sigma^T$  are output. The algorithm used here is given in Ref. [6].

For the *plane* style, if you choose  $\text{dim}=z$ , the averaging-volume along  $z$  direction is given  $\mathcal{V}_i = \{\mathbf{x} \mid i\text{bin} < z - o^z < (i+1)\text{bin}\}$  for  $i = n_{\text{min}}, \dots, n_{\text{max}}$  with  $\text{nbin} = n_{\text{max}} - n_{\text{min}}$ . The maximum bin size "nbin" is determined as  $\text{nbin} = \text{lz}/(2\text{bin})$ . Here,  $o^z$  represent the origin we choose. If we choose group-ID "all" without specifying "coord", then  $o^z = 0$  is chosen. If we choose group-ID "all" and specify "coord z", then the origin will be specified as  $o^z=z$ . If we specify some group-ID, then  $o^z$  is chosen as a center of mass of the group. Three diagonal components along  $z$  direction  $\Sigma^{xx}, \Sigma^{yy}$  and  $\Sigma^{zz}$  are calculated. Then the center of bin  $((i+0.5)\text{bin})$  and these three components are output. The same style is applicable for the cases **dim=x,y**. The algorithm used here is given in Ref. [3]. This method is widely used to calculate the stress profile along the normal direction for the planer surface [7].

For the *field* style, the averaging-volume is given by  $\mathcal{V}_i = \{\mathbf{x} \mid i_\alpha \text{dx}_\alpha < x^\alpha - o^\alpha < (i_\alpha+1)\text{dx}_\alpha, \alpha = x, y, z\}$  where the label  $i$  is a vector given by  $i = (i_x, i_y, i_z)$  and the origin of the bin is set  $\mathbf{o} = (x_0, y_0, z_0)$ .  $\text{dx}_\alpha$  is calculated as  $\text{dx}_\alpha = \text{lx}/\text{nx}$ . Six components  $\Sigma^{xx}, \Sigma^{yy}, \Sigma^{zz}, \Sigma^{xy}, \Sigma^{xz}$  and  $\Sigma^{yz}$  are calculated. Then, the center of bin  $o^x + (i_x - 0.5)\text{lx}/\text{nx}$ ,  $o^y - (i_y + 0.5)\text{ly}/\text{ny}$ ,  $o^z - (i_z + 0.5)\text{dz}$  and these six components are output. **So far, we cannot implement the algorithm to shift the origin of the system for this style even though it might be necessary.**

In the same way of the compute group/group command, the force is calculated by looping over a neighbor list of pairwise interactions in addition to the bond, angle, dihedral and improper list. Thus it can be inefficient to compute this quantity too frequently

## 0.6 Output info:

This compute calculates a global array with the number of rows = nbin, and the number of columns = 1+2 (sphere), 1+3 (plane) and 3+6(field) respectively. The stress tensor are stored ascending order of  $i$  for *sphere* and *plane*. In the case of *field*, they are stored in the order given as  $(i_x, i_y, i_z) = (1,1,1), (1,1,2), \dots, (1,1, \text{nz}), (1,2,1), (1,2,2), \dots, (1,2, \text{nz}), \dots, (1, \text{ny}, \text{nz}), (2,1,1), (2,1,2), \dots, (\text{nx}, \text{ny}, \text{nz})$ . The position will be in distance unit The stress tensor will be in pressure unit.

## 0.7 Restriction:

**For the current version**, long-range interactions due to a `kpace_style` command are also NOT included because the systematic method itself have not been established yet. In addition, we cannot support "SHAKE" type constraint interaction, which is introduced by "fix\_shake" or "fix\_rigid" etc. These constraint interaction will be included in near future. Not all pair potentials can be evaluated in a pairwise mode as required by this compute. For example, 3-body potentials, such as Tersoff and Stillinger-Weber cannot be used. We did not systematically check EAM potentials yet.

newton = yes.

## 0.8 problem and future plan

As long as you use styles *plane* or *sphere* with the reasonable # of bins, you can calculate stress profile in endurable time. For the style *field*, however, even if you use same # of bins for each direction, because the number is multiplied as  $\text{nx}*\text{ny}*\text{nz}$ , the simulation will take much time. This is basically because of the allocation of big array for each time when the compute is called. This problem may be settled by making *fix ave/stress/spatial* program which allocates such a big array only at the beginning of simulation.

# A Theoretical background and notation

## A.1 Microscopic definition of pressure and stress tensor

Let us consider a Newtonian system composed of  $N_f$  particles. The equations of motion for  $N_f$  particles,  $\{\mathbf{r}_i, \mathbf{p}_i\}_{i=1}^{N_f}$ , in the Cartesian coordinate are written as  $\dot{\mathbf{p}}_i = -\nabla_i \Phi(\{\mathbf{r}_j\}_{j=1}^{N_f})$  and  $\dot{\mathbf{r}}_i = \mathbf{p}_i/m_i$ , with the total potential of  $\Phi(\{\mathbf{r}_i\})$

and mass of  $i$ -th particle of  $m_i$ . The microscopic representation of the pressure field  $\Phi(\{\mathbf{r}_j\}_{j=1}^{N_f})$  is given by

$$\frac{\partial}{\partial t} \left[ \sum_{i=1}^{N_f} \mathbf{p}_i(t) \delta(\mathbf{x} - \mathbf{r}_i(t)) \right] = -\nabla \cdot \mathbf{P}, \quad (2)$$

We consider the total potential  $\Phi(\{\mathbf{r}_j\}_{j=1}^{N_f})$  are given as a summation of the translationally symmetric  $m$ -body cluster potentials,  $U^{[m]}$  as  $\Phi(\{\mathbf{r}_j\}_{j=1}^{N_f}) = \sum_m \sum_{\langle j \rangle} U^{[m]}(\mathbf{r}_{\langle j \rangle})$  with  $\sum_{j_k \in \langle j \rangle} \nabla_{j_k} U^{[m]}(\mathbf{r}_{\langle j \rangle}) = \mathbf{0}$ . Here,  $\langle j \rangle$  includes all  $m$ -clusters labeled by  $\langle j \rangle = \{j_1, j_2, \dots, j_m\}$ , and the set of coordinates in the  $m$ -cluster  $\langle j \rangle$  is denoted as  $\mathbf{r}_{\langle j \rangle} \equiv \{\mathbf{r}_{j_1}, \dots, \mathbf{r}_{j_m}\}$ . Namely, we suppose the potential as follows

$$U^{[2]}(\{\mathbf{r}_{j_1}, \mathbf{r}_{j_2}\}) = V^2(r_{j_1 j_2}) \text{ pair} \quad (3)$$

$$U^{[3]}(\{\mathbf{r}_{j_1}, \mathbf{r}_{j_2}, \mathbf{r}_{j_3}\}) = V^3(\mathbf{r}_{j_2 j_1}, \mathbf{r}_{j_2 j_3}) \text{ angle} \quad (4)$$

$$U^{[4]}(\{\mathbf{r}_{j_1}, \mathbf{r}_{j_2}, \mathbf{r}_{j_3}, \mathbf{r}_{j_4}\}) = V^4(\mathbf{r}_{j_2 j_1}, \mathbf{r}_{j_2 j_3}, \mathbf{r}_{j_2 j_4}) \text{ dihedral, improper} \quad (5)$$

Then, the pressure field  $\mathbf{P}$  is represented as

$$\mathbf{P}(\mathbf{x}) = \sum_{i=1}^{N_f} \frac{\mathbf{p}_i \circ \mathbf{p}_i}{m_i} \delta(\mathbf{x} - \mathbf{r}_i) - \boldsymbol{\Sigma}(\mathbf{x}) \quad (6)$$

$$\boldsymbol{\Sigma}(\mathbf{x}) \equiv \sum_{m \geq 2} \sum_{\langle j \rangle} \sum_{k=1}^m \nabla_{j_k} U^{[m]}(\mathbf{r}_{\langle j \rangle}) \circ \int_{C_{j_l j_k}} d\ell \delta(\mathbf{x} - \ell). \quad (7)$$

Here,  $C_{j_l j_k}$ , is the integration contour connecting the  $j_l$ -th particle position  $\mathbf{r}_{j_l}$ , to  $j_k$ -th particle position  $\mathbf{r}_{j_k}$ . [1] The symbol of  $\circ$  denotes a dyadic product.

As discussed in Fig. 2 in our previous paper [6], there are two methods how to choose the set of contours for the many body potential  $m > 2$ . In Eq. (7), we have chosen the reference position  $j_l$  for each cluster  $\langle j \rangle$  and  $m - 1$  contours  $C_{j_l j_k}$  with  $j_k \neq j_l$  in the same way as the our previous paper. Note that we take  $m$  summation in (9), however the contribution from  $C_{j_l j_l}$  is equal to zero. Therefore we only have to calculate the contributions from  $m - 1$  contours.

Then stress tensor is written as

$$\boldsymbol{\Sigma}(\mathbf{x}) = - \sum_{m \geq 2} \sum_{\langle j \rangle} \mathbf{P}_{\langle j \rangle}^{[m]}(\mathbf{x}). \quad (8)$$

where,

$$\mathbf{P}_{\langle j \rangle}^{[m]}(\mathbf{x}) = \sum_{k=1}^m \mathbf{F}_{j_k}^{[m]}(\mathbf{r}_{\langle j \rangle}) \circ \int_{C_{j_l j_k}} d\ell \delta(\mathbf{x} - \ell), \quad (9)$$

where  $\mathbf{F}_{j_k}^{[m]}(\mathbf{r}_{\langle j \rangle}) \equiv -\nabla_{j_k} U^{[m]}(\mathbf{r}_{\langle j \rangle})$  is the force acting on the  $j_k$ -th particle in the  $m$ -cluster  $\langle j \rangle$ .

Hereafter, in order to simplify the expression, we use  $i$  and  $j$  instead of  $j_k$  and  $j_l$  in Eqs. (9), respectively, and the force on the  $i$ th particle in the  $m$ -cluster  $\langle j \rangle$  is denoted by  $\mathbf{F}_{i;j}$ , i.e., for  $\mathbf{F}_{i;j} \equiv \mathbf{F}_{j_k}^{[m]}(\mathbf{r}_{\langle j \rangle})$ . Thus, we can rewrite Eq. (9) as

$$\mathbf{P}_{\langle j \rangle}^{[m]}(\mathbf{x}) = \sum_{i=1, \dots, m(\neq j)} \mathbf{P}_{i;j}(\mathbf{x}) \quad (10)$$

where

$$\mathbf{P}_{i;j}(\mathbf{x}) \equiv \mathbf{F}_{i;j} \circ \int_{C_{j_i}} d\ell \delta(\mathbf{x} - \ell). \quad (11)$$

## References

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