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2.5 Choice of output

TRFDA comes with a wide range of output options. Although internally forces are calculated and stored only in vector form, TRFDA can output pairwise forces as vector or scalar values, and several derived quantities based on them.

A scalar pairwise force is computed as the magnitude of the vector pairwise force, same as in FDA, or as the magnitude of the pairwise force projected onto the distance vector between the two atoms, same as in [4]. In either case, the scalar value carries a sign indicating whether it is a repulsive (plus) or attractive (minus) force. If the angle between the vector pairwise force and the distance vector between the atoms is in the range (- $\Pi/2$, $\Pi/2$), the pairwise force is considered attractive. If the angle between the vector pairwise force and the distance vector between the atoms is in the range ($\Pi/2$, $3\,\Pi/2$), the pairwise force is considered repulsive. If the vector pairwise force is perpendicular to the distance vector, the pairwise force can be considered neither attractive nor repulsive and it is set to zero.

From the absolute values of the scalar pairwise forces acting on an atom, TRFDA can compute the sum and average as well as select the minimum or maximum. The sum of the absolute values of scalar pairwise forces acting on an atom i:

$$S_i = \sum_j |F_{ji}|$$

measures the stress acting on that atom. It is reminiscent of the calculation of stress from continuum models used in mechanical engineering. We denote the stress defined in Eq. 2 as *punctual stress*, emphasizing the action of the force on a dimensionless point instead of an area, which is here ill-defined. As a sum of forces, the punctual stress is expressed in units of force. Such a deviation from the typical definition of stress is also found for the atomic virial stress[10], expressed in units of energy, and stems from the difficulty of defining geometrical properties (area for punctual stress or volume for virial stress) at atomic level. For systems in equilibrium, the sum of scalar pairwise forces from Eq. 2 can converge to non-zero averages over time; in contrast, the sum of vector pairwise forces acting on a single atom i, typically computed in MD simulations, averages to zero in the same conditions. As opposed to the analysis of pairwise forces, which gives a very detailed view of their distribution in or between molecules, the punctual stress expresses in a simple way where pairwise forces accumulate and allows the detection of atomic-level "hot-spots".

For both pairwise forces and per atom quantities, the output consists of simple to parse text files. Their format allows an unlimited number of atoms, pairwise forces and simulation time steps, and is documented in the manual, which accompanies the code. We chose text as opposed to binary file formats to allow for loading the data in various analysis tools at the expense of the size of the files.

TRFDA can also write out scalar pairwise forces in the same format as FDA, preserving compatibility with the FDA R library[1]; however the results should be interpreted with care, as the 3- and 4-body interactions are expressed differently.

4

Shooting Log

Date: _____

Time: _____

Temp / Wind Direction: _____

Firearm Used: _____

Load Specifications

Bullet: _____

Powder / Charge Weight: _____

Primer: _____

Overall Length: _____

Group Size and Comments:

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GATE 2015

Praneeth A S (UG201110023)

B.Tech(Computer Science & Engineering)

Indian Institute of Technology Jodhpur

Jodhpur, Rajasthan 342011, India

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