

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 [19], 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 [16]; however the results should be interpreted with care, as the 3- and 4-body interactions are expressed differently.

2.6. Internal organization

TRFDA defines two groups of atoms between which pairwise forces are computed. A pairwise force is only computed when the two atoms belong to different groups, while pairwise forces between atoms of the same group are not computed. This allows, for example, interactions between a protein and a ligand to be computed efficiently. If the interactions inside the protein and ligand are also of interest, the two groups should comprise the same atoms, namely

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1. Understanding the eBook International Journal Of Mathematics And Computer Applications Research Ijmcarr
 - The Rise of Digital Reading International Journal Of Mathematics And Computer Applications Research Ijmcarr
 - Advantages of eBooks Over Traditional Books
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 - Exploring Different Genres
 - Considering Fiction vs. Non-Fiction
 - Determining Your Reading Goals
3. Choosing the Right eBook Platform
 - Popular eBook Platforms
 - Features to Look for in an International Journal Of Mathematics And Computer Applications Research Ijmcarr
 - User-Friendly Interface
4. Exploring eBook Recommendations from International Journal Of Mathematics And Computer Applications Research Ijmcarr
 - Personalized Recommendations
 - International Journal Of Mathematics And Computer Applications Research Ijmcarr User Reviews and Ratings
 - International Journal Of Mathematics And Computer Applications Research Ijmcarr and Bestseller Lists
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 - International Journal Of Mathematics And Computer Applications Research Ijmcarr eBook Subscription Services

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 - ePub, PDF, MOBI, and More
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 - International Journal Of Mathematics And Computer Applications Research Ijmcarr Enhanced eBook Features
- 7. Enhancing Your Reading Experience
 - Adjustable Fonts and Text Sizes of International Journal Of Mathematics And Computer Applications Research Ijmcarr
 - Highlighting and Note-Taking International Journal Of Mathematics And Computer Applications Research Ijmcarr
 - Interactive Elements International Journal Of Mathematics And Computer Applications Research Ijmcarr
- 8. Staying Engaged with International Journal Of Mathematics And Computer Applications Research Ijmcarr
 - Joining Online Reading Communities
 - Participating in Virtual Book Clubs
 - Following Authors and Publishers International Journal Of Mathematics And Computer Applications Research Ijmcarr
- 9. Balancing eBooks and Physical Books International Journal Of Mathematics And Computer Applications Research Ijmcarr
 - Benefits of a Digital Library
 - Creating a Diverse Reading Collection International Journal Of Mathematics And Computer Applications Research Ijmcarr
- 10. Overcoming Reading Challenges
 - Dealing with Digital Eye Strain
 - Minimizing Distractions
 - Managing Screen Time
- 11. Cultivating a Reading Routine International Journal Of Mathematics And Computer Applications Research Ijmcarr
 - Setting Reading Goals International Journal Of Mathematics And Computer Applications Research Ijmcarr
 - Carving Out Dedicated Reading Time
- 12. Sourcing Reliable Information of International Journal Of Mathematics And Computer Applications Research Ijmcarr
 - Fact-Checking eBook Content of International Journal Of Mathematics And Computer Applications Research Ijmcarr

- Distinguishing Credible Sources
- 13. Promoting Lifelong Learning
 - Utilizing eBooks for Skill Development
 - Exploring Educational eBooks
- 14. Embracing eBook Trends
 - Integration of Multimedia Elements
 - Interactive and Gamified eBooks

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