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 (- II/2, II/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 (II/2, 3 II/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:

$$S_i = \sum_{j} |F_{j+j}|$$

mechanical engineering. We denote the stress defined in Eq. 2 as pasternal 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 purse 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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Neutrosophic Sets and Systems, vol. 14/2016 K Mondal, S. Pramanik , F. Smarandache, S. K. De , I. Beg, M. A. Malik, A. Hassan, S. Broumi, P. J. M. Vera, Neutrosophic Sets and Systems has been created for publications on advanced studies in neutrosophy neutrosophic set neutrosophic logic neutrosophic probability neutrosophic statistics that started in 1995 and their applications in any field such as the neutrosophic structures developed in algebra geometry topology etc

Neutrosophic Operational Research, Vol. I Florentin Smarandache ,Mohamed Abdel-Basset,Yongquan Zhou,2017 This book treats all kind of data in neutrosophic environment with real life applications approaching topics as linear programming problem linear fractional programming integer programming triangular neutrosophic numbers single valued triangular neutrosophic number neutrosophic optimization goal programming problem Taylor series multi objective programming problem neutrosophic geometric programming neutrosophic topology neutrosophic open set neutrosophic semi open set neutrosophic continuous function cylindrical skin plate design neutrosophic MULTIMOORA alternative solutions decision matrix ratio system reference point method full multiplicative form ordinal dominance standard error market research and so on The selected papers deal with the alleviation of world changes including changing demographics accelerating globalization rising environmental concerns evolving societal relationships growing ethical and governance concern expanding the impact of technology some of these changes have impacted negatively the economic growth of private firms governments communities and the whole society Collected Papers. Volume VI Florentin Smarandache, 2022-01-15 This sixth volume of Collected Papers includes 74 papers comprising 974 pages on theoretic and applied neutrosophics written between 2015 2021 by the author alone or in collaboration with the following 121 co authors from 19 countries Mohamed Abdel Basset Abdel Nasser H Zaied Abduallah Gamal Amir Abdullah Firoz Ahmad Nadeem Ahmad Ahmad Yusuf Adhami Ahmed Aboelfetouh Ahmed Mostafa Khalil Shariful Alam W Alharbi Ali Hassan Mumtaz Ali Amira S Ashour Asmaa Atef Assia Bakali Ayoub Bahnasse A A Azzam Willem K M Brauers Bui Cong Cuong Fausto Cavallaro Ahmet evik Robby I

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reanu tefan VI du escu J Vimala Dan Valeriu Voinea Adem Yolcu Yongfei Feng Abd El Nasser H Zaied Edmundas Kazimieras Neutrosophic Sets and Systems, vol. 13/2016 Florentin Smarandache, Mumtaz Ali, Neutrosophic Sets and Zavadskas Systems has been created for publications on advanced studies in neutrosophy neutrosophic set neutrosophic logic neutrosophic probability neutrosophic statistics that started in 1995 and their applications in any field such as the neutrosophic structures developed in algebra geometry topology etc The Encyclopedia of Neutrosophic Researchers, 1st volume Florentin Smarandache, 2016-11-12 This is the first volume of the Encyclopedia of Neutrosophic Researchers edited from materials offered by the authors who responded to the editor s invitation The 78 authors are listed alphabetically The introduction contains a short history of neutrosophics together with links to the main papers and books Neutrosophic set neutrosophic logic neutrosophic probability neutrosophic statistics neutrosophic measure neutrosophic precalculus neutrosophic calculus and so on are gaining significant attention in solving many real life problems that involve uncertainty impreciseness vagueness incompleteness inconsistent and indeterminacy In the past years the fields of neutrosophics have been extended and applied in various fields such as artificial intelligence data mining soft computing decision making in incomplete indeterminate inconsistent information systems image processing computational modelling robotics medical diagnosis biomedical engineering investment problems economic forecasting social science humanistic and practical achievements Neutrosophic Sets and Systems, Vol. I Florentin Smarandache, Mumtaz Ali, This volume is a collection of ten papers written by different authors and co authors listed in the order of the papers F Smarandache Jun Ye M Shabir M Ali M Naz F Yuhua A A Salama S Vladutescu Y Guo A Sengur S Broumi P Chi and P Liu In first paper the author proposed Neutrosophic Measure and neutrosophic Integral Another Form of Correlation Coefficient between Single Valued Neutrosophic Sets and Multiple Attribute Decision Making Method is proposed in the second paper Soft Neutrosophic Group is studied in third paper In fourth paper Neutrosophic Example in Physics is discussed Similarly in fifth paper Filters via Neutrosophic Crisp Sets are discussed In paper six Commnication vs Information an Axiomatic Neutrosophic Solution is presented by the authors A Novel Image Segmentation Algorithm Based on Neutrosophic Filtering and Level Set is given in seventh paper Paper eight is about to Neutrosophic Crisp Points and Neutrosophic Crisp Ideals In the next paper Several Similarity Measures of Neutrosophic Sets are discussed The authors introduced An Extended TOPSIS Method for the Multiple Attribute Decision Making Problems Based on Interval Neutrosophic Sets in the last paper New Neutrosophic Sets via Neutrosophic Topological Spaces Wadei Al-Omeri, Florentin Smarandache, In Geographical information systems GIS there is a need to model spatial regions with indeterminate boundary and under indeterminacy Neutrosophic Sets and Systems, book series, Vol. 13, 2016 Florentin Smarandache, Mumtaz Ali, Abstract Contributors to current issue listed in papers order K Mondal S Pramanik F Smarandache M A Malik A Hassan S Broumi S K De I Beg A N H Zaied H M Naguib N Shah A A Salama M Eisa H E Ghawalby A E Fawzy M Sarkar S Dey T K Roy S Karatas C Kuru P J M Vera C F M Delgado M P

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Collected Papers. Volume XIV Florentin Smarandache, 2022-11-01 This fourteenth volume of Collected Papers is an eclectic tome of 87 papers in Neutrosophics and other fields such as mathematics fuzzy sets intuitionistic fuzzy sets picture fuzzy sets information fusion robotics statistics or extenics comprising 936 pages published between 2008 2022 in different scientific journals or currently in press by the author alone or in collaboration with the following 99 co authors alphabetically ordered from 26 countries Ahmed B Al Nafee Adesina Abdul Akeem Agboola Akbar Rezaei Shariful Alam Marina Alonso Fran Andujar Toshinori Asai Assia Bakali Azmat Hussain Daniela Baran Bijan Davvaz Bilal Hadjadji Carlos D az Bohorquez Robert N Boyd M Caldas Cenap zel Pankaj Chauhan Victor Christianto Salvador Coll Shyamal Dalapati Irfan Deli Balasubramanian Elavarasan Fahad Alsharari Yonfei Feng Daniela G fu Rafael Rojas Gualdr n Haipeng Wang Hemant Kumar Gianey Noel Batista Hern ndez Abdel Nasser Hussein Ibrahim M Hezam Ilanthenral Kandasamy W B Vasantha Kandasamy Muthusamy Karthika Nour Eldeen M Khalifa Madad Khan Kifayat Ullah Valeri Kroumov Tapan Kumar Roy Deepesh Kunwar Le Thi Nhung Pedro L pez Mai Mohamed Manh Van Vu Miguel A Quiroz Mart nez Marcel Migdalovici Kritika Mishra Mohamed Abdel Basset Mohamed Talea Mohammad Hamidi Mohammed Alshumrani Mohamed Loey Muhammad Akram Muhammad Shabir Mumtaz Ali Nassim Abbas Munazza Naz Ngan Thi Roan Nguyen Xuan Thao Rishwanth Mani Parimala Ion P tra cu Surapati Pramanik Quek Shio Gai Qiang Guo Rajab Ali Borzooei Nimitha Rajesh Jes s Estupi an Ricardo Juan Miguel Mart nez Rubio Saeed Mirvakili Arsham Borumand Saeid Saeid Jafari Said Broumi Ahmed A Salama Nirmala Sawan Gheorghe S voiu Ganeshsree Selvachandran Seok Zun Song Shahzaib Ashraf Jayant Singh Rajesh Singh Son Hoang Le Tahir Mahmood Kenta Takaya Mirela Teodorescu Ramalingam Udhayakumar Maikel Y Leyva V zquez V Venkateswara Rao Luige VI d reanu Victor Vl d reanu Gabriela Vl deanu Michael Voskoglou Yaser Saber Yong Deng You He Youcef Chibani Young Bae Jun Wadei F Al Omeri Hongbo Wang Zayen Azzouz Omar Neutrosophic Sets and Systems, Vol. VI Florentin Smarandache, Mumtaz Ali, This volume is a collection of ten papers and a review of a book written by different authors and co authors listed in the

order of the papers F Yuhua P K Maji A A Salama H Elghawalby A Mukherjee M Datta F Smarandache K Mondal S Pramanik M Ali L Vladareanu M Shabir S Broumi S Ye J Ye S Sarkar D Gifu and M Teodorescu In first paper the author proposed Pauli Exclusion Principle and the Law of Included Multiple Middle Weighted Neutrosophic Soft Sets are proposed in the second paper Neutrosophic Crisp Sets and Neutrosophic Crisp Relations are studied in third paper In fourth paper Interval Valued Neutrosophic Soft Topological Spaces are introduced Similarly in fifth paper Multi criteria Group Decision Making Approach for Teacher Recruitment in Higher Education Under Simplified Neutrosophic Environment is discussed In paper six Generalization of Soft Neutrosophic Rings and Soft Neutrosophic Fields are presented by the authors Neutrosophic Refined Similarity Measure Based on Cosine Function is given in seventh paper Paper eight is about to study Similarity Measure between Single Valued Neutrosophic Multisets and Its Application in Medial Diagnosis In the next paper Several Similarity Measures of Interval Valued Neutrosophic Soft Sets and Their Application in Pattern Recognition Problems are discussed The authors introduced Soft Neutrosophic Groupoids and Their Generalization in the tenth paper At the end a book review Neutosophic routes in multiverse of communication is presented by the authors Generalization of Fuzzy C-Means Based on Neutrosophic Logic Aboul Ella HASSANIEN, Sameh H. BASHA, Areeg S. ABDALLA, This article presents a New Neutrosophic C Means NNCMs method for clustering It uses the neutrosophic logic NL to generalize the Fuzzy C Means Neutrosophic Sets and Systems, vol. 5/2014 A. A. Salama, O. M. Khaled, K. M. Mahfouz, S. FCM clustering system Broumi, F. Smarandache, K. Mondal, S. Praminik, M. Eisa, M. Ali, Neutrosophic Sets and Systems has been created for publications on advanced studies in neutrosophy neutrosophic set neutrosophic logic neutrosophic probability neutrosophic statistics that started in 1995 and their applications in any field such as the neutrosophic structures developed in algebra geometry topology etc New Trends in Neutrosophic Theory and Applications Florentin Smarandache (editor), Surapati Pramanik (editor), 2016-11-05 Neutrosophic theory and applications have been expanding in all directions at an astonishing rate especially after the introduction the journal entitled Neutrosophic Sets and Systems New theories techniques algorithms have been rapidly developed One of the most striking trends in the neutrosophic theory is the hybridization of neutrosophic set with other potential sets such as rough set bipolar set soft set hesitant fuzzy set etc The different hybrid structure such as rough neutrosophic set single valued neutrosophic rough set bipolar neutrosophic set single valued neutrosophic hesitant fuzzy set etc are proposed in the literature in a short period of time Neutrosophic set has been a very important tool in all various areas of data mining decision making e learning engineering medicine social science and some more The book New Trends in Neutrosophic Theories and Applications focuses on theories methods algorithms for decision making and also applications involving neutrosophic information Some topics deal with data mining decision making e learning graph theory medical diagnosis probability theory topology and some more 30 papers by 39 authors and coauthors Neutrosophic Sets and Systems, Vol. V Florentin Smarandache, Mumtaz Ali, This book is a collection of nine papers contributed by different

authors and co authors listed in the order of the papers A A Salama O M Khaled K M Mahfouz M Ali F Smarandache M Shabir L Vladareanu S Broumi K Mondal S Pramanik I Arockiarani I R Sumathi M Eisa and I Deli In first paper the authors studied Neutrosophic Correlation and Simple Linear Regression The Generalization of Neutrosophic Rings and Neutrosophic Fields is proposed in the second paper Cosine Similarity Measure of Interval Valued Neutrosophic Sets is studied in third paper In fourth paper A Study on Problems of Hijras in West Bengal Based on Neutrosophic Cognitive Maps is introduced Similarly in fifth paper Neutrosophic Crisp Set Theory is discussed In paper six Interval Valued Fuzzy Neutrosophic Soft Structure Spaces are presented by the authors Soft Neutrosophic Bi LA Semigroup and Soft Neutrosophic N LA Semigroup is given in seventh paper Introduction to Image Processing via Neutrosophic Technique is given in paper eight In the last paper Neutrosophic Soft Multi Set Theory and Its Decision Making is presented by the authors Critical Review, Vol. 12, 2016 S. Broumi, M. Talea, A. Bakali, F. Smarandache, A. Salama, H. E. Khalid, A. K. Essa, M. Ali, A. Elhassouny, The following papers have been published Interval Valued Neutrosophic Graphs Neutrosophic Crisp Probability Theory On Strong Interval Valued Neutrosophic Graphs The Concept of Neutrosophic Less than or Equal A New Insight in Unconstrained Geometric Programming Multi Criteria Decision Making Method for n wise Criteria Comparisons and Inconsistent Problems

Neutrosophic Crisp Probability Theory & Decision Making Process A. A. Salama, Florentin Smarandache, Since the world is full of indeterminacy the neutrosophics found their place into contemporary research Collected Papers. Volume XII Florentin Smarandache, 2022-08-01 This twelfth volume of Collected Papers includes 86 papers comprising 976 pages on Neutrosophics Theory and Applications published between 2013 2021 in the international journal and book series Neutrosophic Sets and Systems by the author alone or in collaboration with the following 112 co authors alphabetically ordered from 21 countries Abdel Nasser H Zaied Muhammad Akram Bobin Albert S A Alblowi S Anitha Guennoun Asmae Assia Bakali Ayman M Manie Abdul Sami Awan Azeddine Elhassouny Erick Gonz lez Caballero D Dafik Mithun Datta Arindam Dey Mamouni Dhar Christopher Dyer Nur Ain Ebas Mohamed Eisa Ahmed K Essa Faruk Karaaslan Jo o Alcione Sganderla Figueiredo Jorge Fernando Goyes Garc a N Ramila Gandhi Sudipta Gayen Gustavo Alvarez G mez Sharon Dinarza lvarez G mez Haitham A El Ghareeb Hamiden Abd El Wahed Khalifa Masooma Raza Hashmi Ibrahim M Hezam German Acurio Hidalgo Le Hoang Son R Jahir Hussain S Satham Hussain Ali Hussein Mahmood Al Obaidi Hays Hatem Imran Nabeela Ishfag Saeid Jafari R Jansi V Jeyanthi M Jeyaraman Sripati Jha Jun Ye W B Vasantha Kandasamy Abdullah Karg n J Kavikumar Kawther Fawzi Hamza Alhasan Huda E Khalid Neha Andalleb Khalid Mohsin Khalid Madad Khan D Koley Valeri Kroumov Manoranjan Kumar Singh Pavan Kumar Prem Kumar Singh Ranjan Kumar Malayalan Lathamaheswari A N Mangayarkkarasi Carlos Rosero Mart nez Marvelio Alfaro Matos Mai Mohamed Nivetha Martin Mohamed Abdel Basset Mohamed Talea K Mohana Muhammad Irfan Ahamad Rana Muhammad Zulgarnain Muhammad Riaz Muhammad Saeed Muhammad Saglain Muhammad Shabir Muhammad Zeeshan Anjan Mukherjee Mumtaz Ali Deivanayagampillai Nagarajan Igra Nawaz Munazza

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