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Software for Extracting Deformation Gradient and Stress from MD Simulations: Simulations using the CHARMM Force Field

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Abstract: Software was developed, and is provided under a general use license, to calculate continuum level deformation gradient and stress for any group of atoms in an MD simulation that uses the CHARMM force fields. This software can also calculate the interaction stress applied by one group of atoms on any other group. To obtain deformation gradient and stress, the user needs to provide the selected group(s) of atoms in an atom group identification file, and provide the associated LAMMPS format files and force field parameter file. An example is included to demonstrate the use of the software.

Keywords: Molecular Dynamics Simulation, Continuum Stress, Interaction Stress, Deformation Gradient, CHARMM Force Field

Contents

Introduction

This document and the associated software are for use with molecular dynamics simulations to calculate, for selected groups of atoms, a continuum level deformation gradient, a continuum level stress, and interaction stresses between different groups. The details of the quantities calculated are provided below and described in detail in associated articles [1, 2]. The attached software is provided for general use under the following license.

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Authors: Mehrdad Negahban, Lili Zhang, Zesheng Zhang, John Jasa, Antoine Jérusalem

Publication references:

1. Zhang, L., Jasa, J., Gazonas, G., Jérusalem, A., and Negahban, M. Extracting continuum-like deformation and stress from molecular dynamics simulations. Computer Methods in Applied Mechanics and Engineering 283, 1010–1031 (2015; DOI 10.1016/j.cma.2014.10.018).
2. Zhang, L., Zhang, Z., Jasa, J., Li, D., Cleveland, R.O., Negahban, M., Jérusalem, A. Molecular dynamics simulations of heterogeneous cell membranes in response to uniaxial membrane stretches at high loading rates. Scientific Reports 7, 8316 (2017; DOI 10.1038/s41598-017-06827-3).

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Calculated quantities

The software calculates the deformation gradient and stress for any group of atoms of a molecular dynamics simulation and also calculates the interaction stress of any group of atoms on another group. The following describes the quantities calculated.

Deformation gradient

The deformation gradient for any part of the MD system (any group of atoms in the system) is calculated using the MinD method [1]. This method minimizes the difference between continuum deformations and discrete atom displacements yielding a relation for calculating the deformation gradient $\mathbf{F}$ given by

$$\mathbf{F} = \left[\sum_{i=1}^{n} m_i (\Delta\mathbf{r}_i \otimes \Delta\mathbf{R}_i) \right] \left[\sum_{i=1}^{n} m_i (\Delta\mathbf{R}_i \otimes \Delta\mathbf{R}_i) \right]^{-1}$$

where, n is the number of particles in the group, m_i is the mass of the ith particle, $\Delta\mathbf{r}_i$ is the relative position of the ith particle with respect to the center of mass of the group in the current configuration, $\Delta\mathbf{R}_i$ is the relative position of the ith particle with respect to the center of mass of the group in the reference configuration. A description of these terms in provided in Fig.1 and details can be found in the associated article [1].
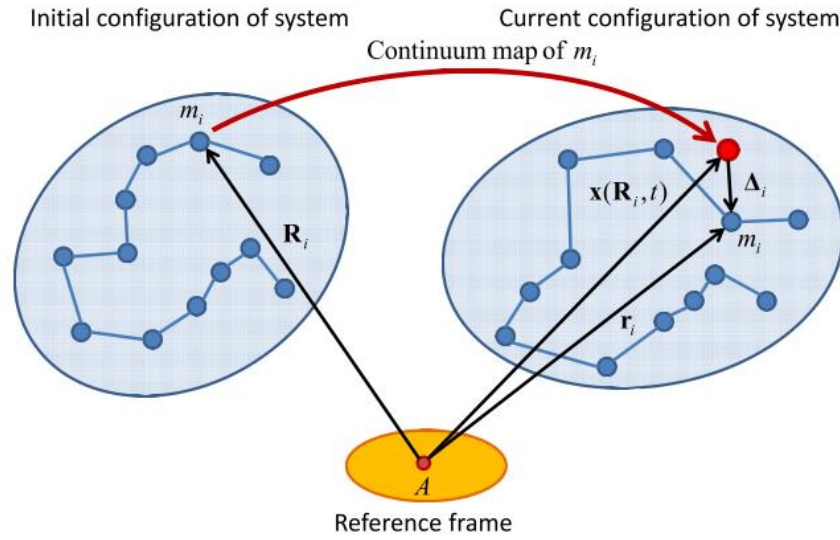
Fig.1 Error between the continuum map and the particle motion that is minimized to get deformation gradient.

Stress

The "internal stress" experienced by any set of interacting particles (atoms), and the "interaction stress" exerted by one group of atoms on another group were calculated as follows. The method is based on constructing a stress field that gives a distribution of traction on a volume's surface such that the traction produces the same resultant force, moment, and power as the interaction forces. The force and moment equivalences are exact, while the power is the same for the stress field if one uses a velocity field constructed from the associated velocity gradient (calculated in a similar manner as the deformation gradient). Details of the process can be found in the associated article [2]. Fig.2 schematically describes a continuous traction distribution over the surface of an equivalent homogeneous continuum body producing the same resultant force, moment and power as the single force does on the particle. The assumption is that for a single force, the traction $\mathbf{t}_i^{(n)}$ on the surface of normal $\mathbf{n}$ is obtained from the associated Cauchy stress $\boldsymbol{\sigma}_i$ through the Cauchy's relation

$$\mathbf{t}_i^{(n)} = \mathbf{n}\boldsymbol{\sigma}_i$$

After generalizing to many particles, and forcing the equivalence, one gets the "internal stress" and the "interaction stress" through calculating the relation

$$\boldsymbol{\sigma} = \frac{1}{V}\sum_{j\in\Omega}\left(\boldsymbol{\rho}_j \otimes \mathbf{f}_j\right)$$

For the "internal stress" calculation, the force $\mathbf{f}_j$ on each particle is the resultant force on particle j from the other particles within the group. For the "interaction stress" calculation, the force $\mathbf{f}_j$ on the particle j is

the resultant force applied by all the particles in the other group. *V* is the volume of the group under consideration, calculated using and equivalent continuum body to this group [1]. The detailed derivation of this method is in the associate article [2].
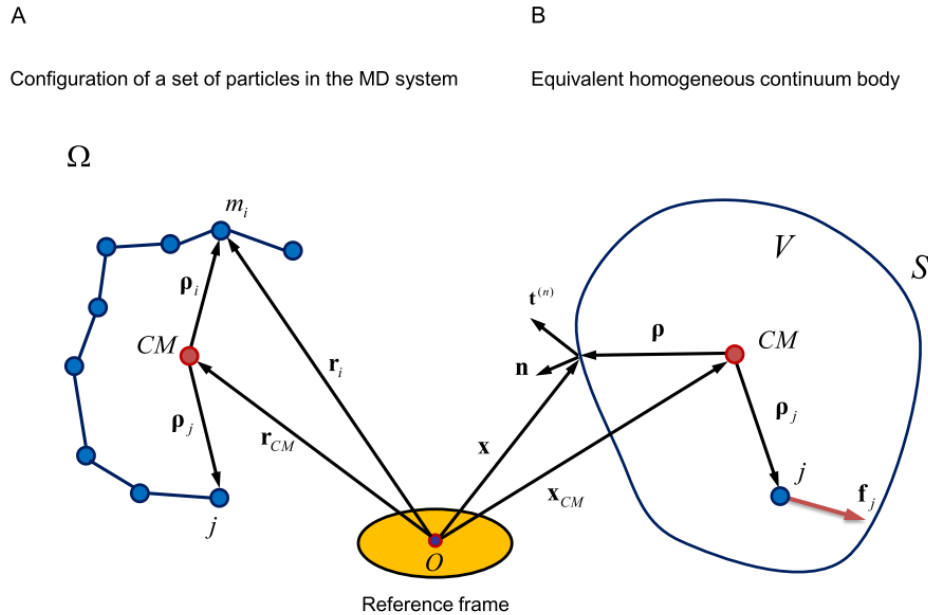

Fig.2 Schematic description of: (A) a set of particles in the MD simulation, and (B) a continuous

traction distribution over the surface of an equivalent homogeneous continuum body.

Code description

The program consists of three pieces of python code (Main.py, ForceCalcSetup.py, and CharmmForceCalc.py). They can be opened by using the Spyder shell from Anaconda Python. The results can be visualized by variable explorer from the Spyder shell. A description of the three Python files are as follows.

Main.py
This program has four functionalities (four flags). The users need to specify what quantity they want to calculate by choosing one the following flags in the main.py.

1. 'DG' means that only deformation gradient in one group of atoms is to be computed.
2. 'NB' means that only pair-wise forces are used in the computation (i.e., the stress is computed based only on pair-wise forces).
3. 'AF' means that all interaction forces including pair-wise, bond, angle, dihedral, improper, etc. of the CHARMM Force Field are computed and the "internal stress" in one group of atoms is computed based on these forces. In this option, the deformation gradient in the group of atoms is also computed.

4. '2B' means that the "interaction stress" is computed based on the using all the interaction forces between the two groups of atoms.

To use main.py, the user need to set up the Lammps data file (name.data), the Lammps step-wise output files (name.txt), the Group names, the flags and the number of processors. The Main.py has detailed comments about the set-up procedure for its user.

The Lammps step-wise output files are created by the Lammps commend "dump ID all custom step-size file-name id mass type mol xu yu zu fx fy fz"

In the example provided, 2K9J.data is the Lammps data file, 2K9J_sss_0/50/100.txt is the Lammps step-wise output files, GroupID.txt is the Group ID file.

ForceCalcSetup.py:

This code is used to read the Group ID and Lammps data and output files, to find the atoms of the designated groups, and to call CharmmForceCalc.py to calculate the forces that will be used in the Main.py.

Only Group ID file (name.txt) needs to be specified in this code. The user needs to create the file GroupID.txt in which the atoms of each group are identified. In the Group ID file, the group name is followed by a block of atom IDs that are separated by spaces. One blank line is used between groups. For an example, see the file GroupID.txt.

CHARMM ForceCalc.py:

The users do not need to change anything here.

This code is used to computed the forces on the atoms in the groups (identified in the Group ID file). These forces include all the CHARMM interaction forces including pair-wise force, bond force, angle force, dihedral force, improper force, etc.

Example

An example is provided in the software package. In the example, the deformation gradient and the internal stress for a small group of atoms using the flag "AF" is calculated. The deformation gradient and the internal stress computed in the third step of this example is given in Tab.1.

Tab.1. The results for the third step: (a) deformation gradient components, (b) internal stress components

1.002	0.004	0.001		2483.484	-693.706	403.841
-0.002	1.004	0.000		-693.706	4860.707	-1008.853
0.002	0.001	1.003		403.841	-1008.853	836.169

(a)   (b)

Software files and citation

The codes for conducting these calculation, this report and the example are placed on the University of Nebraska-Lincoln Digital Commons for free access and download under the license described above. The theoretical development should be cited using the associated articles provided in the reference section. The software and this document are to be cited as:

Mehrdad Negahban, Lili Zhang, Zesheng Zhang, John Jasa, Antoine Jérusalem, "Software for Extracting Deformation Gradient and Stress from MD Simulations: Simulations using the CARMM Force Field" *UNL Digital Commons*, 2017.

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1. Zhang, L., J. Jasa, G. Gazonas, A. Jérusalem, and M. Negahban, *Extracting continuum-like deformation and stress from molecular dynamics simulations.* Computer Methods in Applied Mechanics and Engineering, 2015. **283**: p. 1010-1031.
2. Zhang, L., Z. Zhang, J. Jasa, D. Li, R.O. Cleveland, M. Negahban, and A. Jérusalem, *Molecular dynamics simulations of heterogeneous cell membranes in response to uniaxial membrane stretches at high loading rates.* Scientific Reports, 2017. **7**(1): p. 8316.