

macromolecules, e.g. in equilibrium, under a constant load, a load varying in time, or upon binding of another molecule, can only be characterized by following the changes of the internal forces in time, which cannot be easily achieved with the previous implementation of FDA. We here introduce a Time-Resolved Force Distribution Analysis (TRFDA) method, which adds a temporal component to FDA to enable the analysis of pairwise forces associated with conformational changes.

2. Implementation

2.1. Overview

Time-Resolved Force Distribution Analysis (TRFDA) is based on the same concept of using pairwise forces as FDA, but focuses on their evolution during the MD simulation as well as on the analysis of large molecular systems. To achieve these goals, it stores in memory pairwise forces from only one integration time step at a time, such that the memory usage is independent from the length of the simulation. It also saves output data in new file formats, which are well suited for time series analysis. Similar to FDA, atomic pairwise forces are computed for all types of bonded interactions as well as from Coulomb and Lennard-Jones potentials; long-range electrostatic interactions computed on a grid (e.g. Particle Mesh Ewald Darden et al. (1993); Essmann et al. (1995)) cannot be decomposed in atomic pairwise forces. As in the previous FDA implementation, an MD simulation is first performed to obtain a trajectory, which is then used as the basis for a rerun using the TRFDA code. The core code is completely rewritten for GROMACS 4.5.3 Hess et al. (2008), and VMD Humphrey et al. (1996) plugins are provided for visualization. The implementation includes several notable improvements over FDA, which are discussed below.

2.2. Decomposition of forces from 3- and 4-body potentials

While two-body potentials such as bonds, Coulomb and Lennard-Jones potentials, can be directly used for the analysis of pairwise forces, many-body potentials which act on more than two atoms need to be decomposed into pairwise forces. TRFDA introduces a complete decomposition of the forces resulting from 3- and 4-body potentials (angle, dihedral angle, cross bond-bond, cross bond-angle), as described in the Additional file 1. The pairwise forces resulting from this way of force decomposition can have any direction, *i.e.* do not align with the vector connecting the two atoms involved. To accommodate this, all pairwise forces are stored and handled internally as vectors and are transformed into scalar values only when written to a file, if desired by the user.

The decomposition rectifies the shortcomings of the previous FDA code, which used approximations for computing pairwise forces resulting from 3- or 4-body potentials. For an angle formed by atoms i , j and k (j between i and k), it considered no pairwise forces to act on atom j , and assumed the pairwise force between atoms i and k to act along the distance vector between the two atoms. A similar decomposition has been used for a dihedral angle formed by four atoms. In contrast to these approximations, the decomposition used in TRFDA correctly reproduces the distribution of angle and dihedral forces in a molecule.

Journal Of World Business Submission Guidelines

Jiyuan Zhang



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