

Time-resolved force distribution analysis

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Abstract

Background: Biomolecules or other complex macromolecules undergo conformational transitions upon exposure to an external perturbation such as ligand binding or mechanical force. To follow fluctuations in pairwise forces between atoms or residues during such conformational changes as observed in Molecular Dynamics (MD) simulations, we developed Time-Resolved Force Distribution Analysis (TRFDA).

Results: The implementation focuses on computational efficiency and low-memory usage and, along with the wide range of output options, makes possible time series analysis of pairwise forces variation in long MD simulations and for large molecular systems. It also provides an exact decomposition of pairwise forces resulting from 3- and 4-body potentials and a unified treatment of pairwise forces between atoms or residues. As a proof of concept, we present a stress analysis during unfolding of ubiquitin in a force-clamp MD simulation.

Conclusions: TRFDA can be used, among others, in tracking signal propagation at atomic level, for characterizing dynamical intermolecular interactions (*e.g.* protein-ligand during flexible docking), in development of force fields and for following stress distribution during conformational changes.

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Keywords:

1. Background

Many biomolecular systems or other complex macromolecules can dynamically visit a broad range of conformational states. External perturbations such as a molecular interaction or a mechanical force can cause a molecule to dynamically transit between these conformational states. While the conformational space of biomolecules is typically analyzed by coordinate-based methods such as the detection of correlated motions, Force Distribution

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