Physica A 416 (2014) 21–32

Contents lists available at ScienceDirect

Physica A

journal homepage: www.elsevier.com/locate/physa

Fractal and complex network analyses of protein molecular dynamics☆

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HIGHLIGHTS

- Results of MF-DFA show that the time series from protein dynamics are multifractal.
- We found that the converted horizontal visibility graphs (HVGs) are exponential.
- Our numerical results show that fractality exists in the converted HVGs.
- Estimated parameters from our analyses do not change much for different proteins.
- There is a linear relationship between $\langle h(2)\rangle$ (from MF-DFA) and $\langle d_B\rangle$ of HVGs.

ARTICLE INFO

Article history:
Received 19 March 2014
Received in revised form 11 August 2014
Available online 27 August 2014

Keywords:
Protein molecular dynamics
Multifractal detrended fluctuation analysis
Horizontal visibility graph
Fractal analysis
Degree distribution

ABSTRACT

Based on protein molecular dynamics, we investigate the fractal properties of energy, pressure and volume time series using the multifractal detrended fluctuation analysis (MF-DFA) and the topological and fractal properties of their converted horizontal visibility graphs (HVGs). The energy parameters of protein dynamics we considered are bonded potential, angle potential, dihedral potential, improper potential, kinetic energy, Van der Waals potential, electrostatic potential, total energy and potential energy. The shape of the $h(q)$ curves from MF-DFA indicates that these time series are multifractal. The numerical values of the exponent $h(2)$ of MF-DFA show that the series of total energy and potential energy are non-stationary and anti-persistent; the other time series are stationary and persistent apart from series of pressure (with $H \approx 0.5$ indicating the absence of long-range correlation). The degree distributions of their converted HVGs show that these networks are exponential. The results of fractal analysis show that fractality exists in these converted HVGs. For each energy, pressure or volume parameter, it is found that the values of $h(2)$ of MF-DFA on the time series, exponent λ of the exponential degree distribution and fractal dimension d_B of their converted HVGs do not change much for different proteins (indicating some universality). We also found that after taking average over all proteins, there is a

☆ The contributions of the first two authors are equal, so Jin-Long Liu can be regarded as joint first author.

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http://dx.doi.org/10.1016/j.physa.2014.08.047
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linear relationship between $\langle h(2)\rangle$ (from MF-DFA on time series) and $\langle d_B\rangle$ of the converted HVGs for different energy, pressure and volume.

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1. Introduction

Proteins are among the most important biomacromolecules because they can perform biological functions, which are usually determined by their structures. To date, structures of 97 362 proteins (updated in Protein Data Bank [1] on 2014-01-28) have been obtained by experimental methods, such as X-ray (88.4%), solution NMR (10.6%) and electron microscopy (0.7%). On the other hand, molecular dynamics simulation packages such as NAMD (*Not (just) Another Molecular Dynamics program*) [2] has been developed to learn about different aspects of proteins. Protein molecule energy includes kinetic energy and potential energy, and potential energy can be calculated in quasi-empirical way (such as CHARMM [3] and AMBER [4]). In fact, Rueda et al. [5] used NAMD to analyze the molecular dynamics of 30 real proteins. This paper uses NAMD to simulate protein molecular dynamics, then derives the time series for some corresponding parameters whose features reflect the aspects of protein structures.

Apart from being characterized by an enormous number of degrees of freedom, proteins have multidimensional potential energy surfaces [6]. It is well known that the self-similarity exhibiting in the distributions of their biophysical and biochemical properties can serve as an effective tool to extract the inherently inhomogeneous and nonlinear behaviors of protein structures. Fractal dimension (FD) has been widely used to characterize the self-similarity of fractal objects [7,8]. Many FD-based methods have been proposed to investigate protein structures [6]. Fractal methods can also be used to characterize the scaling properties of time series and then to reveal the self-similarity of the original system [7]. A multifractal system is a generalization of a fractal system in which a single exponent (the fractal dimension) is not enough to describe its dynamics; instead, a continuous spectrum of exponents (the so-called singularity spectrum) is needed [9]. The concept of multifractal phenomena describes that different regions of an object have different fractal properties, and multifractal scaling provides a quantitative description of a broad range of heterogeneous phenomena [10]. Multifractal analysis was initially proposed to treat turbulence data and is a useful way to characterize the spatial heterogeneity of both theoretical and experimental fractal patterns [11]. The multifractal detrended fluctuation analysis (MF-DFA) [12] is an extension of the standard detrended fluctuation analysis (DFA) introduced by Peng et al. [13,14]. DFA can be employed to detect long-range correlations in stationary and nonstationary time series. Hence MF-DFA is a suitable tool to characterize the multifractal property and long-range correlation in time series. Multifractal analysis has been used to study genomes [15–17], protein structures and functions (e.g. Refs. [18–22]). In this paper, we investigate by MF-DFA [12] the scaling property of the associated time series of energy, pressure and volume derived from simulations of protein molecular dynamics.

In last decade, the study of complex networks has gained prominence across many disciplines of science. Studies have shown that complex network theory has become a powerful tool to analyze protein complex structures [23–25]. Single proteins in 3D space can also be considered as biological complex systems emerged through the interactions of their constituent amino acids. These interactions among the amino acids within a protein can be presented as residues interaction network (RIN) (also called residues interaction graphs (RIGs), protein contact network (PCN), protein structure network (PSN), protein contact map (PCM), amino acid network (AAN)), which can be constructed with varying definitions of nodes and edges [23–25].

Recent studies showed that complex network theory (such as recurrence networks) may also be an effective method to analyze time series [26–33]. Lacasa et al. [26] proposed the visibility graph (VG) algorithm to convert time series into complex networks. Then Luque et al. [27] proposed the horizontal visibility algorithm to convert time series into complex networks. It has been shown that these converted networks inherit several properties of time series in the structure of networks [34–36]. Therefore, we can understand time series from a new point of view using the converted networks. In this paper, we hope to reveal some meaningful information in the associated time series of energy, pressure and volume for real proteins from the perspective of the horizontal visibility graphs (HVGs) [27]. This prompts us to further study the fundamental topological and fractal properties of the converted HVGs from different energy, pressure and volume time series of real proteins.

The fractal and self-similarity properties of complex network have also been focused and studied widely in a variety of fields [37–39]. It is found that many complex networks, including the world-wide web (WWW), social networks, protein–protein interaction (PPI) networks and cellular networks, are self-similar under a certain length-scale. Some numerical algorithms have been proposed to calculate the fractal dimensions of complex networks. Song et al. [40] proposed a box-counting algorithm to calculate their fractal dimension. Kim et al. [41] studied the skeleton and fractal scaling in complex networks via an improvement method. Later on, Zhou et al. [42] introduced an alternative algorithm to detect self-similarity of cellular networks. Recently, Li et al. [43] studied the fractal properties of a family of fractal networks using the random sequential box-covering algorithm proposed by Kim et al. [41]. Liu et al. [33] adopted this algorithm to calculate the fractal dimensions of the recurrence networks constructed from fractional Brownian motions. In this paper, we also adopt the random sequential box-covering algorithm to calculate the fractal dimension of the converted HVGs of the time series of energy, pressure and volume for real proteins.

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