Reasonable Non-conventional Generator of Random Linear Chains Based on a Simple Self-avoiding Walking Process: A Statistical and Fractal Analysis

Authors

David R. Avellaneda B., Ramón E. R. González, Carlos Andrés Collazos-Morales, Paola Ariza-Colpas

DOI

https://doi.org/10.1007/978-3-030-86653-2_14

Abstract

Models based on self-excluded walks have been widely used to generate random linear chains. In this work, we present an algorithm capable of generating linear strings in two and three dimensions, in a simple and efficient way. The discrete growth process of the chains takes place in a finite time, in a network without pre-established boundary conditions and without the need to explore the entire configurational space. The computational processing time and the length of the strings depending on the number of trials N′. This number is always less than the real number of steps in the chain, N. From the statistical analysis of the characteristic distances, the radius of gyration (Rg), and the end-to-end distance (Ree), we make a morphological description of the chains and we study the dependence of this quantities on the number of steps, N. The universal critical exponent obtained are in very good agreement with previous values reported in literature. We also study fractal characteristics of the chains using two different methods, Box-Counting Dimension or Capacity Dimension and Correlation Dimension. The studies revealed essential differences between chains of different dimensions, for the two methods used, showing that three-dimensional chains are more correlated than two-dimensional chains.

Keywords

Self-avoiding random walk, Linear chains, Critical exponents, Fractal dimension, Radius of gyration, End-to-end distance