

A Simulation-Based Non-Destructive Framework for Assessing Polymer-Chain Flexibility [†]

Ruogu Tang 

Department of Animal & Food Sciences, University of Delaware, Newark, DE 19713, USA; rgtang@udel.edu

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Abstract

Non-destructive testing (NDT) increasingly incorporates computational and model-assisted approaches to evaluate material behavior without physically altering or damaging samples. In this study, a software-based stochastic simulation framework is presented for the comparative assessment of polymer-chain configurational flexibility within a fully virtual environment. Polymer chains are represented using random-walk (RW) and self-avoiding-walk (SAW) schemes, while directional bias is introduced through prescribed stepping probabilities as a proof-of-concept representation of externally influenced configurational behavior. Chain flexibility is characterized using statistical descriptors including endpoint distributions and end-to-end distance. The simulations show distinct configurational responses among unbiased RW, SAW, and directionally biased conditions, while the baseline RW case exhibits the expected square-root scaling between end-to-end distance and segment number. The framework is intended as an idealized stochastic model for relative configurational assessment and does not directly predict absolute mechanical properties of specific polymer systems. Further molecular-level simulation and experimental validation would therefore be required before extending the observed trends to real polymers. Overall, this study demonstrates the potential of simplified stochastic simulations as complementary digital tools for polymer-chain configurational analysis within emerging model-assisted NDT approaches.

Keywords: non-destructive testing; polymer-chain flexibility; stochastic simulation; random walk; self-avoiding walk; configurational analysis

1. Introduction

Non-destructive testing (NDT) enables evaluation of material behavior without inducing physical damage or failure [1]. While established NDT techniques such as ultrasonic and electromagnetic methods are effective for metals and ceramics, their application to polymeric materials remains challenging due to complex molecular architectures, pronounced thermal motion, and time-dependent responses [2]. Because polymer-chain conformation and configurational flexibility contribute to material behavior at larger length scales, statistical descriptors of chain configuration can provide useful complementary information without directly predicting macroscopic mechanical properties.

Polymer-chain flexibility refers here to the ability of an idealized chain representation to adopt different spatial conformations, whereas conformational mobility describes the statistical variation among accessible configurations [3]. These chain-level descriptors are



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distinct from macroscopic mechanical properties such as tensile strength, elastic modulus, or fracture resistance, which are not directly predicted in the present study. Instead, this work focuses on relative configurational changes characterized through stochastic descriptors such as end-to-end distance and endpoint distributions. A software-based random-walk framework is therefore used to compare unbiased, self-avoiding, and directionally biased chain configurations within a fully virtual environment, providing a simplified model-assisted approach consistent with the broader concept of digital NDT.

2. Simulation Framework

The random-walker-based simulations (TK CMU2001 RandomWalker Simulator) used in this study are conceptually inspired by coarse-grained lattice representations of polymer chains, including the Carmesin–Kremer bond fluctuation model (Figure 1) [4]. The original bond fluctuation model incorporates a defined set of permissible bond vectors, excluded-volume constraints, and stochastic chain moves. The present software-based framework does not implement the complete Carmesin–Kremer algorithm. Instead, it adopts only the broader coarse-grained concepts of discrete chain representation, stochastic configurational sampling, and excluded-volume effects.

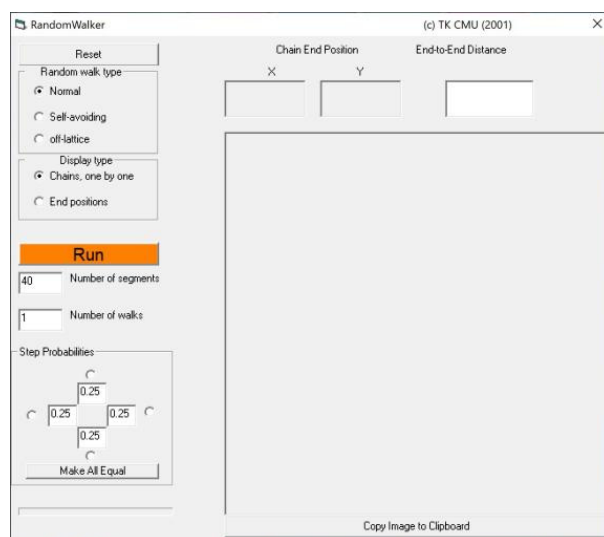


Figure 1. Control panel of random walker software (TK CMU2001 RandomWalker Simulator).

Specifically, the present model represents polymer chains as connected discrete segments generated through random-walk (RW) or self-avoiding-walk (SAW) procedures. In the RW mode, successive segment directions are selected stochastically from four orthogonal directions according to prescribed probabilities. In the SAW mode, self-intersection is additionally prohibited. Thus, the Carmesin–Kremer framework serves as a conceptual reference rather than as a fully implemented bond-fluctuation algorithm.

Based on this conceptual foundation, polymer chains are implemented in a software-based simulation environment using stochastic walking processes [5]. Both random-walk (RW) and self-avoiding-walk (SAW) schemes are employed to represent different degrees of excluded-volume interaction. In the RW scheme, successive steps are selected without restriction, whereas in the SAW scheme, self-intersection of the chain is prohibited.

Each simulation generates a prescribed number of independent stochastic chain realizations. Each realization consists of a fixed number of connected segments, with segment directions selected according to the specified stepping probabilities (Figure 1 and Table 1). These software-defined parameters—walk type, number of independent realizations, number of segments, and directional step probabilities—define the statistical environment

used to evaluate flexibility-related configurational behavior within the present idealized stochastic framework. Together, the RW, SAW, and externally biased simulations constitute a progressive simulation framework for evaluating relative configurational responses under progressively constrained stochastic conditions. This hierarchical design provides the conceptual basis for the statistical analyses presented in the following sections and establishes the foundation for future integration with more physically realistic molecular simulation methods.

Table 1. Directional stepping probability distributions used to represent externally biased polymer chain motion.

Motion Scenario	P(+X)	P(−X)	P(+Y)	P(−Y)
Two quadrants	1/3	0	1/3	1/3

3. Simulation Methodology

For each simulation condition, the walk type was first selected as RW or SAW, followed by specification of the segment number N , number of independent realizations M , and directional stepping probabilities. Independent stochastic chains were then generated using the software, and the resulting endpoint coordinates and end-to-end distances were recorded. The procedure was repeated across the parameter combinations summarized in Table 2, after which ensemble statistics and scaling relationships were analyzed. To provide a clear and reproducible description of the simulation procedure, the software-based workflow is summarized in procedural pseudocode form in Algorithm 1.

Algorithm 1. Procedural pseudocode for the software-based stochastic polymer-chain simulation workflow.

Input:

Walk type (RW or SAW)
Segment number, N
Number of independent realizations, M
Directional stepping probabilities

For each simulation condition:

1. Select the walk type.
2. Set the segment number N .
3. Set the number of independent realizations M .
4. Define the directional stepping probabilities.
5. Generate M independent stochastic chain realizations.
6. Record the endpoint coordinates and end-to-end distance for each realization.
7. Calculate ensemble-averaged quantities and standard deviation (SD).
8. Repeat the procedure for the parameter combinations listed in Table 2.

Output:

Endpoint coordinates/distributions
Ensemble-averaged end-to-end distance
Standard deviation (SD)

Table 2. Summary of simulation scenarios and parameter settings used for random-walk, self-avoiding-walk, and directionally biased polymer-chain simulations.

Simulation Scenario	Walk Type	Segment Number N	Number of Independent Realizations M	Directional Probabilities	Purpose
Baseline: chain-length analysis	RW	10, 20, 50, 100, 200, 500	fixed M = 100	0.25 each	Evaluate R_{ee} vs. chain length
Baseline: ensemble-size analysis	RW	fixed N = 100	10, 20, 50, 100, 200, 500	0.25 each	Evaluate sampling stability
SAW: chain-length analysis	SAW	10, 20, 50, 100, 200, 500	fixed M = 100	0.25 each	Compare excluded-volume effect
SAW: ensemble-size analysis	SAW	fixed N = 100	10, 20, 50, 100, 200, 500	0.25 each	Evaluate ensemble behavior
Directionally biased case	RW	10, 50, 100, 200, 500	10, 50, 100, 200, 500	1/3, 0, 1/3, 1/3	Proof-of-concept directional bias

Note: Ensemble-averaged quantities were calculated from the independent stochastic realizations generated under identical parameter settings, and error bars represent the standard deviation (SD) across those realizations.

3.1. Baseline Condition Without External Force

Polymer-chain configurational behavior was simulated under a force-free condition using a random-walk (RW) scheme. At each walking step, segment displacement was selected from four orthogonal directions with equal probability (25% per direction), resulting in isotropic stochastic motion. No directional bias or external force was applied.

Polymer chains were represented as connected sequences of discrete segments. A prescribed number of independent random-walk realizations was generated for each simulation condition. The number of chain segments controlled the length of each stochastic chain, whereas the number of walks controlled the number of independent realizations used for configurational sampling. This condition served as a reference state for subsequent force-driven simulations.

3.2. Self-Avoiding Walk Without External Force

The SAW simulation followed the same computational procedure described for the RW model. The only additional constraint was that self-intersection of the polymer chain was prohibited throughout the simulation, thereby introducing excluded-volume effects while maintaining identical segment number, number of independent realizations, and stepping probabilities. Polymer chains were represented as connected sequences of discrete segments and a prescribed number of independent SAW realizations was generated. The number of segments defined the chain length, whereas the number of independent walks defined the ensemble size used for statistical sampling. No external force or directional bias was applied in this condition.

3.3. Simulation with External Force Bias

Building upon the RW and SAW simulations, directional-bias effects were incorporated by introducing directional bias into the stepping probabilities. Rather than applying an explicit force field, directional-bias effects were modeled through controlled probability distributions governing segment displacement directions. This probabilistic approach provides a simplified and non-invasive representation of force-driven motion while remaining consistent with the random-walk framework.

At each walking step, segment displacement was restricted to four orthogonal directions along the positive and negative X and Y axes. A two-quadrant directional probability

configuration was selected as a proof-of-concept biased condition toward the positive X direction. The present study focuses on the two-quadrant configuration as a single proof-of-concept directional-bias case (in Table 1).

Due to page and figure limitations associated with conference proceedings, only the two-quadrant bias condition is presented here as a proof-of-concept directionally biased configurational case. This configuration provides a simple proof-of-concept case for examining the effect of directional bias while preserving stochastic lateral motion, allowing the essential effects of externally biased chain motion to be examined. The complete simulation scenarios and parameter settings used throughout this study are summarized in Table 2. For chain-length analyses, the number of independent realizations was held constant while the segment number N was varied. For ensemble-size analyses, the segment number was held constant while the number of independent realizations M was varied. The table also summarizes the corresponding walk type, directional probabilities, and the purpose of each simulation condition. Here, the software parameter “Number of walks” denotes the number of independent stochastic realizations rather than a temporal variable. Because only one directional-bias configuration is analyzed in detail, the present results should not be interpreted as demonstrating general validity across different loading magnitudes or directions. Additional bias conditions will be required to evaluate the broader applicability of the framework.

4. Results

4.1. Baseline Conformational Behavior Without External Force

Under force-free conditions using the random walk (RW) scheme (Section 3.1), polymer chain motion remained isotropic and statistically unbiased. For a fixed number of independent realizations and a given segment number, chain endpoints were distributed across all four quadrants and along both coordinate axes without preferential directional propagation (Figure 2), indicating fully stochastic configurational sampling in the absence of externally imposed constraints. Linear regression of the ensemble-averaged end-to-end distance, R_{ee} , against $\sqrt{N}$, yielded $R_{ee} = 1.1089\sqrt{N}$, with $R^2 = 0.9997$, demonstrating an excellent fit to the expected square-root scaling of the baseline random-walk model.

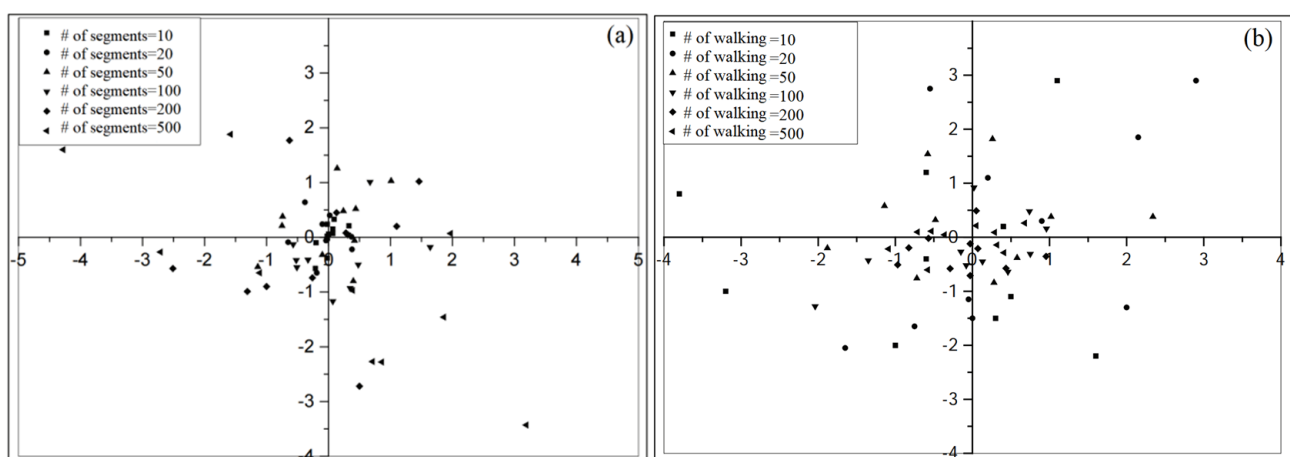


Figure 2. Cont.

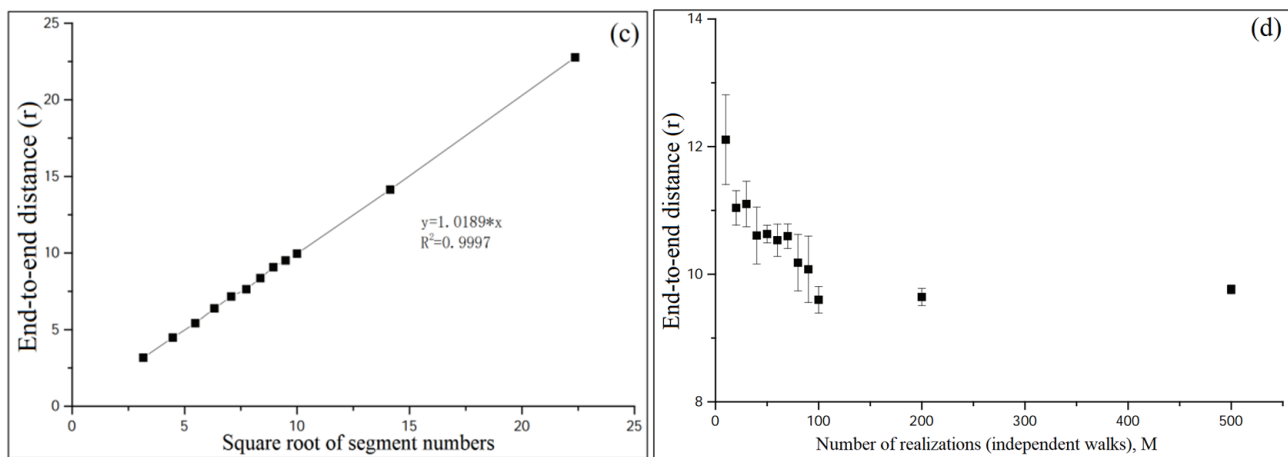


Figure 2. Baseline polymer-chain behavior under force-free random-walk conditions. (a) End-position distributions for varying segment numbers at a fixed number of independent realizations; (b) end-position distributions for varying numbers of independent realizations at a fixed segment number; (c) end-to-end distance versus square root of segment number; (d) end-to-end distance versus number of independent realizations.

When the number of independent realizations was held constant, increasing the number of chain segments produced progressively larger end-to-end distances. The ensemble-averaged end-to-end distance exhibited an overall square-root dependence on chain length, consistent with classical random-walk statistics and freely jointed chain behavior (Figure 2). However, the observed slope exceeded that predicted for an ideal freely jointed chain, suggesting the presence of effective directional correlations during chain propagation. This behavior may be interpreted through bond-angle correlations analogous to a freely rotating chain model, in which the end-to-end distance can be expressed as $r = \sqrt{n} \times l \times \sqrt{\frac{1 + \cos \theta}{1 - \cos \theta}}$, where r is the end-to-end distance, n is the number of segments, l is the segment length, and θ represents an effective bond angle between adjacent segments [6]. Although simplified, this representation provides a useful statistical interpretation of non-ideal configurational behavior within the present simplified stochastic model.

For a fixed number of segments, increasing the number of independent realizations improved the statistical sampling of the configurational ensemble. As the ensemble size increased, the estimated end-to-end distance and endpoint distribution became less sensitive to individual stochastic realizations, providing a more stable representation of the underlying isotropic random-walk statistics. This behavior is consistent with isotropic random-walk statistics and indicates that larger ensemble sizes provide a more stable estimate of the underlying configurational distribution.

4.2. Effect of Self-Avoiding Walk on Chain Conformation

When self-avoiding-walk (SAW) constraints were applied under force-free conditions (Section 3.2), polymer-chain conformations exhibited systematic differences relative to the random-walk (RW) baseline. Chain endpoints remained distributed across all four quadrants, indicating the absence of externally imposed directional bias; however, the overall spatial dispersion increased due to the configurational restrictions imposed by the prohibition of self-intersection. Compared with RW trajectories, SAW chains explored more spatially extended pathways in order to avoid configurational overlap during propagation (Figure 3).

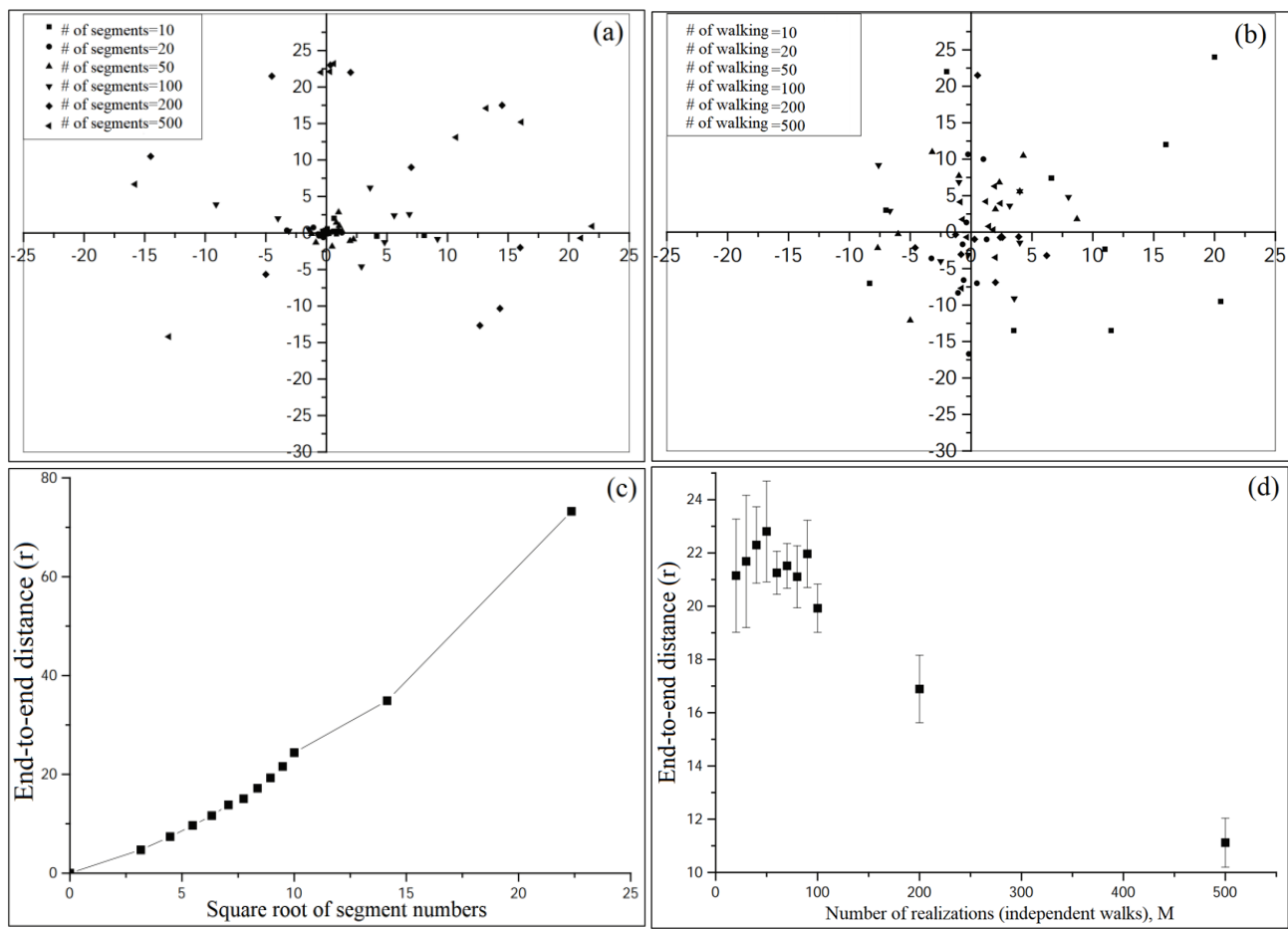


Figure 3. Polymer-chain conformational behavior under force-free self-avoiding walk (SAW) conditions. (a) End-position distributions for varying segment numbers at fixed number of independent realizations; (b) end-position distributions for varying numbers of independent realizations at fixed segment number; (c) end-to-end distance as a function of the square root of segment number; (d) end-to-end distance as a function of the number of independent realizations at fixed segment number.

Within the present idealized stochastic framework, the larger end-to-end distance of SAW chains is attributed to the self-avoidance constraint, which excludes overlapping configurations and thereby reduces the accessibility of compact chain conformations. For a fixed number of independent realizations, SAW chains displayed larger ensemble-averaged end-to-end distances than RW chains at the same segment number. This enhanced extension reflects excluded-volume effects, which reduce configurational accessibility and promote statistically expanded conformations.

For a fixed number of segments, increasing the number of independent realizations improved ensemble sampling and reduced the influence of individual stochastic trajectories on the estimated configurational statistics; however, SAW chains consistently retained larger end-to-end distances than RW chains even at larger ensemble sizes due to persistent excluded-volume restrictions. Within the present idealized model, these observations indicate that self-avoidance enhances configurational extension by restricting overlapping and compact configurations while preserving isotropic, force-free behavior [7]. Consequently, the resulting conformational signatures remain distinguishable from ideal random-walk behavior and provide a useful basis for evaluating excluded-volume effects within the proposed non-destructive stochastic simulation framework.

4.3. Effect of External Force Bias on Chain Conformation

To investigate polymer chain response under externally biased motion, a directional probability scheme corresponding to the two-quadrant condition was applied (Section 3.3). In this configuration, stepping probabilities were preferentially biased toward the positive X direction while preserving stochastic motion in both positive and negative Y directions. Due to page and figure limitations, the two-quadrant bias condition is presented here as a proof-of-concept directionally biased configurational case.

Under this biased condition, polymer chains exhibited clear anisotropic conformational behavior characterized by preferential configurational extension along the positive X direction. End-position distributions shifted systematically toward the imposed bias direction while maintaining lateral dispersion along the Y axis (Figure 4a,b), indicating that stochastic configurational sampling remained active despite directional constraints. Compared with force-free random-walk and self-avoiding-walk cases, the biased trajectories displayed increased configurational asymmetry and directional persistence, reflecting the redistribution of stepping probabilities rather than explicit mechanical deformation.

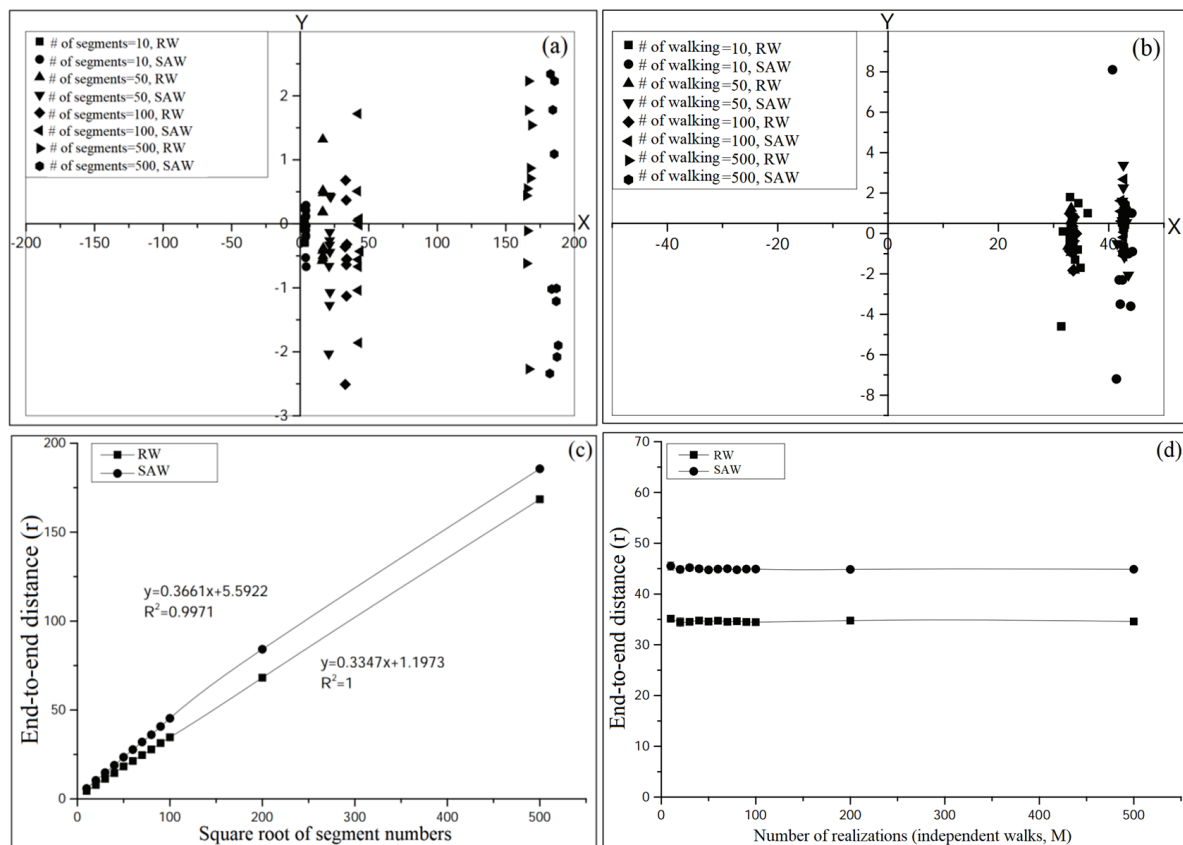


Figure 4. Comparison of polymer chain conformational behavior under force-free random-walk (RW) and self-avoiding-walk (SAW) conditions. (a) End-position distributions for varying segment numbers at a fixed number of independent realizations; (b) end-position distributions for varying numbers of independent realizations at fixed segment number; (c) ensemble-averaged end-to-end distance as a function of the square root of segment number; (d) end-to-end distance as a function of the number of independent realizations at fixed segment number.

The ensemble-averaged end-to-end distance increased relative to both random-walk and self-avoiding-walk baselines (Figure 4c), demonstrating the combined influence of stochastic mobility and externally biased propagation [8]. Although chain extension increased along the preferred direction, trajectories did not collapse into fully aligned paths, confirming that stochastic fluctuations continued to contribute to the configurational distri-

bution throughout the simulation. Increasing the number of independent realizations did not eliminate the anisotropic endpoint distribution induced by the directional probability bias. Instead, the larger ensemble provided a more stable statistical representation of the biased configurational distribution (Figure 4d).

Overall, the two-quadrant bias condition demonstrates that the present stochastic framework is sensitive to this specific form of directional bias. The resulting anisotropic configurational signatures illustrate the response of the model to the prescribed probability distribution while retaining stochastic configurational variability. Because only one directional-bias condition is examined, these results should be interpreted as a proof-of-concept demonstration rather than as evidence of general behavior under external loading.

5. Discussion and Implications

The simulations demonstrate that progressively increasing physical constraints—from random walk (RW) to self-avoiding walk (SAW) and externally biased motion—produce systematic and reproducible changes in polymer-chain conformations [9]. Although the proposed framework employs simplified stochastic models without explicitly considering atomistic interactions, energetic potentials, polymer-specific chain stiffness, entanglement, or chemically specific force fields, it captures statistical descriptors of configurational behavior within the present idealized chain representation. Accordingly, the results should be interpreted as relative configurational trends within this stochastic framework rather than as quantitative predictions for specific real polymers. Transfer of these trends to chemically specific polymer systems would require validation through more physically realistic molecular simulations and/or experiments. These observations indicate that coarse-grained stochastic simulations can preserve essential statistical characteristics governing polymer-chain configurational behavior while remaining computationally efficient.

The RW simulations established an isotropic statistical baseline characterized by the expected square-root scaling relationship between end-to-end distance and chain length [10]. Introducing self-avoidance systematically expanded chain conformations through excluded-volume constraints, while externally biased stepping further generated anisotropic conformational responses without eliminating stochastic fluctuations. Together, these progressively increasing levels of physical constraint demonstrate how simplified stochastic rules can generate characteristic configurational signatures associated with flexibility-related behavior within the present idealized model.

From a non-destructive testing (NDT) perspective, the proposed framework does not aim to directly predict absolute mechanical properties. Instead, it provides a model-assisted digital approach for evaluating relative changes in polymer conformations under different stochastic, geometric, and force-biased conditions. Simulation-derived statistical descriptors therefore offer a complementary means of assessing polymer flexibility in a fully virtual and non-destructive environment, where configurational responses can be systematically analyzed without physical loading, irreversible deformation, or material failure.

More broadly, this proof-of-concept framework illustrates the potential of integrating coarse-grained polymer simulations into emerging digital NDT methodologies. Future developments will incorporate more physically realistic molecular interactions through molecular dynamics simulations, together with polymer entanglement and experimental validation, thereby extending the present framework toward simulation-assisted quantitative polymer characterization.

6. Conclusions

This study establishes a proof-of-concept simulation framework for integrating stochastic polymer-chain modeling into digital non-destructive testing. By progressively incor-

porating random walk, self-avoiding walk, and externally biased motion, the proposed framework demonstrates that simplified stochastic simulations can reproduce distinct configurational signatures within the present idealized chain representation. These signatures should not be interpreted as direct quantitative predictions for specific polymers without further molecular-level or experimental validation. Rather than replacing conventional experimental methods, the framework provides a complementary, computationally efficient, and fully non-destructive approach for investigating idealized polymer-chain configurational behavior within a virtual stochastic framework. The present framework should therefore be interpreted as a preliminary, idealized stochastic model for relative configurational assessment rather than a direct predictor of absolute mechanical properties in specific polymers. Future work will extend this framework through molecular dynamics simulations (e.g., LAMMPS), more realistic intermolecular interactions, polymer entanglement, and experimental validation, ultimately advancing toward simulation-assisted quantitative polymer characterization.

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