“Raindrop” Coalescence of Polymer Chains during Coil—Globule Transition

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ABSTRACT: We approach the problem of coil—globule transition dynamics numerically by Brownian dynamics simulations. This method allows us to study the behavior of polymer chains of varying stiffness and the effects of bending stiffness on chain morphology during the process of coil—globule collapse, imitating globule formation in poor solvent conditions. We record and analyze a three-stage process of globule formation for flexible chains: (1) nucleation, (2) coalescence of nuclei, and (3) collapsed globule formation. Stiffer chains undergo similar formation stages; however, the “raindrops” formed by these chains are elongated (unlike spherical structures formed by flexible chains) and exhibit regular packing of chains into antiparallel hairpin structures. In order to assess the transition dynamics quantitatively, polymer chain configurations were analyzed by generating contact maps and contact frequency histograms for all given configurations. These clusters are initial-configuration-dependent, and their growth and intercluster contacts have direct analogy with the process of raindrop coalescence.

INTRODUCTION

The problem of polymer chain collapse in poor solvents has received much attention over the past decades, from both analytic and numerical approaches. This collapse, often called the “coil—globule transition”, is well-understood as a local version of the polymer demixing Flory has originally formulated for polymer solutions. As the second virial coefficient, representing nonlocal pair interaction between chain segments, becomes sufficiently negative (reflecting an effective attractive pair potential), the chain suddenly shrinks in size and collapses into a condensed globular form with a local structure more like that of a melt than a freely solvated polymer. A generally positive (repulsive) third virial coefficient becomes important in the condensed globule and prevents the chain from nominally collapsing to a point. The coil—globule transition is closely associated with the initial stages of protein folding, particularly secondary structure formation, and DNA condensation. Collapse can occur as a result of effective intrachain interactions, e.g., due to changing solvent quality, but also as a consequence of interactions with a random external potential which localizes the chain within a given region. In this work, we analyze the first classical scenario where collapse takes place due to long-range attractive interaction between monomers.

Langevin and phenomenological models are the main two theoretical directions that have been used to study the kinetics aspect of the polymer collapse. Mostly stemming from the early work of de Gennes, numerous phenomenological kinetic models produce scaling laws for several regime characteristics of collapse. An alternative theoretical model to the one proposed by de Gennes was developed by Halperin and Goldbart; it differs in their interpretation of collapse: the de Gennes model is known as the “expanding sausage model” in which the chain forms an elongated structure that becomes thicker upon collapse, finally condensing into a globular state. The Halperin—Goldbart model is known as the “pearl-necklace model”, reflecting the morphological features of the transition—small nuclei forming globules (pearls) that are randomly formed along the chain (necklace)—and these collapse by collision analogous to droplet coalescence in fluid dynamics. In contrast, Klushin did not view the problem as based on fluid dynamics and nucleation as Halperin and Goldbart describe it later, but from the viewpoint of cluster growth and aggregation where clusters are connected by strands and the aggregation is driven by the entropic tension in the strands. One of the main assumptions that differ in the two interpretations is that a globule subject to end stretching is nonuniformly deformed but partially unfolds through different possible mechanisms segregating into two strands and a spherical core. These models propose varying scaling exponents for collapse time \( \tau \) depending on the degree of polymerization \( N \): The de Gennes model predicts a single scaling exponent \( \tau \sim N^2 \) (ref 18); the Halperin—Goldbart model describes a three-stage nucleation and coalescence process with \( r(1) \sim N^6, r(2) \sim N^{1/5}, \) and \( r(3) \sim N^{6/5} \) (ref 19), while according to Klushin, \( \tau \sim N^{1.6} \). Various inconsistencies also exist between the models, such as whether collapse is a three- or a four-stage process. Our simulations appear to confirm the collapse process.

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as described by Halperin and Goldbart:19 (1) pearlimg, (2) bridge stretching, (3) collapse of the pearl necklace, and (4) equilibrium collapsed configuration in a poor solvent (Figure 1). It is important to mention that there is a possible terminological confusion between theoretical models and numerics—in most numerical simulations, the “pearl necklace” term is used to describe a structure with globules formed by electrostatic contacts,22 whereas a pearl necklace in Halperin–Goldbart terminology19 is one of the stages of polymer collapse that we confirm in simulations; we therefore use the terminology of fluid dynamics, “raindrop formation”, that at least qualitatively appears to describe the physics of the processes that we observe in our work. Despite the fact that equilibrium polymer configurations in good and poor solvents are well understood, important factors that play a critical role in the transition process such as chain length, flexibility of the chain, and viscosity of the solvent have not been well characterized, and we try to address these points here.

According to Halperin and Goldbart terminology, the configurations of a collapsed chain are characterized by a correlation length \( \xi_c \), which is formulated as \( g_c^{-1/2} a \sim \xi_c \), where \( g_c \) is the number of monomers in a blob or a “pearl” and \( a \) is the size of a monomer. The collapsed blobs (pearls), of size \( \xi_c \), attract each other and aggregate densely, so the radius of the final collapsed state is \( R \approx (N/g_c)^{1/3}\xi_c \) (see Figure 8 below). In the early “sausage” model of de Gennes18 the initial state is also represented as a string of blobs which upon coil–globule transition experience attractive forces, hence minimizing the surface energy between an inner domain and solvent. However, in that model, the shape of the intermediate state is believed to be approximated better by a cylinder of length \( L \) and a radius of \( r \). Upon compaction, the “sausage” becomes thicker, finally collapsing into a spherical lowest energy state.18 Our simulation for a flexible chain confirms the Halperin–Goldbart morphology.

Earlier numerical work on polymer collapse can be broadly divided into three approaches: Metropolis Monte Carlo simulations, molecular/Brownian dynamics, and mesoscale simulation techniques. Monte Carlo simulations produce lowest energy state conformations without the time-dependent dynamics that can be observed in other algorithms, which is as a drawback if one needs to study the evolution of the process with time. Molecular and Brownian dynamics techniques are following the motion of particles: molecular dynamics algorithms integrate Newton’s equations of motion, whereas in Brownian dynamics one uses the Langevin equation to describe the effects of thermal noise and Brownian motion. Mesoscale simulation techniques are useful to study hydrodynamic flow phenomena, and there are variations in simulations of this type: (1) dissipative particle dynamics, (2) multiparticle collision dynamics, and (3) the lattice Boltzmann approach.23 These are very efficient considering the time and length scales greatly surpass those that can be studied in molecular dynamics. However, a drawback of this approach is that the concept of a “particle” in simulations of this type represents a whole molecule or fluid regions, and hence the atomistic details are omitted. Mesoscale techniques are flexible and can therefore be coupled to atomistic algorithms such as molecular dynamics, which explains the increasing popularity of the approach in the field of numerical analysis. One of the eminent works in the hybrid simulation approach was performed by Kikuchi et al.24 where it was used to investigate polymer collapse and the role of hydrodynamics on collapse kinetics. In that simulation, solvent was modeled by a mesoscale algorithm known as stochastic rotation dynamics and the polymer by molecular dynamics: this separation of algorithms allows one to overcome the limitation of computationally intensive hydrodynamic time scales. Kikuchi et al. found that hydrodynamic interactions accelerate polymer collapse and appear to change the dynamics of collapse. However, the simulation results are most often presented in terms of time steps, whereas the conversion of these into real time may be quite different in cases of Brownian vs hybrid simulations. In fact, whether the collapse pathway is altered by hydrodynamics is still debated.25 According to Cieplak et al.,26 hydrodynamic interactions are found to affect time characteristics in the vicinity of the native state but have no impact on these characteristics of structural fluctuations around the native state.

Figure 1. The summary of stages of chain coalescence into a globular state, via a sequence of steps resembling the nucleation and growth of liquid out of a gas. Parts A–D are sketches from ref 19, while the series E–G are the snapshots from our simulation at different times of collapse.
Early models gave polymer research a new perspective; however, they also led to numerous diverging interpretations. One of the reasons for misleading results was the fact that the length of the studied chains, $N$, was often not sufficient enough to produce a distinct dynamics behavior. For example, the conclusion of ref 24 that the collapse starts from chain ends may simply be a result of $N < g_c$ (in terminology of Halperin–Goldbart). Another debated argument in the polymer simulations literature is the representation of the solvent. Some argue that implicit and explicit solvent representations produce different results; this might however be an artifact that again arises from an insufficient length of a simulated chain, when solvent molecules can indeed be expected to play a significant role in chain morphology.

In this work, we closely follow the setup of Rosa and Eversen28 and perform numerical simulations using the Large Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS)29 to reproduce the dynamics of a polymer chain over time (Figure 1). For simplicity, our coarse-grained simulations do not include hydrodynamics. In order to obtain a comprehensive interpretation of polymer collapse dynamics, we designed further methods to analyze the collapse-associated processes at a more detailed quantitative level. These include an extensive use of contact and contact-frequency maps, representing graphically the chain segments (monomers, or residues) that are judged to be in direct contact in a folding chain, and the analysis of time evolution of the dense “raindrops” (collapsed blobs separated by regions of a free-fluctuating chain). We performed simulations for a number of different initial configurations of expanded-coil chain in order to avoid confusion of initial-configuration-dependent processes with the real universal dynamics of the polymer. Further, we compare the effects of bending stiffness on the morphology of a collapsing chain and find that above a certain stiffness the semiflexible chain folds into “nematic droplets” with straight segments and sharp hairpins.30 We also demonstrate that the dynamics depends on the viscosity of the solvent—for lower viscosities, the distinct morphological behavior associated with chain stiffness appear to remain intact; however, the process of globule formation takes place on a shorter time scale.

**SIMULATION OF POLYMER CHAINS**

The model used for numerical simulations in this work is based on the bead–spring model described in molecular-dynamic context by Kremer and Grest.31 The system was simulated in a standard way, with a fixed number of particles at a fixed volume in a cubic cell with periodic boundary conditions, which allows particles to exit and re-enter the simulation box. A polymer chain is composed of connected monomeric units consisting of $N = 2000$ monomers—a chain length sufficient to demonstrate the stiffness-dependent dynamics of individual polymer chains during coil–globule transition. Each monomer has a diameter of $\sigma$, and interactions between monomers can be described by the following potentials:

1. Finitely extensible nonlinear elastic (FENE) potential for connected monomers (residues):

   $$
   U_{\text{FENE}} = \begin{cases} 
   -\frac{1}{2}kR_0^{-2}\ln[1 - (r/R_0)^2], & r \leq R_0 \\
   0, & r > R_0 
   \end{cases}
   $$

   The FENE potential is harmonic near its minimum, so that the effective spring constant between monomers is $k$. However, a FENE bond cannot be stretched beyond a maximum length determined by $R_0$ (see below for the discussion of numerical values choice).

2. The Lennard-Jones potential for nonconsecutive pairs of monomers: $U_L = 4\varepsilon \left[ (\sigma/r)^{12} - (\sigma/r)^{6} \right]$, where $\sigma$ is the distance at which the interparticle potential is zero, thus separating the repulsive and attractive regions, and $\varepsilon$ the potential well depth. This potential reaches its minimum $U_L = -\varepsilon$ at $r = 2^{1/6}\sigma$. For numerical simulations, it is common to use a shifted and truncated form of this potential which is set to zero past a certain separation cutoff. For a self-avoiding random-walk chain (i.e., swollen in a good solvent), the potential is set to zero at $r_{\text{cutoff}} = 2^{1/6}\sigma$, representing only the soft repulsion between monomers close-up:

   $$
   U_L = \begin{cases} 
   4\varepsilon \left[ (\sigma/r)^{12} - (\sigma/r)^{6} + \frac{1}{4} \right], & r \leq 2^{1/6}\sigma \\
   0, & r > 2^{1/6}\sigma
   \end{cases}
   $$

   In order to simulate poor solvent conditions when there is an effective attraction between monomers, the cutoff value was set to for $r_{\text{cutoff}} = 3\sigma$ (Figure 2). In each case the potential is also shifted up or down to ensure the continuity at the cutoff radius.

   ![Figure 2. Graphical representation of the shifted and truncated Lennard-Jones potential for good solvent conditions (cutoff $r = 1.12\sigma$, indicated by an arrow), so the effective potential between monomers is purely repulsive, and the poor solvent conditions (cutoff $r = 3\sigma$, also indicated by an arrow), so that there is an attractive potential well of approximately $k_B T$ deep.](dx.doi.org/10.1021/ma302364f)\[Macromolecules 2013, 46, 1239−1247.

3. Bending elasticity of semiflexible chain is described by a potential $U_{\text{bend}} = K_B (1 - \cos \theta)$, where $\theta$ is the angle formed between two consecutive bonds and $K_B$ is the corresponding bending modulus.

For simulated chains for $N = 2000$ monomers, parameters used for simulations are as described in ref 32 with the monomer diameter $\sigma$ chosen to be 0.3 nm (which is a typical size of an aminoacid residue in proteins). Parameters for $k$ and $R_0$ were set so as to avoid any bond crossing. For our simulations, the values used as in ref 31; the maximum bond length $R_0 = 1.5\sigma$, and the spring constant $k = 30\varepsilon/\sigma^2$. The spring constant was studied by Kremer and Grest31 and was found to be strong enough such that the maximum extension of the bond was always less than 1.2$r$ for $k_B T = 1.0\varepsilon$, making the bond breaking energetically unfeasible. The important ratio $K_B/k_B T$, which is the measure of the chain persistence length, $l_p = \sigma(K_B/k_B T)$, was set to vary from $l_p = \sigma$ (or Kuhn’s length of 0.6 nm) to $l_p = 10\sigma$ (or Kuhn’s length of 6 nm) depending on the flexibility of the simulated chain. Integration time step was chosen to be $\tau_{\text{int}} = 0.012\varepsilon$ where $\tau$ is the reduced (Lennard-Jones) time, defined as $\tau = \sigma(m/\varepsilon)^{1/2}$, as discussed in refs 28 and 31. Taking the values of $\sigma$ and $\varepsilon$ above, and the typical...
mass of an aminoacid residue (molecular weight \( \approx 100 \)), we obtain the estimate of \( \tau \approx 0.03 \, \text{s} \). Hence, with \( 10^6 \) time steps of this coarse-grained simulation we are able to follow the dynamics of a polymer chain for \( 360 \, \text{s} \).

In order to study the coil−globule transition, the pair-interaction (Lennard-Jones) potential is altered as shown in Figure 2: at \( t = 0 \) the "good-solvent" repulsive potential with \( r_{\text{cutoff}} = 2^{1/6} \sigma \) is switched to the attractive potential with \( r_{\text{cutoff}} = 3 \sigma \), which represents an instantaneous quenching of the system. We then simulate the process of collapse over time, as discussed, and observe the characteristic "pearling" for both flexible and semiflexible chains (Figure 3).

Figure 3. Flexible chain (A) showing the characteristic "pearling" stage of the collapse process and a semiflexible chain (B) showing characteristic elongated structures formed along the chain.

■ ANALYSIS OF CONFORMATIONS BY CONTACT MAPS

In order to analyze the conformational dynamics of a chain, one needs a method that would let us follow the monomer contact evolution over time. This can be achieved by generating so-called contact maps, which are essentially a representation of the 3D connectivity in a two-dimensional map. This method has been used to represent proteins; however, this type of analysis has not been performed on idealized chains, the conformations of which exist as a result of Brownian dynamics. The algorithm for generating a contact map for a given set of coordinates of all chain units is simple: for each consecutive monomer we list all other monomers that are within the chosen contact radius. Obviously, the choice of this radius is somewhat arbitrary, and we were guided simply by the visual clarity of features on the maps: we regarded a monomer \( m_i \) and a monomer \( m_j \) in contact when they are found within the radius of \( 2 \sigma \). In this way there is always the trivial contact on, or near, the main diagonal, which represents \( m_i = m_j \) and the chain connectivity \( m_i \div m_j \pm 1 \). The off-diagonal contacts, by symmetry always of the square shape symmetric about the main diagonal, represent the essential features of the collapsing structure.

Flexible Chain \( (l_p = \sigma) \). As discussed earlier, our simulations indeed confirm the phenomenological model presented by Klushin,\(^{20} \) as well as Halperin and Goldbart,\(^{19} \) and are in good agreement with earlier simulation work.\(^{24} \) Using our contact map approach, we can further analyze the structures formed within the globule, which, to our knowledge, has not been done before. We demonstrate that for flexible chains first small clusters are formed (Figure 5), and there is no regular packing within a cluster (or a "pearl" in Halperin−Goldbart terminology); these clusters evolve and merge either by coalescence and by various other mechanisms described in detail by Klushin,\(^{20} \) such as one cluster pulling another cluster to unwind and therefore grow. Interestingly, the early processes of coil−globule transition indeed are more likely to demonstrate the process of coalescence, whereas other

Figure 4. Contact map representation of a flexible chain (A) and a semiflexible chain (B): both exhibit cluster formation; however, the semiflexible chain appears to have a more ordered internal structure of each cluster.
mechanisms (pulling/unwinding) are more likely to take place in the final stages of collapse.

Semiﬂexible Chain \((l_p = 10\sigma)\). Perhaps unsurprisingly, the dynamic behavior of collapsing semiflexible chains is different from that of flexible chains (Figures 4, 6, and 7). The chain initially becomes elongated upon compaction, and the pearl-necklace structure is not present as we observe it in flexible chains, even though some characteristics of that behavior are still present, such as cluster formation and merging of clusters. However, simply observing a cylindrically shaped cluster does not reflect how intrachain contacts within the cluster are formed. Using the contact map analysis, we identify a very regular pattern that resembles a diamond shape. Further analysis revealed that each “diamond” represents an antiparallel hairpin structure,\(^{30}\) and these are regularly packed into higher-order structures where multiple antiparallel hairpins merge together in both parallel and antiparallel fashion, depending on the geometric constraints of the complex structure. It has to be noted that there exists a variation in hairpin size as well as in the hairpin density. In order to obtain a clearer representation of the coil–globule transition in this case, we performed analysis of each individual bundle of hairpins (which can be identified as

Figure 5. Series of snapshots for a flexible chain and corresponding representations of the structures in the contact map space. The time scale \(t\) here is represented in units of 1000 simulation time steps.
squares that consist of multiple diamond-like shapes) with respect to time. It is apparent from analysis of this type that a critical bundle size has to be reached before (1) nucleation takes place and (2) two hairpin clusters merge into one larger structure, which will be discussed in the next section.

**BOX-Plot Analysis**

In order to quantify the evolution of contact maps and detect the emergence of clusters, as well as present the process of cluster coalescence, one can perform the following analysis. In a contact map, as described in earlier sections, we can identify a square-shape region that is present around the main diagonal of a given map. Every square that emerges from a small group of contacts known as nucleation points gives us the information about how many monomers are present in a given cluster. The evolution of size $s$ of these clusters ("raindrops") is shown in the box-plot diagrams in Figure 8, and the size of each raindrop is related as $R(s) \approx s^{1/3}$. These raindrops, once formed, will grow and merge with other contact-map squares, producing larger clusters of monomers, until the single collapsed globular state is reached, and the square occupies the whole map ($s = ...
These squares emerge at different times, and each remains relatively constant in size until coalescence with another. We observe that in order to form a bigger cluster and for it to merge with another group of monomers, one requires the initial cluster size of at least $\sim 100$ monomers for flexible chains (Figure 8A) and closer to 200 for stiffer chains (Figure 8B). In this representation, we observe that the critical nucleation occurs when $R_c \approx 3-4\sigma$ for flexible chains and $R_c \approx 6\sigma$ for stiff chains. We also find that cluster formation is initial-configuration-dependent. This was confirmed by studying the evolution of five different initial configurations for each chain quenching episode; in all of these, we observed that the accidental initial off-diagonal contacts gave rise to a square in the region where these contacts existed initially (as one expects in nucleation). From our results, we also find that for flexible chains ($l_p = \sigma$) the number of clusters in the initial stage of the evolution process is higher, and these are also smaller in size compared to the semiflexible chain ($l_p = 10\sigma$), while the late stage is longer and more pronounced for a flexible chain, with just two big droplets persisting for a long time (see Figure 1G or 5 for $t = 300$).

### DYNAMICS OF COIL–GLOBULE TRANSITION

In order to understand the impact of solvent viscosity on the process of coil–globule transition, we performed simulations of polymer chains under different conditions ranging from low to high viscosities. This issue was originally raised in the work of Ansari and Kuznetsov, who experimentally studied the process of hairpin formation in single-stranded nucleotide chains and demonstrated the viscosity dependence of the process of hairpin formation; they conclude that diffusion of the chain through the solvent is involved in the rate-limiting step of hairpin formation. For different viscosities, we studied the time of collapse that is defined by the time at which the final elongated bridge between two globules is no longer detected on corresponding contact maps. On the box plot of Figure 8 this time is clearly visible as the moment when the cluster size jumps to $s = N$. We confirm the observations of Ansari and Kuznetsov (Figure 9) and therefore extend this idea to the fundamental concept of coil–globule transition for all chains.

![Figure 7](image_url)  
**Figure 7.** A closer look at the ordered structures present in the contact maps for semiflexible chains: (A) a series of diamond-like structures each of which represents an antiparallel hairpin as shown in the inset of (B).

![Figure 8](image_url)  
**Figure 8.** An illustration of box-plot analysis for a flexible (A) and a semiflexible (B) chain. The size of the square side $s$ on the contact map is an important parameter equivalent to $g_c$, the number of monomers in a blob, in Halperin–Goldbart terminology. Box-plots demonstrate the evolution of cluster domains with time. Each line represents a separate cluster, which continues until it merges with another.

![Figure 9](image_url)  
**Figure 9.** Power-law dependence of the collapse time on the viscosity of the solvent for a flexible chain. The solid line represents a power law of $-1/2$ (i.e., the time is proportional to the square root of viscosity).
Hairpin formation depends on the viscosity of the solvent and it could be speculated that the corresponding contact map representation of this protein for residue contacts within 15 Å.

**BIOLOGICAL PERSPECTIVE**

In this work, we specifically examined hairpin formation in semiflexible polymers; however, in order to demonstrate the biological importance of this phenomenon, we also introduce the concept of β-hairpin formation in proteins (Figure 10). Hairpin formation is a topic that has received attention from the field of biophysics due to its direct connection to the problem of protein folding. Let us consider the secondary structure features of a generic protein. These can generally be grouped into three categories: (1) β-sheet, (2) α-helices, and (3) unstructured amorphous regions. Each these has their own role in the dynamics and the functionality of a protein, by either stabilizing it or making the structure more flexible (unstructured regions can bring residues that are far apart along the linear chain closer, which will allow the protein to perform a specific function).

For most proteins, the structures of which have been solved experimentally, atomic coordinate data have been made publicly available. In order to show the biological relevance of the contact maps created from simulations in this work, we analyze a widely used, mainly β-sheet protein: the green fluorescent protein (PDB ID 1RXX). In its globular state it is found to form a β-barrel structure that consists of numerous β-hairpins. As with antiparallel hairpin structures described for the simulated chain (Figure 7), these exhibit similar characteristic diamond-shaped form, where the line that crosses the main diagonal represents one of the hairpins.

It is likely that the β-sheet structure, due to stable hydrogen bonding, is less flexible than the α-helical secondary structure, and it could be speculated that β-hairpin formation is a property that follows from this increased stiffness of the chain. From the static representation of the 3-dimensional protein structure, it is not possible to study hairpin formation over time. However, it has been observed experimentally that β-hairpin formation depends on the viscosity of the solvent—the less viscous the solvent, the faster the formation takes place. Our simulations indeed demonstrate this dynamical property. Viscosity gradients vary within the cell, and hence this property might be of biological importance to polymer-associated processes such as DNA folding in the nucleus and protein folding dynamics.

**DISCUSSION**

We have demonstrated that our Brownian dynamics simulations of polymer chains are in agreement with phenomenological models, other existing simulation algorithms such as Monte Carlo and hybrid mesoscale/molecular dynamics methods, and the experimental results available to us. We perform quantitative data analysis of chain configurations by generating dynamic contact maps and study the evolution of cluster sizes with the box-plot analysis to identify the time- and globule-size-dependent properties of the coil—globule transition. This analysis allows us to study the effect of chain bending stiffness on its morphological properties—semiflexible polymer chains undergo the transition process through a number of antiparallel hairpin structures that merge into elongated cylinder-like structures with parallel (nematic-like) folding, which later collapse into a highly anisotropic globular ground state. We also demonstrate a biological connection by highlighting similar properties of contact maps for model semiflexible polymers and for a real β-hairpin protein, which suggests that hairpin formation in proteins is mainly due to the higher stiffness that arises from β-sheet hydrogen bonding properties in polypeptide chains and not necessarily the chemical details of individual amino acids that form the hairpin.

It is important to note that the qualitative nature of our results is quite universal. This is due to the underlying scaling of parameters in the simulation, based on the "monomer" size σ. For instance, Rosa and Everaers used a value for σ = 30 nm, which corresponds to the diameter of experimentally observed chromatin fiber (DNA—protein complex) that would pack into a chromosome in the nucleus of a cell. To simulate a semiflexible nature of such a fiber, they used the persistence length \( l_p = 10\sigma \), which is exactly our semiflexible case. Since all other units are scaled proportionally, for the chromatin simulation, one also has the Lennard-Jones time \( \tau \approx 0.02 \) s, and therefore, our predictions hold quantitatively.
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Notes
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