

# Simulating the Effects of Excluded-Volume Interactions in Polymer Solutions

Elon Langbeheim\*

Cite This: *J. Chem. Educ.* 2020, 97, 1613–1619

Read Online

ACCESS |



Metrics &amp; More



Article Recommendations



Supporting Information

**ABSTRACT:** Excluded-volume interactions are ubiquitous to modeling the average size of polymers in solution. This paper shows how simulations can be used by students to explore the emergence of mathematical scaling relations from excluded-volume interactions. Simulations provide robust visual representations of the system, and can be used to investigate a wide scope of problems and scenarios. The simulations were built with the free VPython coding environment and relatively basic algorithms. The results align with the mathematical theories of Flory and De Gennes and provide access to additional insights that are less obvious in the mathematical treatments. Students with relatively basic programming knowledge were able to extend and modify these models and to examine their alignment with mathematical theories. These examples extend the growing literature on simulation-based approaches for teaching and learning chemistry.

**KEYWORDS:** Upper-Division Undergraduate, First-Year Undergraduate/General, Computer-Based Learning, Molecular Modeling, Statistical Mechanics, Solutions/Solvents, Materials Science



## INTRODUCTION

The theoretical analysis of polymer structure and conformations can be realized with statistical mechanics models or computational models. Several textbooks<sup>1–3</sup> and many courses focus on mathematical models when introducing the equilibrium properties and dynamics of polymer systems. While mathematical models are widespread, the introduction of computational models is still scarce despite their prevalence in research settings. Moreover, interactive, dynamic polymer models can elucidate the complexity of macromolecular behavior, especially if students are able to modify and build their code.<sup>4</sup> However, most texts on computational modeling of polymers are intended for the graduate level, and assume prior knowledge on the subject.<sup>5</sup> The purpose of this paper is thus to suggest a method for introducing polymer simulations to undergraduate level courses or laboratories.

Among the unique properties of polymers, the conformational consequences of excluded-volume interactions are of crucial importance. Excluded-volume interactions are in reality short-ranged repulsions, but can be modeled simply as a forbidden overlap between “rigid” particles. For example, in a model of a hard-sphere gas in a container of volume  $V$ , the volume  $b$  of each of the  $N$  hard sphere particles will be “excluded” from the volume of the container ( $V - Nb$ ). Similarly, in a polymer, excluded-volume interactions are modeled as nonoverlapping chain segments. Excluded-volume interactions influence the conformation of a single polymer molecule in a dilute solution,

but are especially important in dense environments such as living cells, where macromolecular “crowding” occurs.<sup>6,7</sup>

This paper examines two simulation-based activities that illustrate the role of excluded-volume interactions in the emergence of macrolevel polymer properties. The first activity, focuses on a single-chain model in a dilute solution. It uses a simulation of a two-dimensional polymer chain to introduce the probability distribution function of the end-to-end distances of a polymer chain, and the quantitative dependence of the end-to-end distance on the number of monomers. The second activity uses a similar simulation but one with many polymer chains, to examine the effect of concentration on the average end-to-end distances of the model polymers.

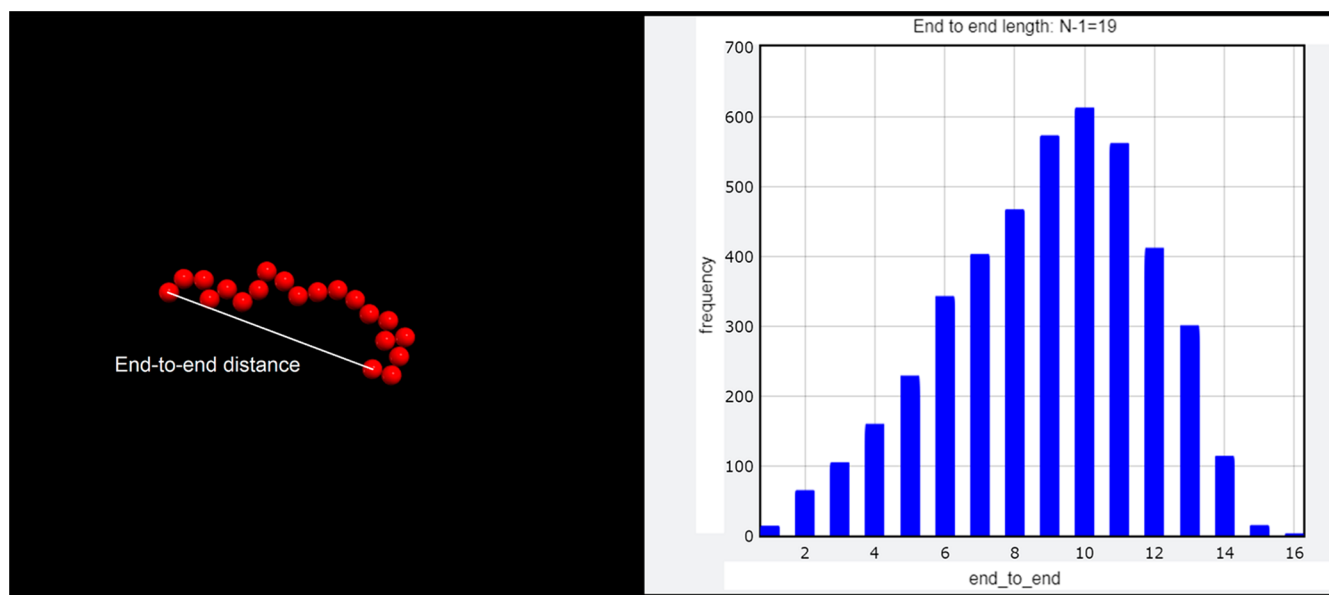
The two models were developed in an extra-credit, project-based course for talented high-school students.<sup>8,9</sup> The computational models were developed using VPython,<sup>10</sup> a free python library for creating three-dimensional graphics for simulations. The new version of VPython, GlowScript, translates the code into JavaScript so that simulations can be written and run on the web-browser.

Received: January 2, 2020

Revised: April 23, 2020

Published: May 11, 2020





**Figure 1.** End-to-end distance illustrated on a screen representing a single chain with  $N = 20$  units (left). The distribution of the end to end distances of the chain (right).

## DESCRIPTION OF THE COURSE AND APPROACH

The polymer simulations were developed for “Computational Science”, an AP level, project-based course for high school seniors.<sup>8,9</sup> The course comprises 15 afternoon sessions that combine a 60 min lecture, and a 90 min recitation in which students construct and modify computational models. Recitations entail worksheets that direct students in coding and mathematical analysis tasks. In addition, the course entails a midterm exam, and a final assignment. The final assignment is a computational inquiry project, in which students extend the models they encounter in course sessions, examine their output, and write a short paper describing their models and their findings. The first model of the single chain described below was studied using a worksheet during one of the sessions, and the second model of the solution, was developed by students in their final project.

The prerequisites for the course are basic knowledge in chemical thermodynamics (e.g., definition of entropy and internal energy) and a basic course in programming. The codes require students to understand “for” and “while” loops, and definition and uses of functions and of list objects. The graphical interface of VPython is introduced in the course itself. Because high school students have a limited background in chemistry and in programming, the scope of systems and computational methods was rather narrow—we focused only on Metropolis-Monte Carlo algorithms<sup>5</sup> and modeled four main systems: elastic-sphere gas, binary mixtures, surfactants, and polymers. A similar course given at our university for third year undergraduates, entails a wider range of computational methods and phenomena.

### Pedagogical Approach to Learning Using Coding

The lectures introduce modeling concepts, such as the end-to-end distance as a measure of the configuration of polymers. The computational models are then explored in the recitations usually by asking students to complete or modify an incomplete “skeleton” model—a useful approach to learn computer programming.<sup>11</sup> Completing and modifying models starts with reading and interpreting an initial “skeleton” computer code and

continues with adding new sections to the code, running the modified code, and checking for errors. This complex task, is scaffolded by detailed instructions both in the skeleton code itself (such as “add a missing line here”) and in the worksheets. Additional guidance is provided by the instructor. The following section introduces a modeling task in which students build a model of the reputation of a single polymer chain. The task duration is two recitation meetings.

## END-TO-END DISTANCE OF A SINGLE CHAIN WITH EXCLUDED VOLUME

### A computational model of a single polymer chain

Polymer models can be implemented on a lattice, where each monomer occupies one site, and the angles between neighboring monomers are determined by the lattice geometry (e.g., square or hexagonal). In an off-lattice model, continuous Cartesian coordinates are used and the angles between neighboring monomers are not fixed. Our computational model is of the latter type, an off-lattice model, which is more appropriate to study dense systems—the topic of the next section. The model utilizes the reptation/slithering snake model.<sup>12</sup> It first creates a nonrandom initial configuration and then drives the chain by moving the first monomer, the “head”, to a new location, and removing the last monomer, the “tail”, from its previous location. The single chain reptation model<sup>13</sup> can be found in the [Supporting Information](#). The algorithm contains an initialization loop in which the chain is created (lines 31–50), and a “reptation” loop that moves the chain along a random path (lines 52–74). The reptation loop starts by randomly choosing an angle  $\theta$  between 0 and  $2\pi$  for the next location of the leading monomer of the chain, the graphical object in the first element in the list “polymer” (in python, the first element is designated as `polymer[0]`). The new location is  $(x + 2r \cos \theta, y + 2r \sin \theta)$  where  $x$  and  $y$  are the current location coordinates of the leading monomer and  $r$  is the radius of each monomer. The program then checks whether the new location overlaps with the chain (lines 55–63), and if it does not, the leading monomer moves to the new position and the other monomers move to the locations

of the monomers in front of them: `polymer[i].pos → polymer[i - 1].pos` (lines 65–69). If the new location is occupied, the polymer list is inverted so that the leading monomer becomes the last monomer, the second monomer becomes one before last etc. (lines 71–74 in the code).

The chain is created in a square with side length  $L = 2N$  where  $N$  is the number of monomers. The radius of each monomer in the chain  $r$  is defined by  $r = \sqrt{\frac{\phi L^2}{N\pi}}$  where  $L^2$  is the size of the square in which the model is contained and  $\phi$  is the two-dimensional area fraction covered by the polymer chain.

The code also uses two functions: the “distance” function that calculates the distance between two monomers (lines 18–24), and the “free-site” function that checks whether a site is occupied or not (lines 9–16). The “free-site” function implements the excluded-volume interaction by calling the “distance” function, that calculates the distance of a location  $(x,y)$  from the center of each monomer of the chain. If the distance is smaller than  $2r$ , the diameter of a monomer, the function returns “False”. If it is larger than  $2r$  it returns “True”.

After running the loop for  $100N$  steps to decorrelate from the initial, nonrandom configuration, the end to end distance is sampled every  $10N$  reptation moves that are necessary to decorrelate from the previous configuration of the chain (lines 76–84). Altogether the algorithm performs  $50,000N$  steps, so it samples 5000 different configurations. The end-to-end distances are binned into a histogram that indicates whether the sample reflects the expected, equilibrium distribution of lengths of a self-avoiding walk.<sup>14</sup> The derivation of the distribution function can be found in ref 2, pp 122–123. The distribution of the end-to-end distance of the polymer chains for  $N = 20$  monomers, at a density  $\phi = 0.02$ , is shown in Figure 1.

### Comparison of Simulation Results and Analytic Theory

The mathematical model for the scaling of the average end-to-end distance of a self-avoiding chain model with its number of monomers in two dimensions can be calculated using the Flory theory (see ref 3, p 41). The theory assumes two entropic terms in the free energy of the polymer chain: one term approximates the entropic contribution of the conformations of a random/intersecting chain with an end-to-end distance  $R$ , and the other approximates the entropic reduction resulting from excluding all of the configurations with overlap between monomers. The minimization of the free energy according to the degree of freedom  $-R$  yields the scaling ratio of a freely jointed chain in two dimensions:

$$\langle R_{2D} \rangle \cong b(N-1)^{0.75} \quad (1)$$

In this equation,  $\langle R_{2D} \rangle$  is the average end-to-end distance,  $b$  is the Kuhn length, and  $N - 1$  is the number of monomer–monomer connections. The power of 0.75 is larger in the two-dimensional case than in the three dimension case (where the power is 0.6) since excluded-volume interactions are more common in two-dimensions forcing the chains to be more elongated. The readers can run the simulation and verify for themselves that the simulation produces relatively elongated chains, and a power law of almost 0.75 which is aligned with the Flory theory of eq 1 as shown in Figure 2. A more detailed description of the assignment administered to the students, can be found in the Supporting Information.

A simple way to verify that the scaling produced by the simulation is indeed due to excluded volume interactions, is by eliminating the forbidden overlap condition in the function

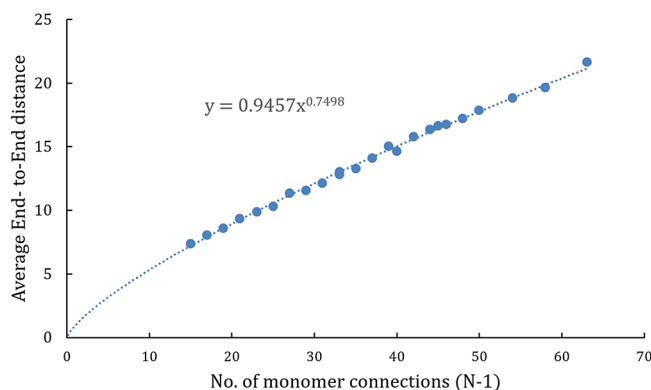


Figure 2. Scaling of the 2D excluded-volume chain.

“free-site”. If lines 11–15 are erased, the “free-site” function will return a “true” value whether the move overlaps or does not. Running the simulation now will yield a “Random-Walk” (RW) chain, that has a shorter average end-to-end distance. The scaling of random-walk chains is described by eq 2:

$$\langle R_{2D,RW} \rangle \cong b(N-1)^{0.5} \quad (2)$$

The comparison of the excluded-volume scaling and the scaling of a chain with self-intersections can be given as an assignment to the students.

### Evidence of Learning to Build the Code of a Single Polymer Chain

Students in the course built the model of the excluded-volume chain, according to the directions in the worksheet that can be found in the Supporting Information. However, most students did not complete the worksheet entirely by themselves. They asked for guidance from the instructor, mainly when debugging errors. In the course, all of the students submitted a working model of a lattice-based self-avoiding chain. Furthermore, in a question given in the midterm exam, students were given a code that did not call the “free-site” function in the reptation loop, and were asked whether the program creates self-avoiding polymers. Most students (89%) correctly recognized that since the code does not include a function that checks whether the site is free, the polymer can intersect with itself. A second question, asked what is the ratio between the end-to-end distance and the number of monomers in this case. A smaller proportion of students (20%) realized that since the code represents an intersecting chain, its average end-to-end distance should be proportional to the square-root of the number of monomer connections, as shown in eq 2. This indicates that while understanding the computer program is relatively straightforward for most students, applying the analytical theory needs more explicit instructional support. The next section, illustrates a more complex example of computational modeling using excluded volume, studied in the final assignment of the course.

### EFFECT OF DENSITY ON THE END-TO-END DISTANCE OF POLYMERS

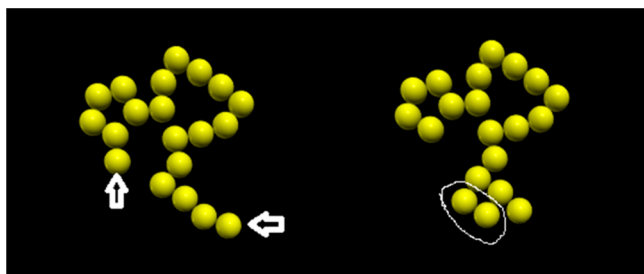
Excluded-volume interactions are important factors in modeling material properties related to changes in density. For example, changing the density a system of liquid crystals, modeled as hard-rods with excluded-volume interactions (no attractive interactions), leads to a spontaneous alignment of the rods and the formation of a “nematic” state.<sup>15</sup> Another example is a binary mixture of hard spheres or squares of two different sizes that



either mixes or phase separates depending on the density and radii ratio.<sup>16</sup>

In a polymer solution, a system of many polymer chains dissolved in a fluid, excluded-volume interactions give rise to a change in scaling of the end-to-end distance (ref 2, pp 176–181). At low concentrations, chains rarely touch each other, and their average size resembles that of the single chain that was discussed in the previous section. This is the “dilute” regime, in which concentration has a negligible effect on the end-to-end distance. However, at higher concentrations, and especially beyond the “overlap concentration”,  $\phi^*$ , the chains touch each other almost all the time, and the interchain excluded-volume interactions decrease the end-to-end distance as the overall concentration increases. This is the “semidilute” regime. At a yet higher concentration,  $\phi^{**}$ , the system reaches the “concentrated” regime in which the chain–chain interactions are so frequent that changing the density does not influence the end-to-end distance very much. A “concentrated” solution in which the concentration of polymer is very high resembles a polymer “melt”—a pure polymer material.

The simulation of a single polymer described in the previous section, can be modified to represent a polymer solution by adding several chains, moving them according to the Metropolis algorithm<sup>17</sup> and monitoring their average end-to-end distance. Building several chains requires changes in the creation of the initial configuration of the system. In the modified simulation,<sup>18</sup> that can be found in the [Supporting Information](#), each chain is placed initially in a folded configuration, with the head and tail neighboring each other. This is a nonequilibrium state, so we must ensure that sampling starts only after sufficient steps that decorrelate the system from its initial configuration. We found that 1500N $\phi$  initial Monte Carlo steps (line 48) suffice for the system to reach a random configuration. A second major modification in the simulation is the addition of a “kink” move option in the algorithm in lines 121–146. This move, shown in [Figure 3](#), creates a kink in the chain, while retracting both its



**Figure 3.** Creation of a “kink” in the chain. The chain before the kink move (left), with the head and tail indicated by arrows. The kinked chain (right), with the two circled monomers sticking out of the chain, and the head and tail retracted.

head and tail. This move is necessary, since the system gets “jammed” and fails to reach equilibrium in dense configurations when only reptation moves are allowed. The [Supporting Information](#) shows that simulations without the kink move do not produce end-to-end distributions that resemble the form of ref 14. In order to prevent the kink move from influencing the scaling of the polymer in dilute solutions, it is only applied at a 0.05 probability and only in cases for which the head move attempt created overlap. One final modification in the program is in the “free-site” function that prevents chain overlap. The revised version of the function first searches which chains have

the middle monomer within a radius of  $Nr$ —half of the chain length—from the current location. Then, only for these chains, it checks whether one of the monomers is within a distance smaller than  $2r$  from the current location. This minor modification in lines 12–13 has a significant impact on the running time of the simulation, and students can verify this by erasing this condition and comparing the running time.

Both the density of the system and the number of monomers in each chain influence the end-to-end distance. [Figure 4](#) shows several system configurations of  $n = 30$  polymer chains at different densities and chain length. Note that while the concentrations in each column are the same, the density seems to be larger in long chains with  $N = 30$  than with the shorter ones with  $N = 10, 20$ . In the next section, we analyze the alignment between the simulation and the analytic theory.

### Comparison of Simulation Results and Analytic Theory

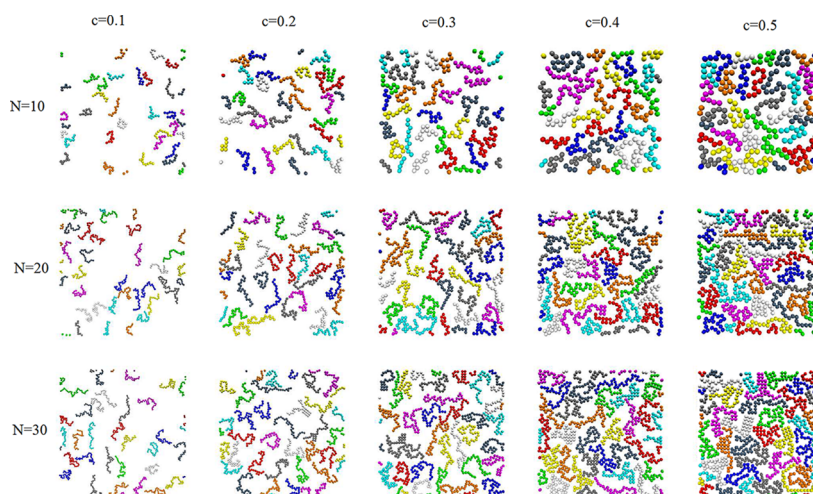
The analytic theory of polymer scaling provides a simple estimate for the “overlap concentration”  $\phi^*$  in good solutions, where bonding with the solvent molecules incurs no energetic costs or losses. The area occupied by each chain can be modeled by a circle or a square. Here we prefer to use squares since the area itself is rectangular and coverage by a circle is not complete. The size of the average square encapsulating the polymer chain can be estimated as

$$s \cong \langle R_{2D} \rangle^2 \cong (b(N-1)^{0.75})^2 \quad (3)$$

The overall area occupied by all  $n$  chains should equal the overall area of the container  $A$ , so that  $A = sn$ , and  $s$  is given by [eq 3](#). The overlap concentration is the ratio between the net area covered by the  $N$  monomers of the  $n$  chains, each with an area of  $\pi(\frac{b}{2})^2$ , and the overall area  $A$ , so that

$$\phi^* = \frac{(N)n\pi(\frac{b}{2})^2}{A} \cong \frac{(N)n\pi(\frac{b}{2})^2}{(b(N-1)^{0.75})^2} \cong \frac{\pi}{4}N^{-0.5} \quad (4)$$

[Equation 4](#) shows that the overlap concentration is inversely proportional to the chain length. The constant  $\frac{\pi}{4}$  reflects the choice of covering the area with squares with sides  $\langle R_{ete} \rangle$  and is therefore an arbitrary approximation—it will be neglected in the subsequent derivation steps. At concentrations larger than the overlap concentration, the end-to-end distance decreases, as chain concentration increases. This has been shown experimentally for various polymers including DNA strands.<sup>19</sup> The most elegant way to estimate the mathematical connection between the end-to-end distance and the concentration in the semidilute regime, is to use a scaling argument. Daoud and De Gennes<sup>20</sup> used two assumptions to deduce the concentration dependence of the end-to-end distance. First, they stated that, at the overlap concentration, the average end-to-end distance should scale like at a single, self-avoiding chain as indicated by [eq 1](#). This assumption maintains continuity between the dilute regime (in which chains rarely interact with other chains) and the semidilute regime. Second, they assume that a chain in the semidilute regime should become more compact than in the dilute regime, since it is confined by neighboring chains. In other words, in the semidilute regime, the “intra-chain” excluded volume interactions that prevent overlap between the chain segments, are balanced by “inter-chain” interactions with the neighboring chains, yielding no excluded-volume swelling. Thus, they assume that the chain should behave in this regime like simple random-walk chains that scale like [eq 2](#). These



**Figure 4.** Configurations of 30 chains with different lengths (vertical) and densities (horizontal)

assumptions are valid only for concentrations below  $\phi^{**}$ , at which the system becomes densely packed, and “concentrated”. They “guess” an expression with the concentration divided by the overlap concentration, and raised to an unknown power  $x$ , that reduces to eq 1 when  $\phi = \phi^*$ .

$$\begin{aligned} \langle R(\phi^{**} > \phi > \phi^*) \rangle &= b(N-1)^{0.75} \left( \frac{\phi^*}{\phi} \right)^x \\ &\cong b(N-1)^{0.75} \left( \frac{N^{-0.5}}{\phi} \right)^x \end{aligned} \quad (5)$$

Since  $R$  should satisfy eq 2 and the concentration  $\phi$  does not depend on  $N$ , the power  $x$  that satisfies this relationship has to be  $x = 0.5$ , and we have

$$\begin{aligned} \langle R(\phi^{**} > \phi > \phi^*) \rangle &\cong b(N-1)^{0.75} \left( \frac{N^{-0.5}}{\phi} \right)^{0.5} \\ &\cong b(N-1)^{0.5} \phi^{-0.5} \end{aligned} \quad (6)$$

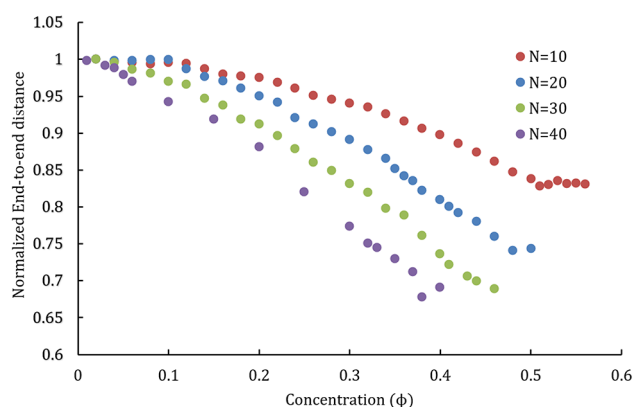
At concentrations higher than  $\phi^{**}$ , the system is in the “concentrated” regime, and the chains are fairly compact. Changes in polymer concentration or chain density do not influence the average radius in the regime, and by inserting  $\phi = \phi^{**}$  into eq 6, we find that the average radius should reach:

$$\langle R(\phi > \phi^{**}) \rangle \cong b(N-1)^{0.5} (\phi^{**})^{-0.5} \quad (7)$$

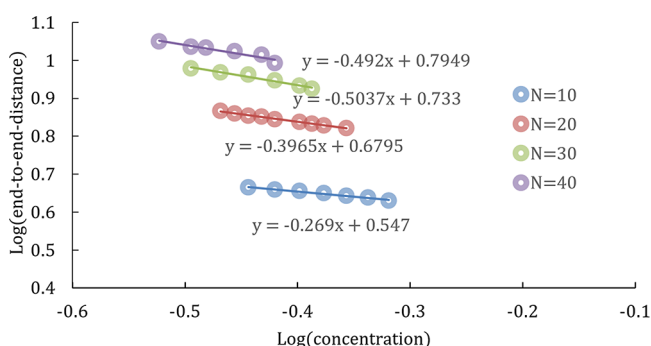
Figure 5 shows the average end-to-end distances of chains of lengths  $N = 10, 20, 30, 40$  at different concentrations. The end-to-end distances were normalized, that is, divided by the initial “dilute” value  $\langle R(\phi \ll 1) \rangle$  in order to compare the trends of the different chain-lengths.

The curves differ in three parameters: the onset of decline in the average chain length at the overlap concentration  $\phi^*$ , the onset of the “concentrated” regime  $\phi^{**}$  in which the end-to-end distances barely change, and the shape of the curves between  $\phi^*$  and  $\phi^{**}$ , in the semidilute regime. The values of  $\phi^*$  and  $\phi^{**}$  clearly decrease with the number of monomers  $N$ , but the values of the overlap concentration seem to be half of the values predicted by eq 4.

The log/log graphs in Figure 6 show the behavior of the system in the semidilute regime. The plot focuses on data points far from the dilute regime, since the theoretical assumption used



**Figure 5.** Simulation results of the end-to-end distance of the chains as a function of concentration at different chain lengths.



**Figure 6.** Log–log plot of the average end-to-end distances in the semidilute regime.

by Daoud and De Gennes in ref 20 was that the polymer lengths scale like eq 2. This assumption is not valid close to the overlap concentration, where the scaling of the chains resembles their size in dilute solutions.

The analytic theory predicts a power of  $\langle R \rangle \propto \phi^{-0.5}$  in the semidilute regime which means a slope of  $(-0.5)$  in the log–log plot, regardless of  $N$ . The simulation data reveal that for  $N = 30$  and  $N = 40$ , the simulation results are indeed very close to the analytic prediction. However, for lower chain lengths ( $N = 10, N = 20$ ) the simulation results do not align with the analytic prediction, and the power dependence of the end-to-end

distance is lower than  $(-0.5)$ . The reason for this discrepancy in short, excluded-volume chains is the correlation between monomer connections in the same chain. That is, the angle between the first monomer and the second is correlated, for example, with the angle between the seventh and eighth monomers. Therefore, the average scaling of these short chains is always larger than predicted by eq 2. This is also evident in the linear equations in Figure 6 for which the intersection of the line with the  $y$  axis should equal  $\log(N-1)^{0.5} = 0.5 \log(N-1)$  according to eq 6. While the values of the  $N = 30$  and  $N = 40$  plots are aligned with the analytical prediction, the values of the  $N = 10$  and  $N = 20$  plots are larger than  $0.5 \log(9)$  and  $0.5 \log(19)$ .

### Model Implementation in the Course

The effect of the polymer's density on its end-to-end distance is an example of a final project assignment in the course. The student who chose this project read the textbook chapter in ref 2 about the different concentration regimes (dilute, semidilute, concentrated) and about the predictions of the analytical theory. Then, the student modified the single chain model into a computational model of a solution with many chains. This entailed several challenges such as the design of the initial configuration of the dense system. The student worked on this project for approximately 3 weeks, during which he consulted the instructor at some key points, but performed most of the programming without help. The student's final paper presented the results of the model and a comparison with the analytical theory, and suggested improvements. Some were implemented in the models shown here. There were other projects that examined excluded-volume topics, for example, assessing the average size of a simulated "star" shaped polymer, or the effect of density on the flow-rate of a polymer solution through a cavity. By and large, students with better programming background were more independent when working on their final assignments; however, some of the best projects were performed by students with almost no background in programming when entering the course.

### CONCLUDING REMARKS

The simulations presented in this paper illustrate the effect of excluded-volume interactions on the size of polymers in a two-dimensional model of a solution. Excluded-volume is implemented through the "free-site" function that prevents overlap between monomers. This simple model produces results aligned with the mathematical theory of Flory and De Gennes and promotes discussion of the effects of excluded-volume on the size of the chain. This modeling approach extends the recent interest in implementing simulation-based learning for introducing polymer properties.<sup>4</sup> The limitation of this approach is shown by the midterm exam results. While students comprehended the computational model well, their ability to apply the analytical theory was limited. Nevertheless, this example of supporting students in building models in this AP level high-school course indicates the feasibility of this approach at the college level.

### ASSOCIATED CONTENT

#### Supporting Information

The Supporting Information is available at <https://pubs.acs.org/doi/10.1021/acs.jchemed.0c00003>.

Single polymer VPython code (PDF, DOCX)

Polymer solution VPython code (PDF, DOCX)

Justification for including the "kink" procedure (PDF, DOCX)

Student worksheet for constructing the single polymer model (PDF, DOCX)

### AUTHOR INFORMATION

#### Corresponding Author

Elon Langbeheim – Graduate Program for Science and Technology Education, Ben Gurion University of the Negev, 84105 Beer Sheva, Israel; [orcid.org/0000-0001-8063-3999](https://orcid.org/0000-0001-8063-3999); Email: [elonlang@bgu.ac.il](mailto:elonlang@bgu.ac.il)

Complete contact information is available at: <https://pubs.acs.org/10.1021/acs.jchemed.0c00003>

#### Notes

The author declares no competing financial interest.

### ACKNOWLEDGMENTS

I want to thank my mentors Samuel Safran and Edit Yerushalmi from the Weizmann Institute of Science for giving me the opportunity to develop this course. A special thanks goes to Ohad Cohen, who cotaught the course with me, for reading and commenting on the manuscript.

### REFERENCES

- (1) Doi, M. *Introduction to polymer physics*; Oxford University Press: New York, NY, 1996.
- (2) Rubinstein, M.; Colby, R. H. *Polymer Physics*; Oxford University Press: New York NY, 2003; Vol. 23.
- (3) Teraoka, I. *Polymer Solutions: An Introduction to Physical Properties*; John Wiley & Sons: New York, NY, 2002.
- (4) Al-Moameri, H. H.; Jaf, L. A.; Suppes, G. J. Simulation Approach to Learning Polymer Science. *J. Chem. Educ.* **2018**, 95 (9), 1554–1561.
- (5) Binder, K. Ed. *Monte Carlo and Molecular Dynamics Simulations in Polymer Science*; Oxford University Press: New York, NY, 1995.
- (6) Ralston, G. B. Effects of "Crowding" in Protein Solutions. *J. Chem. Educ.* **1990**, 67 (10), 857.
- (7) Silverstein, T. P.; Slade, K. Effects of Macromolecular Crowding on Biochemical Systems. *J. Chem. Educ.* **2019**, 96 (11), 2476–2487.
- (8) Langbeheim, E.; Edri, H.; Schulmann, N.; Safran, S. A.; Yerushalmi, E. Extending the boundaries of High School Physics: Talented Students Develop Computer Models of Physical Processes in Matter. In *Research in Science Education (RISE) Series - Vol. 8, Physics Teaching and Learning: Challenging the Paradigm*; Dennis, W. S., Ed.; Information Age Publishing, 2019.
- (9) Langbeheim, E.; Abrashkin, A.; Steiner, A.; Edri, H.; Safran, S. A.; Yerushalmi, E. Shifting the learning gears: redesigning a project-based course on soft matter through the perspective of constructionism. *Phys. Rev. Phys. Educ. Res.* **2020**.
- (10) Scherer, D.; Dubois, P.; Sherwood, B. A. Vpython: 3d interactive scientific graphics for students. *Comput. Sci. Eng.* **2000**, 2 (5), 56–62.
- (11) Van Merriënboer, J. J.; De Croock, M. B. Strategies for computer-based programming instruction: Program completion vs. program generation. *J. Ed. Comp. Res.* **1992**, 8 (3), 365–394.
- (12) Wall, F. T.; Mandel, F. Macromolecular dimensions obtained by an efficient Monte Carlo method without sample attrition. *J. Chem. Phys.* **1975**, 63 (11), 4592–4595.
- (13) Glowscript. Single Polymer Program. <https://www.glowscript.org/#/user/matmid19/folder/Public/program/singlepolymer> (accessed 2020–03–18).
- (14) Mazur, J. On the Limiting Shape of the Distribution Function of Lengths of a Single Polymer Molecule with Excluded-Volume Effects. *J. Chem. Phys.* **1965**, 43 (12), 4354–4356.

- (15) Frenkel, D.; Eppenga, R. Evidence for algebraic orientational order in a two-dimensional hard-core nematic. *Phys. Rev. A: At, Mol, Opt. Phys.* **1985**, 31 (3), 1776.
- (16) Buhot, A.; Krauth, W. Phase separation in two-dimensional additive mixtures. *Phys. Rev. E: Stat. Phys., Plasmas, Fluids, Relat. Interdiscip. Top.* **1997**, 159, 2939–2941.
- (17) Metropolis, N.; Rosenbluth, A.; Rosenbluth, M.; Teller, A.; Teller, E. Equation of state calculations by fast computing machines. *J. Chem. Phys.* **1953**, 21 (6), 1087–1092.
- (18) Glowscript. Polymer Solution Program. <https://www.glowscript.org/#/user/matmid19/folder/Public/program/polymersolution> (accessed 2020–03–18).
- (19) Nepal, M.; Yaniv, A.; Shafran, E.; Krichinsky, O. Structure of DNA coils in dilute and semidilute solutions. *Phys. Rev. Lett.* **2013**, 110, 058102.
- (20) Daoud, M.; De Gennes, P. G. Statistics of macromolecular solutions trapped in small pores. *J. Phys.* **1977**, 38 (1), 85–93.