

Section	Criteria	Points
<b>1. Implementation</b> (80 Points)		
<b>A. Molecular Dynamics Simulation of Polymer Chain</b> (50 Points)		
	Correct Initialization of Positions and Velocities	15
	– Properly sets up initial positions without overlaps	8
	– Applies periodic boundary conditions correctly	7
	– Initializes velocities from Maxwell-Boltzmann distribution	
	Implementation of Harmonic Bond Potentials and Forces	10
	– Correctly codes the harmonic bond potential	5
	– Accurately computes forces from the harmonic potential	5
	Implementation of Lennard-Jones Non-Bonded Interactions	10
	– Correctly codes repulsive LJ potential and forces	5
	– Correctly codes attractive LJ potential and forces	5
	Integration Using Velocity Verlet Algorithm	10
	– Correctly implements the velocity Verlet integration	10
	Temperature Control Using Velocity Rescaling Thermostat	5
	– Accurately maintains constant temperature using velocity rescaling	
<b>B. Data Collection and Storage</b> (10 Points)		
	Storage of Trajectories for Analysis	5
	– Efficiently stores positions and velocities over time	
	Calculation and Storage of Properties	5
	– Correctly calculates $R_g$ , $R_{ee}$ , and potential energy	
	– Stores computed properties for analysis	
<b>C. Simulation Parameters</b> (20 Points)		
	Simulation at Different Temperatures	10
	– Correctly sets up simulations across specified temperature range	
	– Ensures stability and accuracy at each temperature	
	Identification of Suitable Parameters	10
	– Determines values of $k$ and $\epsilon_{\text{repulsive}}$ to prevent folding	
	– Justifies choices based on simulation results	
<b>2. Analysis</b> (60 Points)		
<b>A. Calculation of Properties</b> (20 Points)		
	Calculation of Radius of Gyration ( $R_g$ )	10

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	<ul style="list-style-type: none"> <li>– Implements correct formula for <math>R_g</math></li> <li>– Accurately computes <math>R_g</math> from simulation data</li> </ul>	
	Calculation of End-to-End Distance ( $R_{ee}$ )	10
	<ul style="list-style-type: none"> <li>– Implements correct formula for <math>R_{ee}</math></li> <li>– Accurately computes <math>R_{ee}</math> from simulation data</li> </ul>	
	<b>B. Phase Transition Identification</b> (20 Points)	
	Observation of Phase Transition	10
	<ul style="list-style-type: none"> <li>– Identifies folding and unfolding behaviors in simulations</li> <li>– Provides evidence of phase transition from data</li> </ul>	
	Determination of Transition Temperature	10
	<ul style="list-style-type: none"> <li>– Accurately determines the temperature of phase transition</li> <li>– Supports findings with appropriate analysis and plots</li> </ul>	
	<b>C. Visualization</b> (20 Points)	
	Plots of $R_g$ vs. Temperature	7
	<ul style="list-style-type: none"> <li>– Clear and accurate plot of <math>R_g</math> as a function of temperature</li> </ul>	
	Plots of $R_{ee}$ vs. Temperature	7
	<ul style="list-style-type: none"> <li>– Clear and accurate plot of <math>R_{ee}</math> as a function of temperature</li> </ul>	
	Plots of Potential Energy vs. Temperature	6
	<ul style="list-style-type: none"> <li>– Clear and accurate plot of potential energy as a function of temperature</li> </ul>	
	Visualization of Polymer Configurations	5
	<ul style="list-style-type: none"> <li>– Provides visualizations at different temperatures</li> <li>– Illustrates differences between folded and unfolded states</li> </ul>	
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<b>3. Report</b> (50 Points)		
	<b>A. Quality of Writing</b> (15 Points)	
	Clarity and Conciseness	5
	<ul style="list-style-type: none"> <li>– Presents information logically and coherently</li> <li>– Explains technical terms clearly</li> </ul>	
	Grammar and Spelling	5
	<ul style="list-style-type: none"> <li>– Uses correct grammar and spelling throughout</li> </ul>	
	Structure and Organization	5
	<ul style="list-style-type: none"> <li>– Includes all required sections (Introduction, Methods, Results, Discussion, Conclusion)</li> <li>– Uses headings and subheadings effectively</li> </ul>	

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Section	Criteria	Points
	<b>B. Inclusion of Figures and Visualizations</b> (15 Points)	
	Inclusion of All Required Figures	5
	– All plots and visualizations are included as specified	
	Figure Quality and Formatting	5
	– High-resolution images with clear labels and legends	
	– Consistent formatting across all figures	
	Proper Referencing of Figures	5
	– Figures are properly referenced and discussed in the text	
	<b>C. Interpretation and Implications</b> (20 Points)	
	Explanation of Results	10
	– Provides insightful interpretation of simulation data	
	– Explains how temperature affects polymer behavior	
	Discussion of Phase Transition and Material Design	10
	– Discusses implications for polymer design in space applications	
	– Connects findings to the prevention of folding at low temperatures	
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<b>4. Submission</b> (10 Points)		
	<b>A. Code Submission</b> (6 Points)	
	Code Organization and Documentation	4
	– Code is well-organized with appropriate directories and files	
	– Includes comments and documentation for clarity	
	Code Repository	2
	– Code is pushed to GitHub repository	
	<b>B. Submission of Repository Link</b> (4 Points)	
	Timely Submission	2
	– Repository link submitted before the deadline	
	Accessibility	2
	– Repository is public and accessible	
	– Link directs to the correct repository	
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<b>5. Optional Enhancements</b> (Up to 10 Bonus Points)		
	<b>A. Chain Length Effects</b>	5
	– Investigates how polymer length affects folding behavior	

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Section	Criteria	Points
	– Presents analysis and discussion of findings	
	<b>B. Energy Minimization Before MD Simulation</b>	5
	– Performs energy minimization to find stable initial configuration	
	– Describes methodology and impact on results	