## **Introduction**

Stimuli-responsive polymers (SRPs), also known as "smart" or "intelligent" polymers, are materials that undergo significant and reversible changes in response to environmental stimuli. These stimuli can be physical, such as temperature, ionic strength, solvents, radiation (UV, visible light), electric fields, mechanical stress, high pressure, sonic radiation, and magnetic fields; chemical, like pH, specific ions, and chemical agents; or biochemical, such as enzyme substrates and affinity ligands [1-3]. The ability of SRPs to adapt to environmental conditions allows for dynamic functionality across various applications. Their versatility lies in the design and fine-tuning of polymers' physical, chemical, or mechanical properties to respond to one or more stimuli, making SRPs essential in sectors ranging from healthcare to energy and electronics.

In particular, SRPs have garnered significant attention in the medical field, where their ability to respond to specific triggers proves invaluable. For example, in drug delivery systems, the inability to precisely control when and where medications are released can lead to side effects and reduced therapeutic efficacy. SRPs address this challenge by releasing drugs in response to specific triggers, such as temperature or pH, ensuring targeted and controlled delivery and thereby improving efficacy while reducing side effects [4-7]. Beyond drug delivery, SRPs are instrumental in diagnostics [1, 8-10], tissue engineering and regenerative medicine [11-13], and cell culture applications [14-17], where their responsive nature enhances functionality and outcomes.

Similarly, in energy storage and conversion, conventional materials rely on external regulation for efficiency, whereas SRPs can autonomously adjust energy release or conversion based on environmental conditions. For instance, SRPs enhance the performance of batteries, supercapacitors, and solar cells by adjusting energy storage and release in real-time in response to changes in temperature or light [18-20]. This adaptability not only improves efficiency but also contributes to the development of more sustainable energy systems.

In environmental remediation, the need for materials that can target specific pollutants is critical. SRPs respond to changes in pH or the presence of certain chemicals, enabling selective pollutant capture and degradation, thereby improving the effectiveness of clean-up efforts [21-25]. Applications include air purification and water treatment and purification processes, where SRPs can selectively bind and neutralize contaminants [26-28].

SRPs have also found promising applications in textiles, enabling the creation of flexible sensors and smart displays for use in fields such as healthcare and environmental monitoring. These textiles can adjust moisture-wicking and breathability in response to temperature fluctuations, display color changes triggered by pH levels [29], magnetic fields [30], UV exposure, or the presence of volatile organic compounds [31]. Such developments highlight the growing potential of SRPs in producing textiles that are not only highly functional but also sustainable, as they incorporate environmentally friendly materials [32].

SRPs are advancing electronics by enabling more adaptive and responsive devices. Soft fiber and textile actuators respond to stimuli, exhibiting versatile deformations like bending and contraction. This makes them suitable for applications like artificial muscles and smart textiles. Additionally, water-responsive polymers have been developed to provide rapid contraction for bioelectronic interfaces, allowing conformity to irregularly shaped tissues, which is essential for medical implants and flexible electronics [33, 34].

Understanding the behavior of stimuli-responsive polymers requires simulation techniques that can accurately capture their dynamic and structural properties across different scales. These simulations have also explored the structure-property relationship, which is essential for predicting how SRPs will perform under various conditions. Particle-based simulation methods are pivotal in this endeavor, as they model systems at the level of individual particles or groups of particles. The primary methods include Molecular Dynamics (MD), Monte Carlo (MC), Brownian Dynamics (BD), and Dissipative Particle Dynamics (DPD). Each method has its theoretical foundations, strengths, and limitations.

MD is one of the most widely used particle-based simulation methods, frequently applied to study the structure and dynamic evolution of biomolecules, proteins, and polymers. MD works by solving Newton’s equations of motion iteratively, using predefined interaction potentials, commonly referred to as force-field parameters [35, 36]. These interactions are categorized into bonded and nonbonded forces. Bonded interactions, typically modeled by harmonic potentials, include bond lengths, bond angles, dihedral angles, and improper angles. Nonbonded interactions account for electrostatic and van der Waals forces [37]. MD can be performed at both atomic (all-atom or AA) and molecular (coarse-grained or CG) levels, depending on the scale and complexity of the system being studied. In all-atom MD simulations, every atom in the system is explicitly modeled, allowing for high-resolution studies of molecular interactions. While all-atom MD offers an accurate depiction of atomic-level behavior, it comes with significant computational costs, especially when applied to large systems involving millions of atoms. Despite its detailed insights, simulating extensive time scales or complex environments, such as solvated polymers, can be highly resource-intensive, limiting its practicality for large-scale or long-duration simulations.

MC uses a stochastic approach, relying on random numbers to predict particle positions [38, 39]. In this method, particle positions are updated iteratively, and changes in potential energy determine whether the new configurations are accepted or rejected. If the new configuration results in lower potential energy, it is accepted; otherwise, it may still be accepted based on a probability related to the system's temperature and energy difference [40]. UnlikeMD, MC does not calculate forces and is better suited for analyzing the equilibrium properties of systems rather than their dynamic behavior. Since MC relies on mathematical approximations, it is often employed to study the equilibrium configurations of complex systems. However, MC simulations can become computationally demanding due to the long time needed to reach equilibrium, particularly in larger systems. In contrast, MD has a key advantage over MC, as it can simulate systems both in and out of equilibrium, providing insights into dynamic behaviors that MC cannot capture [41].

BDsimulations rely on a simplified version of Langevin dynamics, incorporating random forces and dissipation to mimic the effects of a surrounding solvent. In BD, the solvent is modeled implicitly, meaning the interactions between particles are influenced by random fluctuations and drag forces rather than explicit solvent molecules [41, 42]. One of the key benefits of BD is its ability to efficiently simulate large, multicomponent systems over long simulation periods, which is particularly useful for exploring the behaviours of SRPs in diverse environments. However, a limitation of this method is its inability to conserve energy or momentum, which reduces its accuracy in capturing hydrodynamic interactions, the fluid flow effects that occur between particles [43]. Although techniques such as the Rotne-Prager-Yamakawa tensor have been developed to approximate these interactions [44, 45], they remain challenging to fully implement in BD simulations. Despite these drawbacks, BD simulations are effective for studying the self-assembly and equilibrium behavior of polymers, particularly in solution, and become more effective when combined with the Monte Carlo method. This combination offers a computationally efficient approach to predicting polymer structures and dynamics. [37].

DPD is a coarse-grained molecular dynamics approach appropriate for simulations at larger time and length scales [46]. Coarse-grained methods are specifically designed to simplify complex molecular systems, which facilitate the study of mesoscale phenomena. These techniques reduce the number of degrees of freedom by grouping atoms into single interaction sites and deriving effective interaction potentials. They provide a balance between computational efficiency and the ability to capture essential physical behaviors, making them invaluable tools in both theoretical and applied research [47].

The simplicity of the DPD algorithm, along with its impressive adaptability for mesoscale modeling, makes it a great tool for testing models of different molecules, especially in complex fluids and soft materials [48]. **Mesoscale modeling occupies the intermediate domain between atomistic and macroscopic scales, generally described as the spatio-temporal range from** 10 to 10^4 nanometers **and** 1 to 10^6 nanoseconds[49, 50]**.** In the realm of polymers, mesoscale simulations are crucial for capturing critical phenomena such as micelle formation [51, 52], polymer brush formation [53], and stimuli-responsive structural change [54-57] that are not effectively represented at other scales. DPD’s main advantage over other coarse-grained techniques lies in its computational efficiency and the availability of various parametrization schemes, all while preserving essential system properties [58]. Moreover, DPD excels at incorporating hydrodynamic interactions and accurately modeling solvent effects, surpassing traditional methods such as BD. Unlike all-atom MD, which becomes computationally expensive due to the explicit modeling of each atom, DPD's coarse-grained approach enables the simulation of large and complex systems, including stimuli-responsive polymers (SRPs), with significantly reduced computational costs. DPD is particularly well-suited for simulating soft matter systems such as polymers, membranes, and colloids, making it an essential tool for investigating the structural changes of SRPs in various environments, including both solution and melt states.

Given its ability to model large systems while accounting for hydrodynamic interactions and other essential forces, DPD is particularly valuable in understanding the behavior of SRPs under a range of conditions. For these reasons, this review focuses on studies utilizing DPD to simulate the structural changes and dynamics of SRPs in response to changes in pH, temperature, and light, offering valuable insights into how these materials can be optimized for specific applications.

**Methods ( I am working on in this new branch)**

The original DPD model, introduced by Hoogerbrugge and Koelman [59], was later refined by Español and Warren [60] into a proper statistical mechanics model.

In DPD, the system is represented by a set of particles called beads, interacting through three main types of forces: conservative, dissipative, and random forces. The particle (bead) dynamics is controlled through Newton’s equations of motion:

|  |  |
| --- | --- |
| = , = | (1) |

where all masses are normalized to 1 for simplicity. The position and velocity of particle *i*, are denoted by ri and , respectively, and is the total force acting on particle *i*, given by:

|  |  |
| --- | --- |
|  | (2) |

The expression within the brackets represents the force arising from the interaction between bead *i* and its neighboring bead *j*, regardless of whether the beads are bonded.

This interaction force is made up of three parts: a purely repulsive conservative force , a dissipative force ​, and a random (stochastic) force ​. Each of these forces is pairwise additive and operates within a cutoff radius ​, beyond which all forces vanish, defining the system's length scale. The other terms refer to forces generated from bonded interactions, specifically from springs () and angular constraints ().

The conservative, dissipative, and random pair forces share a unified structure:

|  |  |
| --- | --- |
| , | (3) |

Where (= ) represents the symmetric force amplitude, and is the unit direction vector which determines the direction of the force. The function defines the radial dependence of the force, remaining continuous and positive for *r* < , and zero for *r* ≥ . This function serves to distribute the force amplitude C across an interaction region with radius . As indicated by Eq. 3, these forces are consistent with Newton's third law, = −. Consequently, they do not contribute to the system's total force. Since the net force is zero, the total momentum remains constant, which is a crucial element for hydrodynamics simulations.

As previously mentioned, the conservative force is a soft repulsive force acting between particles *i* and *j*, serving to prevent them from overlapping. It is defined as follows:

|  |  |
| --- | --- |
| , | (4) |

where is the maximum repulsion parameter between particles *i* and *j*, and a simple linear weight function for the conservative force is denoted by .

|  |  |
| --- | --- |
|  | (5) |

The dissipative force corresponds to a frictional force dependent on both the position and relative velocities of the particles and acts to remove kinetic energy from the system, simulating the effect of viscosity and thermal fluctuations at the mesoscale. The random force represents a random interaction between bead *i* and its neighboring bead *j* and introduces thermal fluctuations into the system. It works in conjunction with the dissipative force to maintain the system's temperature, ensuring compliance with the fluctuation-dissipation theorem, as reflected in the following equations:

|  |  |
| --- | --- |
| *,* | (6) |

and

|  |  |
| --- | --- |
| . | (7) |

Where and are the friction and noise amplitudes, respectively, and are weight functions,  = vi - vj represents the relative velocity, and a randomly fluctuating variable with zero mean and unit variances is denoted by . Noise and dissipation both stem from the fast atomic motions not captured by the mesoscale model, often referred to as the "bath." The bath generates rapidly fluctuating forces that contribute to the thermal motion of the beads. Simultaneously, it restricts the beads' movement by dissipating kinetic energy. Together, noise and dissipation act as a thermostat, regulating the system’s temperature. To achieve the correct canonical equilibrium state, the weight functions and amplitudes are related through the fluctuation-dissipation theorem [60].

|  |  |
| --- | --- |
|  | (8) |

|  |  |
| --- | --- |
|  | (9) |

*(how to have a comma after the eqn 8)*

Where *T* is the system's equilibrium temperature and represents the Boltzmann constant. These forces maintain local momentum conservation, ensuring accurate hydrodynamic behavior, even in systems with only a few hundred beads.

Additional bonded interactions come into play, when a mesomolecule consists of multiple beads. The spring force acting on bead *i* is determined by:

|  |  |
| --- | --- |
| , | (10) |

where represents the total bonded potential.

|  |  |
| --- | --- |
|  | (11) |

With the sum accounting for all bonds involved. In this equation, a spring constant *C* and a length are used to parameterize each spring and signifies the equilibrium bond length.

The force on bead *i* from angular interactions to account for chain stiffness is determined by:

|  |  |
| --- | --- |
| , | (12) |

where is the total angular potential.

|  |  |
| --- | --- |
|  | (13) |

Where the sum runs over all angles and the angle potential is parameterized by the modulus, *k*, and the equilibrium angle, .

**Numerical Integration (more references) (to be checked)**

In molecular dynamics simulations, the time evolution of the system is typically computed using numerical integration algorithms. The velocity-Verlet algorithm is commonly employed due to its simplicity and good energy conservation properties. However, in DPD simulations, the forces depend explicitly on velocities because of the dissipative and random forces, complicating the integration process.

Early DPD simulations used the Euler algorithm, but this method can introduce significant numerical errors and lacks time reversibility. To address these issues, Groot and Warren used a modified version of the velocity-Verlet algorithm [61] specifically for DPD simulations [48]. Their approach incorporates a predictor-corrector scheme with a tuning parameter λ, optimizing the integration for systems where forces depend on velocities. The modified algorithm proceeds as follows:

|  |  |
| --- | --- |
| *(t +*  *(t +*  *(t + )*  *(t + )* | (14) |

The interaction parameter *aij* is derived from the Flory-Huggins interaction parameter , ​which quantifies the compatibility between different species:

|  |  |
| --- | --- |
|  | (15) |

This establishes a connection between the molecular characteristics of the coarse-grained model and the DPD parameter. For compatible species ( ), ​ approaches the baseline value of 25 in DPD unit.

To calculate values, the Hildebrand relation is used for determining the Flory-Huggins parameter :

|  |  |
| --- | --- |
|  | (16) |

Where is the volume to which refers and are the solubility parameters of components *A* and *B*, respectively. The solubility parameter is defined as:

|  |  |
| --- | --- |
|  | (17) |

Here, is the volume of the bead and is the cohesive energy, which is the energy needed to evaporate a system to an ideal gas at constant temperature. The cohesive energy can be calculated from atomistic molecular dynamic simulation as the average intermolecular energy.[62] (It should be noted that there are alternative routes to the derivation of a¯AB , including experimental solubility parameters, pair-interaction calculations,22 experimental vapor-pressures,23 or solubilities.)

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