Draft for the thesis

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Summary Document for the draft of the Thesis.

Introduction

Acknowledge

Objectives

Justification

Theoretical framework

Theory of simple liquids Computational Physics[**?**]

Most realistic physical systems are tractable only in a model, in which the interesting features of the system are highlighted and in which the less relevant parts are either eliminated or treated in an approximate way.

In this spirit we have for example eliminated molecular degrees of freedom by considering (parts of) molecules to be rigid. Another example of this approach is the Langevin dynamics technique.

Consider a solution containing polymers or ions which are much heavier than the solvent molecules. As the kinetic energy is on average divided equally over the degrees of freedom, the ions or polymers will move much more slowly than the solvent molecules. Moreover, because of their large mass, they will change their momenta only after many collisions with the solvent molecules and the picture which emerges is that of the heavy particles forming a system with a much longer time scale than the solvent molecules. This difference in time scale can be employed to eliminate the details of the degrees of freedom of the solvent particles and represent their effect by forces that can be treated in a simple way. This process can be carried out analytically through a projection procedure (see chapter 9 of Ref. [11] and references therein) but here we shall sketch the method in a heuristic way.

How can we model the effect of the solvent particles without taking into account their degrees of freedom explicitly? When a heavy particle is moving through the solvent, it will encounter more solvent particles at the front than at the back. Therefore, the collisions with the solvent particles will on average have the effect of a friction force proportional and opposite to the velocity of the heavy particle. This suggests the following equation of motion for the heavy particle:

[11] J. P. Hansen and I. R. McDonald, Theory of Simple Liquids 2nd edn. New York, Academic Press, 1986.

To make the model more realistic we must include the rapid variations in the force due to the frequent collisions with solvent particles on top of the coarse-grained friction force. We then arrive at the following equation:

where $R(t)$ is a “random force”. Again, the time correlations present in the fluid should show up in this force, but they are neglected once more and the force is subject to the following conditions - Average 0 - No time correlation - Gaussian distribution

The opposite situation is given by a system thatremains in strong thermal contact with another system at thermal equilib-equilibrium. The prototype of such behavior is provided by small particles that interact among them-selves with a given force (which may be electrical,magnetic, gravitational, etc., in origin) suspended in a highly viscousliquid (i.e., oil) at a given temperature. In the high-viscosity limit the equation of motion of the ith particle is

The missing term in Eq.A9.1 is the force acting on the particles due to the collisions of themolecules of oil: they produce an extra random force $b(t)$, which shouldbe added to A9.2. We have This new force prevents the particles from remaining at the minimumposition (xim), and it is the origin of the Brownian motion.

In the simplest case, each collision gives a contribution to theforce, and contributions coming from different collisions are uncorre-lated: the forces acting on the same particle at different times (or ondifferent particles at the same time) are practically uncorrelated. We canthuswrite

where the bar denotes the average over many repeated experiments: i.e.,we have M identical copies of the same system (or a single system onwhich M measurements are taken at widely separated time intervals) andwe average the B't) over these M replicas. The bar denotes theaverage when M goes to infinity. If the number of collisions in a time e isquite large, the B'(t) will be Gaussian-distributed variables with avariance[1]

[1] Explanaition of why gaussian in page 25

[Parisi, 1988]

Its basis is the stochastic theory used by Langevin to describe the brow-nian motion of a large and massive particle in a bath of particles that are much smaller and lighter than itself. The problem is characterised by two very different timescales, one associated with the slow relaxation of the initial velocity of the brownian particle and another linked to the frequent collisions that the brownian particle suffers with particles of the bath. Langevin assumed that the force acting on the brownian particle consists of two parts: a systematic, frictional force proportional to the velocity u(t), but acting in the opposite sense, and a randomly fluctuating force, R(t), which arises from collisions with surrounding particles.

$$m\frac{\mathrm{d}\vec{v}(t)}{\mathrm{d}t} = -\gamma v(t) - \nabla_{\vec{r}}U(\vec{r},t) + \vec{R}(t) \tag{1}$$

[Paquet and Viktor, 2015]

“The dynamics of a macromolecular system is entirely determined by the potential U(rN) associated with the process. For computational and practical reasons, this potential is virtually always an approximation of the real physical potential.”

the correction is formed of two terms: a friction term, which introduces an artificial viscosity, and a stochastic term, which takes into account the unknown nature of the correction

One should notice that the frictional term depends on the previous history of the trajectory (Markovian process). The friction term is important in obtaining realistic simulations, as it takes into account the viscosity of the solvent (a feature, which is absent from both MD and MC). If one assumes that the frictional term is constant (no history), one obtains the celebrated Langevin equation (LE):

The Langevin equation improves conformational sampling over standard molecular dynamics.

[Wang et al., 2025]

In the processes of polymerization and depolymerization, polymers exhibit Brownian nonGaussian kinetic characteristics [9].

To elucidate the essence of these natural phenomena and uncover the underlying physical mechanisms, scientists employ statistical and mathematical tools to quantify the dynamical behaviors. Methods for quantitative modeling across multiple scales are primarily categorized into two types: one focused on simulating dynamics at the microscale, and the other dedicated to deriving or establishing evolutionary equations at the macroscale.

There are two commonly used modeling frameworks, the continuous time random walk (CTRW) model and the Langevin equation.

Reference [34] presents the Langevin equation for polymers engaged in polymerization/depolymerization reactions, by establishing a random diffusion coefficient that correlates with particle size. Reference [35] presents the Langevin equations for continuous time Lévy walks. X. D. Wang et al. present the Langevin description of the Lévy walk [36]. Y. Chen et al. then provide the Langevin description of the Lévy walk with memory [37] and examine the impact of an external force [38,39].

[Lü et al., 2019] The Langevin equation has been widely used to describe the dynamics of open systems interacting with an environment (bath). Their interaction introduces dissipation and fluctuations to the system [1–3], which are incorporated into the Langevin equation as friction and noise terms. When the time scales of the particle and the environmental degrees of freedom (DoF) are comparable, the frictional force felt by the particle will have a memory kernel, meaning that the friction acting on the particle depends on the velocity at an earlier time.

[Pastor, 1994] As the name implies, Langevin dynamics is based on the Langevin equation [1,2]. It differs from molecular dynamics simulations (based on Newton's equation) in that the solvent is modelled by stochastic and dissipative forces. This approximation allows substantially longer simulations than would be possible if the solvent were explicitly included, and Langevin dynamics is an excellent alternative to molecular dynamics for certain systems.

The intra-solute [3,4] terms of the force field used for molecular dynamics generally can be carried over for a Langevin dynamics simulation; the critical new parameter is the friction constant, which parametrises the effect of solvent damping and activation.

The generalised Langevin equation can be simplified by assuming that (i) the friction kernel is delta correlated in time, and (ii) it is not a function of the position of any of the particles:

Assumption (i) is equivalent to assuming that the viscoelastic relaxation of the solvent is very rapid with respect to solute motions, and, in fact, (is just the zero frequency value of the friction kernel.

Grote land Hynes [26] have investigated this assumption for motions involving barrier crossing and hav found that while it is seriously in error for passage over sharp barriers (such as 12 recombination); it is quite adequate for conformational transitions such as might be found in polymer motions.

Assumption (ii) involves the neglect of hydrodynamic interaction or spatial correlation in the friction kernel.

(y is commonly referred to as the collision frequency in the simulation literature, even though formally a Langevin description implies that the solute suffers an infInite number of collisions with infInitesimally small momentum transfer. In comparing the results of Langevin dynamics with those of other stochastic methods [28-31], the relevant variable is the velocity relaxation time, 'tv> which equals y.1.)

Brownian dynamics

Brief explanation of what is Brwonian motion, what is trying to represent/-model, how this can modeld the microgel.

Even though there are different mathematical representations that describes the brownian motion, we use the langevin equation[2] described with increments of Wiener process,

$$\begin{cases} \mathrm{d}r = v\ \mathrm{d}t \\ \mathrm{d}v = -\frac{\gamma}{m} v\ \mathrm{d}t - \frac{1}{m}\nabla U(r)\ \mathrm{d}t + \sqrt{\frac{2\gamma k_B T}{m}}\mathrm{d}W_t \end{cases} . \tag{2}$$

The Wiener process has the correlation property of $\left\langle \mathrm{d}W_i \mathrm{d}W_j \right\rangle = \delta_{ij}\mathrm{d}t$. γ represent the viscosity of the implicity medium, k_B is the Boltzmann constant and T the tempereture of the system.[3]

formullations of the Langeving equation[4], we choose to described the brownian motion using

Here explain the Langevin equation.

Stress

Introductory paragraph To characterize the behaviour of materials, constitutive relations serve as an input to the continuum theory. . . [5]

This derivation can be found in the apendix of[Admal and Tadmor, 2010][6].[7] Consider a system of N interacting particles with each particle position given by

$$\vec{r}_\alpha = \vec{r} + \vec{s}_\alpha, \tag{3}$$

where $\vec{r}$ is the position of the center of mass of the system and $\vec{s}_\alpha$ is the position of each point relative to the center of mass. Hence, we can express the momentum of each particle as

$$\vec{p}_\alpha = m_\alpha\left(\dot{\vec{r}} + \dot{\vec{s}}_\alpha\right) = m_\alpha\left(\dot{\vec{r}} + \vec{v}_\alpha^{\mathrm{rel}}\right). \tag{4}$$

[2] No se que más decir a parte de “porque está implementado en lammps”, jsjs

[3] En lammps está cómo

$$F_c - \frac{m}{\mathrm{damp}} v + \propto \sqrt{\frac{k_B T m}{dt\mathrm{damp}}}$$

[4] No estoy muy seguro si decir el resto de formalismos

[5] Capaz e ir introduciendo ideas del Clausius[Clausius, 1870]

[6] Describe more if what is done in this article

[7] (Eventualmente pondré esto en párrafo) Notation: $\boldsymbol{\sigma}$ Tensor, $\vec{\sigma}$ vector, $\sigma_{i,j}$ tensor, $\overline{\sigma}$ time average,

Before starting the procedure, lets take into account that the center of mass of the system is given by

$$\vec{r} = \frac{\sum_\alpha m_\alpha \vec{s}_\alpha}{\sum_\alpha m_\alpha}, \tag{5}$$

and by replacing (3) in (4) we get the following relations, which will be used later,

$$\sum_\alpha m_\alpha \vec{r}_\alpha = \vec{0}, \quad \sum_\alpha m_\alpha \vec{\upsilon}_\alpha^{\text{rel}} = \vec{0}. \tag{6}$$

Now we can start by computing the time derivative of tensorial product $\vec{r}_\alpha \otimes \vec{p}_\alpha$[8],

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\vec{r}_\alpha \otimes \vec{p}_\alpha\right) = \underbrace{\vec{\upsilon}_\alpha^{\text{rel}} \otimes \vec{p}_\alpha}_{\text{Kinetic term}} + \underbrace{\vec{r}_\alpha \otimes \vec{f}_\alpha}_{\text{Virial term}}, \tag{7}$$

[8] It is interesting to note that the tensorial product $\vec{r}_\alpha \otimes \vec{p}_\alpha$ has units of action and by tacking the time derivative we are dealing with terms that has units of energy.

which is known as the *dynamical tensor virial theorem* and it is simply an alternative form to express the balance of linear momentum. This theorem becomes useful after making the assumption that there existis a time scale τ, which is short relative to macroscopic processes but long relative to the characteristic time of the particles in the system, over which the particles remain close to their original positions with bounded positions and velocities. Taking advantage of this property we can compute the time average of (7),

$$\frac{1}{\tau}\left(\vec{r}_\alpha \otimes \vec{p}_\alpha\right)\Big|_0^\tau = \overline{\vec{\upsilon}_\alpha^{\text{rel}} \otimes \vec{p}_\alpha} + \overline{\vec{r}_\alpha \otimes \vec{f}_\alpha}. \tag{8}$$

Assuming that $\vec{r}_\alpha \otimes \vec{p}_\alpha$ is bounded, and the time scales between microscopic and continuum processes are large enough, the term on the left-hand side can be as small as desired by tacking τ sufficiently large and by summing over all particles we achieve the *tensor virial theorem*:

$$\overline{\mathbf{W}} = -2\overline{\mathbf{T}}, \tag{9}$$

where

$$\overline{\mathbf{W}} = \sum_\alpha \overline{\vec{r}_\alpha \otimes \vec{f}_\alpha} \tag{10}$$

is the time-average virial tensor and

$$\overline{\mathbf{T}} = \frac{1}{2}\sum_\alpha \overline{\vec{\upsilon}_\alpha^{\text{rel}} \otimes \vec{p}_\alpha} \tag{11}$$

is the time-average kinetic tensor. This expression for the tensor virial theorem applies equally to continuum systems that are not in macroscopic equilibrium as well as those that are at rest.

The assumption of the difference between the time scales allow us to simplify the relation by replacing (4) in (11), so that,

$$\overline{\mathbf{T}} = \frac{1}{2}\sum_\alpha m_\alpha \overline{\vec{\upsilon}_\alpha^{\text{rel}} \otimes \vec{v}_\alpha^{\text{rel}}} + \frac{1}{2}\left[\overline{\sum_\alpha m_\alpha \vec{\upsilon}_\alpha^{\text{rel}}}\right] \otimes \dot{\vec{r}}, \tag{12}$$

which is not the simplification we expected, however, by the relations from (6), equation (12) simplifies to[9]

$$\overline{\mathbf{T}} = \frac{1}{2}\sum_\alpha m_\alpha \overline{\vec{\upsilon}_\alpha^{\text{rel}} \otimes \vec{\upsilon}_\alpha^{\text{rel}}}. \tag{13}$$

[9] No estoy muy seguro si incluir una discusión acerca del término cinético en la expresión del virial. Posiblemente un párrafo... posiblemente lo ponga en la interpretación del teorema. También, no se si ir metiendo interpretación durante la derivación o no, pero bueno.

On the other hand, instead of reducing the expression, we start to create the conection with the Cauchy stress tensor by distributing (10) into an internal and external contributions,

$$\overline{\mathbf{W}} = \underbrace{\sum_{\alpha} \overline{\vec{r}_\alpha \otimes \vec{f}_\alpha^{\text{int}}}}_{\overline{\mathbf{W}}_{\text{int}}} + \underbrace{\sum_{\alpha} \overline{\vec{r}_\alpha \otimes \vec{f}_\alpha^{\text{ext}}}}_{\overline{\mathbf{W}}_{\text{ext}}}. \tag{14}$$

The time-average internal virial tensor takes into account the interaction between particle α with the other particles in the system, meanwhile, the time-average external virial tensor considers the interaction with atoms outside the system, via a traction vector $\vec{t}$ and external fields acting on the system represented by $\rho\vec{b}$, where ρ is the mass density of it and $\vec{b}$ is the body force per unit mass applied by the external field. Therefore we can express the following,

$$\sum_{\alpha} \overline{\vec{r}_\alpha \otimes \vec{f}_\alpha^{\text{ext}}} := \int_{\delta\Omega} \vec{\xi} \otimes \vec{t} dA + \int_{\Omega} \vec{\xi} \otimes \rho \vec{b} dV. \tag{15}$$

Where $\vec{\xi}$ is a position vector within the domain Ω occupied by the system of particles with a continuous closed surface $\delta\Omega$. Assuming that Ω is large enough to express the external forces acting on it in the form of the continuum traction vector $\vec{t}$.

With this we can substitute the traction vector with $\vec{t} = \boldsymbol{\sigma}\vec{n}$, where $\boldsymbol{\sigma}$ represent the Cauchy stress tensor and applying the divergence theorem in (15), we have

$$\overline{\mathbf{W}}_{\text{ext}} = \int_{\Omega} \left[\vec{\xi} \otimes \rho\vec{b} + \operatorname{div}_{\vec{\xi}} \left(\vec{\xi} \otimes \boldsymbol{\sigma} \right) \right] dV = \int_{\Omega} \left[\boldsymbol{\sigma}^{\mathrm{T}} + \vec{\xi} \otimes \left(\operatorname{div}_{\vec{\xi}} \boldsymbol{\sigma} + \rho\vec{b} \right) \right] dV \tag{16}$$

Since we assume that we are under equilibrium conditions, the term $\operatorname{div}_{\vec{\xi}} \boldsymbol{\sigma} + \rho\vec{b}$ is zero (16) it simplifies to

$$\overline{\mathbf{W}}_{\text{ext}} = V\boldsymbol{\sigma}^{\mathrm{T}}. \tag{17}$$

By tacking into account that we integrate over the domain Ω we can say that we compute the spatial average of the Cauchy stress tensor,

$$\boldsymbol{\sigma}_{\text{av}} = \frac{1}{V} \int_{\Omega} \boldsymbol{\sigma} dV, \tag{18}$$

in which V is the volume of the domain Ω. Replacing (17) into (14), the tensor virial theorem (9) can be expressed as,

$$\sum_{\alpha} \overline{\vec{r}_\alpha \otimes \vec{f}_\alpha^{\text{int}}} + V\boldsymbol{\sigma}_{\text{av}}^{\mathrm{T}} = -\sum_{\alpha} m_\alpha \overline{\vec{v}_\alpha^{\text{rel}} \otimes \vec{v}_\alpha^{\text{rel}}}. \tag{19}$$

Finally, solving for the Cauchy Stress tensor we get,

$$\boldsymbol{\sigma}_{\text{av}} = -\frac{1}{V} \left[\sum_{\alpha} \overline{\vec{f}_\alpha^{\text{int}} \otimes \vec{r}_\alpha} + \sum_{\alpha} m_\alpha \overline{\vec{v}_\alpha^{\text{rel}} \otimes \vec{v}_\alpha^{\text{rel}}} \right], \tag{20}$$

an expression that describe the macroscopic stress tensor in terms of microscopic variables[10].

To end the section it is important to show that (20) is symmetric. Therefore, we rewrite the internal force as the sum of forces between the particles,

$$\vec{f}_\alpha^{\text{int}} = \sum_{\beta_{\beta \neq \alpha}} \vec{f}_{\alpha\beta}, \tag{21}$$

[10] It is important to acknowledge that several mathematical subtleties were not taken into consideration, however all the mathematical formality is adressed by Nikhil Chandra Admal and E. B. Tadmor in [Admal and Tadmor, 2010]

and substituting (21) into (20), we have

$$\boldsymbol{\sigma}_{\text{av}} = -\frac{1}{V}\left[\sum_{\alpha,\beta_{\beta\neq\alpha}} \overline{\vec{f}_{\alpha\beta}\otimes\vec{r}_{\alpha}} + \sum_{\alpha} m_{\alpha}\overline{\vec{\upsilon}^{\text{rel}}_{\alpha}\otimes\vec{\upsilon}^{\text{rel}}_{\alpha}}\right]. \tag{22}$$

Due to the property $\vec{f}_{\alpha\beta} = -\vec{f}_{\beta\alpha}$ we obtain the following identity

$$\sum_{\alpha,\beta_{\beta\neq\alpha}} \vec{f}_{\alpha\beta}\otimes\vec{r}_{\alpha} = \frac{1}{2}\sum_{\alpha,\beta_{\beta\neq\alpha}}\left(\vec{f}_{\alpha\beta}\otimes\vec{r}_{\alpha} + \vec{f}_{\beta\alpha}\otimes\vec{r}_{\beta}\right) = \frac{1}{2}\sum_{\alpha,\beta_{\beta\neq\alpha}} \vec{f}_{\alpha\beta}\otimes\left(\vec{r}_{\alpha}-\vec{r}_{\beta}\right). \tag{23}$$

Therefore, by replacing the identity of (23) into (22), we have

$$\boldsymbol{\sigma}_{\text{av}} = -\frac{1}{V}\left[\frac{1}{2}\sum_{\alpha,\beta_{\beta\neq\alpha}} \overline{\vec{f}_{\alpha\beta}\otimes\left(\vec{r}_{\alpha}-\vec{r}_{\beta}\right)} + \sum_{\alpha} m_{\alpha}\overline{\vec{\upsilon}^{\text{rel}}_{\alpha}\otimes\vec{\upsilon}^{\text{rel}}_{\alpha}}\right], \tag{24}$$

expressed with indexical notation and using the eistein summation convention,

$$\sigma^{\text{av}}_{ij} = -\frac{1}{V}\left[\frac{1}{2}\sum_{\alpha,\beta_{\beta\neq\alpha}} \overline{f^{\alpha\beta}_{i} r^{\alpha}_{j} + f^{\beta\alpha}_{i} r^{\beta}_{j}} + \sum_{\alpha} m_{\alpha}\overline{\upsilon^{\alpha\ \text{rel}}_{i}\upsilon^{\alpha\text{rel}}_{j}}\right], \tag{25}$$

which is the same expression implemented in LAMMPS[Thompson et al., 2022].[11]

[11] No se si poner la referencia a la pagina de documentacionhttps://docs.lammps.org/compute_stress_atom.html

Computational Implementation

General description

The simulation methodology is based on the work presented in[Gnan et al., 2017] and[Sorichetti et al., 2023], with the objective of create a representative polymer structure of a microgel and characterize the mechanical response under shear deformation. This methodology creates the structure by using a mixture of two types of patchy particles. The patchy particles are spheres of identical size and mass decorated by patches to represent interaction sites. One type represent a *Crosslinker* and is define by 1 central particle with 4 patches placed at the vertices of a circumscribed tetrahedron. The other one represent a *Monomer* define by 1 central particle and 2 patches placed at the poles.

- $\vec{r}_i$: Position of Crosslinker central particle
- $\vec{r}_j$: Position of Monomer central particle
- $\{\vec{r}^{\,i}_{\mu}\}$ Set of positions of the patches in the crosslinker patchy particle
- $\{\vec{r}^{\,j}_{\upsilon}\}$ Set of positions of the patches in the monomer patchy particle

The interaction between the central particles is modeled with a Weeks-Chandler-Andersen repulsive potential,

$$U_{WCA}(r_{i,j}) = \begin{cases} 4\varepsilon_{i,j}\left[\left(\frac{\sigma}{r_{i,j}}\right)^{12} - \left(\frac{\sigma}{r_{i,j}}\right)^{6}\right] + \varepsilon_{i,j}, & r_{i,j}\in[0,2^{1/6}\sigma], \\ 0, & r_{i,j} > 2^{1/6}\sigma \end{cases}, \tag{26}$$

where $r_{i,j}$ is the distance between the center of the central particles, σ is the diameter of the particles and $\varepsilon_{i,j}$ is the energy of the interacton. The patch-patch interaction is modeled with an attractive potential,

$$U_{\text{patchy}}(r_{\mu\upsilon}) = \begin{cases} 2\varepsilon_{\mu\upsilon}\left(\frac{\sigma_p^4}{2r^4_{\mu\upsilon}} - 1\right)\exp\left[\frac{\sigma_p}{(r_{\mu\upsilon}-r_c)} + 2\right], & r_{\mu\upsilon}\in[0,r_c], \\ 0, & r_{\mu,\upsilon} > r_c, \end{cases} \tag{27}$$

where $r_{\mu\upsilon}$ is the distance between two patches, σ_p is the diameter of the patches, r_c is the cut distance of interaction set to $1.5\sigma_p$ and $\varepsilon_{\mu,\upsilon}$ is the interaction energy between the patches. Moreover, the interaction between patches is complemented by a three-body repulsive potential, defined in terms of (27), that provides an efficient bond-swapping mechanism making possible to easily equilibrate the system at extremely low temperatures, while at the same time, reataining the single-bond-per-patch condition[Sciortino, 2017],

$$U_{\text{swap}}(r_{l,m}, r_{l,n}) = w \sum_{l,m,n} \varepsilon_{m,n} U_3(r_{l,m}) U_3(r_{l,n}), \quad r_{l,n} \in [0, r_c], \tag{28}$$

where

$$U_3(r) = \begin{cases} 1 & r \in [0, r_{\min}], \\ -U_{\text{patchy}}(r)/\varepsilon_{m,n}, & r \in [r_{\min}, r_c] \end{cases} . \tag{29}$$

The sum in (28) runs over all triples of bonded patches (patch l bonded both with m and n). $r_{l,m}$ and $r_{l,n}$ are the distances between the reference patch and the other two patches. The parameter $\varepsilon_{m,n}$ is the energy of repulsion and w is used to tuned the swapping ($w = 1$) and non-swapping bonds ($w \gg 1$). The cut off distance r_c is the same as in the potential of interaction between patches, meanwhile the minimum distance $r_{\min}$ is the distance at the minimum of (27), *i.e.* $\varepsilon_{m,n} \equiv \left|U_{\text{patchy}}(r_{\min})\right|$. Finally, the energy of interaction between crosslinker patches ($\varepsilon_{\mu^i,\mu^i}$) are set to 0 to allow only crosslinker-monomer and monomer-monomer bonding (figure 2).

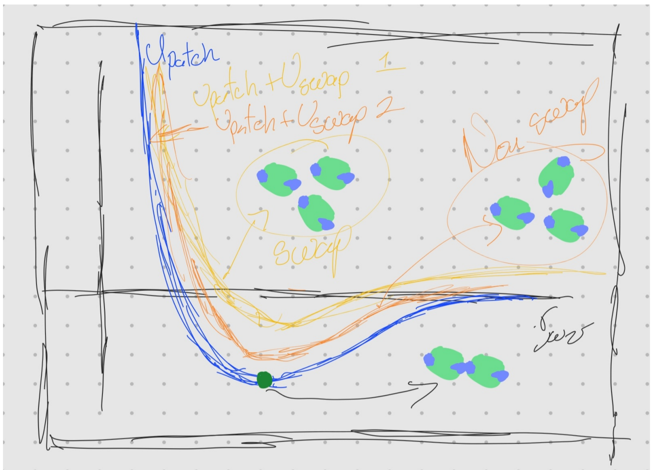

Figure 1: La idea de la figura es poner el pontecial de interacción entre paches y ver el efecto del pontecial de 3 cuerpos cuando $w = 1$ y cuando $w \gg 1$.

Assembly of the network

We perform molecular dynamics (MD) simulations at fixed temperature $T = kBT/\varepsilon = 0.05$, where kB is the Boltzmann constant. Thanks to such a low temperature, the system tends to maximize the number of bonds. In addition, owing to the bondswapping mechanism, the system is able to continuously restructure itself, until the large majority of possible bonds are formed. It is important to said that the main difference between the articles cited and the implementation in this htesis are the absence of FENE bonds and the swelling potential.

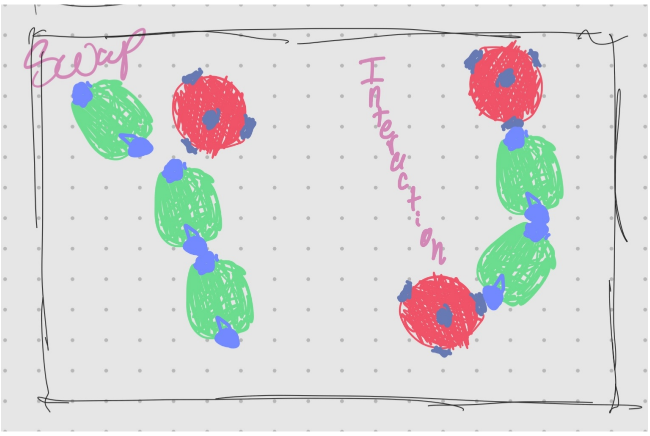

Figure 2: La idea de esta es mostrar las posibles configuraciones (monomero-monomero, monomero-crosslinker y un poco de pontecial de 3 cuerpos)

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