Finite Element Method

Dr. Antonio Ortiz Ambriz

Francisco Javier Vázquez Tavares A00827546

Contents

1 Description of the simulation . . . 1
1.1 Poisson equation . . . 1
1.2 Bar of steel . . . 1
2 Poisson equation . . . 1
2.1 Weak form . . . 1
2.2 Shape function . . . 3
2.3 Evaluation of the weak form . . . 4
2.4 Compute the solution . . . 4
3 Bar of steel . . . 6

1 Description of the simulation

A 100 particles interacts with each other through a Lennard-Jones potential with parameters ε and σ inside a box modeled using Lennard-Jones potential with sides of 20σ. The system has an initial temperature $T = 2\varepsilon/\kappa_B$.

1.1 Equations of motion

The movement of the particles are going to be describe using Newton's second law of motion and the relation between a force and a conservative potential,

$$m_i\vec{a}_i = \sum_{j\neq i} -\nabla U_{j\to i}, \tag{1}$$

where $m_i\vec{a}_i$ is the change in momentum of the particle i and is set to be equal to the sum of the forces applied by a particle j over the particle i through a potential U. Knowing that the interactions between the particles are going to be modeled using the Lennard-Jones potential, U can be expressed as,

$$U_{j\to i}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right], \tag{2}$$

where r_{ij} is the distance between the particles i and j, σ represent a distance in which a repulsive effect is predominant, usually associated with particle size and $epsilon$ is a constant with units of energy [research later the interpretation].

In this case, the force is the derivative of the potential with respect the distance between particles,

$$\vec{F}_{j\to i}(r) = \frac{4\varepsilon}{r}\left[12\left(\frac{\sigma}{r_{ij}}\right)^{12} - 6\left(\frac{\sigma}{r_{ij}}\right)^{6}\right]\hat{r},$$

and the equation(**??**) can be rewritten as,

$$m_i\vec{a}_i = \frac{4\varepsilon}{r}\left[12\left(\frac{\sigma}{r_{ij}}\right)^{12} - 6\left(\frac{\sigma}{r_{ij}}\right)^{6}\right]\hat{r}. \tag{3}$$

With this expression, the force is multiplied by the unit vectors of the distance between the particles to get the the x and y component of the force leading to,

$$m_i\vec{a}_{xi} = \frac{4\varepsilon}{r}\left[12\left(\frac{\sigma}{r_{ij}}\right)^{12} - 6\left(\frac{\sigma}{r_{ij}}\right)^{6}\right]\frac{x_i - x_j}{r_{ij}}\,\hat{x}, \tag{4}$$

$$m_i\vec{a}_{yi} = \frac{4\varepsilon}{r}\left[12\left(\frac{\sigma}{r_{ij}}\right)^{12} - 6\left(\frac{\sigma}{r_{ij}}\right)^{6}\right]\frac{y_i - y_j}{r_{ij}}\,\hat{y}. \tag{5}$$

In the next section it will be explained the implementation of the boundary conditions, the algorithm to establish initial conditions and the numerical method to solve the equations of motion.

1.2 Boundary condition

To confine the particles in a box with size of 20σ, it is use the Lennard-Jones potential. In which the variable r is the distance between the particle and the limit of the box, and the parameter σ_w can be related with the width of the edge of the box.

To simplify the implementation of the force, the potential is evaluate in a one spatial dimension, hence, there are 4 extras forces in the particles due to the boundaries conditions,

$$U_{w_x\to i}(r) = 4\varepsilon\left[\left(\frac{\sigma_w}{x_i - w_x}\right)^{12} - \left(\frac{\sigma_w}{x_i - w_x}\right)^{6}\right], \tag{6}$$

$$U_{w_y\to i}(r) = 4\varepsilon\left[\left(\frac{\sigma_w}{y_i - w_y}\right)^{12} - \left(\frac{\sigma_w}{y_i - w_y}\right)^{6}\right]. \tag{7}$$

1.3 Initial conditions

Knowing that the potential is proportional to the inverse of the distance between particles is important to set a minimum distance between the particles to avoid infinite values in the force and prevent particles

from escaping the box. For that, the space is partitioned by segments of 1.5σ of length and the size of the space is reduce by $20\sigma - 2\sigma_w$ to prevent placing a particle near the wall. This implementation create an evenly particle placement at the initial condition, as shown in figure **??**

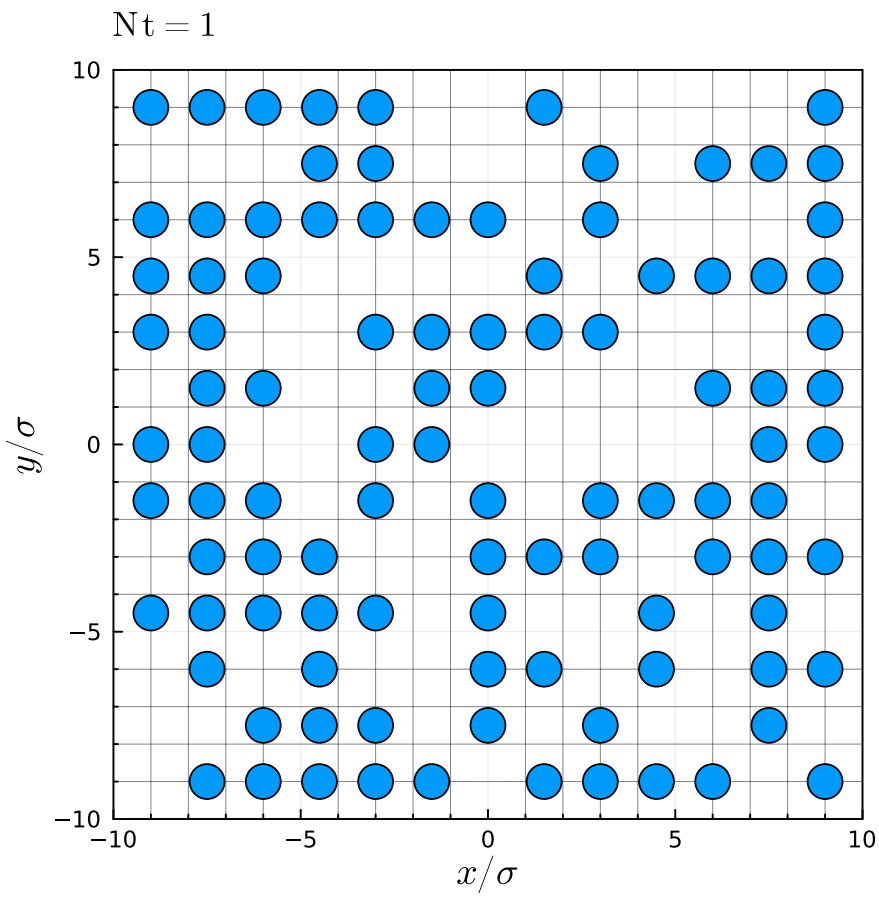


Figure 1: Initial position for 100 particles uniformly spaced.

To the set of initial velocities, the Maxwell-Boltzmann distribution for molecular velocity components is used,

$$P(\upsilon_x) = \left(\frac{m}{2\pi kT}\right)^{1/2} \exp\left[-\frac{m}{2kT}\upsilon_x^2\right], \tag{8}$$

which is a normal distribution with standard deviation of $\sqrt{k_b T/m}$ and mean 0.

1.4 Numerical method

With the boundary and initial conditions set, the equations of movement (**??**),(**??**) can be solved using the Velocity Verlet algorithm,

$$\vec{v}_i(t+\Delta t/2) = \vec{v}_i(t) + \frac{\Delta t}{2}\frac{1}{m_i}\vec{F_{j\to i}}\left(\vec{r_{i,j}}(t)\right), \tag{9}$$

$$\vec{r}_i(t+\Delta t) = \vec{r}_i(t) + \Delta t\vec{v}_i(t+\Delta t/2), \tag{10}$$

$$\vec{v}_i(t+\Delta t) = \vec{v}_i(t+\Delta t/2) + \frac{\Delta t}{2}\frac{1}{m_i}\vec{F_{j\to i}}\left(\vec{r_{i,j}}(t+\Delta t)\right). \tag{11}$$

2 Results

The numerical method is implemented in Julia and the scripts can be access in the following git-hub repository: FranVT Repository . It is important to mention that almost all physical parameters are set to 1 in all the simulations to simplify the analysis and focus in the overall phenomena of the system, the energy for the innerparticle interaction is equal to 5, causing a initial temperature of 10.

In the figure **??** it is shown the trajectories of 10 particles with Nt steps with the purpose of showing the collision with the boundaries, ensuring the correct implementation of the boundary conditions, force and numerical method. Also, it can be observed the collision between particles and the change of momentumm.

Beside the position of the particles, it is useful to observed the evolution of the temperature of the system, which is related with the average kinetic energy of the system by the following equation,

$$T = \frac{2}{3}\frac{1}{k_B}\left[\overline{\frac{1}{2}mv^2}\right]. \tag{12}$$

In the figure **??** is shown the evolution of the temperature of the system with 100 particles and in the following link Link to the animation it can be access and animation of the evolution of the system. In that gif is shown the time node and the temperature in that time step.

Knowing the relation between the temperature and the kinetic energy with equation (**??**), it is possible to assure that the numerical implementation converges, because the value of the variable oscillates around a constant temperature. However, that value is above the initial temperature, which is $T = 10$, this issue can be related with the quantity of particles and size of the box or the values assign to the physical parameters.

In conclusion, it can be said that a correct implementation of the algorithm of Velocity Verlet to simulate the evolution of a characteristic basic system of molecular dynamics with hard boundary conditions is achieve. Also, the fact that the evolution of the temperature of the system tends to a constant value shows that the algorithm converges. Finally,it can be improved the definition of the physical parameters to relate the system with experimental systems.

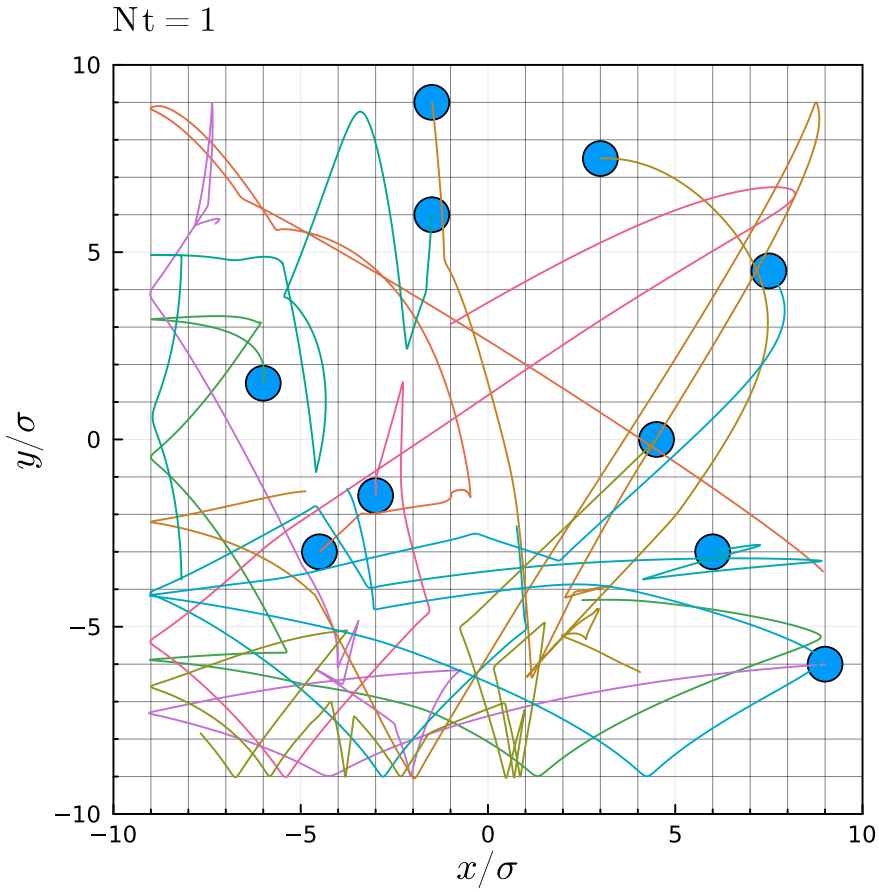


Figure 2: Position of 10 particles for Nt steps.

3 Description of the simulation

Modify the simulation done in assignment 1 to include Periodic Boundary Conditions. Remember that for this to work, you will need to add a cutoff to your interaction function.

3.1 Periodic Boundary condition

The idea of periodic boundary conditions is to use a limited number of atoms due to computational constrains, with the intention of imitating a wider system. This type of boundary condition treats a the simulation box like a tillable pattern, creating finite copies surrounding the original box, creating "ghost particles". The advantage to create finite copies is that is not necessary to compute the trajectories of the ghost particles, but just the interaction between "ghost" and "real" particles.

In the following sections is a discussion to set a cut distance in the potential that helps to reduce the computational requirements, then a brief explanation on the implementation of the periodic boundary

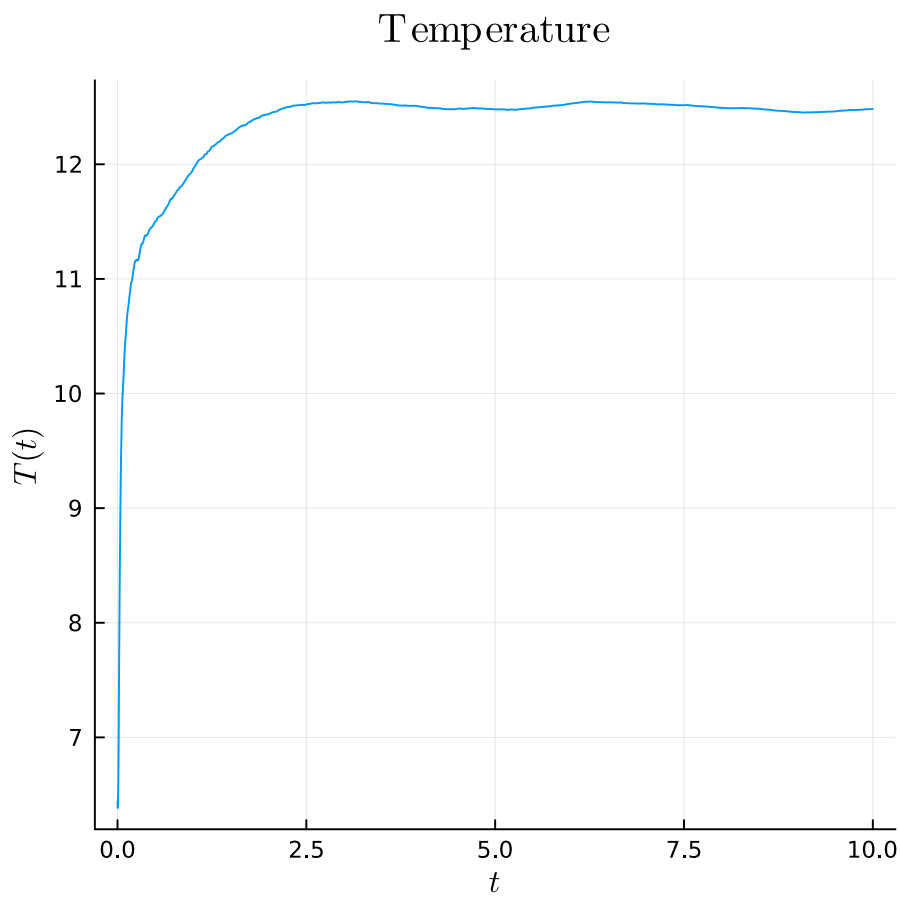


Figure 3: Temperature over time froma system of 100 particles

conditions and finally the results.

3.1.1 Cut off distance

The first issue to analyses at consider periodic boundary conditions is the interaction between the real and ghost particles. Adding a huge amount of ghost particles will help to improve the accuracy of the simulation, however it would cost time and computational capacity, therefore, a strategy to tackle this issue is to cut the range of the potential.

To set the cut off distance we equal the Lennard-Jones potential to a constant, η, and resolve for the distance. To do that, the following change of variable is introduce, $\gamma = \sigma^6/r^6$, hence,

$$4\varepsilon\left(\gamma^2 - \gamma\right) = \eta,$$

solving for γ, we get,

$$\gamma = \frac{\varepsilon \pm \sqrt{\varepsilon^2 + \varepsilon\eta}}{2\varepsilon},$$
$$\frac{\sigma^6}{r^6} = \frac{\varepsilon \pm \sqrt{\varepsilon^2 + \varepsilon\eta}}{2\varepsilon},$$

introducing a new change of variable, the expression can be written as,

$$r^6 = \frac{\sigma^6}{\alpha}, \qquad \alpha = \frac{\varepsilon \pm \sqrt{\varepsilon^2 + \varepsilon\eta}}{2\varepsilon}.$$

Knowing that this polynomial has 6 roots, 4 of them are in the complex plane and 2 in the real set of numbers, we select the real positive root, because it has physical interpretation, since we need a positive distance of cut off,

$$r = \frac{\sigma}{\alpha^{1/6}}.$$

Substituting the change of variable and a recommendation of terms,

$$r_{cut} = \sigma \frac{\sqrt[6]{2\varepsilon}}{\sqrt[6]{\varepsilon \pm \sqrt{\varepsilon(\varepsilon + \eta)}}}. \tag{13}$$

To prove that the result makes physical sense, we can set $\eta = 0$, expecting to get σ as the root of the function,

$$r_{cut} = \sigma \frac{\sqrt[6]{2\varepsilon}}{\sqrt[6]{\varepsilon \pm \sqrt{\varepsilon(\varepsilon)}}},$$
$$= \sigma \frac{\sqrt[6]{2\varepsilon}}{\sqrt[6]{\varepsilon \pm \varepsilon}},$$

in these case, we consider the positive root, hence

$$r_{cut} = \sigma \frac{\sqrt[6]{2\varepsilon}}{\sqrt[6]{2\varepsilon}},$$
$$r_{cut} = \sigma.$$

Therefore, we can associate the positive root near to σ, and the negative root with the largest root of the polynomial.

An interesting approach to defining η is $\eta = \alpha\varepsilon, \alpha[-1, 0]$. This definition helps to define the distance of cut off in terms of the energy of the particles and equation **??** simplifies to,

$$r_{cut} = \sigma \frac{\sqrt[6]{2}}{\sqrt[6]{1 \pm \sqrt{1 + \alpha}}}, \tag{14}$$

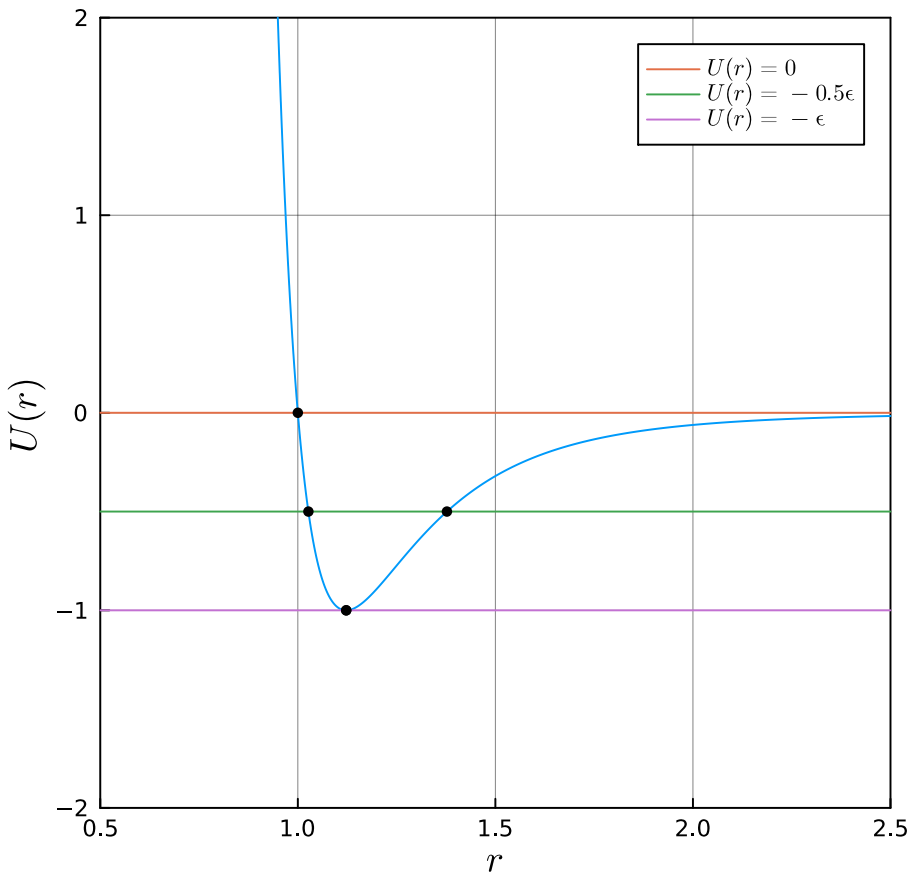


Figure 4: Lennard-Jones potential with intersection at energy equals to $0, 1/2\varepsilon$ and $-\varepsilon$.

when $\alpha = 0$, then $r = \sigma$ and when $\alpha = -1$, then $r = \sqrt[6]{2}\sigma$.

In figure **??** we can see when $\alpha = 0, \alpha = -0.5, \alpha = -1$.

Finally, to give a physical meaning to $\eta = \alpha\varepsilon$, we can relate the parameter ε with temperature using the equipartition theorem,

$$\varepsilon = \frac{3}{2} k_B T. \tag{15}$$

At relating the temperature with the energy of the particles, we are relating the average kinetic of the system with the potential energy between particles. It is important to notice that in equation **??**, $\eta \in [0, \varepsilon]$, leading to have a system in which the potential energy between the particles needs to be greater than the average of the kinetic energy of the system, as shown in figure **??**.

3.2 Implementation

To implement the cutoff in the system, it is needed to modify the potential to avoid a discontinuity at the cut off distance. For that, in the book (**libroClase**) shows the expression to avoid discontinuity in the potential and the force,

$$U_{rcut}(r) = U_{LJ}(r) - (r - r_{cut})\frac{\mathrm{d}}{\mathrm{d}r}U(r_{cut}) - U(r_{cut}). \tag{16}$$

In figure **??** it shows the comparison of the Lennard-Jones potential with the potential with cutoff **??**. In which both potentials achieve the same minimum point, preserving the energy of the particle, however, the cut off potential decays to 0 faster than the Lennard-Jones potential, getting the desire behavior.

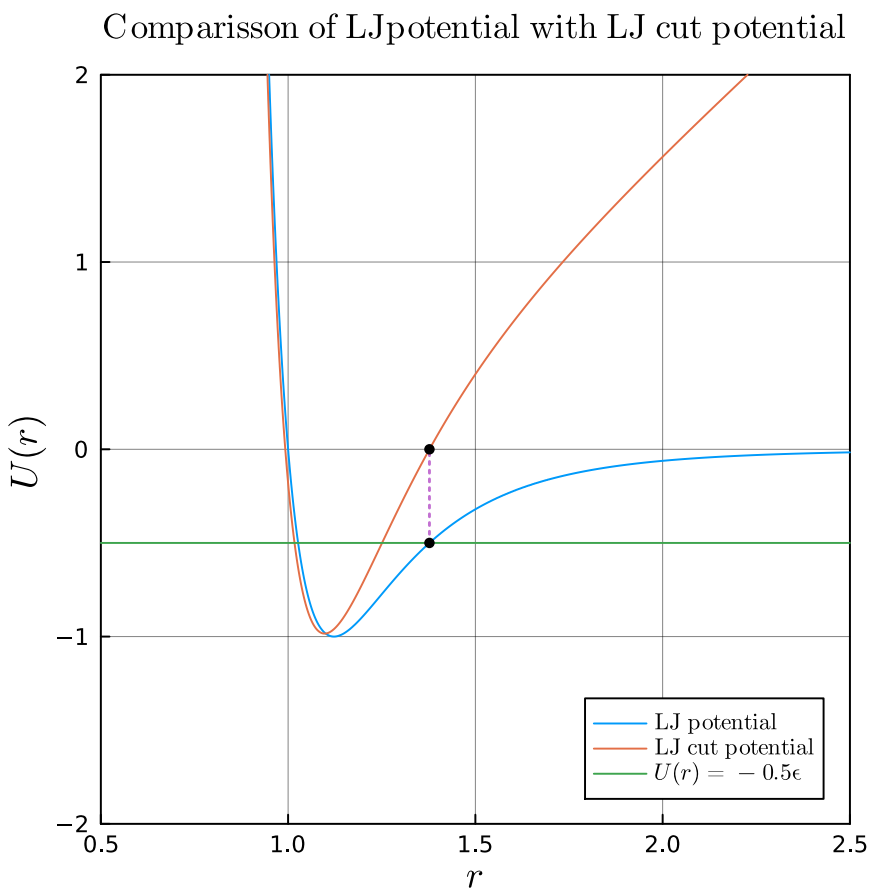


Figure 5: Comparison between the Lennard-Jones potential with the cut off Lennard-Jones potential. The cut off energy is obtain with equation (**??**) and $\alpha = -0.5$.

On the other hand, the quantity of copies for the boundary conditions can be set in relation with the r_{cut}. Taking into account equation (**??**) and setting $\alpha = -0.001$, the value for $r_{cut} = 3.98405$ and the size of the box are 20σ, with just one copy of the system in every direction is sufficient to use the periodic boundary condition. In figure **??** is an example of the initial condition with the ghost particles.

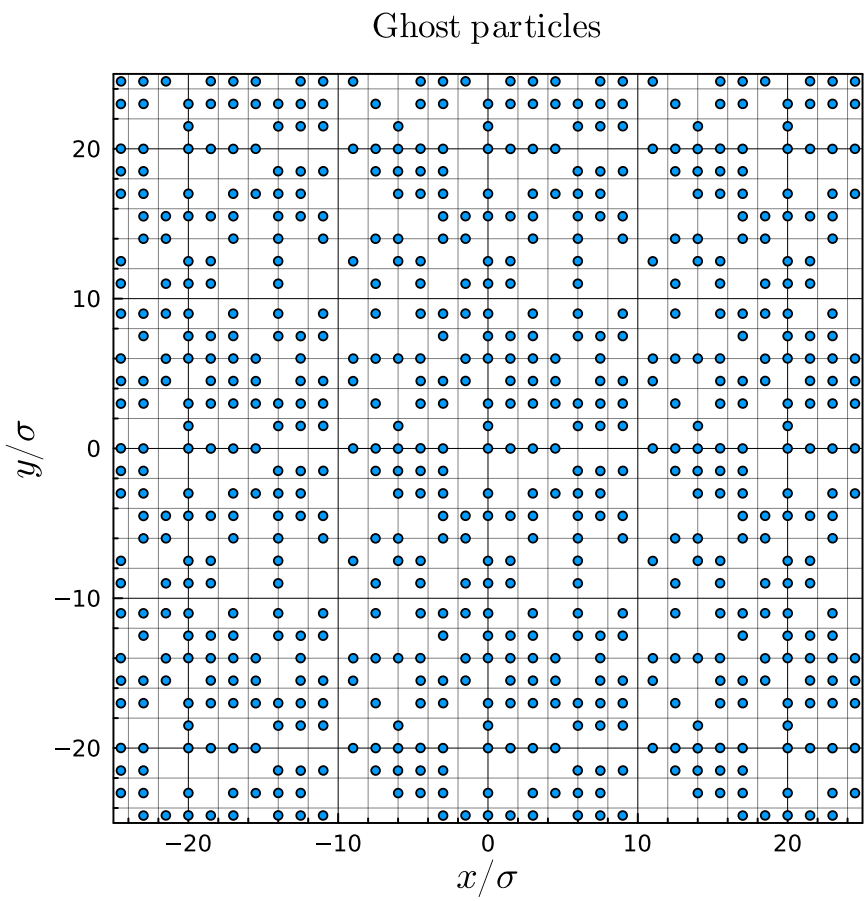


Figure 6: Initial condition with ghost particles.

4 Results

Finally in figure **??** is shown the evolution of the temperature in a simulation with 100 particles in a box of 20σ by 20σ and a numerical value of 1 for the temperature and 5 for ε. It can be observed a stabilization above 3.8. The access to the animation is thru the following link Access to the animation.

5 Description of the simulation

Use LAMMPS to make a 3D simulation of a binary mixture of two types of particles interacting through a Lennard-Jones force. Type 1 particles should have a radius of 1σ and type 2 should have a radius of 2σ. The particles are connected to a bath, and therefore have a Langevin thermostat.

Use OVITO to visualize the results of the simulation. Make an animation, for three different values of the density, trying to get qualitatively different behaviors. Also make a report where you show a snapshot

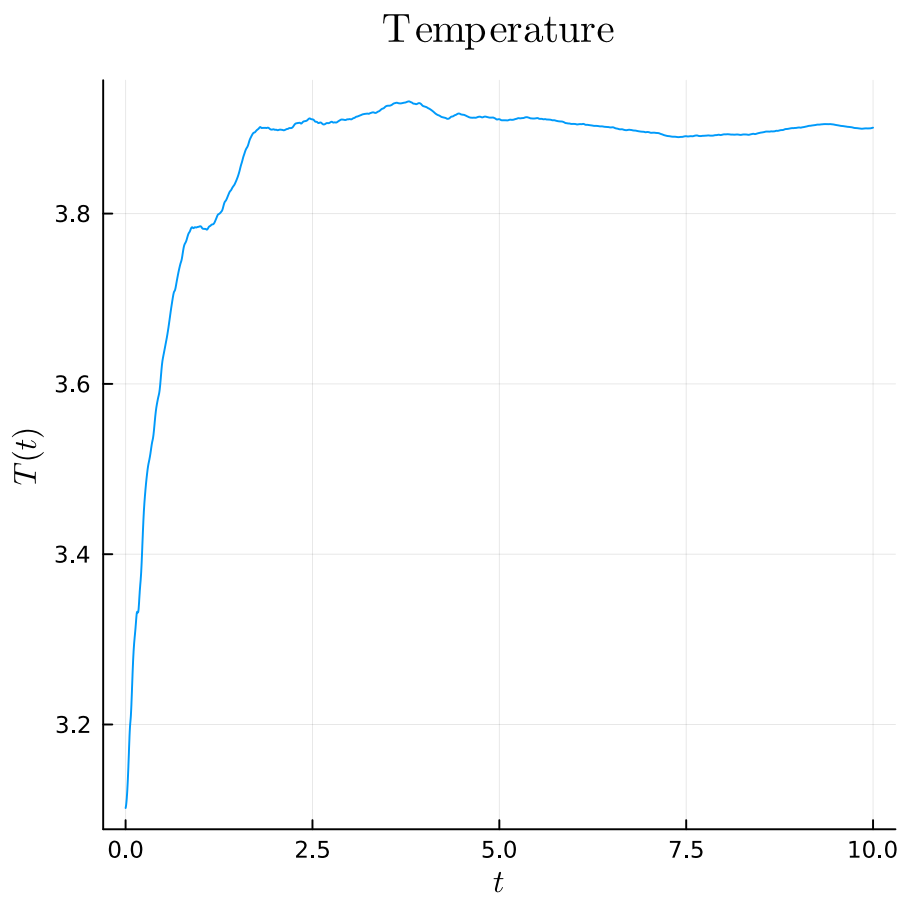


Figure 7: Temperature of a simulation of 100 particles in abox with periodic boundary conditions.

of the animation and discuss your results.

5.1 Langevin thermostat

According with (**Langevin_equation**) the Langevin equation provided a conceptual and quantitative improvement on the description of the phenomenon of Brownian motion. This equation is a stochastic differential equation written as follows

$$dv(t) = -\gamma v(t) + D dw(t), \tag{17}$$

where $v(t)$ is the velocity, γ is a friction coefficient due to the viscosity of the liquid, D is the diffusion coefficient and $w(t)$ is the Wiener process. Finally, the friction coefficient γ and the diffusion coefficient D are related by: $D = 2\gamma kT$, where k is the Boltzmann's constant and T is temperature.

This equation can be interpreted as the description of a heavy particle moving through a solvent. While is moving it will encounter more solvent particles in the front than in 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 (**libroClase**). However, the solvent is modeled by a stochastic and dissipative force, allowing substantially longer simulations that would be possible if the solvent were explicitly included (**Luckhurst_Veracini_2012**).

In the following section is a brief description of the software LAMMPS and how it was set the simulation for a binary mixture with Lennard-Jones force and langevin thermostat.

5.2 LAMMPS

LAMMPS is an acronym for Large-scale Atomic/Molecular Massively Parallel Simulator and on the LAMMPS website it describes its program as a classical molecular dynamics code with a focus on materials modeling and has potentials for solid-state materials (metals, semiconductors) and soft matter (biomolecules, polymers) and coarse-grained or mesoscopic systems. It can be used to model atoms or, more generically, as a parallel particle simulator at the atomic, meso, or continuum scale (**LAMMPS**).

For the simulation of the binary mixture a tutorial by Simon Gravelle (**Gravelle**). The objective of that tutorial is to set set, launch and analyze a molecular dynamics simulations of a binary Lennard-Jones fluid made of neutral particles with two different diameters in a cubic box with periodic boundary conditions and the temperature if the system is imposed using a Langevin thermostat. In the following sections are shown the results from the simulations.

6 Results

In figure **??** is shown a snapshot of the initial conditions for the binary mixture displayed using Ovito. As it is shown in the figure the particles are set up at a random position inside the box. At setting this configuration as the initial condition is necessary to run a minimization procedure before initialize the molecular dynamics to prevent the simulation from diverging.

From the simulation is retrieved the temperature, potential, kinetic and total energy of the system as a tool to analyze the simulation. In figure **??** is shown the evolution of the temperature thru the time steps and it is observed that converges to a value, indicating a stable system. Also in figure **??**, are shown the potential, kinetic and potential energy of the system thru all the simulation. As expected, the kinetic energy has a similar curve as the temperature, tending towards a constant value. On the other hand, the potential energy can be neglect from the total energy, due to the difference in magnitude with the kinetic energy.

Finally in appendix **??** is the script used for the simulation and in the following link is the access to the animation of the system: Access to the animation

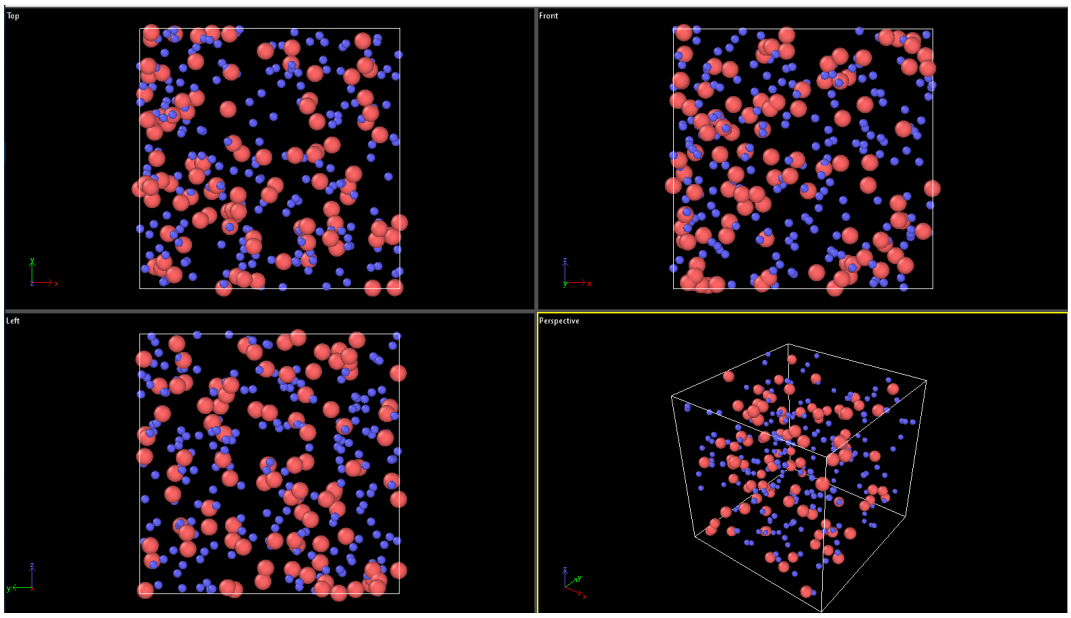


Figure 8: Snapshot of the initial conditions viewed in Ovito.

7 Description of the simulation

Simulate a polymer chain by bonding ten or more atoms together using a FENE potential. Use a Langevin thermostat. Observe how the chain curls with the fluctuations. Modify the interactions using angles and dihedrals so that the polymer remains closer to a straight line (some fluctuations are ok). Add several similar chains to your program. Make all particles interact through a Lennard Jones potential.

8 FENE potential

The finite extensible nonlinear elastic (FENE) potential (**bond_style_FENE_LAMMPSdoc**) is used for bead-spring polymer models with the following equation,

$$E = -\frac{1}{2}KR_0^2 \ln\left[1-\left(\frac{r}{R_0}\right)^2\right] + 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] + \varepsilon. \tag{18}$$

The first term models an attractive force with energy K over a distance R_0, the second term is a Lennard-Jones potential with inner-particle energy ε and σ particle size. Finally, the third term is the inner-particle energy causing that the minimum for the Lennard-Jones potential is 0.

Knowing that R_o has units of distance, it is intuitive to be proportional to the particle size, $R_0 = \alpha\sigma$. This can be interpreted as the length of the "bond", whereas K, with units of energy over distance, can be set as $K = \varepsilon/R_0$ and represent the energy of the "bond".

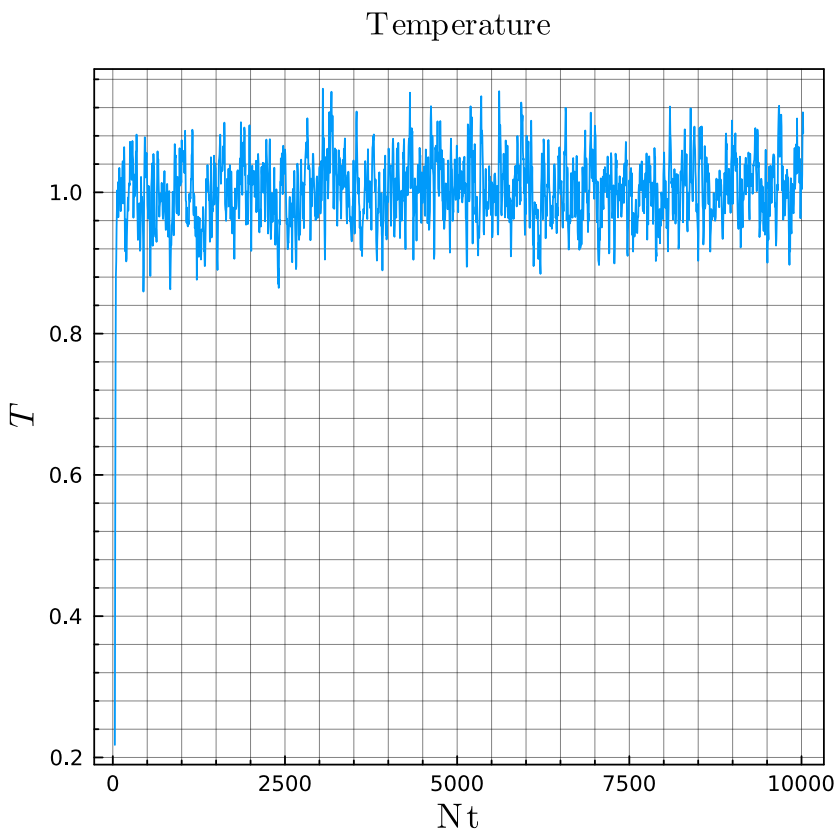


Figure 9: Temperature of the system

In figure **??** it is shown a comparison of 3 FENE potentials with $R_0 = 3\sigma$, 5σ and 7σ. At a increasing R_0, the potential tends to infinity as the distance tends to R_0 and goes to infinity at $r = \sigma$. This potential is desire to create a huge repulsive force when the distance between is small, and a strong attractive force when the distance increments.

For completeness, a comparison between a force due to a Lennard-Jones potential and a FENE potential is shown in figure **??**. As is expected from a Lennard-Jones force, the force tends to zero when the distance tends to infinity, on the other hand, the force from the FENE potential tends to $-\infty$ when the distance approaches R_0.

9 Angular potentials

Knowing that the FENE potential is going to cause a strong attractive force at a certain distance it is needed to add a restriction in order to prevent the particle chain collapse in a small cluster. For that potentials with angular dependence are introduce in the script.

As mention in class, the potential with angular dependence used in the simulation are harmonic angle

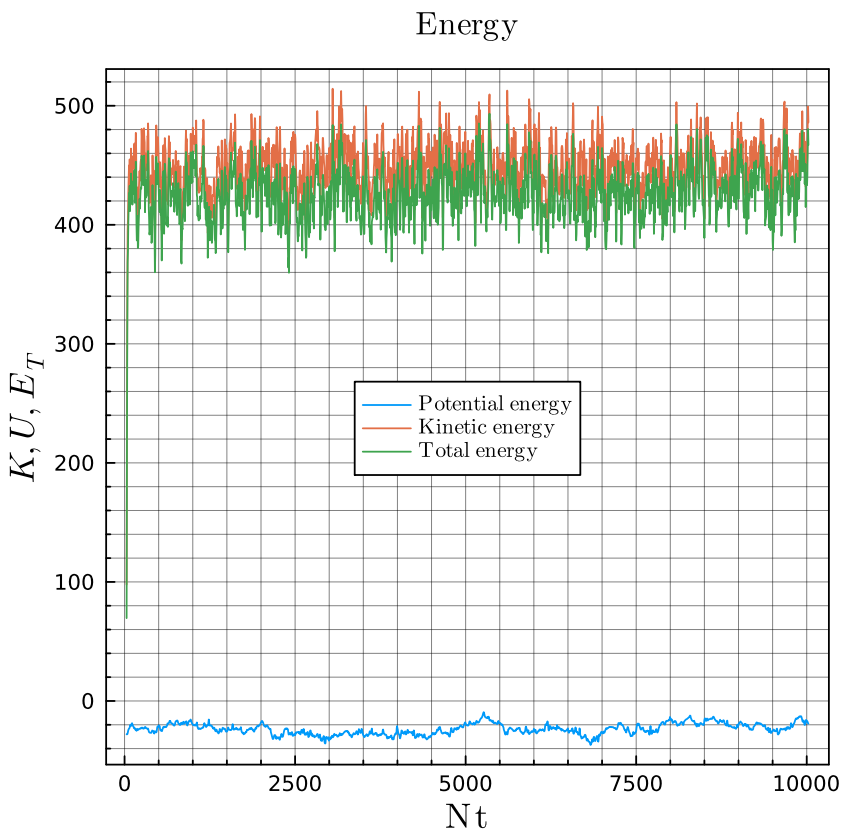


Figure 10: Potential, kinetic and total energy of the binary fluid.

(**angle_style_Harmonic_LAMMPSdoc**) and dihedral harmonic (**dihedral_style_Harmonic_LAMMPSdoc**). The angle harmonic potential is described with the following equation,

$$E(\theta) = K(\theta - \theta_o)^2, \tag{19}$$

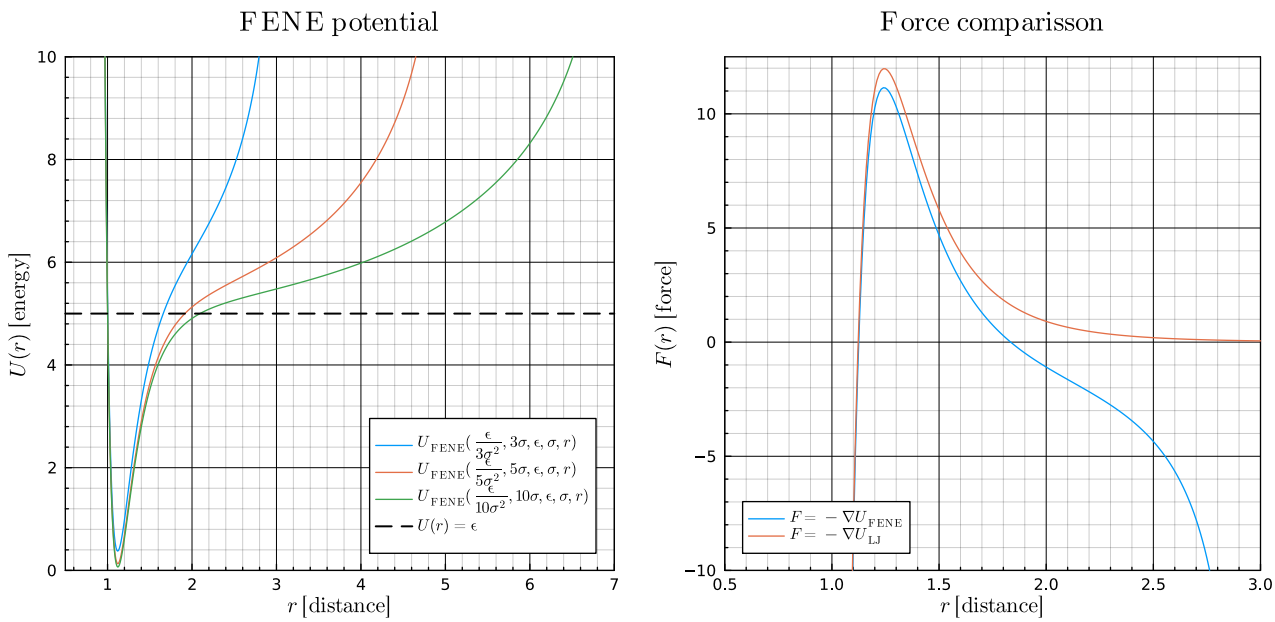
where K is the energy with units of energy over radian squared and θ_o is the angle of equilibrium. On the other hand, the dihedral harmonic potential is modeled as,

$$E(\phi) = K[1 + d\cos(n\phi)], \quad d \in \{1, -1\},\ n \in \mathbb{Z} \tag{20}$$

where K is the energy. The parameter d change the maximum of the function to a minimum when $\phi = \pi$ and the parameter n change the frequency.

Is important to acknowledge that the angle θ refers to the polar angle and ϕ to the azimuth angle in spherical coordinates, hence, introducing both angular potentials will help to introduce restrictions in the behavior of the particle chain.

In figure **??** is a comparison of both angular potentials in the angular domain of 0 to 2π, taking advantage of the periodic pattern of the cos function. The angle of equilibrium for the angle harmonic potential is set to π and n is set to 1 for the dihedral harmonic potential for visualization purposes.



(a) (b)

Figure 11: **??** Comparison of the FENE potential with different R_o and K in terms of ε and σ. **??** Comparison of the force due to a FENE potential with a force due to a Lennard-Jones potential with $R_o = 3\sigma$ and $K = \varepsilon/(3\sigma)^2$.

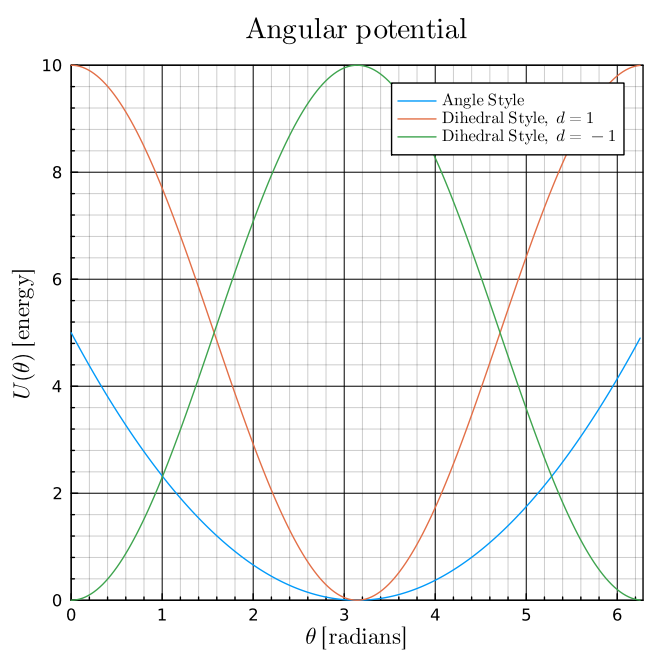


Figure 12: Comparison between angular and dihedral style potentials, with $\theta_o = \pi$ and $n = 1$.

10 Results

The main result of the simulation are the trajectories of the polymer chains, hence, in the following link you can access to the animations of the polymer chains: Access to the animation. On the other hand, in figure **??** it is shown a comparison of kinetic, potential and total energy of the simulations with polymer chains modeled with angle restriction and angle with dihedral restriction.

As a global characteristic of both systems the tendency of the energies are the same, however the polymers chains modeled with just the angle restriction has more energy than the chains modeled with angle and dihedral restrictions. This difference makes sense because the second polymer chain has less degrees of fredoom than the first one.

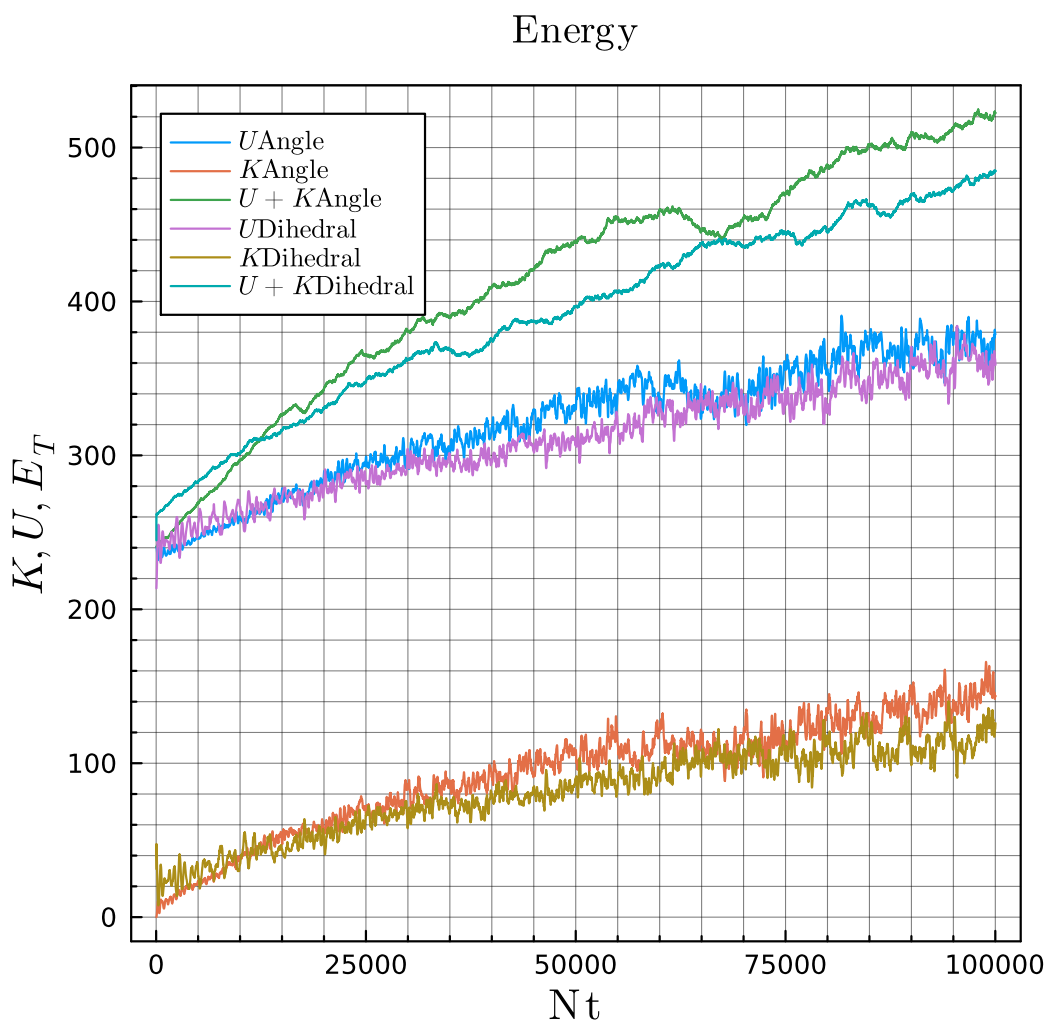


Figure 13: Comparison of kinetic, potential and total energy for simulations of a polymer chain modeled with angle restriction (U_{Angle}, K_{Angle}) and a polymer chain with angle and dihedral restriction (U_{Dihedral}, K_{Dihedral}).