A Coarse-grained Molecular Dynamics for Crystalline Solids

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Contents

1   Introduction

Molecular Dynamics has applications in Chemistry, Engineering, and Medicine. For example in Engineering it can be used to model and predict how a material can possibly deform after you apply a force to certain positions of a material. Furthermore, in medicine it has been successfully applied to modelling chemical structures and in drug design. A striking example of this took place at the University of Illinois in 2013, where researchers were able to model the structure of the HIV-1 virus capsid [5].

To understand goals of this paper it is necessary to understand the motivations behind the study of Molecular Dynamics. Molecular Dynamics aims to study the behaviour of Molecular Systems [1] . These are systems comprised of individual molecules interacting with one another. By studying Molecular Dynamics, we gain deeper insights into the reasons why some objects behave the way they do.

Despite the power of the applications of Molecular Dynamics, the simulations can be computationally expensive. Even objects we would consider small, like a strand of hair, contain a number molecules on the order of 10^{15}. This is beyond the capacity of even the most powerful computers available today, and there is therefore a tradeoff between the complexity of simulations that can be run and the amount of processing power needed for these simulations. As such, our focus will be on a specific type of solid which requires a modest amount of computational power. I aim to review methods outlined by Xiantao Li for estimating the dynamics of crystaline solids in source [3] and also test the accuracy of the claims he makes in the example of a 1D particle chain and a 2D lattice with different intermolecular potentials.

1.1   Mathematical Formulation

In this paper we will model all particle interactions using Classical Mechanics. This is partly because Classical Mechanics gives an accurate enough description of most scenarios in Molecular Dynamics. It is also partly because Schrödinger's equation is a 2nd order partial differential equation in each molecules spatial direction and in time [1]. The complexity of solving Schrödinger's equation in each variables requires a large amount of computing power added on top of the computing power required to simulate many molecules, making it a unsuitable method for modelling a system of molecules.

To model the behaviour of molecule i we will describe all interactions in terms of the momentum of a particle $\mathbf{p}_i(t)$, its position $\mathbf{q}_i(t)$ and an inter-particle potential $V(\mathbf{q}_1, \mathbf{q}_2, ..., \mathbf{q}_n)$, with $1 \leq i \leq n$ and n being the number of particles we are modelling. The main behaviours of the model are determined by the inter-particle potential. Here we need to note the importance of the inter particle potential. The potential is what determines what kind of model we are investigating. Once we have a potential we aim to solve the equation given

by newtons second law

$$\mathbf{M}\ddot{\mathbf{q}} = -\nabla V(\mathbf{q}). \tag{1}$$

$\mathbf{M}$ is the mass matrix defined by $(\mathbf{M})_{ij} = m_i$ if $i = j$, and 0 otherwise. m_i is the mass of particle i.
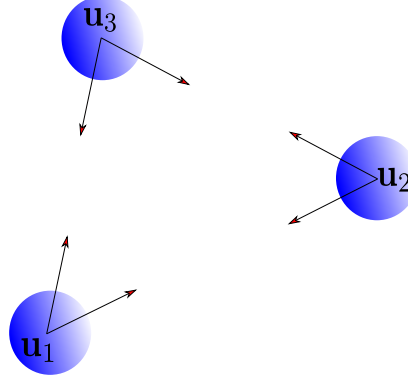

Figure 1: This figure shows 3 masses interacting with each other with respect to just the gravitational potential $V(\mathbf{u_j}) = \sum_{i=1}^{3} \frac{-(1-\delta_{ij})Gm_i m_j}{\|\mathbf{u_j}-\mathbf{u}_i\|}$.

1.2 The Hamiltonian Operator and the Verlet Method

It is most natural to use the Hamiltonian formulation of Classical Mechanics to determine the trajectory of the system. This is because it's based directly on the assumption of a closed system, meaning that the total energy in the system is always conserved [1]. The Hamiltonian is defined as

$$H(\mathbf{p}, \mathbf{q}) = \frac{1}{2}\mathbf{p}^{\mathsf{T}}\mathbf{M}^{-1}\mathbf{p} + V(\mathbf{q}).$$

Note that the first term of the Hamiltonian describes the kinetic energy of the system. We also define the momentum of the system as

$$\mathbf{p} = \mathbf{M}\dot{\mathbf{q}}.$$

Furthermore, notice that

$$\dot{\mathbf{q}} = \mathbf{M}^{-1}\mathbf{p},$$
$$\dot{\mathbf{p}} = -\nabla V(\mathbf{q}).$$

With the current definition of the Hamiltonian and momentum the equation of motion given by (1) becomes [1]

$$\dot{\mathbf{q}} = \frac{\partial H}{\partial \mathbf{p}}, \tag{2}$$

$$\dot{\mathbf{p}} = -\frac{\partial H}{\partial \mathbf{q}}. \tag{3}$$

This way of writing (1) is a lot easier to deal with because, instead of trying to solve one 2nd order ordinary differential equation we are now trying to solve a first order system of ordinary differential equations.

Furthermore, the Hamiltonian is always conserved. This fits the law of conservation of energy as the Hamiltonian is the total energy of the system of particles. The result can be shown by direct calculation of the derivative of the Hamiltonian in time.

Proposition 1. *The Hamiltonian of a system is always conserved. Meaning that*

$$\dot{H} = 0.$$

Now that we have the Hamiltonian formulation of the system we can start to think about trying to find a solution to (2) and (3). Since we are trying to find a solution to a partial differential equation in several variables it is unlikely that we will find an exact analytical solution to the problem, so we must employ a numerical approximation. To do this r will use a numerical scheme called the Verlet Method which for which there is a clear derivation in [1].

Let $[0, \tau]$ be a interval for which we want to find a solution for the equations of motion (2) and (3). Let N be the maximum number of steps we are taking to find the solution of the partial differential equation and $h = \tau/N$. Define initial conditions $\mathbf{q}_0 = \mathbf{q}(0)$ and $\mathbf{p}_0 = \mathbf{p}(0)$ and let $\mathbf{q}_i = \mathbf{q}(ih)$ and $\mathbf{p}_i = \mathbf{p}(ih)$. Then the next iteration of the momentum and the position of the system are given by

$$\mathbf{p}_{i+\frac{1}{2}} = \mathbf{p}_i - \frac{h}{2}\nabla V(\mathbf{q}_i),$$

$$\mathbf{q}_{i+1} = \mathbf{q}_i + h\mathbf{M}^{-1}\mathbf{p}_{i+\frac{1}{2}},$$

$$\mathbf{p}_{i+1} = \mathbf{p}_i - \frac{h}{2}\nabla V(\mathbf{q}_{i+1}).$$

This is the Verlet Scheme. We will use this to find numerical solutions the the equations given above in the examples of the 1D particle chain and the 2D lattice.

2 The Mori-Zwanzig Projection

A way to combat the difficulty of implementing the dynamics of a system of molecules is to simply simulate an observable of the molecules. The observable can be a projection onto a local region of molecules, or it can be the mean of a local region of molecules and so on. However, this is not so simple as it sounds, since we still need to take into account the rest of system of molecules. The Mori-Zwanzig projection allows us to do this. This is because it gives us a method to express an observable of a system of molecules that we are interested in exactly, whilst taking into account the contributions from the rest of the system.

In [3] Li defines position and momentum of a system, maps to a subset of the position and momenta of the system. He then uses the Mori-Zwanzig projection to estimate how and observable of the system evolves in time while also taking into account the contributions from the rest of the system. In this following section we will summarise Li's paper.

Let $\mathbf{u}$, $\mathbf{v}$ be the position and the velocity of the system respectively. Assuming each molecule has the same mass m we define coarse grain variables

$$
\mathbf{p} = m\mathbf{B}\mathbf{v},
$$
$$
\mathbf{q} = \mathbf{B}\mathbf{u}.
$$

Where $\mathbf{B}$ is the observable which maps us to our coarse grained variables. Note that $\mathbf{B}$ is a $k \times n$ matrix with rank dn where d is the dimension of the space and k is the number of molecules in the coarse grained model. The coarse grained variables could for example be a selection of particular molecules like in figure 2, or it can be the average of a cluster of molecules.
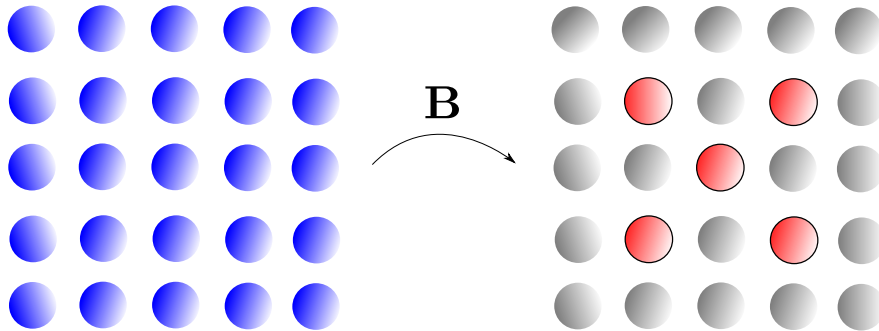

Figure 2: An example of the kind of map $\mathbf{B}$ can be. In this example B would select the position and momenta of the red molecules in the Lattice.

To apply the Mori-Zwanzig projection we first need to define the Liouville operator by

$$\mathcal{L} = \mathbf{v} \cdot \nabla_{\mathbf{u}} - \frac{1}{m} \nabla V \cdot \nabla_{\mathbf{v}}.$$

We also define a projection operator on $\mathbf{v}$ and $\mathbf{u}$ by

$$\mathcal{P} = \mathbb{E}[\cdot \,|\, (\mathbf{p}, \mathbf{q})].$$

Where the expectation is given with respect to Gibbs distribution. We also define $\mathcal{Q}$ to be the operator orthogonal to $\mathcal{P}$. Given that $\mathbf{p}(t)$ is a dynamic variable Li writes $\mathbf{p}(t) = e^{tL}\mathbf{p}(0)$ [3], And applies the Mori-Zwanzig procedure to give us

$$\dot{\mathbf{p}}(t) = e^{t\mathcal{L}}\mathcal{P}\mathcal{L}\mathbf{p}(0) + \int_0^t e^{(t-s)\mathcal{L}}\mathbf{K}(s)\,\mathrm{d}s + \mathbf{F}(t), \tag{4}$$

$$\mathbf{K}(t) = \mathcal{P}\mathcal{L}\mathbf{F}(t), \tag{5}$$

$$\mathbf{F}(t) = e^{t\mathcal{Q}\mathcal{L}}\mathcal{Q}\mathcal{L}\mathbf{p}(0). \tag{6}$$

This is an equation of motion for coarse grain variable $\mathbf{p}$ which implicitly considers the rest of the system of molecules [3] [2]. This is a great result because it means that we can simulate local regions of a molecular dynamics model exactly whilst being able to take into consideration the rest of the model. However, there is one problem, as the equation is currently it is still too difficult to implement.

2.1 An approximation of the Dynamics

Due to the difficulty of implementing (4), (5) and (6) Li assumes that the system is in mechanical equilibrium. Then he uses this to approximate the positions and momenta of the molecules in the system. This is a very fair assumption to make considering that we assume that we are modelling the molecules of a Crystalline solid.

First of all, to begin the approximation we need to define the matrix $\mathbf{D}$ which is given by the linearisation of the forces at the reference state. We call $\mathbf{D}$ the force constant matrix.

Suppose the positions of each molecule $\mathbf{u}_i \in \mathbb{R}^3$ for $1 \leq i \leq n$. Assuming that $\mathbf{u} = (\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3, ..., \mathbf{u}_n)^{\mathsf{T}} = (u_{11}, u_{12}, u_{13}, u_{21}, u_{22}, u_{23}, ..., u_{n1}, u_{n2}, u_{n3})^{\mathsf{T}}$. Let $\mathbf{u}_i^*$ be the position where the inter-molecular potential of the ith molecule is minimized. Let $\mathbf{f}$ be the vector function whose i^{th} entries $\mathbf{f}_i = (f_{i1}, f_{i2}, f_{i3})$ is the force at the ith molecule. Then we can

write the force constant matrix $\mathbf{D}$ as block matrix whose block entries are given by

$$(\mathbf{D})_{ij} = \mathscr{D}_{\mathbf{u}_i}\mathbf{f}_j(\mathbf{u})|_{\mathbf{u}=\mathbf{u}_i^*},$$

where $1 \le i, j \le n$ and $\mathscr{D}_{\mathbf{u}_i}$ is the vector derivative with respect to $\mathbf{u}_i$. Note that in the 1D and 2D cases $\mathbf{D}$ is defined analogously.

Using this he came to an approximation of $\mathbf{u}$ by

$$\mathbf{u} = \mathbf{Rq}, \quad \text{where} \quad \mathbf{R} = \mathbf{D}^{-1}\mathbf{B}^{\mathsf{T}}\left(\mathbf{B}\mathbf{D}^{-1}\mathbf{B}^{\mathsf{T}}\right)^{-1}. \tag{7}$$

Li also calculates that the projection operators operator $\mathcal{P}$ applied to $\mathbf{u}$ and $\mathbf{v}$ will give

$$\mathcal{P}\mathbf{u} = \bar{\mathbf{u}} + \mathbf{P}_u(\mathbf{u} - \bar{\mathbf{u}}), \tag{8}$$

$$\mathcal{P}\mathbf{v} = \bar{\mathbf{v}} + \mathbf{P}_u(\mathbf{v} - \bar{\mathbf{v}}), \tag{9}$$

Where $\bar{\mathbf{u}}$ and $\bar{\mathbf{v}}$ are the mean values of $\mathbf{u}$ and $\mathbf{v}$ in the reference state, $\mathbf{P}_u = \mathbf{RB}$, and $\mathbf{P}_v = \mathbf{B}^{\mathsf{T}}\left(\mathbf{B}\mathbf{B}^{\mathsf{T}}\right)^{-1}\mathbf{B}$. We also define complimentary matrices $\mathbf{Q}_u = \mathbf{I} - \mathbf{P}_u$, $\mathbf{Q}_v = \mathbf{I} - \mathbf{P}_v$.

In addition to this when $\mathcal{L}$, and $\mathcal{Q}$ are applied to the random force $\mathbf{F}$ we get

$$\mathcal{L}F = \mathbf{C}\left(t\right)\mathbf{v}\left(0\right) - \frac{1}{m}\mathbf{S}\left(t\right)D\mathbf{u}\left(0\right), \tag{10}$$

$$\mathcal{Q}\mathcal{L}\mathbf{F} = \mathbf{C}\left(t\right)\mathbf{Q}_v\left(\mathbf{v}\left(0\right) - \bar{\mathbf{v}}\right) - \frac{1}{m}\mathbf{S}\left(t\right)\mathbf{D}\mathbf{Q}_u\left(\mathbf{u}\left(0\right) - \bar{\mathbf{u}}\right). \tag{11}$$

Now we have all of the tools ready to understand the simplified version of equation (4). Looking at the first term $e^{t\mathcal{L}}\mathcal{P}\mathcal{L}\mathbf{p}(0)$ Li noticed that this term is usually written as a mean force with respect to the Gibbs distribution

$$e^{t\mathcal{L}}\mathcal{P}\mathcal{L}\mathbf{p}(0) = -\langle\nabla_{\mathbf{q}}\mathcal{F}\rangle,$$

and then proceeded to use a Harmonic approximation to write the mean force as

$$\langle\nabla_{\mathbf{q}}\mathcal{F}\rangle = \mathbf{B}\mathbf{P}_u^{\mathsf{T}}\nabla V(\mathbf{Rq}) + \mathbf{B}\mathbf{D}\mathbf{Q}_u(\mathbf{u}(0) - \bar{\mathbf{u}}). \tag{12}$$

After Li approximated the first term in (4) to get (12) he then proceeds to approximate the second term of (4). To do this he found an approximation for $\mathbf{F}$ (6) the random force felt by particles in the system. This is given by

$$\mathbf{F}(t) = \mathbf{C}(t)\left(\mathbf{u}(0) - \bar{\mathbf{u}}\right) + \mathbf{S}(t)\left(\mathbf{v}(0) - \bar{\mathbf{v}}\right), \tag{13}$$

where both $\mathbf{C}(t)$ and $\mathbf{S}(t)$ are given by the initial value problem. They can be solved using the Verlet Method given in the introduction.

$$\mathbf{S}(0) = \mathbf{0}, \quad \dot{\mathbf{S}}(0) = -\mathbf{BDQ}_v,$$
$$\dot{\mathbf{S}}(t) = \mathbf{C}(t)\mathbf{Q}_v, \quad m\ddot{\mathbf{S}}(t) = -\mathbf{S}(t)\mathbf{DQ}_v,$$

$$\mathbf{C}(0) = -\mathbf{BDQ}_u, \quad \dot{\mathbf{C}}(0) = \mathbf{0},$$
$$m\dot{\mathbf{C}}(t) = -\mathbf{S}(t)\mathbf{DQ}_u, \quad m\ddot{\mathbf{C}}(t) = -\mathbf{C}(t)\mathbf{Q}_v\mathbf{D},$$

which is based off of (10) and (11).

In addition to this using (10) and (11) he further approximates the term $\mathbf{K}$ by

$$\mathbf{K}(t) = \mathbf{C}(t)\,\mathbf{P}_v\mathbf{v}(0) + \mathbf{C}(t)\,\mathbf{Q}_v\bar{\mathbf{v}} - \mathbf{S}(t)\,\mathbf{DQ}_u\bar{\mathbf{u}}. \tag{14}$$

$$\tag{15}$$

Using this the second term of the of (4) can be expressed as

$$\int_0^t e^{(t-s)\mathcal{L}}\mathbf{K}(s)\,\mathrm{d}s = -\int_0^t \theta(t)\left(\mathbf{BB}^\mathsf{T}\right)^{-1}\mathbf{p}(t-s)\,\mathrm{d}s + \mathbf{C}(t)\,\bar{\mathbf{u}} + \mathbf{S}(t)\,\bar{\mathbf{v}} + \mathbf{BDQ}_u\bar{\mathbf{u}}, \tag{16}$$

$$\theta(t) = -\mathbf{C}(t)\,\mathbf{B}^\mathsf{T}.$$

Now using (16) and (12) and also defining $\mathbf{M} = m\left(\mathbf{BB}^\mathsf{T}\right)^{-1}$ and $\mathbf{G}(t) = \left(\mathbf{BB}^\mathsf{T}\right)^{-1}\mathbf{F}(t)$ he expresses the equations of motion (2) and (3) by

$$\dot{\mathbf{q}} = \frac{1}{m}\mathbf{p}, \tag{17}$$

$$\mathbf{M}\dot{\mathbf{p}} = -\mathbf{R}^\mathsf{T}\nabla V\left(\mathbf{Rq}\right) - \int_0^t \Theta(\tau)\,\mathbf{p}(t-\tau)\,\mathrm{d}\tau + \mathbf{G}(t) + \mathbf{f}_0(t), \tag{18}$$

where

$$\Theta(t) = \left(\mathbf{BB}^\mathsf{T}\right)^{-1}\theta(t)\left(\mathbf{BB}^\mathsf{T}\right)^{-1}, \quad \mathbf{f}_0(t) = \mathbf{C}(t)\,\bar{\mathbf{u}} + \mathbf{S}(t)\,\bar{\mathbf{v}}. \tag{19}$$

This is an approximation of the dynamics of the coarse-grain variables that we have selected

3   A 1-Dimensional Example

In this section I will be testing the claims made by Li in [3]. To do this I've written 20 MATLAB files which describe a Hamiltonian system, use numerical methods such as the Verlet method to solve the system of ordinary differential equations which describe the system(2) (3), and solve the system of ordinary differential equations which describe its coarse-grained counterpart (18) (17). The first set of differential equations which describe the motion of the entire Hamiltonian system were implemented in order to be compared against the coarse-grained dynamics. We do this by finding the observable of the full scale system at each time step and then compare that against the coarse-grained dynamics at each time step. Doing this gives an insight to just how accurately the coarse-grained dynamics simulate the observable the Hamiltonian system.

3.1   The Model

To begin with the example we must first describe the model we are choosing to implement. We will be considering a 1-Dimensional particle chain consisting of 8 particles each with a mass of 1. The particle chain will model pairwise interactions according to the Lennard-Jones potential given by

$$\phi(r) = \frac{1}{r^{12}} - \frac{2}{r^6}.$$

Notice that in figure 5 and the equation for the potential indicate $\lim_{r \to 0} \phi(r) = \infty$. This is to try and model the repulsive forces between the particles at close distances [1]. The figure and the equation for the potential also indicate that $\lim_{r \to \infty} \phi(r) = 0$. This is to try and show that if two particles are far from each other then they will feel less of an attractive force to each other. In addition to this the minimum potential is achieved at a distance of 1 between the particles. In other words, the greatest attraction between two particles is achieved at 1. On top of all of this, the Lennard Jones potential is not very computationally expensive to compute since the 12th of r is achieved by squaring the 6th power[1]. From this we see that the Lennard Jones potential is a good choice to model the inter molecular potential of two molecules.

Taking the intermolecular potential into account we write the equations of motion of the
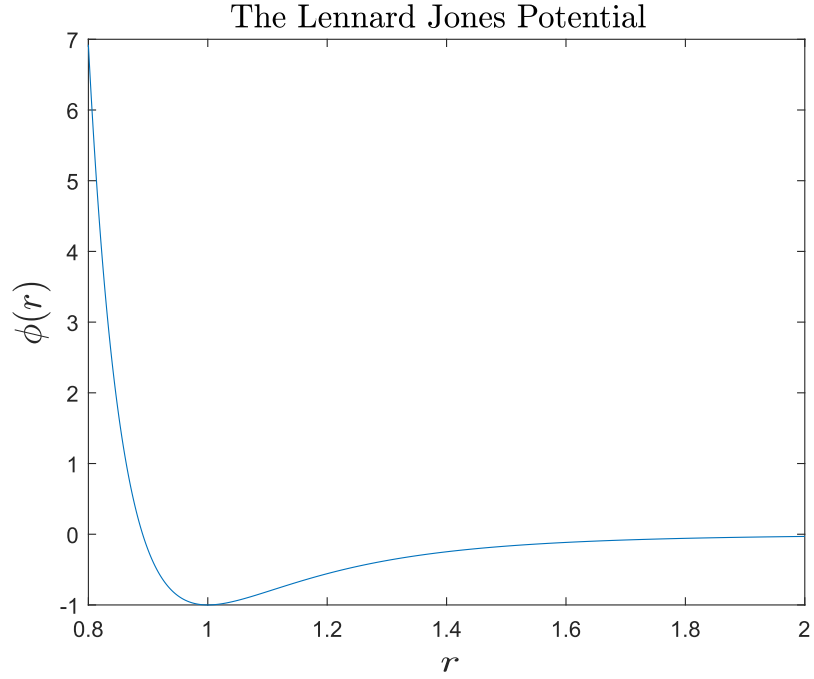
Figure 3: A graph of the Lennard Jones Potential

Hamiltonian system (2) and (3) as

$$\dot{\mathbf{u}} = \mathbf{v},$$

$$\dot{\mathbf{v}} = -\nabla V(\mathbf{u}), \quad \text{where} \quad V(\mathbf{u}) = \sum_{i=1}^{8} \phi(u_{i+1} - u_i).$$

Notice that since the mass of each particle is 1 that the momentum and velocity of the system are equal.
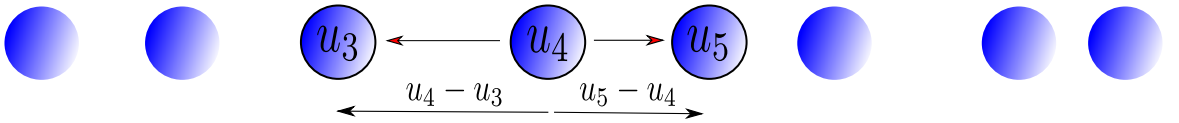

Figure 4: This figure depicts the arrangement of the Model. The contribution to the potential of the molecule at position u_4 is given by $\phi(u_5 - u_4) + \phi(u_4 - u_3)$. Under the Lennard jones potential each particle oscilates around its initial position.

The only thing left to define for the model is the initial conditions of the particle chain. Both the velocity and positions of the particle chain are randomly generated. Each element of the initial velocity vector $\mathbf{v}(0)$ is uniformly distributed in $[-1, 1]$. To also ensure that average velocity at time 0 is 0 we subtract the mean velocity from each element in the

velocity vector. In other words if $\mathbf{z}$ is the vector of elements given by

$$z_i = 2x_i - 1, \quad \text{where} \quad x_i \in X \sim U(-1, 1) \quad \text{for} \quad 1 \le i \le 8,$$

then $\mathbf{v}(0)$ is given by

$$v_i(0) = z_i - \bar{\mathbf{z}}.$$

This is all to ensure that the mean velocity of the entire system of molecules is 0 relative to its original position.

The position vector is a little bit harder to assign an initial value to. This is because if some of the particles start too closely together then the intermolecular potential would dictate that the force acting on the particles could be large enough for the chain to break in possibly more than 1 place. Furthermore, if some of the particles start too far away from each other then the intermolecular potential between the particles would be too small for the particles to come together again. This case means that the chain would be broken to begin with. To get around this I assigned the initial position $\mathbf{u}(0)$ to be given by

$$u_1 = y_1,$$
$$u_{i+1}(0) = u_i + 1 + \frac{y_i}{100}, \quad \text{where} \quad 2 \le i \le 7,$$

and

$$y_i \in Y \sim N(0, 1) \quad \text{for} \quad 1 \le i \le 8.$$

3.2 Coarse-grained Dynamics Of The 1D Chain

Now that the Hamiltonian system is clearly defined it is time to select the coarse grained variables $\mathbf{p}$ and $\mathbf{q}$. To do this we must pick an observable $\mathbf{B}$. The one I have chosen for the example is

$$\mathbf{B} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

This observable selects the first, last, and one of the middle particles. Following in suit of the previous section we define coarse-grain variables

$$\mathbf{p} = \mathbf{Bv},$$
$$\mathbf{q} = \mathbf{Bu}.$$

p and **q** describe the momentum and position of the first, last, and one of the middle. Similarly if you want to find the dynamics of the sum of all the particles one can select the observable to be $\mathbf{B} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix}$.
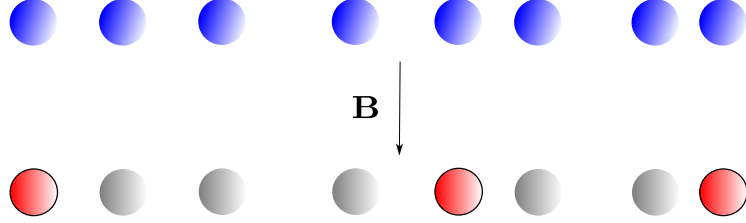

Figure 5: A depiction of the coarse-grain arrangement.

Now to proceed with implementing the simplified coarse-grained dynamics we need to define the force constant matrix **D**. In this case

$$\mathbf{D} = \begin{pmatrix}
-2\phi''(1) & \phi''(1) & 0 & 0 & 0 & 0 & 0 & 0 \\
\phi''(1) & -2\phi''(1) & \phi''(1) & 0 & 0 & 0 & 0 & 0 \\
0 & \phi''(1) & -2\phi''(1) & \phi''(1) & 0 & 0 & 0 & 0 \\
0 & 0 & \phi''(1) & -2\phi'(1) & \phi''(1) & 0 & 0 & 0 \\
0 & 0 & 0 & \phi''(1) & -2\phi'(1) & \phi''(1) & 0 & 0 \\
0 & 0 & 0 & 0 & \phi''(1) & -2\phi'(1) & \phi''(1) & 0 \\
0 & 0 & 0 & 0 & 0 & \phi''(1) & -2\phi'(1) & \phi''(1) \\
0 & 0 & 0 & 0 & 0 & 0 & \phi''(1) & -2\phi''(1)
\end{pmatrix}.$$

Now that **D** is defined we find all the other matrices such as $\mathbf{R}$, $\mathbf{P}_u$, $\mathbf{Q}_u$, and so on by just computing them from the formulas given in the previous section. After these matrices are found the next step is to find $\bar{\mathbf{u}}$, $\bar{\mathbf{v}}$, $\mathbf{S}(t)$, $\mathbf{C}(t)$ and use these to compute $\mathbf{F}(t)$, $t \in [0, \tau]$. From the initial condition of **v** we can see that the mean velocity of all the particles would be 0. This is because they all oscillate around the same positions. This also means that the mean positions of the particles would be given by $\bar{u}_1 = u_1(0)$, and $\bar{u}_i = \bar{u}_{i-1} + 1$ for $2 \leq i \leq 8$. All of the MATLAB files to compute the matrices are in the appendix.

To find $\mathbf{S}(t)$ and $\mathbf{C}(t)$, $t \in [0, \tau]$ we implement the Verlet method given in section 1.2. To find **C** we do this by setting $\mathbf{p} = \dot{\mathbf{C}}$, $\mathbf{q} = \mathbf{C}$, $\nabla V(\mathbf{q}) = q\mathbf{Q}_v \mathbf{D}$ in the Verlet Method. To find **S** we do this by setting $\mathbf{p} = \dot{\mathbf{S}}$, $\mathbf{q} = \mathbf{S}$ and $\nabla V(\mathbf{q}) = q\mathbf{D}\mathbf{Q}_v$ in the Verlet method. I implemented the Verlet time stepping scheme in MATLAB.

After every every quantity has been defined to implement (18), and (17) we can use the Verlet scheme to find $\mathbf{p}(t)$ and $\mathbf{q}(t)$ for $t \in [0, \tau]$. We only need to take care when dealing with the second term from (18). To calculate this term I implemented the trapezoidal rule given in [4]. Using this we can write the second term of (18) as

$$\int_0^t \Theta\left(\tau\right) \mathbf{p}\left(t - \tau\right) \mathrm{d}\tau \approx \frac{\Delta\tau}{2}\left(\Theta_j \mathbf{p}_0 + \Theta_0 \mathbf{p}_j\right) + \Delta\tau \sum_{i=1}^{j-1} \Theta i \mathbf{p}_{j-i},$$

where $j = \left\lfloor \frac{t}{h} \right\rfloor$, and h is the step size in the Verlet Scheme.

4 Conclusion

In summary, this has been a very successful project.

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