main.m

%% Initialize particles

| **Variable** | **value** | **Type of variable** | **What it represents in real life** |
| --- | --- | --- | --- |
| DIM | 2 | 1x1 double | Dimension of space to observe |
| N | 32 | 1x1 double | Number of particles |
| BoxSize | 10.0 | 1x1 double | Length of one side of the space to observe (2D space in this case) |
| volume | 100 | 1x1 double, global variable | Area of space to observe (since DIM=2 in this case) |
| density | 0.32 | 1x1 double, global variable | Particles per unit of space (particle/area unit) |
| position |  | 32x2 double | Starting position of particles (x,y) |
| pos (line 17) |  | 32x2 double | Position divided by box size, to scale to 1x1 space |
| MassCenter | [-0.0150, 0.0126] | 1x2 double | Average position of all particles combined |
| pos (line 22) |  | 32x2 double | Positions, with (0,0) located at the mass center of all particles |

%% setting up the simulation

| **Variable** | **value** | **Type of variable** | **What it represents in real life** |
| --- | --- | --- | --- |
| NSteps | 10000 | 1x1 double | Number of frames to take new positions, avg potential energy, avg kinetic energy, pressure, and temp measurements |
| deltat | 0.0032 | 1x1 double | Time between each NStep |
| TRequested | 0.5 | 1x1 double | Reduced temperature (units not specified) |
| DumpFreq | 100 | 1x1 double | Every 100 frames, an image would be uploaded for the animation |
| epsilon | 1.0 | 1x1 double | Depth of the potential well (dispersion energy), basically an energy scaling constant that says how strongly two particles attract each other |
| ene\_kin\_aver |  | 1x10000 double | Avg kinetic energy for all 32 particles per frame |
| ene\_pot\_aver |  | 1x10000 double | Avg potential energy |
| pressure |  | 1x10000 double | Pressure at each frame |
| temperature |  | 1x10000 double | Temperature at each frame |
| pos (line 42) |  | 32x2 double | Position of the particles at the 10000th frame |

MD.m

| **Variable** | **value** | **Type of variable** | **What it represents in real life** |
| --- | --- | --- | --- |
| pos (input) |  | 32x2 double |  |
| NSteps | 10000 | 1x1 double |  |
| deltat | 0.0032 | 1x1 double |  |
| TRequested | 0.5 | 1x1 double | Reduced temp |
| DumpFreq | 100 | 1x1 double |  |
| epsilon | 1.0 | 1x1 double |  |
| BoxSize | 10.0 | 1x1 double |  |
| DIM | 2 | 1x1 double |  |
| density | 0.32 | 1x1 double | Particles per unit of space |
| volume | 100 | 1x1 double | Area of space |
| N | 32 | 1x1 double | Number of positions (number of particles) |
| vel (line 16) |  | 32x2 double | Randomly generated velocity from normally distributed numbers (distribution centered at zero), idk why -0.5. Only for initial (frame 1) velocity. |
| acc (line 17) |  | 32x2 double | Randomly generated acceleration for initial velocity |
| fid |  | file: ‘traj.xyz’ column ‘w’ |  |
| period |  | 1x1 double | (period, i) locates values on the 32x2 position array that are out of bounds |
| pos (line 31) |  | 32x2 double | Position at the next frame point, based on xt=x0+v0t +(½)at2 |
| chi |  | 1x1 double | Scaling temperatures to TRequested (looking at relative temp instead of actual temp) |
| vel (line 39) |  | 32x2 double | Next frame’s velocity calculated |
| acc (line 42) |  | 32x2 double | New acceleration calculated considering force-force interactions between particles |
| ene\_pot\_aver (line 42) |  | 1x10000 double | Avg potential energy per frame, calculated from amount of energy suppressed. Calculated one-by-one using compute\_forces function |
| virial (line 42) |  | 1x10000 double | Virial represents the attraction and repulsion between particles. Compute\_forces calculates one virial at a time. |
| vel (line 45) |  | 32x2 double | Next frame’s velocity updated using new acceleration |
| Ene\_kin\_aver (line 48) |  | 1x10000 double | Avg kinetic energy, calculated using Calculate\_Temperature function, one position at a time |
| temperature (line 48) |  | 1x10000 double | Temperature using Calculate\_Temperature function, one position at a time |
| Pressure (line 51) |  | 1x10000 double | Pressure |

Calculate\_Temperature.m

| **Variable** | **value** | **Type of variable** | **What it represents in real life** |
| --- | --- | --- | --- |
| vel |  | 32x2 double | Current frame’s velocity |
| BoxSize | 10.0 | 1x1 double |  |
| DIM | 2 | 1x1 double |  |
| N | 32 | 1x1 double |  |
| real\_vel |  | 32x2 double | Velocity rescaled to 10x10 space |
| ene\_kin |  | 1x1 double | KE=(½)mv2. Cumulative KE from all 32 particles |
| ene\_kin\_aver |  | 1x1 double | Average kinetic energy for that frame |
| temperature |  | 1x1 double | T=(2\*KE)/(3\*k) for 3D system, where k is constant. Since it is 2D, T=2\*KE/2 |

compute\_force.m

| **Variable** | **value** | **Type of variable** | **What it represents in real life** |
| --- | --- | --- | --- |
| pos |  | 32x2 double |  |
| epsilon | 1.0 | 1x1 double |  |
| BoxSize | 10.0 | 1x1 double |  |
| DIM | 2 | 1x1 double |  |
| N | 32 | 1x1 double |  |
| Rcutoff | 2.5 | 1x1 double | The lennard-jones potential contains r (distance between interacting particles) and σ (distance where potential energy is zero). Setting an Rcutoff makes sure the particles don’t go too far apart, and we don’t need to consider those interactions. |
| phicutoff | -0.0163 | 1x1 double | Phi represents the intermolecular potential when σ=1 (σ is measure of how close atoms can get without bonding), and r=Rcutoff. This makes sure that any interactions between far-apart particles (distance between them is greater than Rcutoff) can be subtracted out of the final potential energy. |
| Sij (line 17) |  | 1x2 double | Difference of one point’s coordinates and the next point’s coordinate, in order listed on pos |
| Sij (line 20) |  | 1x2 double | Made sure Sij is within bounds (1x1 square, from -0.5 to 0.5) |
| Rij (line 23) |  | 1x2 double | Sij x 10.0 (scaled back to 10x10 square) |
| Rsqij (line 24) |  | 1x1 double | Sum of squared values from Rij. Squaring helps normalize negative and positive distances between two points. |
| rm2 |  | 1x1 double | (σ/r)^2, where σ=1, and r=Rsqij. |
| rm6 |  | 1x1 double | (σ/r)^6, where σ=1, and r=Rsqij. |
| rm12 |  | 1x1 double | (σ/r)^12, where σ=1, and r=Rsqij. |
| phi |  | 1x1 double | Represents V (intermolecular potential between two particles) in the official L-J equation. |
| dphi |  | 1x1 double | Rate at which the intermolecular potential changes as distance changes. Usually, dV/dr would be fine, but we used [-1/r][dV/dr] in this case, because we multiply by r^2 later on (instead of just multiplying by r) when using the rate (i.e. dphi) to find virial forces. |
| ene\_pot |  | 1x32 double | Potential energy each particle feels. As the for loop repeats, more energy is added if the particle is within Rcutoff of the others. Only add 0.5phi to each, because total potential energy split among the two interacting particles. |
| virial |  | 1x1 double | Virial also represents the attraction and repulsion between particles, but it is more cumulative when looking at potential forces. Since this is in the same units as phi (unit of force), we need to multiply dphi by Rij^2 |
| acc |  | 32x2 double | One of the particles gets a positive acceleration added, the other feels a negative and equal acceleration. dphi\*Sij represents acceleration, because dphi is with respect to how fast the distance between the atoms is changing. Phi is a unit of energy, so its derivative should be force. Since mass is not considered in phi, its derivative would just be ***a*** instead of ***ma*** |
| ave\_ene |  | 1x1 double | Average potential energy |
| virial\_coeff |  | 1x1 double | Virial stresses scaled for each dimension |

LJ\_plot

| **Variable** | **value** | **Type of variable** | **What it represents in real life** |
| --- | --- | --- | --- |
| r |  | 1x500 double | Various distances between two particles |
| epsilon | 1.0 | 1x1 double | Depth of the potential well; how strongly two particles attract each other |
| sigma | 1.0 | 1x1 double | σ is measure of how close atoms can get without bonding; distance where potential energy is zero (not negative or positive) |
| E\_LJ |  | 1x500 double | Lennard-jones potential energy calculated for each value of r |
| Rcutoff | 2.0 | 1x1 double | Closest distance at which particles would show interaction |
| phicutoff | -0.0615 | 1x1 double | Potential energy felt by particles at Rcutoff distance apart |
| E\_LJ\_shift |  |  |  |