
Molecular Dynamics Simulation

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An introduction to soft-particle Molecular Dynamics (MD) simulation. This file is also a working MD simulator. A companion file introMDpbc.m is also available with fewer comments.

- [[MDIntro.pdf](#)] pdf version.
- [[MDIntro.php](#)] html version.

Theory I: Solving Newtons Laws for collection of particles

A Molecular Dynamics (MD) simulation is a computer simulation of Newton's Laws for a collection of N particles. The n -th particle at initial position $\vec{x}_n(0)$ with velocity $\vec{v}_n(0)$ moves according to Newton's Law:

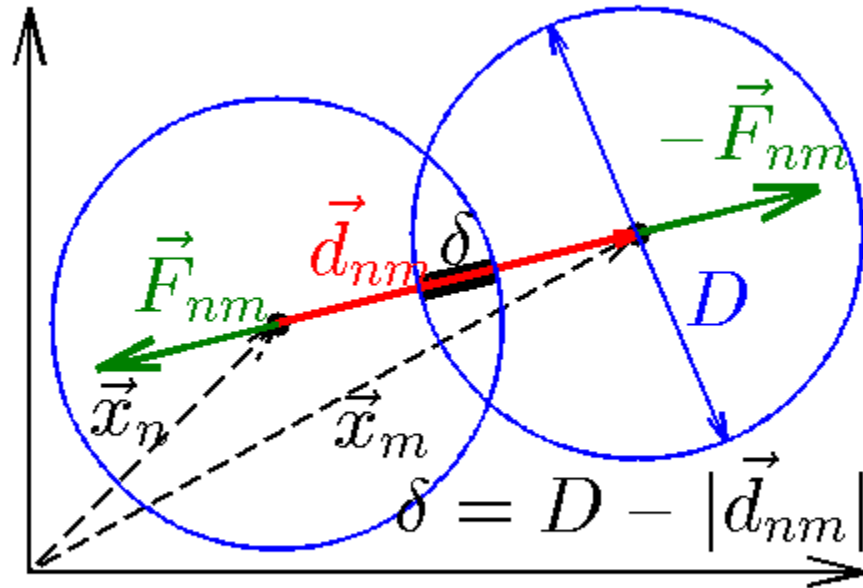
$$M_n \frac{d^2}{dt^2} \vec{x}_n(t) = \vec{F}_n(t) = \sum_{m=1}^N \vec{F}_{nm}(t) + \vec{F}_n^e(t), \quad [1]$$

where M_n is the mass of particle n , $\vec{F}_n(t)$ is the force on particle n , $\vec{F}_{nm}(t)$ is the force on particle n from particle m , and $\vec{F}_n^e(t)$ is the sum of all external forces. For this introduction, we assume that the force is obtained from a scalar potential $\Phi(\vec{x}_n)$ such that

$$\vec{F}_{nm} = -\frac{\partial}{\partial \vec{x}_n} \Phi(\vec{x}_m, \vec{x}_n). \quad [2]$$

Figure 1: Diagram defining particle-particle interaction variables.

MDfigures(1);



We will further assume the particles are disks with a simple harmonic potential:

$$V(\vec{x}_m, \vec{x}_n) = \Phi(|\vec{x}_m - \vec{x}_n|) = \Phi(d_{nm}) = \frac{1}{2}K(D - d_{nm})^2 = \frac{1}{2}K\delta^2, \quad [3a]$$

where

$$\vec{d}_{nm} = \vec{x}_m - \vec{x}_n \quad [3b]$$

is the vector pointing from the center of particle n to the center of particle m and

$$d_{nm} = |\vec{d}_{nm}|; \quad [3c]$$

K is a material constant that determines how hard the material is, D is the particle diameter, and

$$\delta = D - |\vec{d}_{nm}| \quad [3d]$$

is the particle overlap. (See Figure 1.) Differentiating the potential, the force

$$\vec{F}_{nm} = -K\delta\hat{d}_{nm}. \quad [3e]$$

The direction of the force is opposite to the unit vector \hat{d}_{nm} pointing from particle n to m , which pushes the particles apart. From Newton's third law the force on particle m from n is

$$\vec{F}_{mn} = -\vec{F}_{nm}. \quad [3f]$$

In this introduction we use a contact force, which only acts when the particles are in contact. That is, the force is zero if

$$\delta \leq 0. \quad [3g]$$

Simple Molecular Dynamics Simulation

introMDpbc.m contains the same code without the explanation:

Experimental Parameters (particle)

Here we define all of the particle parameters needed to determine the forces between particle pairs:

```
N=80; % number of particles
D=2; % diameter of particles
K=100; % force vector n<-m Fnm=-K*(D/|dnm|-1)*dnm, where vect dnm=Xm-Xn
M=3; % mass of particles
```

Experimental Parameters (space-domain)

This simulation uses a [periodic domain](#). In a periodic domain there are copies or images of each particle separated by L_x and L_y such that for each particle a positions (x, y) there are also particles at

$$(x + kL_x, y + lL_y),$$

for all integers k and l . In the main simulation box $k = 0$ and $l = 0$. For this simulation we need the distance between all particle pairs, but since we have a short range potential [3g] we only need the [nearest image distance](#). This calculation is done below in the main loop.

Here we define parameters needed to determine the space-domain for the particles in a periodic box of size L_x by L_y .

```
Lx=10*D; % size of box
Ly=10*D;
```

Experimental Parameters (initial conditions)

We choose random velocities with the property that the total kinetic energy: $M/2 * \sum(v_x.^2 + v_y.^2) = KE_{set}$.

```
KEset=5; % initial total Kinetic Energy (KE)
```

Experimental Parameters (time-domain)

The time-domain is from 0 to TT .

```
TT=1; % total simulation time (short for demo).
```

Display Parameters

This section controls the simulation plotting animation

```
demo=true; % true for this demo
plotit=false; % plot ? off for this demo
Nplotskip=50; % number of time steps to skip before plotting
```

Theory II: Numeric integration of Newton's laws Part I

To solve [1] we first rewrite it as two first-order equations:

$$\begin{aligned} \frac{d}{dt} \vec{x}_n(t) &= \vec{v}_n(t). \\ \frac{d}{dt} \vec{v}_n(t) &= \vec{F}_n(t)/M_n. \end{aligned} \quad [4]$$

When solving [4] numerically, time is broken up into discrete steps of size Δt (i.e., $t = k\Delta t$, where k is an integer). If Δt is small we can approximate [4] with:

$$[\vec{x}_n((k+1)\Delta t) - \vec{x}_n(k\Delta t)] / \Delta t \simeq \vec{v}_n(k\Delta t). \quad [5]$$

$$[\vec{v}_n((k+1)\Delta t) - \vec{v}_n(k\Delta t)] / \Delta t \simeq \vec{F}_n(t) / M_n.$$

Solving for the later times $(k+1)\Delta t$ in terms of earlier times $k\Delta t$:

$$\vec{x}_n^{(k+1)} \equiv \vec{x}_n((k+1)\Delta t) \simeq \vec{x}_n^{(k)} + \vec{v}_n^{(k)} \Delta t \quad [6]$$

$$\vec{v}_n^{(k+1)} \equiv \vec{v}_n((k+1)\Delta t) \simeq \vec{v}_n^{(k)} + \vec{F}_n^{(k)} / M_n \Delta t$$

Equation [6] discovered by L. Euler is called the [Euler Method](#) and could be used to integrate the system to get the new positions $\vec{x}_n^{(k+1)}$ and velocities $\vec{v}_n^{(k+1)}$ from the old positions $\vec{x}_n^{(k)}$, velocities $\vec{v}_n^{(k)}$, and forces $\vec{F}_n^{(k)}(\vec{x}_n^{(k)})$, which only depends on $\vec{x}_n^{(k)}$. However [6] is not recommended. If we use [6] the energy of the system will grow without bounds as seen in Figure 2. To make a useful integration scheme we can change the order of integration. If we calculate $\vec{v}_n^{(k+1)}$ first we can use it to calculate $\vec{x}_n^{(k+1)}$. These equations are an enhanced version of Euler's method called the [Semi-implicit Euler Method](#):

$$\vec{v}_n^{(k+1)} \simeq \vec{v}_n^{(k)} + \vec{F}_n^{(k)} / M_n \Delta t. \quad [7]$$

$$\vec{x}_n^{(k+1)} \simeq \vec{x}_n^{(k)} + \vec{v}_n^{(k+1)} \Delta t.$$

Figure 2 compares an Euler simulation from [eulerMDpbc.m](#) with an semi-implicit Euler simulation from [eEulerMDpbc.m](#). The semi-implicit Euler method is the simplest example of a general method called [Symplectic Integration](#), which is designed to conserve energy.

Figure 2: Euler vs. Semi-implicit Euler Integration.

The following code is used to produce figure 2. External files [eulerMDpbc.m](#) and [eEulerMDpbc.m](#) are used.

```

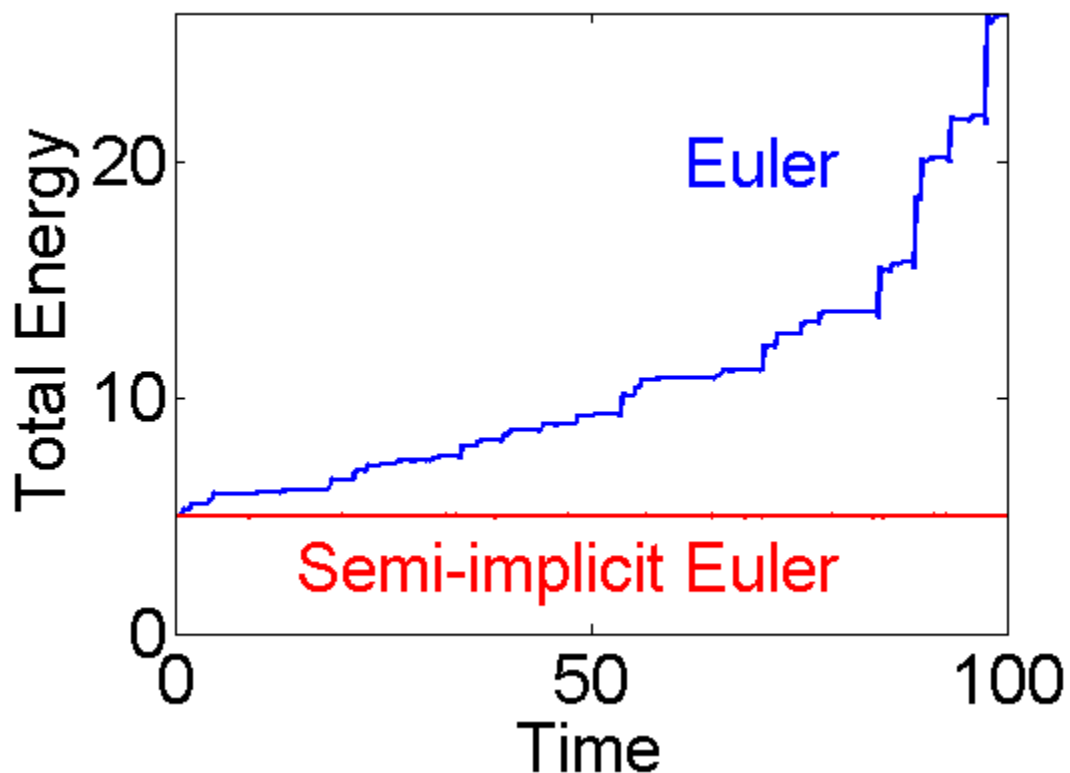
KE=5; % initial Kinetic Energy
Ts=100; % total simulation time
[Ek Ep]=eulerMDpbc(10,KE,Ts,false); % 10 particle--Euler integration
eTe=Ek+Ep; % save total energy for Euler;
[Ek Ep]=eEulerMDpbc(10,KE,Ts,false); % 10 particle--Semi-implicit Euler
eTse=Ek+Ep; % save total energy for semi-implicit Euler

```

```

Nt=length(Ek); % number of time steps
t=(0:Nt-1)/Nt*Ts; % simulation time
fs=25;
plot(t,eTe,t,eTse,'r','linewidth',2); % plot total energy
axis([0 Ts 0 inf]);
set(gca,'fontsize',fs);
xlabel('Time');
ylabel('Total Energy');
text(80,eTe(fix(90/Ts*Nt)),'Euler',...
     'color','b','fontsize',fs,'horizontal','right');
text(80,.9*KE,'Semi-implicit Euler',...
     'color','r','fontsize',fs,...
     'horizontal','right','vertical','top');

```



Theory II: Numeric integration of Newton's laws Part II

It is clear that energy conservation is poor using the (blue) Euler method. In principle Equation [7] could be used for simple MD simulations. However, both methods are only accurate to first order in Δt , and this limits the usefulness of the semi-implicit Euler method.

In this introduction we use a [Symplectic Integrator](#) with errors proportional to $(\Delta t)^2$ and good energy conservation due to L. Verlet called [Velocity Verlet integration](#). The main drawback of the semi-implicit

Euler method the error is proportional to Δt . Since we used $\Delta t=0.01$, we can expect errors of order 1% (see Figure 3). Sometimes that is not sufficient. One option is to decrease Δt , but the drawback is that the simulation time is increase proportionally. So with $\Delta t=0.01/100=0.0001$ semi-implicit Euler would give error of order 0.01% the simulation time would increase by a factor of 100. To overcome this deficiency Verlet devised a different integration scheme based on a second order approximation to [4] as follows:

$$\vec{x}_n^{(k+1)} \simeq \vec{x}_n^{(k)} + \vec{v}_n^{(k)} \Delta t + \frac{1}{2} \vec{a}_n^{(k-1)} (\Delta t)^2. \quad [8]$$

$$\vec{a}_n^{(k)} = \frac{1}{M_n} \sum_{m=1}^N \vec{F}_{nm} (|\vec{x}_m^{(k+1)} - \vec{x}_n^{(k+1)}|) \quad [9]$$

$$\vec{v}_n^{(k+1)} \simeq \vec{v}_n^{(k)} + \frac{1}{2} (\vec{a}_n^{(k)} + \vec{a}_n^{(k-1)}) \Delta t. \quad [10]$$

Figure 3: Velocity Verlet vs. Semi-implicit Euler Integration.

The following code is used to produce figure 3. External files [verletMDpbc.m](#) and [eEulerMDpbc.m](#) are used.

```

KE=5; % initial Kinetic Energy
Ts=100; % total simulation time
[Ek Ep]=verletMDpbc(10,KE,Ts,false); % 10 particle--Verlet integration
eTv=Ek+Ep; % save total energy for Verlet;
Nt=length(Ek); % number of time steps
t=(0:Nt-1)/Nt*Ts; % simulation time
fs=25;
plot(t,eTv,t,eTse,'r','linewidth',2); % plot total energy
hold on;
plot(t,[0*t+1.01*KE;0*t+.99*KE],'r--','linewidth',2); % 1% error
plot([73 85],[1.014 1]*KE,'linewidth',2);
hold off;
axis([0 Ts 5*(1+[-.02 .0201])]);
set(gca,'fontsize',fs);
xlabel('Time');
ylabel('Total Energy');
text(50,1.014*KE,'Velocity Verlet',...
'color','b','fontsize',fs,'horizontal','center');
text(50,.988*KE,'Semi-implicit Euler \pm 1%',...
'color','r','fontsize',fs,...
'horizontal','center','vertical','top');

```

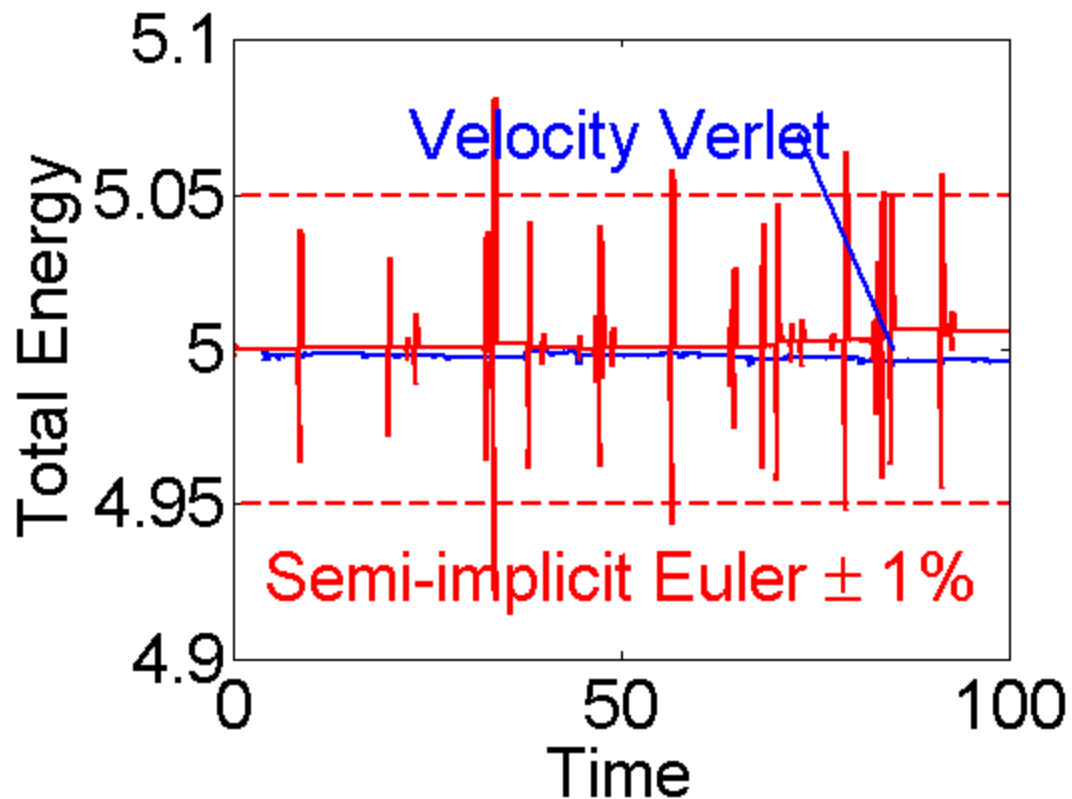


Figure 3: Velocity Verlet vs. Semi-implicit Euler Integration (caption).

Figure 3 shows the total energy over time for a 10 particle system using the Semi-implicit Euler integration method from [7] (red) and Velocity Verlet from [8-10] (blue). Red dashed lines show a range of $\pm 1\%$. The error for the Velocity Verlet is ≈ 100 times smaller.

Simulation Parameters

Regardless of the integration method Δt (dt in code) must be determined. Here we use a fixed time step $dt=0.01 \approx \sqrt{M/K}/20$. The total number of time steps Nt is determined from the total simulation time TT .

```
dt=1e-2;           % integration time step
Nt=fix(TT/dt);    % number of time steps
```

Initial Conditions (Positions)

The particles need to be placed in the box with minimal overlap to avoid excess potential energy at the beginning of the simulation. For moderately dense systems a square grid can be used. The matlab command `ndgrid` creates D spaced points on a grid inside of the L_x by L_y box. `randperm` randomly chooses N

positions from all [numel\(x\)](#) available locations. The final result is a pair of matlab vectors x and y each with `size(x)=[1,N]` that represents $\vec{x}_n^{(k)}$ at each time $k\Delta t$. Here, for the initial conditions before the simulation starts $k = 0$. In the code k is represented in matlab as `nt`, the time step number.

```
[x y]=ndgrid(D/2:D:Lx-D/2,D/2:D:Ly-D/2); % place particles on grid
ii=randperm(numel(x),N); % N random position on grid
x=x(ii); % set x-positions
y=y(ii); % set y-positions
```

Initial Conditions (Velocities)

The velocities v_x and v_y each with `size(vx)=[1,N]` represent $\vec{v}_n^{(k)}$ at time $k\Delta t$. Here, for the initial conditions before the simulation starts $k = 0$. The velocities are chosen randomly from a normal distribution using [randn](#). The mean velocity is removed to avoid center of mass drift. The variance of the distribution is set so that the total kinetic energy: $M/2*\sum(vx.^2+vy.^2)=KE_{set}$.

```
vx=randn(1,N)/3; % normal (Maxwell) distribution of velocities
vy=randn(1,N)/3;

vx=vx-mean(vx); % remove center of mass drift
vy=vy-mean(vy);

tmp=sqrt(2*KEset/M/sum((vx.^2+vy.^2))); % set Kinetic energy
vx=vx*tmp;
vy=vy*tmp;
```

Initial Conditions (Accelerations)

The accelerations from the $k - 1$ previous time step is need for Verlet's second order integration scheme.

```
ax_old=0*x; % need initial condition for velocity Verlet integration
ay_old=0*y;
```

Save variables

List of quantities to be saved at each time step.

```
Ek=zeros(Nt,1); % Kinetic Energy
Ep=zeros(Nt,1); % particle-particle potential
xs=zeros(Nt,N); % x-position
ys=zeros(Nt,N); % y-position
vxs=zeros(Nt,N); % x-velocity
vys=zeros(Nt,N); % y-velocity
```

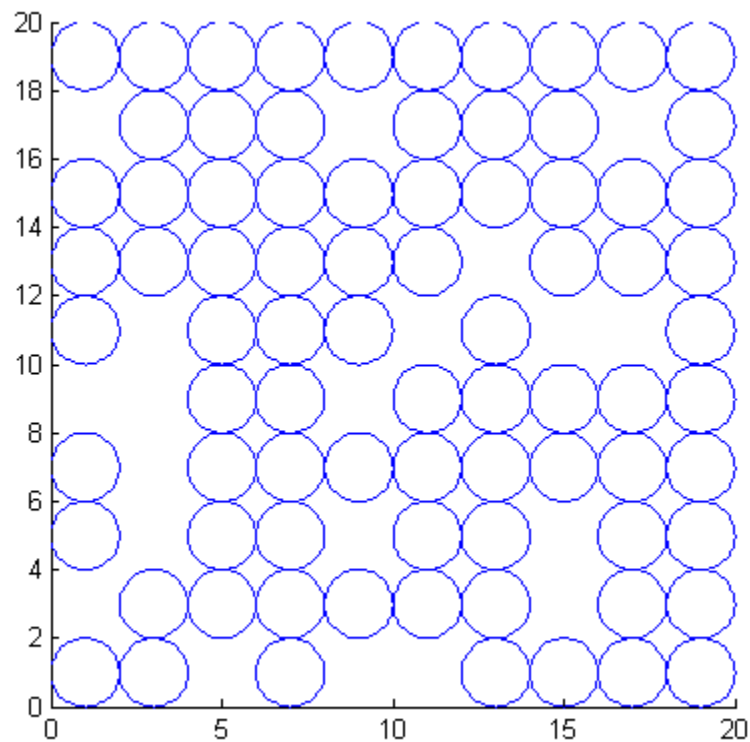
Figure 3: Setup Plotting

Here we use an external function [plotNCirc.m](#) to create an animation of the simulations progress. `plotNCirc` returns an array of handles h to a [rectangle](#) object for each of the N particles. Matlab rectangles

contain a curvature property with turns them into circles. The handles are used later to animate the particle positions. An example initial condition is shown here.

NB: periodic images of particles are not shown

```
if(plotit || demo)           % only if plotit true
  clf;                       % clear figure
  h=plotNCirc(x,y,D,'none'); % plot particles no color; store handle h
  axis('equal');             % square pixels
  axis([0 Lx 0 Ly]);        % plotting range
end
```



Main Loop

In the main loop the simulation steps through N_t time steps, advancing time, the particle positions, forces, and velocities. Comments refer back to sections and equations above.

```
for nt=1:Nt
  % plot particles
  if(plotit && rem(nt-1,Nplotskip+1)==0) % nt-1 divides Nplotskip+1
    xp=mod(x,Lx);
    yp=mod(y,Ly);
    for np=1:N
      set(h(np),'Position',[xp(np)-.5*D yp(np)-.5*D D D]); % update handle
    end
    drawnow;
  end
end
```

```

end

x=x+vx*dt+ax_old*dt^2/2; % first step in Verlet integration eq.[8]
y=y+vy*dt+ay_old*dt^2/2;

% position dependent calculations
xs(nt,:)=x; % save positions
ys(nt,:)=y;

% Force between particles eq. [9] and [3a-g]
Fx=zeros(1,N); % zero forces
Fy=zeros(1,N);

for nn=1:N % check particle n
    for mm=nn+1:N % against particle m from n+1->N
        dy=y(mm)-y(nn); % [3b] y-comp dnm vector from from n->m
        dy=dy-round(dy/Ly)*Ly; % closest periodic image
        if(abs(dy)<D) % [3g] y-distance close enough?
            dx=x(mm)-x(nn); % [3b] x-comp dnm vector from from n->m
            dx=dx-round(dx/Lx)*Lx; % closest periodic image
            dnm=dx.^2+dy.^2; % [3c] squared distance between n and m
            if(dnm<D^2) % [3g] overlapping?
                dnm=sqrt(dnm); % [3c] distance
                F=-K*(D/dnm-1); % [3d-e] force magnitude
                Fx(nn)=Fx(nn)+F.*dx; % [9,3e] accumulate x force on n
                Fx(mm)=Fx(mm)-F.*dx; % [9,3ef] x force on m (equal opposite)
                Fy(nn)=Fy(nn)+F.*dy; % [9,3e] accumulate y force on n
                Fy(mm)=Fy(mm)-F.*dy; % [9,3ef] y force on m (equal opposite)
                Ep(nt)=Ep(nt)+(D-dnm).^2;% [3a] particle-particle potential I
            end
        end
    end
end
end
end
Ep(nt)=K/2*Ep(nt); % eq [3a] particle particle potential II

ax=Fx./M; % eq [9] calc a from F=Ma
ay=Fy./M;

vx=vx+(ax_old+ax)*dt/2; % eq [10] second step in Verlet integration
vy=vy+(ay_old+ay)*dt/2;

% velocity dependent calculations
Ek(nt)=M*sum((vx.^2+vy.^2))/2; % Kinetic energy
vxs(nt,:)=vx; % save velocities
vys(nt,:)=vy;

ax_old=ax; % need for eqs [8-10] save for next step
ay_old=ay;
end

```

m-files

- [MDIntro.zip](#) All files in one zip file.

- [MDIntro.m](#) Introduction to Molecular dynamics (This File).
- [MDIntro.pdf](#) (pdf version).
- [introMDpbc.m](#) Version of this file without discussion.
- [introMDwalls.m](#) Version with walls instead of periodic boundaries.
- [eulerMDpbc.m](#) Function to demonstrate Euler Integration.
- [eEulerMDpbc.m](#) Function to demonstrate Semi-implicit Euler Integration.
- [verletMDpbc.m](#) Function to demonstrate Velocity Verlet Integration.
- [MDfigures.m](#) Create figures.
- [plotNCirc.m](#) Plot N circles and return handles.

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