009x_53

March 18, 2017

Stochastic Processes: Data Analysis and Computer Simulation

Brownian motion 3: data analyses and applications
-Interacting Brownian particles-

1 Necessary changes for interacting Brownian particles

1.1 Periodic boundary conditions

1.2 Inter-particle interaction

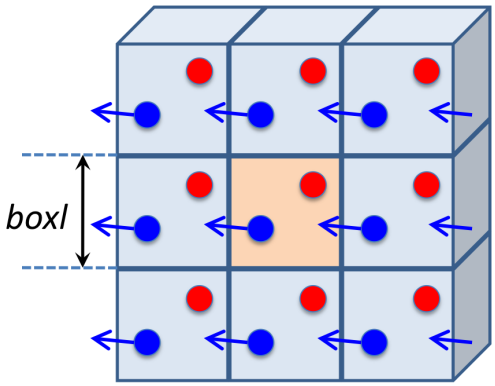
$$U = \sum_{r_{ij}<2\sigma} \phi(r_{ij}) = \sum_{r_{ij}<2\sigma} 4\epsilon \left(\frac{\sigma}{r_{ij}}\right)^{12}, \quad \mathbf{F}_i = -\frac{dU}{d\mathbf{r}_{ij}} = \sum_{r_{ij}<2\sigma} 48\epsilon \left(\frac{\sigma}{r_{ij}}\right)^{12} \frac{\mathbf{r}_{ij}}{r_{ij}^2} \qquad \text{(I1, I2)}$$

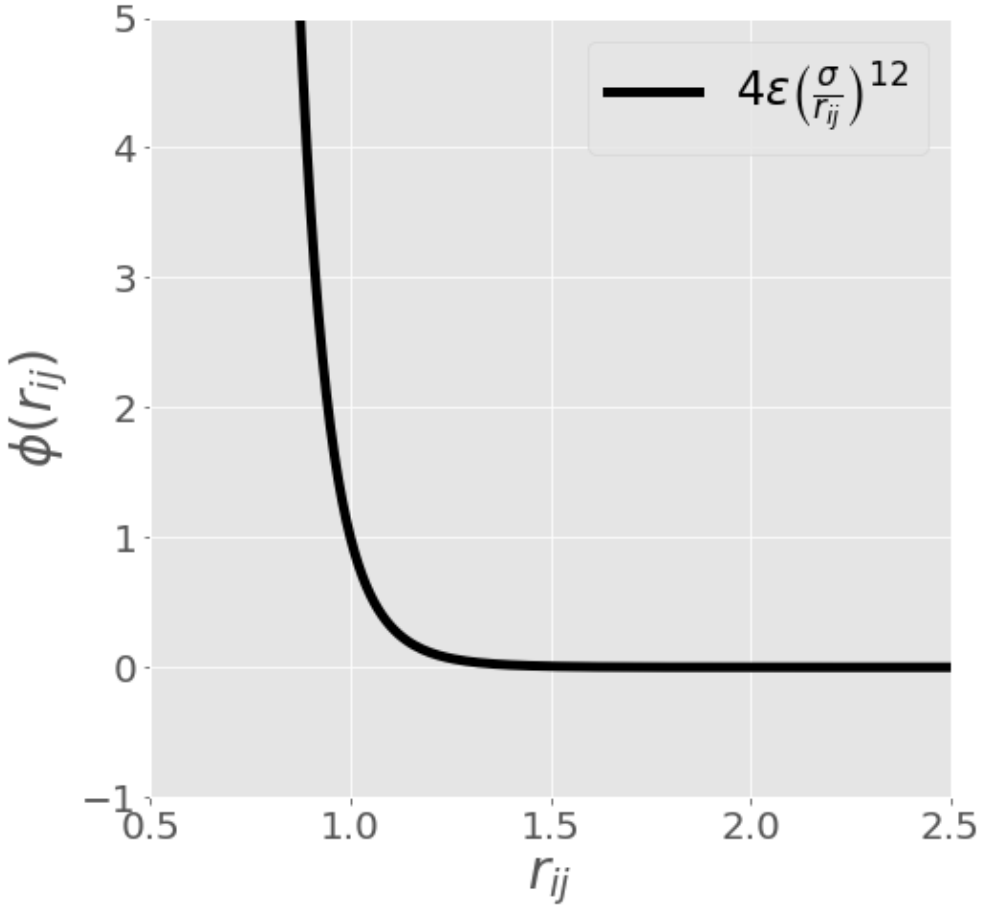
$$\mathbf{r}_{ij} = \mathbf{r}_j - \mathbf{r}_i, \quad r_{ij} = |\mathbf{r}_{ij}|$$

2 Simulation code for interacting Brownian particles with animation

2.1 Import libraries

```
In [1]: % matplotlib nbagg
        import numpy as np # import numpy library as np
        import matplotlib.pyplot as plt # import pyplot library as plt
```




$4\varepsilon\left(\frac{\sigma}{r_{ij}}\right)^{12}$
$\phi(r_{ij})$
r_{ij}
5
4
3
2
1
0
−1
0.5
1.0
1.5
2.0
2.5

```
import matplotlib.animation as animation # import animation modules from ma
from   mpl_toolkits.mplot3d import Axes3D # import Axes3D from mpl_toolkits
from   numpy import newaxis # import newaxis used for inter-particle force
plt.style.use('ggplot') # use "ggplot" style for graphs
```

2.2 Define `init` function for `FuncAnimation`

```
In [2]: def init():
            global R,V,W,F,Rs,Vs,Ws,time # define global variables
            initconf()           # create random particle configuration without over
            V[:,:] = 0.0         # initialize all the variables to zero
            W[:,:] = 0.0         # initialize all the variables to zero
            F[:,:] = 0.0         # initialize all the variables to zero
            Rs[:,:,:] = 0.0      # initialize all the variables to zero
            Rs[0,:,:] = R[:,:]   # store initial particle positions in Rs
            Vs[:,:,:] = 0.0      # initialize all the variables to zero
            Ws[:,:,:] = 0.0      # initialize all the variables to zero
            time[:]   = 0.0      # initialize all the variables to zero
            title.set_text(r'') # empty title
            line.set_data([],[]) # set line data to show the trajectory of particle
            line.set_3d_properties([]) # add z-data separately for 3d plot
            particles.set_data([],[]) # set position current (x,y) position data fo
            particles.set_3d_properties([]) # add current z data of particles to ge
            return particles,title,line # return listed objects that will be drawn
```

2.3 Define `animate` function for `FuncAnimation`

```
In [3]: def animate(i):
            global R,V,W,F,Rs,Vs,Ws,time # define global variables
            time[i]=i*dt # store time in each step in an array time
            particleforces() # compute inter-particle force F by examining all nump
            W = std*np.random.randn(nump,dim) # generate an array of random forces
            V = V*(1-zeta/m*dt)+F/m*dt+W/m # update velocity via Eq.(F9) with inter
            R = R+V*dt # update position via Eq.(F5)
            Rs[i,:,:]=R # accumulate particle positions at each step in an array Rs
            Vs[i,:,:]=V # accumulate particle velocitys at each step in an array Vs
            Ws[i,:,:]=W # accumulate random forces at each step in an array Ws
            title.set_text(r"t = "+str(time[i])+"/"+str((nums-1)*dt))  # set the ti
            line.set_data(Rs[:i+1,n,0],Rs[:i+1,n,1]) # set the line in 2D (x,y)
            line.set_3d_properties(Rs[:i+1,n,2]) # add z axis to set the line in 3D
            particles.set_data(pbc(R[:,0],box[0]), pbc(R[:,1],box[1])) # set the cu
            particles.set_3d_properties(pbc(R[:,2],box[2])) # add z axis to set the
            return particles,title,line # return listed objects that will be drawn
```

2.4 Newly defined functions for interacting Brownian particles

```
In [4]: def pbc(r, lbox): # enforce Periodic Boundary Conditions for all positions
            return np.fmod(r+lbox,lbox)
```

```
        def distance(r1,r2,lbox): # Compute distance vector R2 - R1 with PBC
            return r2-r1-np.around((r2-r1)/lbox)*lbox
        def fij(r2,rij): # calculate Fij=dU/drij
        #    f=-24*eps*(2*(r2/sig**2)**(-6)-(r2/sig**2)**(-3))/r2*rij # Lennard-Jon
            f=-48*eps*((r2/sig**2)**(-6))/r2*rij # soft-core potential
            return f
        def particleforces(): # compute inter-particle force F by examining all num
            global F
            F[:,:] = 0.0
            for n in range(nump): # repeat below for all particles
                rij = distance(R[n,:], R, box) # distance vectors rij=R_i-R_j for a
                r2  = np.linalg.norm(rij, axis=1)**2 # square distance rij**2
                nei = (r2 < (2.0*sig)**2)  # list neighbor particles of j
                nei[n] = False # ignore self pair (i=j)
                F[n,:] = np.sum(fij(r2[nei, newaxis], rij[nei,:]), axis=0) # total
        def initconf():  # create random particle configuration without overlapping
            global R,V,W,F,Rs,Vs,Ws,time
            for n in range(nump): # repeat below from n=0 to nump-1
                nn=0 # set overlap true to perform while loop below for the n-th pa
                while nn == 0: # repeat the loop below while overlap is true (nn==0
                    R[n,:]=np.random.rand(dim)*box # generate a position candidate
                    nn = 1 # initialize overlap as false
                    for l in range(n): # examine overlap generated positions (from
                        rij = distance(R[n,:],R[l,:],box) # calculate distance vect
                        r2  = np.linalg.norm(rij)**2 # calculate the squared distan
                        if r2 < (0.90*sig)**2: # check if the distance is smaller t
                        # Yes -> perform below (nn=0) -> repeat while loop, No (nn=
                            nn = 0 # set overlap true
```

2.5 Set parameters and initialize variables

```
In [5]: dim  = 3    # system dimension (x,y,z)
        nump = 100  # number of interacting Brownian particles to simulate
        nums = 4096 # number of simulation steps
        dt   = 0.01 # set time increment, \Delta t
        zeta = 1.0  # set friction constant, \zeta
        m    = 1.0  # set particle mass, m
        kBT  = 1.0  # set thermal energy, k_B T
        std  = np.sqrt(2*kBT*zeta*dt) # calculate std for \Delta W via Eq.(F11)
        sig  = 1.0  # unit of length of inter-particle potential
        eps  = 1.0  # unit of energy inter-particle potential
        vf   = 0.001 ##volume fraction of particles < 0.45
        boxl = np.power(nump*np.pi/6/vf,1/3) # calculate the side length of unit ce
        print('Volume fraction =',vf,'  boxl =',boxl) # print vf and boxl
        box  = np.array([boxl,boxl,boxl])*sig # set array box[dim]
        np.random.seed(0) # initialize random number generator with a seed=0
        R = np.zeros([nump,dim]) # array to store current positions and set initial
        V = np.zeros([nump,dim]) # array to store current velocities and set initia
```

```
        W = np.zeros([nump,dim]) # array to store current random forcces
        F = np.zeros([nump,dim]) # rray to store current particle orcces
        Rs = np.zeros([nums,nump,dim]) # array to store positions at all steps
        Vs = np.zeros([nums,nump,dim]) # array to store velocities at all steps
        Ws = np.zeros([nums,nump,dim]) # array to store random forces at all steps
        time = np.zeros([nums]) # an array to store time at all steps
```

```
Volume fraction = 0.001   boxl = 37.4110192682
```

2.6 Perform and animate the simulation using `FuncAnimation`

```
In [6]: fig = plt.figure(figsize=(10,10)) # set fig with its size 10 x 10 inch
        ax = fig.add_subplot(111,projection='3d') # creates an additional axis to t
        ax.set_xlim(0.0,box[0]) # set x-range
        ax.set_ylim(0.0,box[1]) # set y-range
        ax.set_zlim(0.0,box[2]) # set z-range
        ax.set_xlabel(r"x",fontsize=20) # set x-lavel
        ax.set_ylabel(r"y",fontsize=20) # set y-lavel
        ax.set_zlabel(r"z",fontsize=20) # set z-lavel
        ax.view_init(elev=12,azim=120)  # set view point
        particles, = ax.plot([],[],[],linestyle='None',color='r',marker='o',ms=250/
        title = ax.text(0.,0.,0.,r'',transform=ax.transAxes,va='center') # define o
        line, = ax.plot([],[],[],'b',lw=2,alpha=0.8) # define object line
        n = 0  # trajectry line is plotted for the n-th particle
        anim = animation.FuncAnimation(fig,func=animate,init_func=init,
                    frames=nums,interval=5,blit=True,repeat=False)
        ## If you have ffmpeg installed on your machine
        ## you can save the animation by uncomment the last line
        ## You may install ffmpeg by typing the following command in command prompt
        ## conda install -c menpo ffmpeg
        ##
        #anim.save('movie.mp4',fps=20,dpi=400)
```

```
<IPython.core.display.Javascript object>
```

```
<IPython.core.display.HTML object>
```

2.7 The mean square displacement and the diffusion constant

```
In [7]: # mean square displacement vs time
        msd = np.zeros([nums])
        for i in range(nums):
            for n in range(nump):
                msd[i]=msd[i]+np.linalg.norm(Rs[i,n,:]-Rs[0,n,:])**2 # (R(t) - R(0)
            msd[i] = msd[i]/nump
        dmsd = np.trapz(msd, dx=dt)/(3*(nums*dt)**2)
```

```
        print('D =',kBT/zeta,'(Theoretical)')
        print('D =',dmsd,'(Simulation via MSD)')
        print('Volume fraction =',vf) ### print vf
        fig, ax = plt.subplots(figsize=(7.5,7.5))
        ax.set_xlabel(r"$t$", fontsize=20)
        ax.set_ylabel(r"mean square displacement", fontsize=16)
        ax.plot(time,6*kBT/zeta*time,'r',lw=6,label=r'$6Dt={6k_BT t}/{\zeta}$')
        ax.plot(time,msd,'b',lw=4, label=r'$\langle R^2(t)\rangle$')
        ax.legend(fontsize=16, loc=4)
        plt.show()
```

```
D = 1.0 (Theoretical)
D = 0.885552952684 (Simulation via MSD)
Volume fraction = 0.001
```

```
<IPython.core.display.Javascript object>
```

```
<IPython.core.display.HTML object>
```

3 Reference

- The SciPy.org website, https://docs.scipy.org/doc/numpy/user/basics.broadcasting.html
- Listed in the major unsolved problems in physics, https://en.wikipedia.org/wiki/List_of_unsolved_proble