

KyotoUx-009x (/github/ryo0921/KyotoUx-009x/tree/master)
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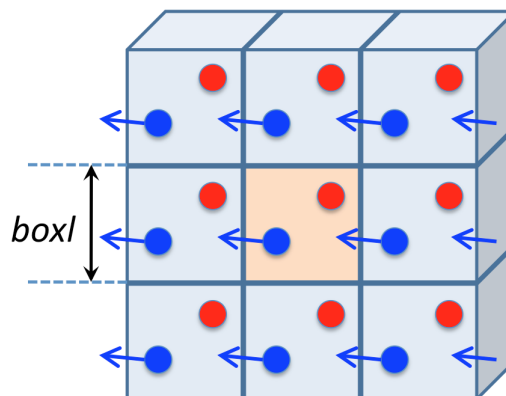
Stochastic Processes: Data Analysis and Computer Simulation

Brownian motion 3: data analysis

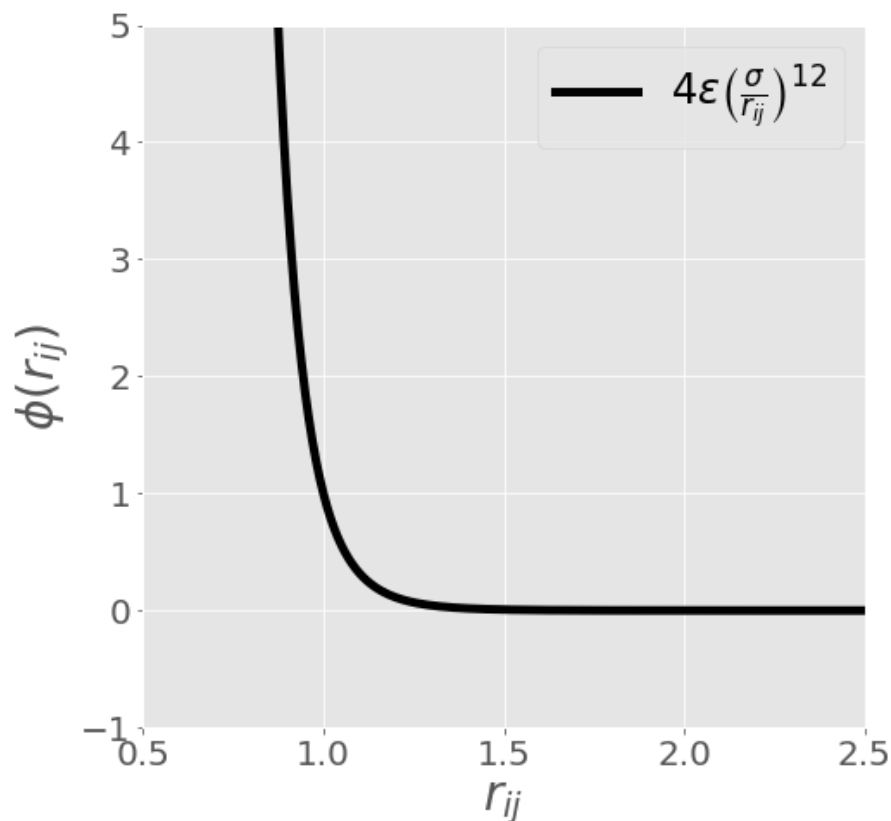
3. Interacting Brownian particles

3.1. Necessary changes for interacting Brownian particles

Periodic boundary conditions



Inter-particle interaction



$$U = \sum_{r_{ij} < 2\sigma} \phi(r_{ij}) = \sum_{r_{ij} < 2\sigma} 4\epsilon \left(\frac{\sigma}{r_{ij}} \right)^{12}, \quad \mathbf{F}_i = -\frac{\partial U}{\partial \mathbf{r}_{ij}} = \sum_{r_{ij} < 2\sigma} 48\epsilon \left(\frac{\sigma}{r_{ij}} \right)^{12} \frac{\mathbf{r}_{ij}}{r_{ij}^2} \quad (\Pi, I)$$

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

3.2. Simulation code for interacting Brownian particles with animation

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

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 c
    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 parti
    line.set_3d_properties([]) # add z-data separately for 3d plot
    particles.set_data([],[]) # set position current (x,y) position data
    particles.set_3d_properties([]) # add current z data of particles to
    return particles,title,line # return listed objects that will be dra
```

Define animate function for FuncAnimation

The Euler method used in previous animate function is replaced with the Leap-Frog method in the following new animate function because of the numerical instability taking place with the former method for the present case of interacting Brownian particles.

```
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 n
    W = std*np.random.randn(nump,dim) # generate an array of random forc
#    V = V*(1-zeta/m*dt)+F/m*dt+W/m # update velocity via Eq.(I11) using
    V = (V*(1-zeta/2/m*dt)+F/m*dt+W/m)/(1+zeta/2/m*dt) # update velocity
    R = R+V*dt # update position via Eq.(I12) using the L-F method
    Rs[i,:,:]=R # accumulate particle positions at each step in an array
    Vs[i,:,:]=V # accumulate particle velocitys at each step in an array
    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
    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
    particles.set_data(pbc(R[:,0],box[0]), pbc(R[:,1],box[1])) # set the
    particles.set_3d_properties(pbc(R[:,2],box[2])) # add z axis to set
    return particles,title,line # return listed objects that will be dra
```

Newly defined functions for interacting Brownian particles

```
In [4]: def pbc(r, lbox): # enforce Periodic Boundary Conditions for all positio
        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-
    f=-48*eps*((r2/sig**2)**(-6))/r2*rij # soft-core potential
    return f
def particleforces(): # compute inter-particle force F by examining all
    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 fc
        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) # tot
def initconf(): # create random particle configuration without overlap
    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
        while nn == 0: # repeat the loop below while overlap is true (nn
            R[n,:]=np.random.rand(dim)*box # generate a position candida
            nn = 1 # initialize overlap as false
            for l in range(n): # examine overlap generated positions (fr
                rij = distance(R[n,:],R[l,:],box) # calculate distance v
                r2 = np.linalg.norm(rij)**2 # calculate the squared dis
                if r2 < (0.90*sig)**2: # check if the distance is smalle
                    # Yes -> perform below (nn=0) -> repeat while loop, No (
                    nn = 0 # set overlap true
```

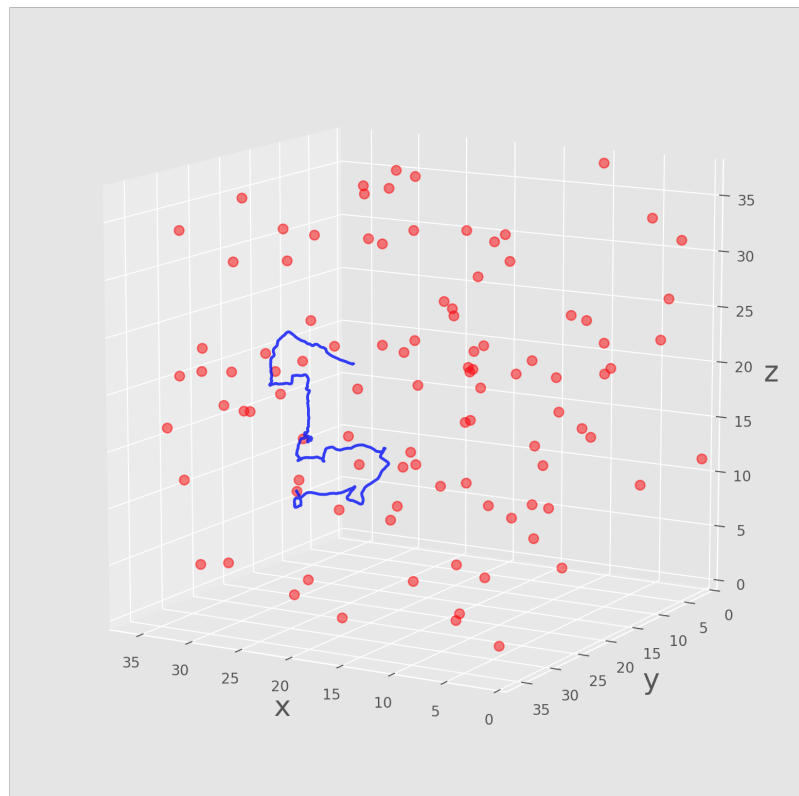
Set parameters and initialize variables

```
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
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 init
V = np.zeros([nump,dim]) # array to store current velocities and set ini
W = np.zeros([nump,dim]) # array to store current random forces
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 ste
time = np.zeros([nums]) # an array to store time at all steps
```

Volume fraction = 0.001 boxl = 37.4110192682

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 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=2)
title = ax.text(0.,0.,0.,r'',transform=ax.transAxes,va='center') # defin
line, = ax.plot([],[],[],'b',lw=2,alpha=0.8) # define object line
n = 0 # trajectory 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 prc
## conda install -c menpo ffmpeg
##
#anim.save('movie.mp4',fps=20,dpi=400)
```



t = 40.95/40.95

3.3. The mean square displacement and the diffusion constant

```

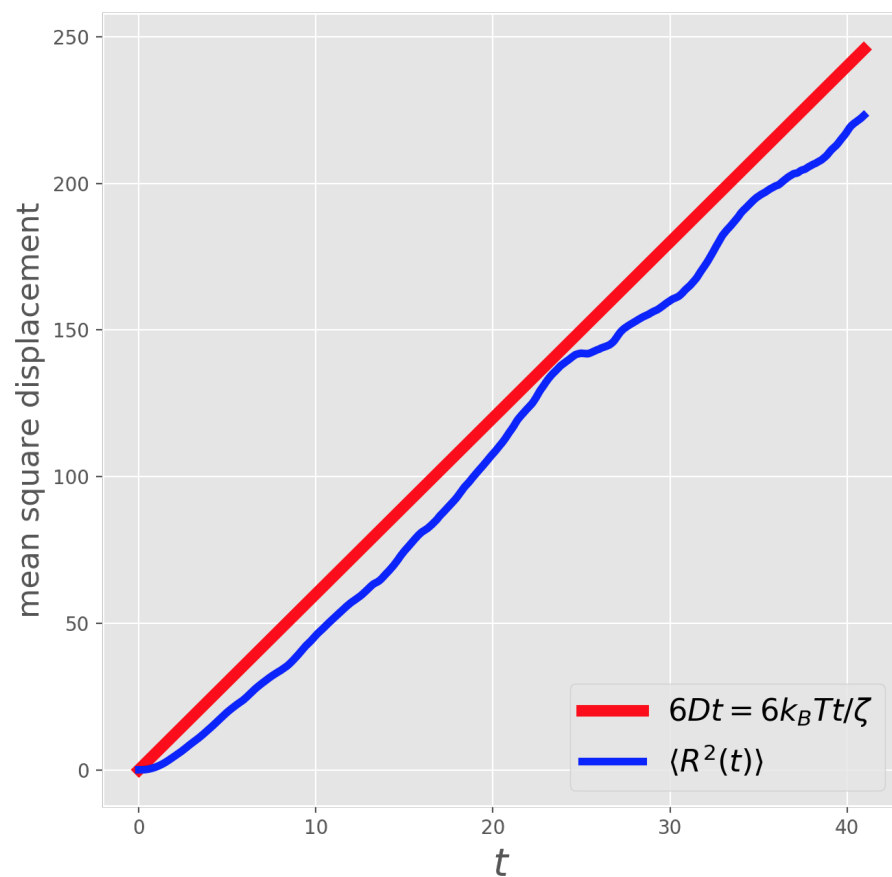
In [7]: # mean square displacement vs time
msd = np.zeros([nums])
for i in range(nums):
    for n in range(nump):
        msd[i]=msd[i]+np.linalg.norm(Rs[i,n,:]-Rs[0,n,:])**2 #  $\langle R(t) - R(0) \rangle^2$ 
    msd[i] = msd[i]/nump
dmsd = np.trapz(msd, dx=dt)/(3*(nums*dt)**2)
print('D_0 =',kBT/zeta,'(Theoretical)')
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_0 = 1.0 (Theoretical)
D = 0.885382884029 (Simulation via MSD)
Volume fraction = 0.001

```



References

- The SciPy.org website, <https://docs.scipy.org/doc/numpy/user/basics.broadcasting.html>
(<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_problems_in_physics#Condensed_matter_physics
(https://en.wikipedia.org/wiki/List_of_unsolved_problems_in_physics#Condensed_matter_physics)

Summary of simulation method

Original differential equation

i : particle index

$$\frac{d\mathbf{R}_i(t)}{dt} = \mathbf{V}_i(t) \quad (I3)$$

$$m \frac{d\mathbf{V}_i(t)}{dt} = -\zeta \mathbf{V}_i(t) + \mathbf{F}_i(t) + \mathbf{F}_R(t) \quad (I4)$$

with

$$\langle \mathbf{F}_R(t) \rangle = \mathbf{0} \quad (I5)$$

$$\langle \mathbf{F}_R(t) \mathbf{F}_R(0) \rangle = 2k_B T \zeta \mathbf{I} \delta(t) \quad (I6)$$

Euler method

i : index of particles, n : time step

$$\mathbf{V}_{i,n+1} = \left(1 - \frac{\zeta}{m} \Delta t\right) \mathbf{V}_{i,n} + \frac{1}{m} \mathbf{F}_{i,n} \Delta t + \frac{1}{m} \Delta \mathbf{W}_n \quad (I7)$$

$$\mathbf{R}_{i,n+1} = \mathbf{R}_{i,n} + \mathbf{V}_{i,n} \Delta t \quad (I8)$$

with

$$\langle \Delta \mathbf{W}_n \rangle = \mathbf{0} \quad (I9)$$

$$\langle \Delta \mathbf{W}_n \Delta \mathbf{W}_l \rangle = 2k_B T \zeta \Delta t \mathbf{I} \delta_{nl} \quad (I10)$$

Leap-Frog method

i : index of particles, n : time step

$$\begin{aligned} \mathbf{V}_{i,n+\frac{1}{2}} &= \mathbf{V}_{i,n-\frac{1}{2}} - \frac{\zeta}{m} \Delta t \mathbf{V}_{i,n} + \frac{1}{m} \mathbf{F}_{i,n} \Delta t + \frac{1}{m} \Delta \mathbf{W}_n \\ &= \mathbf{V}_{i,n-\frac{1}{2}} - \frac{\zeta}{m} \Delta t \frac{1}{2} \left(\mathbf{V}_{i,n+\frac{1}{2}} + \mathbf{V}_{i,n-\frac{1}{2}} \right) + \frac{1}{m} \mathbf{F}_{i,n} \Delta t + \frac{1}{m} \Delta \mathbf{W}_n \end{aligned}$$

$$\therefore \mathbf{V}_{i,n+\frac{1}{2}} = \left(\left(1 - \frac{\zeta}{2m} \Delta t\right) \mathbf{V}_{i,n-\frac{1}{2}} + \frac{1}{m} \mathbf{F}_{i,n} \Delta t + \frac{1}{m} \Delta \mathbf{W}_n \right) \left(1 + \frac{\zeta}{2m} \Delta t\right)^{-1} \quad (I11)$$

$$\mathbf{R}_{i,n+1} = \mathbf{R}_{i,n} + \mathbf{V}_{i,n+\frac{1}{2}} \Delta t \quad (I12)$$

with

$$\langle \Delta \mathbf{W}_n \rangle = \mathbf{0} \quad (I13)$$

$$\langle \Delta \mathbf{W}_n \Delta \mathbf{W}_l \rangle = 2k_B T \zeta \Delta t \mathbf{I} \delta_{nl} \quad (I14)$$

2nd order Runge-Kutta method

i : index of particles, n : time step

$$\mathbf{V}'_{i,n+\frac{1}{2}} = \mathbf{V}_{i,n} - \frac{\zeta}{m} \frac{\Delta t}{2} \mathbf{V}_{i,n} + \frac{1}{m} \mathbf{F}_{i,n} \frac{\Delta t}{2} = \left(1 - \frac{\zeta}{m} \frac{\Delta t}{2}\right) \mathbf{V}_{i,n} + \frac{1}{m} \mathbf{F}_{i,n} \frac{\Delta t}{2} \quad (\text{I15})$$

$$\mathbf{R}'_{i,n+\frac{1}{2}} = \mathbf{R}_{i,n} + \mathbf{V}_{i,n} \frac{\Delta t}{2} \quad (\text{I16})$$

$$\mathbf{V}_{n,i+1} = \mathbf{V}_{i,n} - \frac{\zeta}{m} \Delta t \mathbf{V}'_{n,i+\frac{1}{2}} + \frac{1}{m} \Delta t \mathbf{F}_{i,n+\frac{1}{2}} + \frac{1}{m} \Delta \mathbf{W}_i \quad (\text{I17})$$

$$\mathbf{R}_{n,i+1} = \mathbf{R}_{n,i} + \mathbf{V}'_{n,i+\frac{1}{2}} \Delta t \quad (\text{I18})$$

$$\text{with} \quad \langle \Delta \mathbf{W}_n \rangle = \mathbf{0} \quad (\text{I19})$$

$$\langle \Delta \mathbf{W}_n \Delta \mathbf{W}_l \rangle = 2k_B T \zeta \Delta t \mathbf{I} \delta_{nl} \quad (\text{I20})$$