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Stochastic Processes: Data Analysis and Computer Simulation

Brownian motion 2: computer simulation

3. Simulations with on-the-fly animation

3.1. Simulation code with on-the-fly 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.mlab as mlab # import mlab module to use MATLAB comman
import matplotlib.animation as animation # import animation modules from
from mpl_toolkits.mplot3d import Axes3D # import Axes3D from mpl_toolkit
plt.style.use('ggplot') # use "ggplot" style for graphs
```

Define `init` function for `FuncAnimation`

In [2]:
```
def init():
    global R,V,W,Rs,Vs,Ws,time
    R[:,:] = 0.0 # initialize all the variables to zero
    V[:,:] = 0.0 # initialize all the variables to zero
    W[:,:] = 0.0 # initialize all the variables to zero
    Rs[:,:,:] = 0.0 # initialize all the variables to zero
    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 tc
    return particles,title,line # return listed objects that will be dra
```

Define `animate` function for `FuncAnimation`

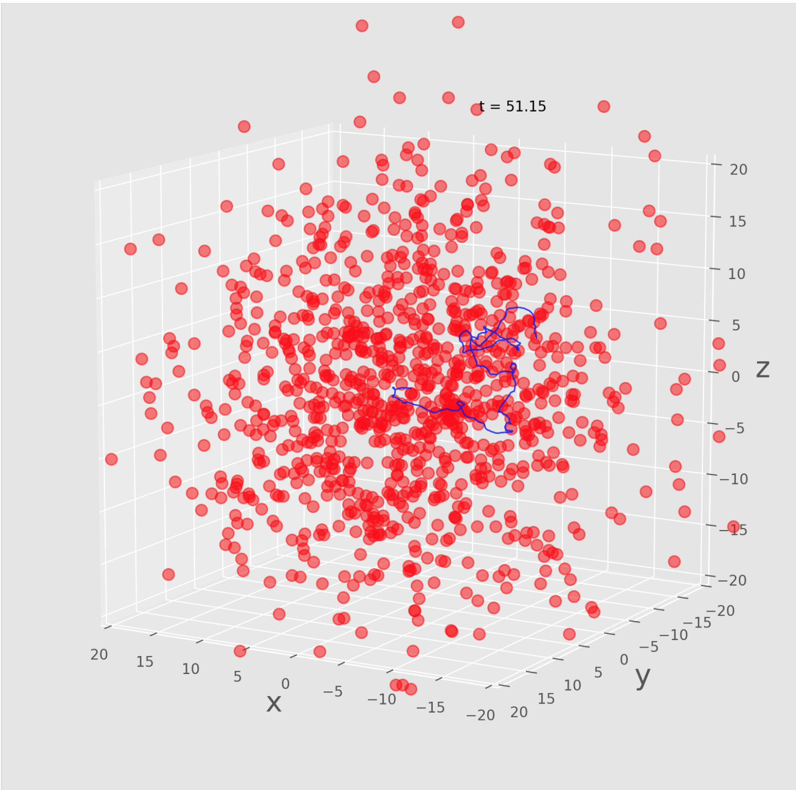
In [3]:
```
def animate(i):
    global R,V,W,Rs,Vs,Ws,time # define global variables
    time[i]=i*dt # store time in each step in an array time
    W = std*np.random.randn(nump,dim) # generate an array of random forc
    R, V = R + V*dt, V*(1-zeta/m*dt)+W/m # update R & V via Eqs.(F5)&(F9
    Rs[i,:,:]=R # 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])) # set the title to display 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(R[:,0],R[:,1]) # set the current position of all
    particles.set_3d_properties(R[:,2]) # add z axis to set the particle
    return particles,title,line # return listed objects that will be dra
```

Set parameters and initialize variables

In [4]:
```
dim  = 3 # system dimension (x,y,z)
nump = 1000 # number of independent Brownian particles to simulate
nums = 1024 # number of simulation steps
dt   = 0.05 # set time increment, \Delta t
zeta = 1.0 # set friction constant, \zeta
m    = 1.0 # set particle mass, m
kBT  = 1.0 # set temperatute, k_B T
std  = np.sqrt(2*kBT*zeta*dt) # calculate std for \Delta W via Eq.(F11)
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 forcces
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
```

Perform and animate the simulation using `FuncAnimation`

In [5]:
```
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
box = 40 # set draw area as box^3
ax.set_xlim(-box/2,box/2) # set x-range
ax.set_ylim(-box/2,box/2) # set y-range
ax.set_zlim(-box/2,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([],[],[],'ro',ms=8,alpha=0.5) # define object parti
title = ax.text(-180.,0.,250.,r'',transform=ax.transAxes,va='center') #
line, = ax.plot([],[],[],'b',lw=1,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 prc
## conda install -c menpo ffmpeg
##
# anim.save('movie.mp4',fps=50,dpi=100)
```



Summary of simulation methods

Original differential equation

$$\frac{d\mathbf{R}(t)}{dt} = \mathbf{V}(t) \tag{F1}$$

$$m\frac{d\mathbf{V}(t)}{dt} = -\zeta\mathbf{V}(t) + \mathbf{F}(t) \tag{F2}$$

with

$$\langle \mathbf{F}(t) \rangle = \mathbf{0} \tag{F3}$$

$$\langle \mathbf{F}(t)\mathbf{F}(0) \rangle = 2k_BT\zeta\mathbf{I}\delta(t) \tag{F4}$$

Euler method

$$\mathbf{V}_{i+1} = \left(1 - \frac{\zeta}{m}\Delta t\right)\mathbf{V}_i + \frac{1}{m}\Delta\mathbf{W}_i \tag{F9}$$

$$\mathbf{R}_{i+1} = \mathbf{R}_i + \mathbf{V}_i\Delta t \tag{B3}$$

with

$$\langle \Delta\mathbf{W}_i \rangle = \mathbf{0} \tag{F10}$$

$$\langle \Delta\mathbf{W}_i\Delta\mathbf{W}_j \rangle = 2k_BT\zeta\Delta t\mathbf{I}\delta_{ij} \tag{F11}$$

2nd order Runge-Kutta method

$$\mathbf{V}'_{i+\frac{1}{2}} = \mathbf{V}_i - \frac{\zeta}{m}\frac{\Delta t}{2}\mathbf{V}_i = \left(1 - \frac{\zeta}{m}\frac{\Delta t}{2}\right)\mathbf{V}_i \tag{F12}$$

$$\mathbf{V}_{i+1} = \mathbf{V}_i - \frac{\zeta}{m}\Delta t\mathbf{V}'_{i+\frac{1}{2}} + \frac{1}{m}\Delta\mathbf{W}_i \tag{F13}$$

$$\mathbf{R}_{i+1} = \mathbf{R}_i + \mathbf{V}'_{i+\frac{1}{2}}\Delta t \tag{F14}$$

4th order Runge-Kutta method

$$\mathbf{V}'_{i+\frac{1}{2}} = \mathbf{V}_i - \frac{\zeta}{m}\frac{\Delta t}{2}\mathbf{V}_i \tag{F15}$$

$$\mathbf{V}''_{i+\frac{1}{2}} = \mathbf{V}_i - \frac{\zeta}{m}\frac{\Delta t}{2}\mathbf{V}'_{i+\frac{1}{2}} \tag{F16}$$

$$\mathbf{V}'''_{i+1} = \mathbf{V}_i - \frac{\zeta}{m}\Delta t\mathbf{V}''_{i+\frac{1}{2}} \tag{F17}$$

$$\mathbf{V}_{i+1} = \mathbf{V}_i - \frac{\zeta}{m}\frac{\Delta t}{6}\left(\mathbf{V} + \mathbf{V}'_{i+\frac{1}{2}} + \mathbf{V}''_{i+\frac{1}{2}} + \mathbf{V}'''_{i+1}\right) + \frac{1}{m}\Delta\mathbf{W}_i \tag{F18}$$

$$\mathbf{R}_{i+1} = \mathbf{R}_i + \frac{\Delta t}{6}\left(\mathbf{V} + \mathbf{V}'_{i+\frac{1}{2}} + \mathbf{V}''_{i+\frac{1}{2}} + \mathbf{V}'''_{i+1}\right) \tag{F19}$$