009x_52

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Stochastic Processes: Data Analysis and Computer Simulation

Brownian motion 3: data analyses
-Mean square displacement and diffusion constant-

1 Calculating the diffusion constant from simulation data

1.1 Perform simulation (at equilibrium)

```
In [1]: % matplotlib inline
        import numpy as np
        import matplotlib.pyplot as plt
        import matplotlib as mpl
        plt.style.use('ggplot')
        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 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
        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
        for i in range(nums): # repeat the following operations from i=0 to nums-1
            W = std*np.random.randn(nump,dim) # generate an array of random forces
            V = V*(1-zeta/m*dt)+W/m # update velocity via Eq.(F9)
            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
            time[i]=i*dt # store time in each step in an array time
```

1.2 Mean square displacement vs. time

- Calculate the mean square displacement, and compare it with the following theoretical result (see the derivation for Eq.(30)).

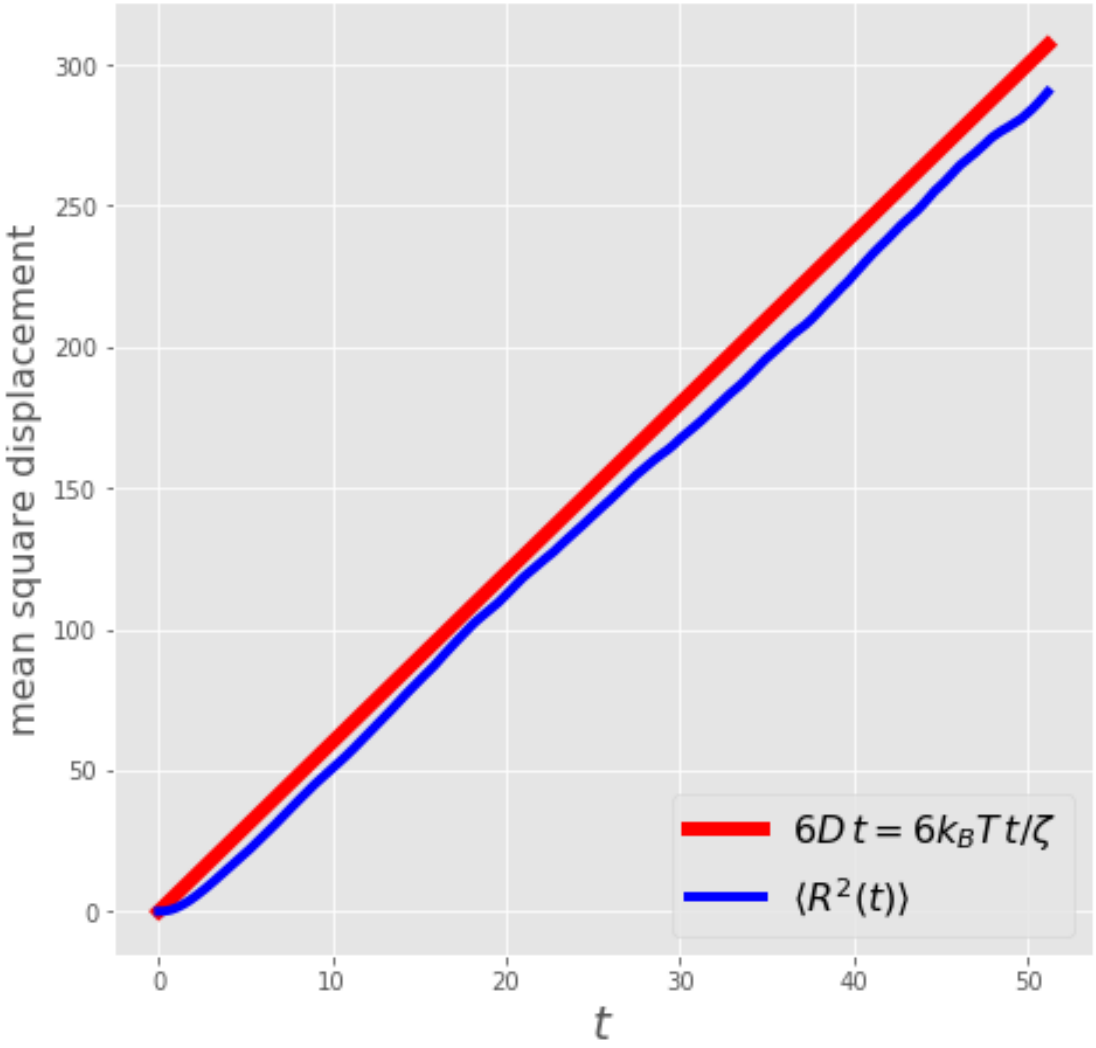
$$\langle [\mathbf{R}(t) - \mathbf{R}(0)]^2 \rangle = 6Dt \tag{H1}$$

- Note that the diffusion coefficient can be easily calculated from the mean square displacement by integrating both sides of Eq.(H1) with respect to time

$$D = \frac{1}{3T^2} \int_0^T \mathrm{d}t \, \langle [\mathbf{R}(t) - \mathbf{R}(0)]^2 \rangle \tag{H2}$$

```
In [2]: # mean square displacement vs time
        msd = np.zeros([nums])
        for i in range(nums): # loop over time steps
            for n in range(nump): # loop over particles
                msd[i]=msd[i]+np.linalg.norm(Rs[i,n,:])**2 # (R(t) - R(0))^2 = R(t)
            msd[i] = msd[i]/nump  # average over particles
        dmsd = np.trapz(msd, dx=dt)/ (3*(nums*dt)**2) # integrate using trapezoidal
        print('D =',kBT/zeta,'(Theoretical)')
        print('D =',dmsd,'(Simulation via MSD)')
        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'$6D\,t={6k_BT \,t}/{\zeta}$'
        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 = 0.926874089843 (Simulation via MSD)
```



1.3 Diffusion constant and Velocity auto-correlation function

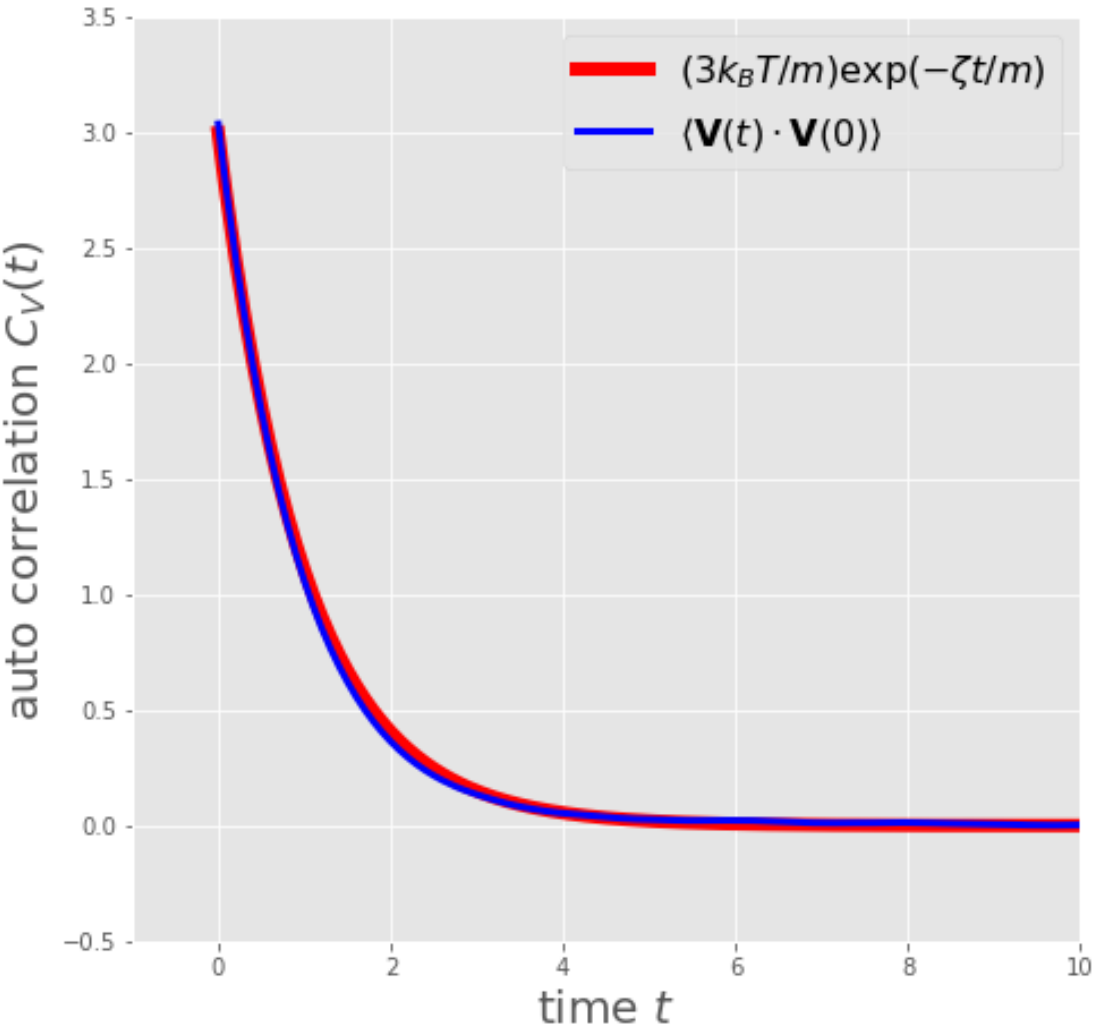
- Calculate the velocity auto-correlation function, and evaluate the diffusion constant using the Green-Kubo formula (see the derivation for Eq.(49)).

$$D = \frac{1}{3}\int_o^\infty \varphi_V(t)dt \tag{H3}$$

```
In [3]: # compute self-correlation of vector v
        def auto_correlate(v):
            # np.correlate computes C_{v}[k] = sum_n v[n+k] * v[n]
            corr = np.correlate(v,v,mode="full") # correlate returns even array [0
            return corr[len(v)-1:]/len(v) # take positive values and normalize by n
        corr = np.zeros([nums])
```

```
        for n in range(nump):
            for d in range(dim):
                corr = corr + auto_correlate(Vs[:,n,d]) # correlation of d-componer
        corr=corr/nump #average over all particles
        print('D =',kBT/zeta,'(Theoretical)')
        print('D =',np.trapz(corr,dx=dt)/3,'(Simulation via Green-Kubo)')
        fig, ax = plt.subplots(figsize=(7.5,7.5))
        ax.plot(time,dim*kBT/m*np.exp(-zeta/m*time),'r',lw=6, label=r'$(3k_BT/m)\ex
        ax.plot(time,corr,'b',lw=3,label=r'$\langle\mathbf{V}(t)\cdot \mathbf{V}(0)
        ax.set_xlabel(r"time $t$", fontsize=20)
        ax.set_ylabel(r"auto correlation $C_V(t)$", fontsize=20)
        ax.set_xlim(-1,10)
        ax.set_ylim(-0.5,3.5)
        ax.legend(fontsize=16)
        plt.show()
```

```
D = 1.0 (Theoretical)
D = 0.944777284634 (Simulation via Green-Kubo)
```



1.4 Perform simulation under external force (out of equilibrium)

```
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
        F0   = 1.0  # set external drift force
        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 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]) # array to store external force
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
F[:,0]=F0 # constant force along x, zero force in y and z
for i in range(nums): # repeat the following operations from i=0 to nums-1
    W = std*np.random.randn(nump,dim) # generate an array of random forces
    V = V*(1-zeta/m*dt)+W/m+F/m*dt # update velocity via Eq.(F9)
    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
    time[i]=i*dt # store time in each step in an array time
```

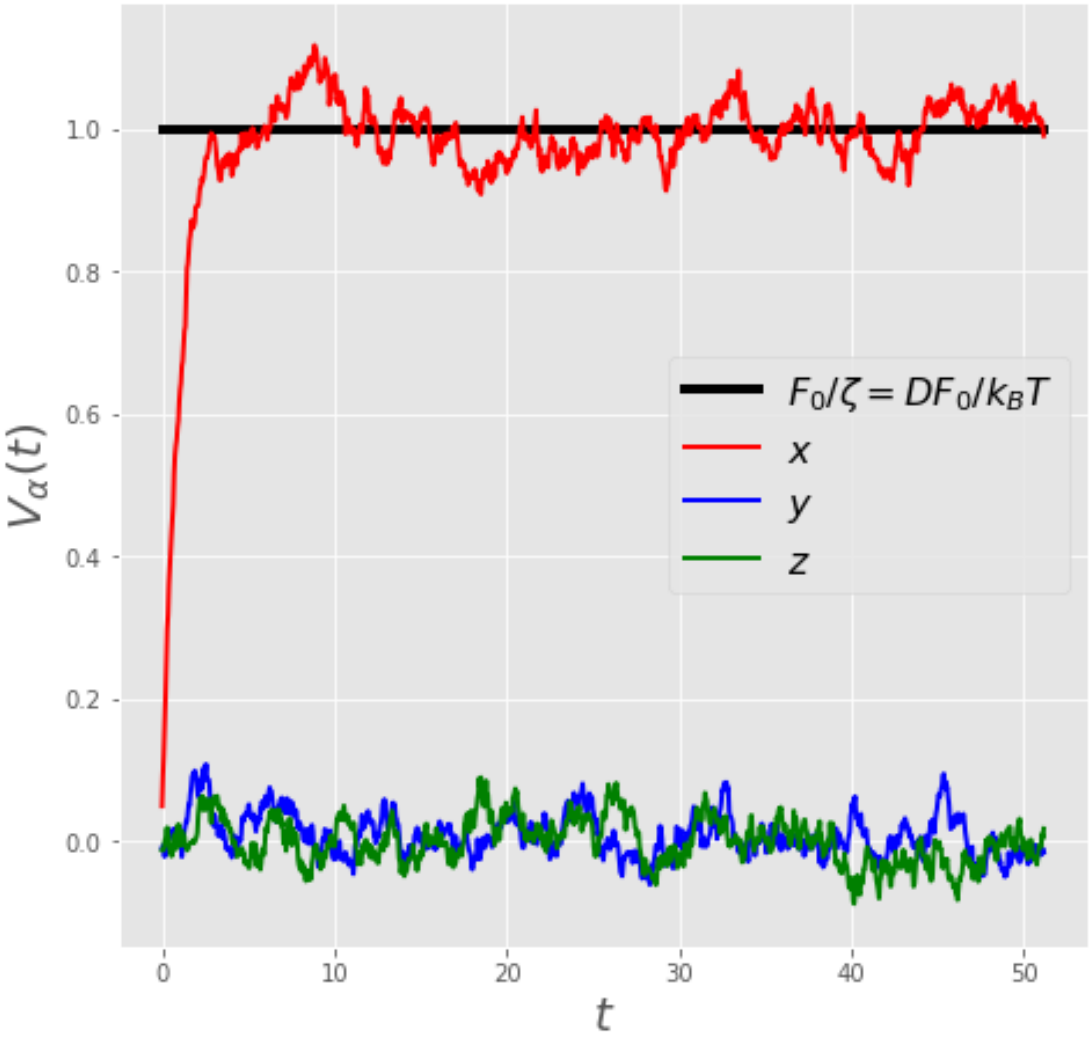
1.5 Drift velocity under external force

- Calculate the drift velocity $\langle V_x \rangle_{ext}$, and evaluate the diffusion constant using the equation shown here (see the derivation for Eq.(43)).

$$D = \frac{\langle V_x \rangle_{ext} k_B T}{F_0} \tag{H4}$$

```
In [5]: Vsa = np.average(Vs,axis=1) # average over particles (0-axis is time, 1-axi
        Vx  = np.average(Vsa[:,0]) # time average of (particle averaged) x-velocity
        print('D =',kBT/zeta, '(Theoretical)')
        print('D =',Vx*kBT/F0,'(Simulation with external force)')
        fig, ax = plt.subplots(figsize=(7.5,7.5))
        ax.set_ylabel(r"$V_{\alpha}(t)$", fontsize=20)
        ax.set_xlabel(r"$t$", fontsize=20)
        ax.plot(time,F0/zeta*np.ones(nums),'k',lw=4,label=r"$F_0/\zeta=DF_0/k_B T$"
        ax.plot(time,Vsa[:,0],'r',lw=2,label="$x$")
        ax.plot(time,Vsa[:,1],'b',lw=2,label="$y$")
        ax.plot(time,Vsa[:,2],'g',lw=2,label="$z$")
        ax.legend(fontsize=16,loc=5)
        plt.show()

D = 1.0 (Theoretical)
D = 0.980302218583 (Simulation with external force)
```


1.0
0.8
0.6
0.4
0.2
0.0
$V_\alpha(t)$
0
10
20
30
40
50
t
$F_0/\zeta = DF_0/k_BT$
x
y
z