Droplet_MD_Util

July 13, 2020

0.1 Utility functions for Droplet MD Simulation Post-Processing

The following Notebook contains all functions for making use of the MD simulation trajectory files in PDB Format to obtain spatial density profile which is used to obtain the droplet diameter and droplet contact angle. The key parameters that need to specified in the cells that follows are : **N_molecules, N_timesteps, xlim, ylim, zlim and the filename passed to get_txt function which converts a PDB file to txt format**.

In the computation of density, the user may choose to specify any other cell_size. dx and dz determine the grid spacing in the X and Z directions on which the computation is made approximating each dx.dz sized box as a cuboid.

As long as the standard PDB format file is used, none of the functions may be changed internally.

Note - The drop is assumed to be resting on a substrate on the X-Y plane and the Z direction is normal to the substrate. This tutorial was used for a water droplet.

[1]:
```
import numpy as np
import matplotlib.pyplot as plt
from mpl_toolkits import mplot3d
from numba import jit
```

[2]:
```
N_molecules = 1981 #Number of molecules having atom : atomname
N_timesteps = 200  #Number of time steps for which N_molecules trajectory was␣
 ↪stored
xlim = [0,240] #Max Limits on X coord
ylim = [0,240] #Max Limits on Y coord
zlim = [0,90]  #Max Limits on Z coord
```

[3]:
```
#Use mask and apply it over all arrays
def get_clean_coord(X,Y,Z,timestep):
    i = timestep
    X_clean = np.ma.masked_where(X[:,i]>xlim[1], X[:,i])
    Y_clean = np.ma.masked_where(X[:,i]>xlim[1], Y[:,i])
    Z_clean = np.ma.masked_where(X[:,i]>xlim[1], Z[:,i])

    X_clean = np.ma.masked_where(X_clean[:]<xlim[0], X_clean[:])
    Y_clean = np.ma.masked_where(X_clean[:]<xlim[0], Y_clean[:])
    Z_clean = np.ma.masked_where(X_clean[:]<xlim[0], Z_clean[:])

    X_clean = np.ma.masked_where(Y_clean[:]>ylim[1], X_clean[:])
```

```
    Y_clean = np.ma.masked_where(Y_clean[:]>ylim[1], Y_clean[:])
    Z_clean = np.ma.masked_where(Y_clean[:]>ylim[1], Z_clean[:])

    X_clean = np.ma.masked_where(Y_clean[:]<ylim[0], X_clean[:])
    Y_clean = np.ma.masked_where(Y_clean[:]<ylim[0], Y_clean[:])
    Z_clean = np.ma.masked_where(Y_clean[:]<ylim[0], Z_clean[:])


    X_clean = np.ma.masked_where(Z_clean[:]>zlim[1], X_clean[:])
    Y_clean = np.ma.masked_where(Z_clean[:]>zlim[1], Y_clean[:])
    Z_clean = np.ma.masked_where(Z_clean[:]>zlim[1], Z_clean[:])

    X_clean = np.ma.masked_where(Z_clean[:]<zlim[0], X_clean[:])
    Y_clean = np.ma.masked_where(Z_clean[:]<zlim[0], Y_clean[:])
    Z_clean = np.ma.masked_where(Z_clean[:]<zlim[0], Z_clean[:])

    return X_clean, Y_clean, Z_clean
```

[4]:
```
# Get coordinates of atom having name : atomname from file named : filename and␣
 ↪store in a local txt file

def gen_txt(filename, atomname):
    pdb = open('./PDB/'+filename+'.pdb')
    trimmed_pdb = open('Coord_'+filename+'.txt',"w")
    for line in pdb:
        if line[0] == 'A' and line[13] == atomname:
            trimmed_pdb.write(line[31:45]+' '+line[47:55] +'\n')
    pdb.close()
    trimmed_pdb.close()

def get_coordinates(filename):
    trimmed_pdb = open('Coord_'+filename+'.txt')
    x = []
    for line in trimmed_pdb:
        x.append(line)

    X = np.zeros((N_molecules,N_timesteps))
    Y = np.zeros((N_molecules,N_timesteps))
    Z = np.zeros((N_molecules,N_timesteps))
    for j in range(0,N_molecules*N_timesteps):
        c = [float(i) for i in x[j].split()]
        i1 = j%N_molecules
        j1 = int(j/N_molecules)
        X[i1][j1] = c[0]
        Y[i1][j1] = c[1]
        Z[i1][j1] = c[2]
```

```
    return X,Y,Z

def plot_snapshot(X, Y, Z, timestep):
    plt.scatter(X[:,timestep],Z[:,timestep])
```

[5]:
```
@jit
def find_nearest(array, value):
    array = np.asarray(array)
    idx = (np.abs(array - value)).argmin()
    return idx
```

[6]:
```
@jit
def get_rho(cell_size,xlim,ylim,zlim,x0,y0,z0,padding,dx,dz):

    p = cell_size/2
    q = padding
    Nx = int(1/dx)
    Nz = int(1/dz)
    #Populate Density Matrix for each cell
    rho = np.zeros(((xlim[1]-xlim[0]+2*q)*Nx,(zlim[1]-zlim[0]+2*q)*Nz))

    for x in range(-q*Nx,(xlim[1]-xlim[0]+q)*Nx):
        for z in range(-q*Nz,(zlim[1]-zlim[0]+q)*Nz):
            y_temp = y0[(x0>x/Nx+xlim[0]-p) & (x0<x/Nx+xlim[0]+p) & (z0>z/
↪Nz+zlim[0]-p) & (z0<z/Nz+zlim[0]+p)]
            if y_temp.size != 0 and y_temp.max() != y_temp.min():
                rho[x+q*Nx][z+q*Nz] = y_temp.shape[0]/(y_temp.max()-y_temp.
↪min())
    return rho
```

[7]:
```
def plot_rho(rho,padding,xlim,zlim,dx,dz):
    q = padding
    Nx = int(1/dx)
    Nz = int(1/dz)
    z_ax = np.linspace((zlim[0]-q)*Nz, (zlim[1]+q-1)*Nz, ␣
↪(zlim[1]+2*q-zlim[0])*Nz)
    x_ax = np.linspace((xlim[0]-q)*Nx, (xlim[1]+q-1)*Nx, ␣
↪(xlim[1]+2*q-xlim[0])*Nx)
    x_ax, z_ax = np.meshgrid(x_ax,z_ax)
    fig = plt.figure()
    ax = plt.axes(projection='3d')
    surf = ax.plot_surface(z_ax, x_ax, rho.T,cmap='viridis')
    ax.set_xlabel('Z')
    ax.set_ylabel('X')
    ax.set_title(r'Level Plot of $ \rho $')
    fig.colorbar(surf)
    ax.view_init(-90, 0)
```

```
    fig
```

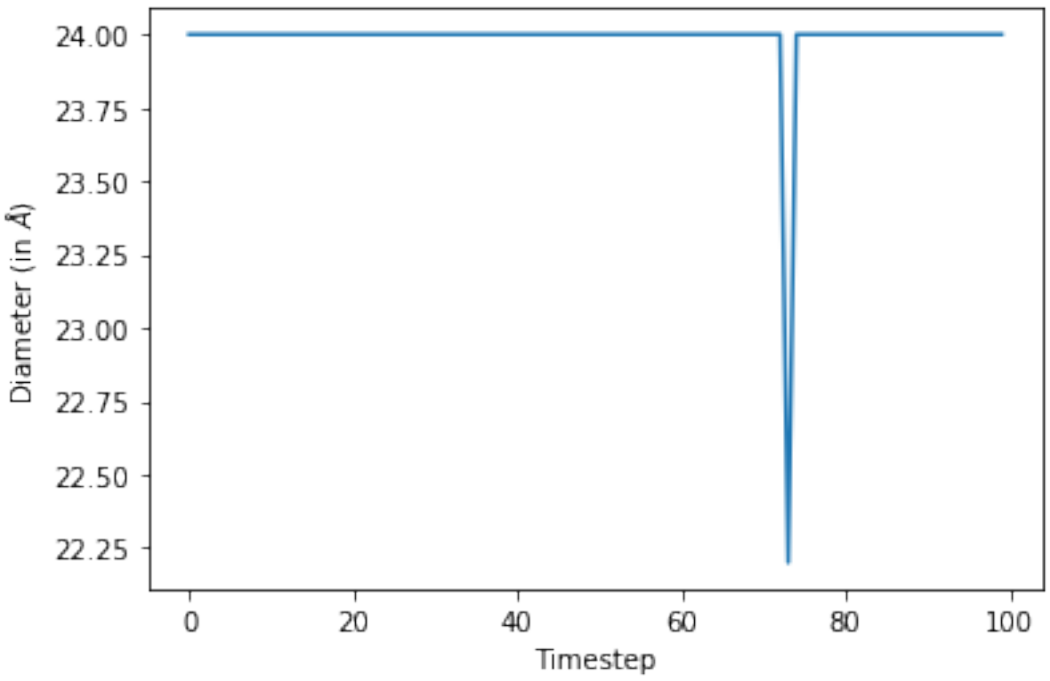
[8]:
```
#Example : Generate txt file of coordinates of oxygen ('O') from pdb file with␣
 ↪name 'e=0.5_E=0'
gen_txt('e=2.5_E=0','O')
```

[9]:
```
X,Y,Z = get_coordinates('e=2.5_E=0')
q = 5 #Padding
dx = 0.1
dz = 0.1
Nx = int(1/dx)
Nz = int(1/dz)
cell_size = 6.8
```

[15]:
```
#Get the Diameter List (this is slow!)
D = [] #Dia List
dx = 0.1
dz = 0.1
Nx = int(1/dx)
Nz = int(1/dz)
for t in range(50,150):
    x0,y0,z0 = get_clean_coord(X,Y,Z,t)
    xlim = [int(x0.min()),int(np.ceil(x0.max()))] #New Limits
    ylim = [int(y0.min()),int(np.ceil(y0.max()))] #New Limits
    zlim = [int(z0.min()),int(np.ceil(z0.max()))] #New Limits
    rho = get_rho(6.8,np.asarray(xlim),np.asarray(ylim),np.
 ↪asarray(zlim),x0,y0,z0,q,dx,dz) #Get rho Cell_Size of 6.8
    r = rho.flatten()
    r = np.median(r)
    d = find_nearest(rho[:,(4+q)*Nz][int(rho.shape[0]/2):],r/2)+int(rho.
 ↪shape[0]/2) -find_nearest(rho[:,(4+q)*Nz][0:int(rho.shape[0]/2)],r/2)
    D.append(d*dx)
```

[16]:
```
plt.plot(D)
plt.ylabel(r'Diameter (in $\AA$)')
plt.xlabel('Timestep')
```

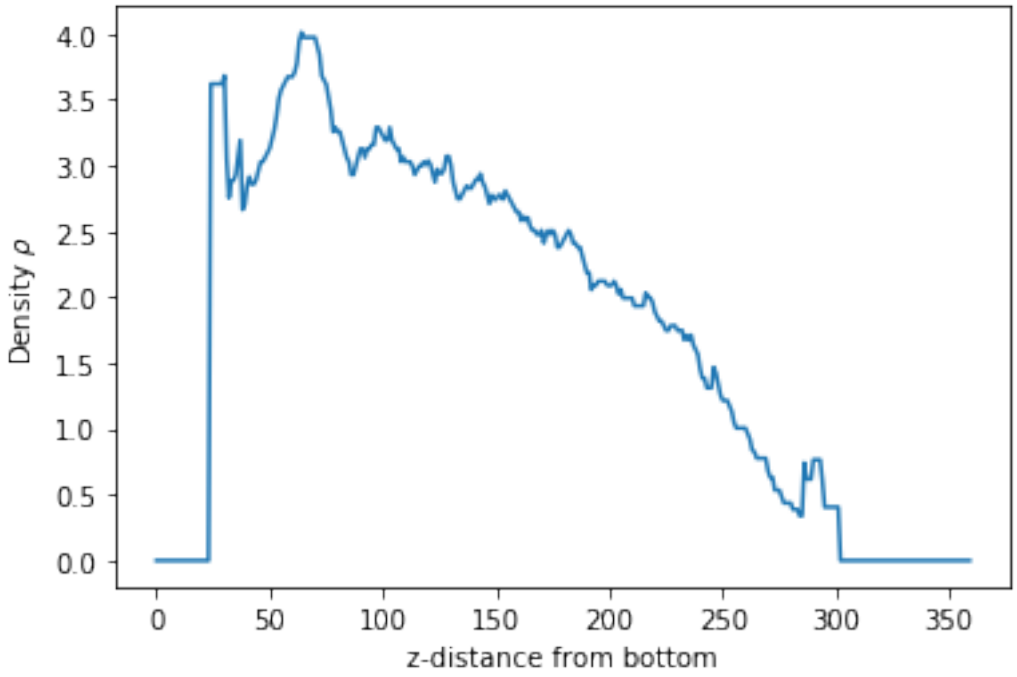
[16]:
```
Text(0.5, 0, 'Timestep')
```



[15]:
```
x0,y0,z0 = get_clean_coord(X,Y,Z,100)
```

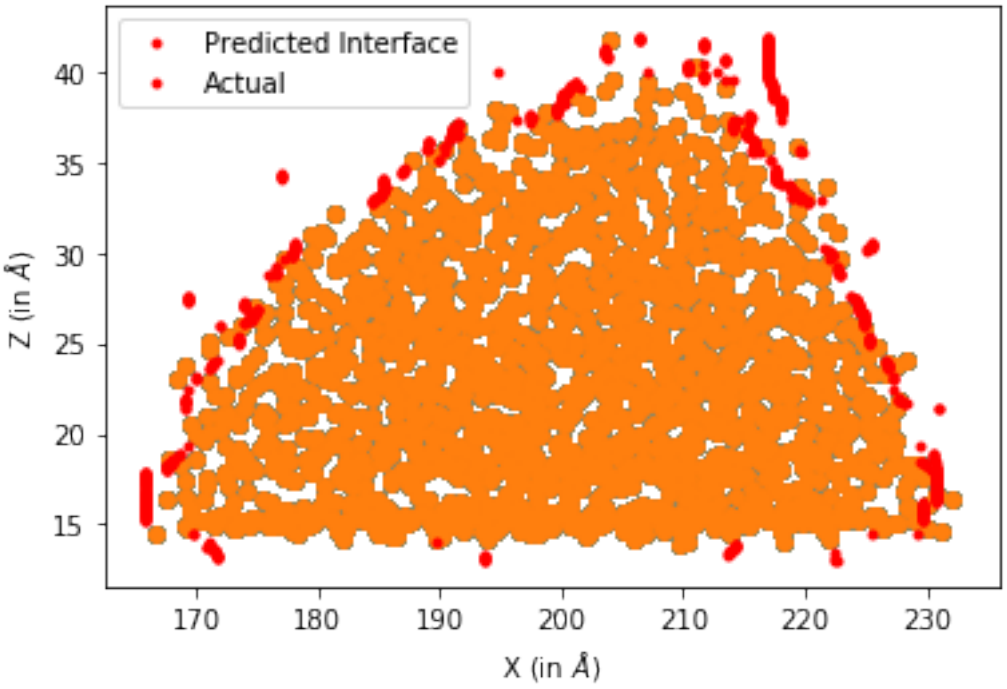
[37]:
```
plt.plot(rho[int(rho.shape[0]*0.5),:])
plt.ylabel(r'Density $ \rho $')
plt.xlabel('z-distance from bottom')
```

[37]:
```
Text(0.5, 0, 'z-distance from bottom')
```

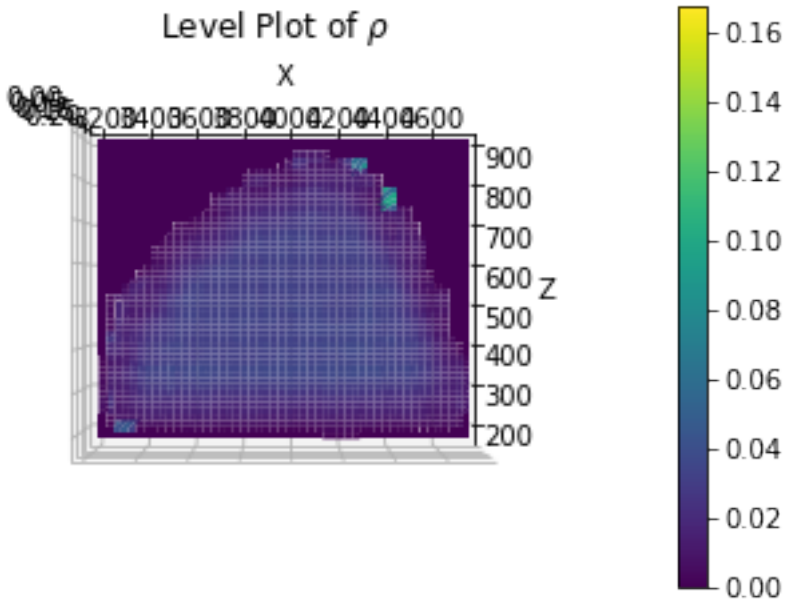


[10]:
```
dx = 0.05
dz = 0.05
Nx = int(1/dx)
Nz = int(1/dz)
q = 3
cell_size = 6.8
x0,y0,z0 = get_clean_coord(X,Y,Z,100)
xlim = [int(x0.min()),int(np.ceil(x0.max()))]
ylim = [int(y0.min()),int(np.ceil(y0.max()))]
zlim = [int(z0.min()),int(np.ceil(z0.max()))]
rho = get_rho(6.8,np.asarray(xlim),np.asarray(ylim),np.
 ↪asarray(zlim),x0,y0,z0,q,dx,dz) #Get rho Cell_Size of 6.8
r = rho.flatten()
r = np.median(r)*2
left_pts = []
right_pts = []
for z in range(0,rho.shape[1]-q*Nz-3*Nz):
    p1 = find_nearest(rho[:,int(z+q*Nz)],r/2)
    temp_idx = min(p1+int(rho.shape[0]*0.25),int(rho.shape[0]*0.75))
    p2 = find_nearest(rho[:,int(z+q*Nz)][temp_idx:],r/2)+temp_idx
    if p2 > p1:
        plt.plot(p1/Nx+xlim[0]-q, z/Nz+zlim[0],'r.')
        left_pts.append([p1/Nx+xlim[0]-q, z/Nz+zlim[0]])
        plt.plot(p2/Nx+xlim[0]-q, z/Nz+zlim[0],'r.')
        right_pts.append([p2/Nx+xlim[0]-q, z/Nz+zlim[0]])
```

```
        plt.scatter(x0,z0)
        plt.xlabel(r'X (in $\AA$)')
        plt.ylabel(r'Z (in $\AA$)')
        plt.legend(['Predicted Interface','Actual'])
```



[100]:
```
#Level Plot of Rho
plot_rho(rho/(cell_size*cell_size),q,xlim,zlim,dx,dz)
```



[13]:
```
n = np.median(rho.flatten())*2/(cell_size**2)

N_A = 6.022*1e23 # Avogadro's Number
L_c = 1e-10 # 1 Angstorm to meter
M_Mass = 18 # Molecular Mass of Water

print('Predicted # Density of Water : ',n, '\n')
print('Predicted Density of Water:', n*18*1e-3/(N_A*L_c**3),'kg/m^3')
```

```
Predicted # Density of Water :  0.03183939620748707

Predicted Density of Water: 951.6923476166842 kg/m^3
```

[16]:
```
left_arr = np.squeeze(np.asarray(left_pts))
right_arr = np.squeeze(np.asarray(right_pts))
```

[80]:
```
from scipy.optimize import curve_fit
def func(x,a,b,c):
    return a*x**2+b*x+c
def func_prime(x,a,b,c):
    return 2*a*x+b

zlevel = 20 #zlevel at which contact angle is measured


xdata = left_arr[:,0]
ydata = left_arr[:,1]
popt, pcov = curve_fit(func, xdata, ydata)

x_at_zlevel = (-popt[1]+np.sqrt(popt[1]**2-4*popt[0]*(popt[2]-zlevel)))/
 ↪(2*popt[0])

v = np.array([1,func_prime(x_at_zlevel,*popt)])
origin = [x_at_zlevel],[zlevel]
right_angle = int(np.arctan(v[1]/v[0])*180/np.pi*100)/100
plt.quiver(*origin, v[0], v[1], color=['k'], scale=10, width=0.016)
plt.plot(xdata,func(xdata,*popt),'r.')
plt.text(x_at_zlevel+10,zlevel+5,'Right Angle:'+str(right_angle))

xdata = right_arr[:,0]
ydata = right_arr[:,1]
popt, pcov = curve_fit(func, xdata, ydata) #Fitting to get polynomial␣
 ↪coefficients in popt

x_at_zlevel = (-popt[1]-np.sqrt(popt[1]**2-4*popt[0]*(popt[2]-zlevel)))/
 ↪(2*popt[0])
```

```
v = np.array([-1,-func_prime(x_at_zlevel,*popt)])
origin = [x_at_zlevel],[zlevel]
left_angle = int(-np.arctan(v[1]/v[0])*180/np.pi*100)/100
plt.quiver(*origin, v[0], v[1], color=['k'], scale=15,width=0.016)

plt.plot(xdata,func(xdata,*popt),'b.')
plt.xlabel(r'X (in $\AA$)')
plt.ylabel(r'Z (in $\AA$)')
plt.title('Contact Angle Plot')
plt.legend(['Left Half Fit','Right Half Fit'])

plt.text(x_at_zlevel-25,zlevel+5,'Left Angle:'+str(left_angle))
```

[80]: `Text(203.91971985862875, 25, 'Left Angle:63.94')`