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import numpy as np
import matplotlib.pyplot as plt
N = 100          # number of molecules
D = 100         # side dimension of box
T = 15*10**3    # number of timesteps
B = 50         # location of initial distribution

# initialize variables
nx = 0; ny = 0; s = 0; wallflag = 0
x = np.zeros(N, dtype=int)
y = np.zeros(N, dtype=int)
d = np.zeros(N, dtype=int)
for i in range(N):
    x[i] = np.random.choice(B, 1)
    y[i] = np.random.choice(D, 1)
f = open('workfile', 'w')

for t in range(T):
    R = 0
    for i in range(N):
        if d[i] == 0:
            s = np.random.choice(8, 1); d[i] = s + 1           # random walk 8
directions
            s = d[i]; wallflag = 0                               # inertia
            if s == 1:
                nx = x[i]
                if y[i] + 1 <= D: ny = y[i] + 1; d[i] = s
                else: ny = y[i]; d[i] = 2; wallflag = 1
            if s == 2:
                nx = x[i]
                if y[i] - 1 >= 0: ny = y[i] - 1; d[i] = s
                else: ny = y[i]; d[i] = 1; wallflag = 1
            if s == 3:
                ny = y[i]
                if x[i] + 1 <= D: nx = x[i] + 1; d[i] = s
                else: nx = x[i]; d[i] = 4; wallflag = 1
            if s == 4:
                ny = y[i]
                if x[i] - 1 >= 0: nx = x[i] - 1; d[i] = s
                else: nx = x[i]; d[i] = 3; wallflag = 1
            if s == 5:
                if y[i] + 1 <= D and x[i] + 1 <= D:
                    ny = y[i] + 1; nx = x[i] + 1; d[i] = s
                else: ny = y[i]; nx = x[i]; wallflag = 1
                if y[i] + 1 > D: d[i] = 7
                if x[i] + 1 > D: d[i] = 8
            if s == 6:
                if y[i] - 1 >= 0 and x[i] - 1 >= 0:
                    ny = y[i] - 1; nx = x[i] - 1; d[i] = s
                else: ny = y[i]; nx = x[i]; wallflag = 1

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        if y[i] - 1 < 0: d[i] = 8
        if x[i] - 1 < 0: d[i] = 7
    if s == 7:
        if y[i] - 1 >= 0 and x[i] + 1 <= D:
            ny = y[i] - 1; nx = x[i] + 1; d[i] = s
        else: ny = y[i]; nx = x[i]; wallflag = 1
        if y[i] - 1 < 0: d[i] = 5
        if x[i] + 1 > D: d[i] = 6
    if s == 8:
        if y[i] + 1 <= D and x[i] - 1 >= 0:
            ny = y[i] + 1; nx = x[i] - 1; d[i] = s
        else: ny = y[i]; nx = x[i]; wallflag = 1
        if y[i] + 1 > D: d[i] = 6
        if x[i] - 1 < 0: d[i] = 5

    if wallflag == 0:
        for j in range(N):
            if x[j] == nx and y[j] == ny and not(j == i):
                d[i] = 0 # collision
                x[i] = nx; y[i] = ny # inertia

    if x[i] >= int(D/2): R = R + 1

print(t, R)
f.write(str(R)+" ")

f.close()

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