ME 7953: Simulations in Materials

Fall 2002

Problem Set 3 (Friday, 9/13/2002)

Problems are due at the beginning of the class, Friday, 9/20/2002.

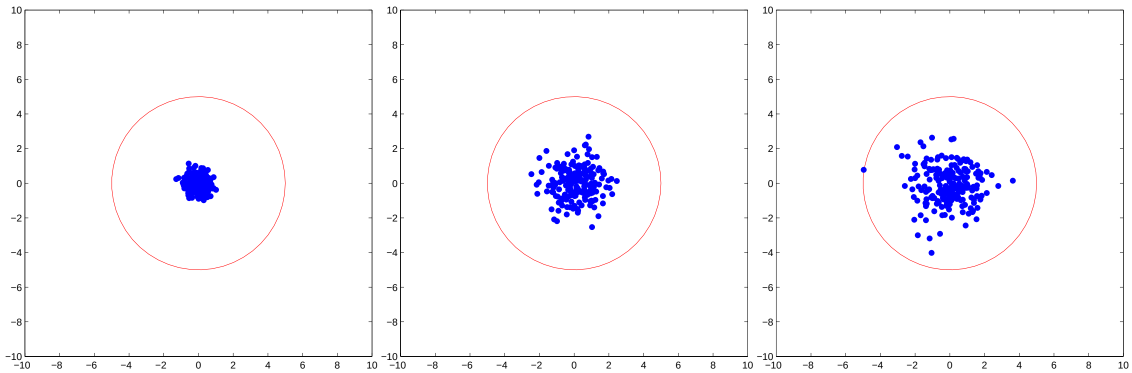
Stochastic simulation is the focus of this week's problems. The basic assumption underlying the stochastic model that we will consider is that the motion of the particles is such that their trajectory is random. For simplicity, we assume that the particles do not interact with each other.

1) Diffusion

Here is an MATLAB example simulating 2D diffusion. Listed below is the Brownian motion example code. Initial particle positions are generated at the center within an 1×1 area with uniform random distribution.

```
nPart = 400; %number of particles
sizeRandomStep = .02; %temperature related parameter
rMax = 10;

%initial particles
x = rand(nPart,1)-0.5;
y = rand(nPart,1)-0.5;

h = plot(x,y,'.'); %plot particles as dots
hold on
axis([-20 20 -20 20])
axis square
grid off
set(h,'EraseMode','xor','MarkerSize',18)

% draw the circle the diffusion will finally reach to
theta = linspace( 0, pi*2, 50 );
plot(rMax*cos(theta),rMax*sin(theta),'r-');

nStep = 0;
while ( max(sqrt(x.^2+y.^2)) < rMax )
    drawnow
    x = x + sizeRandomStep * randn(nPart,1);
    y = y + sizeRandomStep * randn(nPart,1);
    nStep = nStep + 1;
    set(h,'XData',x,'YData',y)
end
nStep % display how many steps cost to reach to the circle
```

The following three snapshots show the spreading of the particles till one of them first reaches the circle of radius $rMax = 10$.



(A) Modify the code, let the code stop when half of the total particles ($n/2$) are out of the circle of radius $rMax$. Print out three snapshots showing particles are moving out of the circle till half of them move out.

(B) Write a MATLAB function:

```
function [halfOutSteps] = halfOut(rMax,sizeRandomStep)
```

The input data for the function is rMax and sizeRandomStep. The sizeRandomStep can be related to the temperature of the system. At higher temperature, particles have larger size of random movement for a fixed evolution time step. In the simulation we assume each step cost 1 unit time. The rMax is the radius of the circle that particles are spreading to.

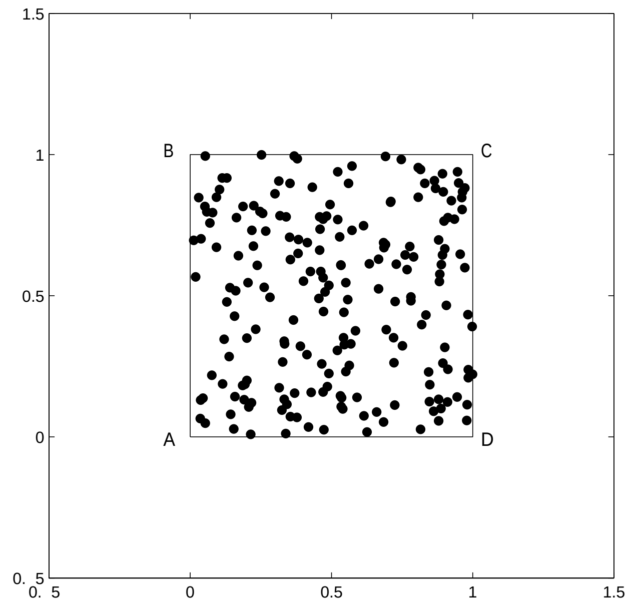
The function will find how many steps to take for half of the total particles diffuse out of the circle with radius of $rMax$. This number is the output of the function. Through this function, we can easily change the values of those two variables, and run the code to see the responses.

(C) Show the relationship between (rMax/halfOutSteps) and sizeRandomStep. The physical meaning can be explained as the diffusion rate versus temperature of the system. Take *np* = 10 points to draw the curve, as shown in the bellow.

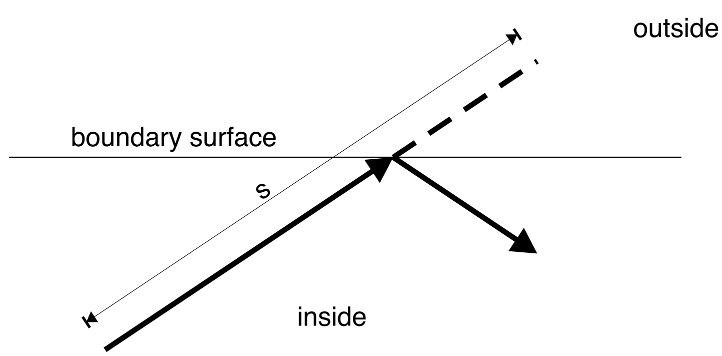
```
np = 10;
rMax = 10;
sizeRandomStep = linespace(0.005,0.08,np);
for i=1:np
      rate(i) = rMax / halfOut(rMax,sizeRandomStep(i));
end
plot(sizeRandomStep,rate);
```

2) Brownian motion in a closed box

As shown in the following figure, this is a two-dimensional simulation of the Brownian motion in a closed box.



Particles cannot move out of the box. When a particle's random movement hits on the boundary and tries to move out, the boundary surface will reflect the particle back to the box. This boundary reflection process can be better shown in the following figure.

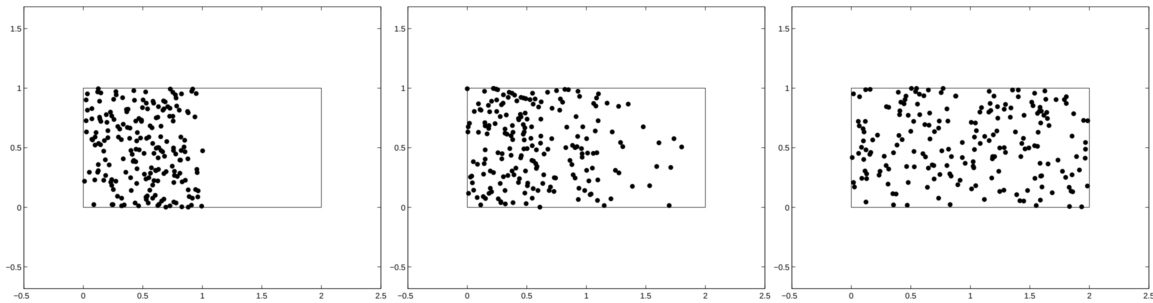


A) Write the details about how are you going to deal with the boundary at AB, BC, CD, and DA.
B) Write a code to simulate Brownian motion of 400 particles in a close box (1×1). Print out two snapshots of the simulation.
C) Calculate the average of pressure on the walls. How are you going to define the pressure in the box ABCD? Find the relation curve of pressure versus temperature. The temperature can be represent by sizeRandomStep. You can take

```
sizeRandomStep = linespace(0.005,0.08,10);
```

and calculate the ***average*** pressure for each sizeRandomStep.

3) Extension of particles from one room to two rooms
Imagine a closed box that is divided into two parts of equal volume. Initially all particles are in the left half, and the right half is empty. This problem simulates the extension of particles from one room to two rooms, as shown in the following figure.



A) The particles will spread from left to right till the system reaches equilibrium. How to define that system has reached equilibrium?

B) Write a code to simulate Brownian motion of 400 particles in a closed box (1×2), as shown in the above figures. Print out four snapshots to show the propagation of particles from left to right, till system reaches equilibrium.

C) Plot a curve to show the changes of pressure at the right side face of the box.

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Problem Set 2, error correction

In problem 4, the equivalent stress should be

$$\sigma_e = \frac{\sqrt{2}}{2}\left[(\sigma_x - \sigma_y)^2 + (\sigma_y - \sigma_z)^2 + (\sigma_z - \sigma_x)^2 + 6(\tau_{xy}^2 + \tau_{yz}^2 + \tau_{zx}^2)\right]^{1/2}.$$

For this reason, problems are due at the beginning of the class, Monday, 9/16/2002. If you can turn in the homework today, I will give you 2 extra points.