NATIONAL AND KAPODISTRIAN UNIVERSITY OF ATHENS

School of Science

Information Technologies in Medicine and Biology

Direction: ***Bioinformatics***

Simulation Methods in Medicine and Biology

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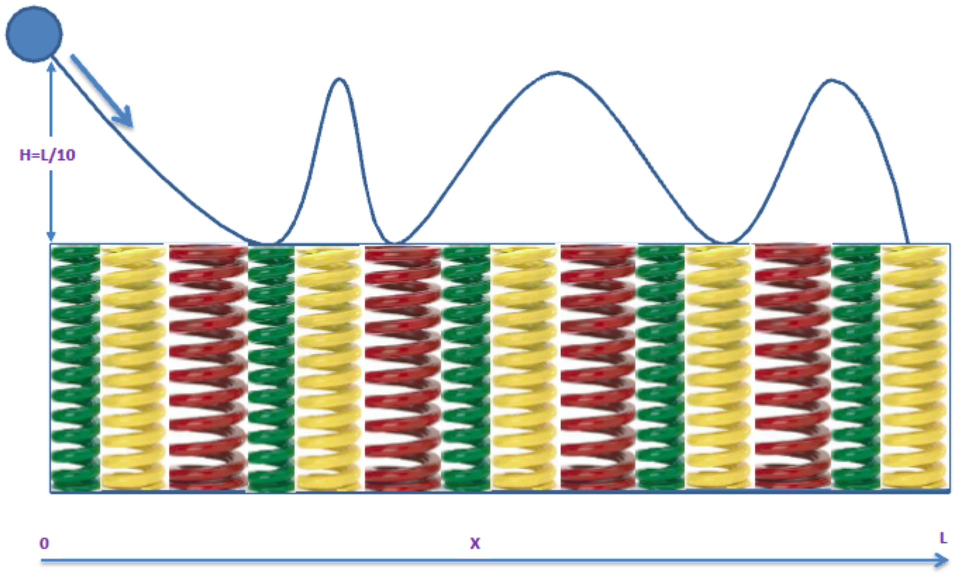
Assignment 1



E: Sphere energy

k: Spring constant (k1,k2,k3)

L: Length of elastic layer, L=90

x: Route between two collisions (sphere-string) with PDF:

$x \alpha e^{-kEx}$

10^6 spheres with angles ϑ in [0^o,45^o] following uniform PDF and energies *E* varying in [5J,25J] with frequency appearance of the inverse square power PDF.

Springs constants are k1=1, k2=2, k3=3

Springs positions alternate every L/30 steps beginning with the k1 constant.

1.1.

We are assigned to find how many collisions are going to occur in the elastic layer.

To do this first we have to find the cumulative distribution functions of the angles ϑ and energies *E.*

Angles (ϑ)

Using the equation of uniform PDFs we have:

$$\mathbf{f}(\boldsymbol{\theta}) = \frac{1}{\beta - \alpha} = \frac{1}{\frac{\pi}{4} - 0} = \frac{\mathbf{4}}{\boldsymbol{\pi}}$$

So the cumulative distribution function of the angles ϑ is*:*

$$F(\theta 1) = \int_0^{\theta 1} p(\theta) d\theta = \int_0^{\theta 1} \frac{4}{\pi} d\theta = \frac{4}{\pi}\int_0^{\theta 1} d\theta = \frac{4}{\pi}(\theta 1 - 0) = \frac{\mathbf{4\theta 1}}{\boldsymbol{\pi}}$$

Suppose $\frac{\mathbf{4\theta 1}}{\boldsymbol{\pi}} = \boldsymbol{R1} \rightarrow \boldsymbol{\theta 1} = \frac{\boldsymbol{\pi R1}}{\mathbf{4}}$

Energies (E)

Using the equation of inverse square power PDFs we have:

$$\mathbf{f}(\boldsymbol{E}) = \frac{a}{\mathrm{E}^2}, \alpha\ constant$$

In order to find α we have:

$$\int_5^{25} f(E) dE = 1 \ \rightarrow \ a\int_5^{25} \frac{1}{E^2} dE = 1 \rightarrow -a\int_5^{25} \left(\frac{1}{E}\right)' dE = 1 \rightarrow -a\left(\frac{1}{25} - \frac{1}{5}\right) = 1 \rightarrow 4a = 25 \rightarrow \boldsymbol{a} = \frac{\mathbf{25}}{\mathbf{4}}$$

So, $\mathbf{f}(\boldsymbol{E}) = \frac{25}{\mathrm{E}^2}$

The cumulative distribution function of the Energy *E* is*:*

$$F(E1) = \int_5^{E1} \frac{25}{4E^2} dE = -\frac{25}{4}\int_5^{E1} \left(\frac{1}{E}\right)' dE = -\frac{25}{4}\left(\frac{1}{\mathrm{E1}} - \frac{1}{5}\right) = -\frac{\mathbf{125 - 25E1}}{\mathbf{20}\boldsymbol{E}\mathbf{1}}$$

Suppose $-\frac{\mathbf{125-25E1}}{\mathbf{20}\boldsymbol{E}\mathbf{1}} = \boldsymbol{R2} \rightarrow \boldsymbol{E1} = \frac{\mathbf{25}}{\mathbf{5-4}\boldsymbol{R}\mathbf{2}}$

Route (λ)

Using the equation of inverse square power PDFs we have:

$$\mathbf{f}(\boldsymbol{x}) = x\alpha e^{-kEx}$$

In order to find λα we have:

$$\int_0^{90} x\alpha e^{-kEx} dx = 1 \;\rightarrow\; -\frac{1}{kE} x\alpha \int_0^{90} \left(e^{-kEx}\right)' dx = 1 \rightarrow -\frac{1}{kE} x\alpha\left(e^{-90kE} - 1\right) = 1$$

$$\rightarrow \quad \boldsymbol{xa} = \frac{\boldsymbol{kE}}{\mathbf{1} - \boldsymbol{e}^{-\mathbf{90}\boldsymbol{kE}}}$$

So, $\mathbf{f}(\boldsymbol{x}) = \frac{\boldsymbol{kE}}{\mathbf{1}-\boldsymbol{e}^{-\mathbf{90}\boldsymbol{kE}}} \frac{\mathbf{25}}{\mathbf{E}^2} \boldsymbol{e}^{-\boldsymbol{kEx}}$

The cumulative distribution function of the route λ is*:*

$$F(x1) = \int_0^{x1} \frac{kE}{1 - e^{-90kE}} e^{-kEx} dx = -\frac{1}{kE} \frac{kE}{1 - e^{-90kE}} \left(\mathrm{e}^{-\mathrm{x1kE}} - 1\right)$$

$$= -\frac{\mathbf{1}}{\mathbf{1} - \boldsymbol{e}^{-\mathbf{90}\boldsymbol{kE}}} \left(\mathbf{e}^{-\mathbf{x1kE}} - \mathbf{1}\right)$$

Suppose $-\frac{\mathbf{1}}{\mathbf{1}-\boldsymbol{e}^{-\mathbf{90}\boldsymbol{kE}}}\left(\mathbf{e}^{-\mathbf{x1kE}} - \mathbf{1}\right) = \boldsymbol{R} \rightarrow \boldsymbol{x1} = \frac{\boldsymbol{ln}(\mathbf{1}-\boldsymbol{R}(\mathbf{1}-\boldsymbol{e}^{-\mathbf{90}\boldsymbol{kE}}))}{-\boldsymbol{kE}}$

In order to produce 10^6 spheres and produce collisions among them, which we are going to count, we use the above equation results in the *R* (ass1_1.r) shown below:

```
Nspheres = 10^3
k1 = 1
k2 = 2
k3 = 3
L = 90
H = L/10
R1 = runif(Nspheres, min=0, max=1)
theta = (pi*R1)/4
R2 = runif(Nspheres, min=0, max=1)
E = 25/(5-4*R2)
collisions = 0
spheres = matrix(0, nrow=1, ncol=Nspheres)   # collisions per sphere
x0 = tan(theta)*H                       # distance until the first collision to the strings
for(i in 1:Nspheres){
        if(x0[i] <= L){                 # if distance <= length of elastic layer ==> collision occurs
                x = x0[i]
                repeat{
                        collisions = collisions + 1
                        spheres[i] = spheres[i] + 1
                        y = (x/3) %% 3   # with x position in the elastic layer known, the
```

```
string that it collides with is found using the molulo 3
                              R = runif(1, min=0, max=1)
                              if((y >= 0) & (y < 1)){               # string with k1
                                        k=k1
                              }
                              else if((y >= 1) & (y < 2)){          #string with k2
                                        k=k2
                              }
                              else{                                                    #string  with
k3
                                        k=k3
                              }
                              xi = log(1-R*(1-exp(-k*E[i]*90)))/(-k*E[i])

                              x = x + xi   # adding distance to previous distance of each sphere
                              if(x > L){          #  do  until  sphere  reaches  the  end  of  the  elastic
layer
                                        break
                              }
                    }
          }
}
print(paste("The total number of collisions on the elastic layer is: ",collisions))
```

After running the above *R* code in R console the printed results for the total number of collisions on the elastic layer was:

```
[1] "The total number of collisions on the elastic layer is:  1734762552"
```

<u>1.2.</u>

To find the median number of collisions per sphere we just have to do the computation

$$\frac{Collisions}{Nsphere}$$

So we appended the above code in the *R* (ass1_1.r) with the following lines:

```
median_collisions = collisions/Nspheres
print(paste("The   median   number   of   collisions   per   sphere   on   the   elastic   layer   is:
",median_collisions))
```

and the result found was:

```
[1] "The median number of collisions per sphere on the elastic layer is: 1734.762552"
```

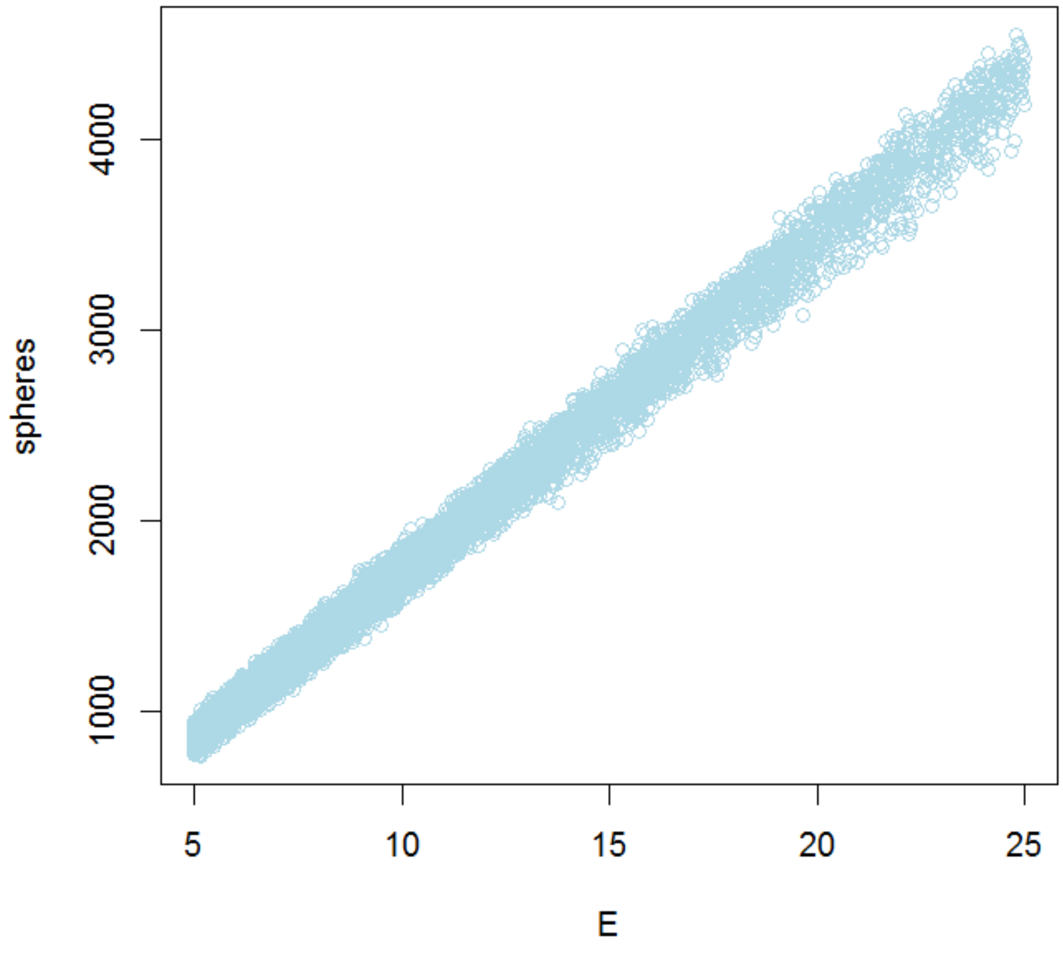
1.3.

In order to find how the total number of collisions per sphere is affected from the sphere's energy we plotted each **sphere[i] energy** *per* **the total collisions of sphere[i]**, by appending the above code in the *R* (ass1_1.r) with the following lines:

```
print("The plot of sphere's energy per sphere collisions is: ")
plot(E,spheres,col="lightblue")
```

and the result returned the graph below:

```
[1] "The plot of sphere's energy per sphere collisions is: "
```



1.4.

In order to find how the total number of collisions per sphere is affected from the sphere's angle we plotted each **sphere[i] angle** *per* **the total collisions of sphere[i]**, by appending the above code in the *R* (ass1_1.r) with the following lines of the next page:

```
print("The plot of sphere's angle per sphere collisions is: ")
windows()         # Windows
#X11()            # Unix
#quartz()         # Mac
plot(theta,spheres,col="blue")
```

and the result returned the graph below:

```
[1] "The plot of sphere's angle per sphere collisions is: "
```