NE451 Solution: Homework assignment 2

Fall 2019. Instructor: Dr. Jeff Chen

Prob. 1. [3-3. Computational]
[Pseudo code]

```
N=10    XL=20
DEFINE X(N), Y(N), ISEED
* J LOOP FROM 1 TO N
****************************************
5
X0=RAN(ISEED)*XL
Y0=RAN(ISEED)*XL
IF(J.EQ.1)GOTO NEXT J
****************************
K LOOP FROM 1 TO J-1
R2=(X0-X(K))**2+(Y0-Y(K))**2
IF (R2 is less or equal to 1.5**2 )GO BACK TO 5
END K LOOP
****************************
X(J)=X0
Y(J)=Y0
WRITE X0,Y0 FOR PLOTTING
TH=RAN(ISEED)*2PI
COSTH = COS(TH)
SINTH = SIN(TH)
WRITE COSTH,SINTH FOR PLOTTING
* END J LOOP
****************************************
```

[Plot]

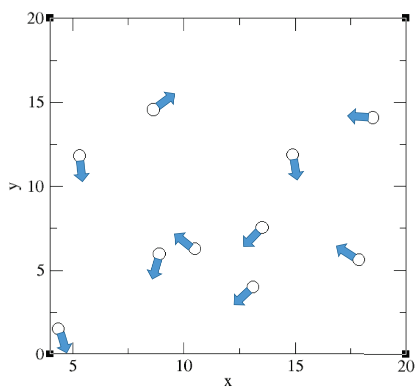

FIG. 1: Generating 10 positions randomly in a xy box. The arrows represent u_x and u_y required.

Prob. 2. [3-4. Computational]
[Pseudo code]

```
Initializing  XL =20,  X0=XL/2.0,  V=1,  M=10**5,
H=0.001
X1=X0+V*H
****************************************
J LOOP from 1 to M
T=T+H
F = 10.0/X1**11 - 10.0/(XL-X1)**11
X=2.0*X1-X0 + F*H*H
V=(X-X1)/H
POT = 1/X1**10 + 1/(XL-X1)**10
EN=0.5*V*V+POT
WRITE T,X
WRITE T,EN
X0=X1
X1=X
END J LOOP
****************************************
```

[Plot]

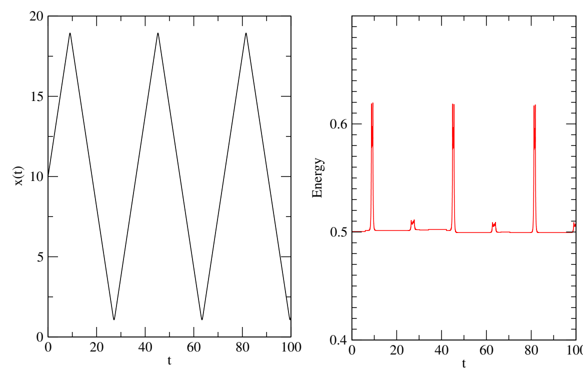

FIG. 2: Trajectory $x(t)$ and the total energy $E(t)$ as functions of t in 10^5 steps.

Prob. 3. [3-7. Computational]
[**Pseudo code**] (Brief version)
Initialization: same as in the previous two.
Add: Loop through $I = 1, N$ to obtain

$$\vec{r}_1(i) = \vec{r}_0(i) + h\vec{v}(i)$$

****
J LOOP from 1 to M (time loop)
T=T+H
I LOOP from 1 to N (particle loop)
FX calculated, FY calculated (need another loop to go through all particles and all walls)
Then

$$\vec{r}_{\rm new}(i) = 2\vec{r}_1(i) - \vec{r}_0(i) + h^2\vec{F}$$

END I Loop (particle loop)
WRITE the coordinates as required.
END J Loop (time loop)
****

[**Plot**]

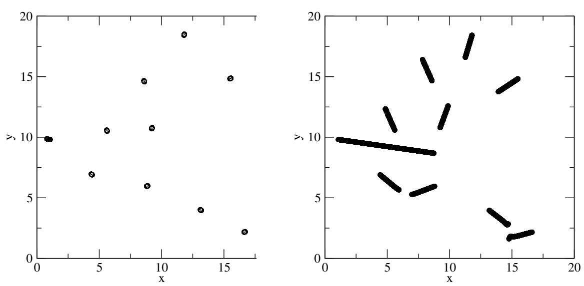

FIG. 3: Trajectories of the particles in $t \leq 0.1$ and $0.1 \leq t \leq 2$.

Prob. 4. [3-9. Analytical]
[**Write down...**] From a statistical mechanics book, one has

$$f(\vec{v}) = \exp\left(-m\vec{v}^2/2k_BT\right). \tag{1}$$

[**Reduced version**]
Using the reduced temperature, then

$$m\vec{v}^2/2k_BT = \frac{mk_B\sigma^2\vec{\tilde{v}}^2}{2\tau^2\epsilon\tilde{T}}$$

Now $\tau^2 = \sigma^2 m/\epsilon$, hence

$$f(\vec{\tilde{v}}) = \exp\left(-\vec{\tilde{v}}^2/2\tilde{T}\right). \tag{2}$$

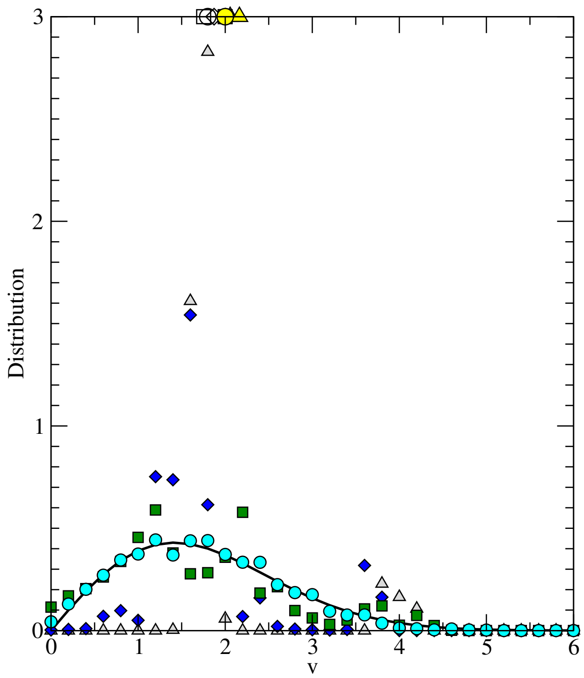

FIG. 4: Comparison of the distribution functions. The solid curve is plotted according to the Maxwell speed distribution for a 2D system. The cyan circles, green squares, blue diamonds, and grey triangles are the historgrams collected for this distribution when $M = 10^6, 10^5, 10^4, 10^3$, respectively. Added to the top of the graph are the results for $\bar{v}$ (unfilled) and $\sqrt{\bar{v^2}}$ (yellow), where again, $M = 10^6, 10^5, 10^4, 10^3$ are represented by circles, squares, diamonds, and triangles.

Prob. 5. [3-10, Numerical]
[Pseudo code 1: running MD]

1. **Initialization**. Declare array sizes for $\mathbf{r}_0$ (old-old coordinates), $\mathbf{r}_1$ (old coordinates), $\mathbf{v}$ (velocity), and H (histogram); set M (total steps), L (box size), N (number of particles), h (time step), γ (Berendson coefficient), Δ (used in collecting histogram; I set $\Delta = 0.2$) and $\tilde{T}$ (temperature).

2. **Preparation**. Set $\mathbf{r}_0$; Based on $\tilde{T}$, estimate $v2$, set $\mathbf{v}$ to magnitude $\sqrt{v2}$ according to Prob. 3-3; Define K_0 using $\tilde{T}$; Initializing H to zero if needed. Set $\mathbf{r}_1$ by using one-step Euler.

3. **Start time loop**.

4. **First particle loop**. Start first particle loop; calculate $\mathbf{v}$; add to K (kinetic energy); collect average for $\bar{v}$ and $\bar{v^2}$; collect statistics for H based on each molecule's speed. End first particle loop. Calculate $B = \gamma(K_0/K - 1)$ as a coefficient.

5. **Second particle loop**. Start second particle loop; Calculate auxiliary forces (wall and Berendson force). Start another particle loop to calculate interaction force based on LJ expression. End of another particle loop. Update the coordinates $\vec{r}_{\rm new}$ using Verlet. Let $\mathbf{r}_0 = \mathbf{r}_1$ and $\mathbf{r}_1 = \mathbf{r}_{\rm new}$. End of second particle loop.

6. **End time loop**.

7. **Finalizing...**. Calculate $\bar{v}$, $\bar{v^2}$; write these and the histogram.

[Pseudo code 2: Normalization of the histogram]

1. **Initialization**. Define Δ; read the H histogram; Define a function $f = v\exp(-v^2/2\tilde{T})$ — note the equal sign and the extra v.

2. **Finding the area**. Adding $H * \Delta$ to produce A_H. Adding $f * \Delta$ to produce A_f.

3. **Normalization**. Let H/A_H and $f = f/A_f$. Record your data for plotting.