

Since our experiment is similar to LISA, we also want to obtain the 'ForceSqr' variable. As you mentioned before, you defined it as the sums of $m \cdot v^2$ components. It makes me confused. I give my calculation below.

#	Area	Temperature [K]	Imping rate	Pressure [mbar]	v.mol speed [m/s]	MC Hits	Equiv hits	Force	Force^2
1	21.16	293.15	3.60862e+22	0.00995376	584.948	31330179	3.13302e+07	0.002106 N (-3.486e-07, -2.953e-07, -0.002106)	4.531e-26 N^2 (1.851e-26, 1.85e-26, 3.699e-26)

Fig 1

As shown in fig 1, a screenshot at a certain time. Firstly, I make a simple check to the Force result. According to the document, the force should be calculated by eq. (1).

$$F_i = \frac{\sum dI}{dt} = \frac{\sum_{j=1}^{N_{hit,j}} I_{\perp,i,j} \cdot K_{\frac{real}{virtual}}}{t_{window}} \approx \frac{N_{hit,i} \langle I_{\perp,i} \rangle \cdot K_{\frac{real}{virtual}}}{t_{window}} \quad (1)$$

In this moment, the hits are 31330179, $t_{window} = 1e-4$. Since the collision type is diffuse, so the average momentum is about $m_0 \cdot \sqrt{2 \cdot \pi \cdot k_B \cdot T / m_0}$ in the normal direction.

$$\text{In}[2] := \int_0^\infty \int_0^\infty \left(e^{-\frac{y^2}{v^2}} \frac{2y}{v^2} e^{-\frac{z^2}{v^2}} \frac{2z}{v^2} (y+z) \right) dy dz$$

$$\text{Out}[2] = \text{ConditionalExpression}\left[\frac{\sqrt{\pi}}{\sqrt{\frac{1}{v^2}}}, \text{Re}[v^2] > 0\right] \quad (v = \sqrt{\frac{2k_B T}{m}})$$

The velocities in the normal direction obey the Rayleigh distribution. $K_{\{real/test\}}$ can be calculated by the imping rate.

$$K_{\frac{real}{virtual}} = \frac{z t_{window} A}{N_{hit,i}}$$

The I obtain 0.00210153 N, closed to the simulated result.

$$\text{In}[5] := k_B = 1.3806503 \times 10^{-23}; T = 293.15; m = 18 \times 1.670539066 \times 10^{-27}; A = 21.16 \times 10^{-4};$$

$$F = \frac{31330179}{10^{-4}} m \sqrt{\frac{2 \pi k_B T}{m}} \frac{3.60862 \times 10^{22} \times 10^{-4}}{31330179} A$$

$$\text{Out}[6] = 0.00211153$$

For the calculation of ForceSqr, I list two possible equation that you may used.

$$F_i^2 = \frac{\sum dI^2}{dt^2} = \frac{\sum_{j=1}^{N_{hit,j}} I_{\perp,i,j}^2 \cdot K_{\frac{real}{virtual}}}{t_{window}^2} \approx \frac{N_{hit,i} \langle I_{\perp,i}^2 \rangle \cdot K_{\frac{real}{virtual}}}{t_{window}^2} \quad (3)$$

$$F_i^2 = \frac{\sum dI^2}{dt^2} = \frac{\sum_{j=1}^{N_{hit,j}} I_{\perp,i,j}^2 \cdot K_{\frac{real}{virtual}}}{t_{window}^2} \approx \frac{N_{hit,i} \langle I_{\perp,i}^2 \rangle \cdot K_{\frac{real}{virtual}}}{t_{window}^2} \quad (4)$$

Similar to the above calculation, the $\langle I_{\perp,i}^2 \rangle$ is about $m_0^2 \cdot \{(4+\pi) \cdot k_B \cdot T / m_0\}$.

$$\int_0^\infty \int_0^\infty \left(e^{-\frac{y^2}{v^2}} \frac{2y}{v^2} e^{-\frac{z^2}{v^2}} \frac{2z}{v^2} (y+z)^2 \right) dy dz$$

$$\text{ConditionalExpression}\left[\frac{1}{2} (4 + \pi) v^2, \text{Re}[v^2] > 0\right]$$

Inserting these parameters into eqs. (3) and (4), the result is

$$\text{In[12]:= FSqr1} = \frac{31\,330\,179}{10^{-8}} \text{ m}^2 (4 + \pi) \frac{k_B T}{m} \frac{3.60862 \times 10^{22} \times 10^{-4}}{31\,330\,179} \text{ A}$$

$$\text{FSqr2} = \frac{31\,330\,179}{10^{-4}} \text{ m}^2 (4 + \pi) \frac{k_B T}{m} \frac{3.60862 \times 10^{22} \times 10^{-4}}{31\,330\,179} \text{ A}$$

$$\text{Out[12]= } 6.63674 \times 10^{-22}$$

$$\text{Out[13]= } 6.63674 \times 10^{-26}$$

Therefore, Eq. (4) may be the possible method in your code. But I'm not sure the discrepancy between 6.63674e-26 and 3.699e-26.

In fact, Eq. (3) should be more suitable. For example, from a quantitative point of view

$$F_i = \frac{N_{hit,i} \langle I_{\perp,i} \rangle \cdot K_{\frac{real}{virtual}}}{t_{window}} \Leftrightarrow \frac{1 \cdot \text{kg} \cdot \text{m} / \text{s} \cdot 1}{s} = \text{kg} \cdot \frac{\text{m}}{\text{s}^2} = \text{Newton}$$

But

$$F_i^2 = \frac{N_{hit,i} \langle I_{\perp,i}^2 \rangle \cdot K_{\frac{real}{virtual}}}{t_{window}^2} \Leftrightarrow \frac{1 \cdot (\text{kg} \cdot \text{m} / \text{s})^2 \cdot 1}{s^2} = \left(\text{kg} \cdot \frac{\text{m}}{\text{s}^2} \right)^2 = \text{Newton}^2$$

$$F_i^2 = \frac{N_{hit,i} \langle I_{\perp,i}^2 \rangle \cdot K_{\frac{real}{virtual}}}{t_{window}} \Leftrightarrow \frac{1 \cdot (\text{kg} \cdot \text{m} / \text{s})^2 \cdot 1}{s} = \left(\text{kg} \cdot \frac{\text{m}}{\text{s}^2} \right)^2 s = \text{Newton}^2 \cdot s$$