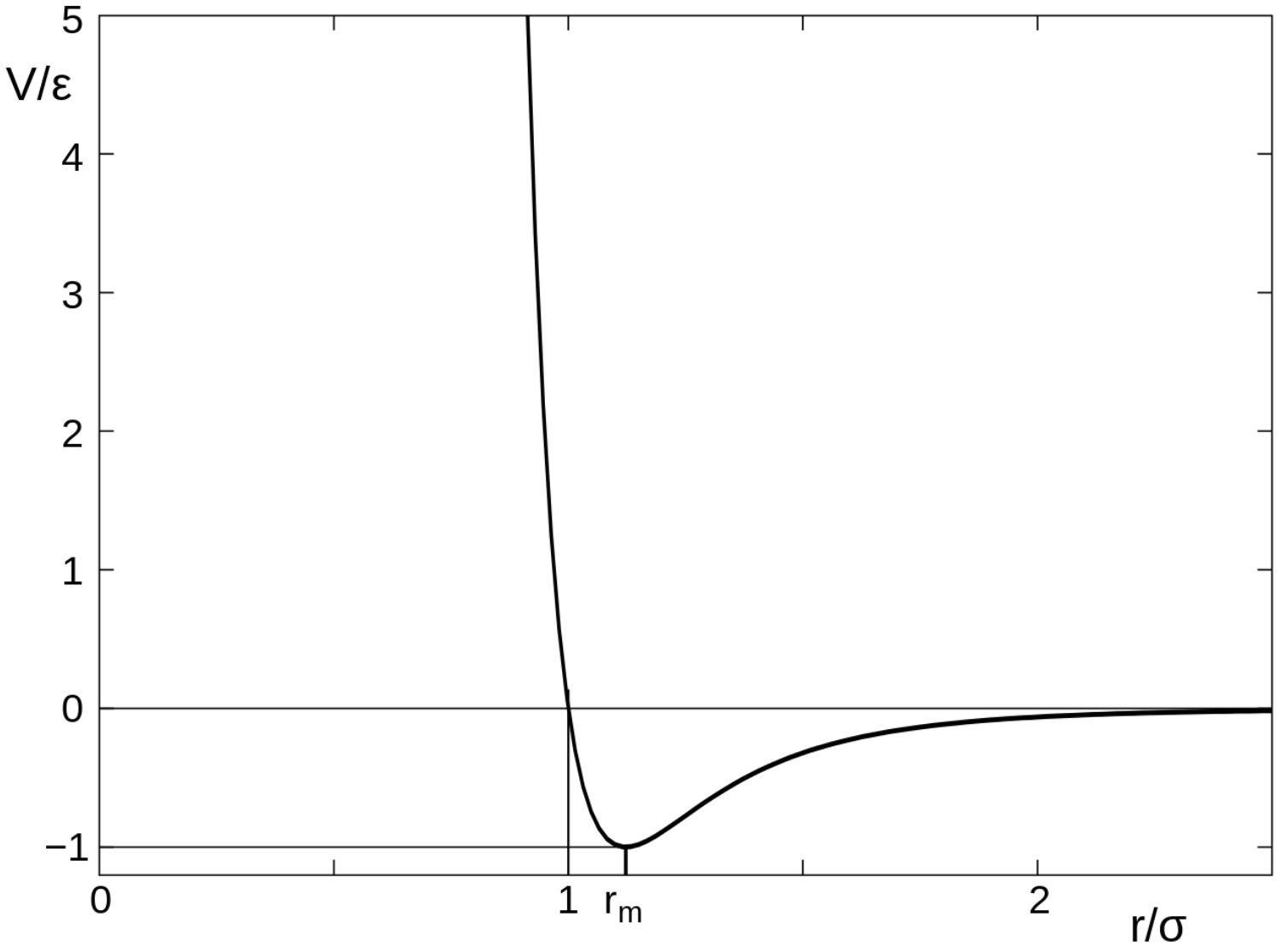
期末專題
氣體分子位能場模擬

組員
陳宗恩
鄭篤容
張哲維

目的

- 理想氣體模型
- 加入位能場
- 觀測機率分布圖
- 觀測方程式是否符合
- 在低溫狀態下相變

Lennard-Jones Potential



Lennard-Jones Potential

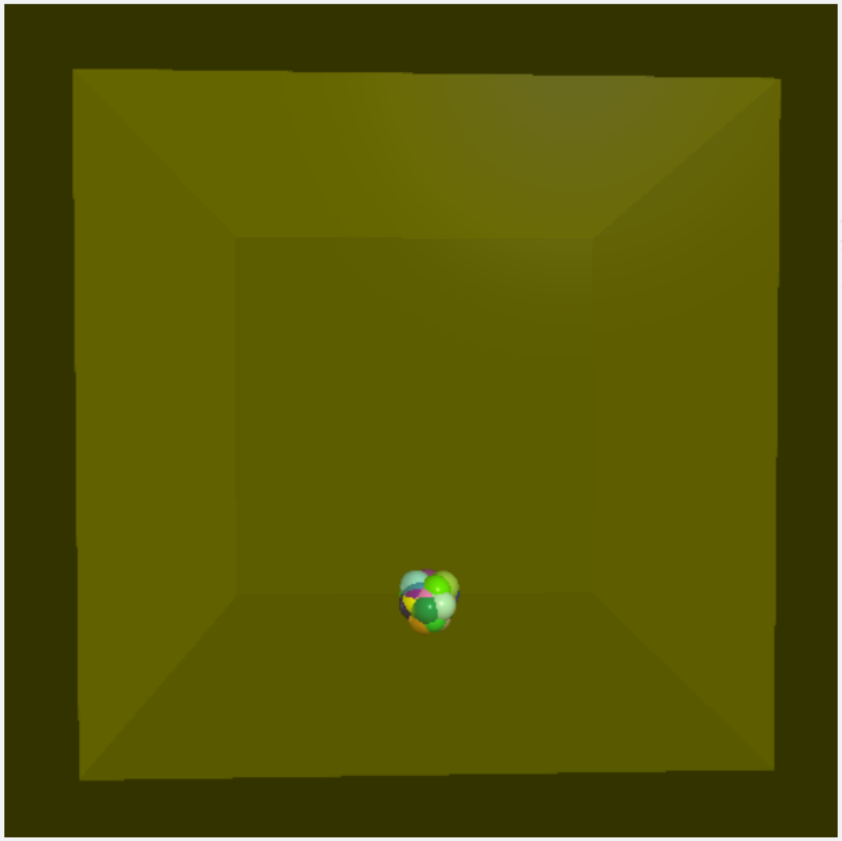
- 位能場 (6-12 potential)
- $V_{LJ} = 4\varepsilon[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}]$
- 位能場作用力
- $\vec{F}_{LJ} = -\vec{\nabla}V = 4\varepsilon(\frac{12\sigma^{12}}{r^{14}} - \frac{6\sigma^{6}}{r^{8}})\vec{r}$

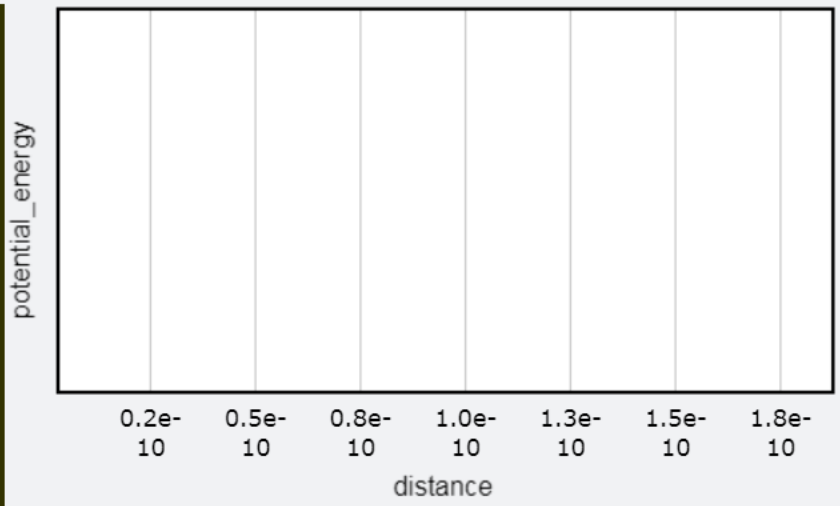
模擬方法

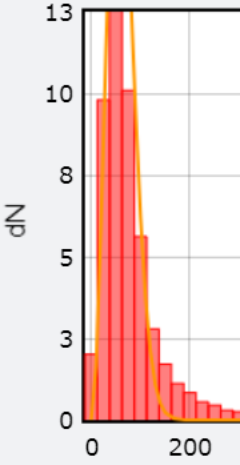
```
for i in range(N-1):
    a_a[i] += np.array([0,-9.8,0])          #consider gravity
    for j in range(i+1,N):
        distance = sum((p_a[i]-p_a[j])**2)**0.5
        if distance > 10*sigma:
            continue
        if distance < 3*sigma:
            continue
        force = (LJ_force_on_particle(p_a[i],p_a[j]))
        a_a[i] += force/m
        a_a[j] += -1*force/m
```

模擬方法

```
#算kk次
  for i in range(N-1):
     for j in range(i+1,N):
        distance = sum((p_a[i]-p_a[j])**2)**0.5
        if distance <= (2**(1/6))*sigma:
           v_a[i],v_a[j] = vcollision(p_a[i],p_a[j],v_a[i],v_a[j])
  elif distance <= 2*sigma:
```





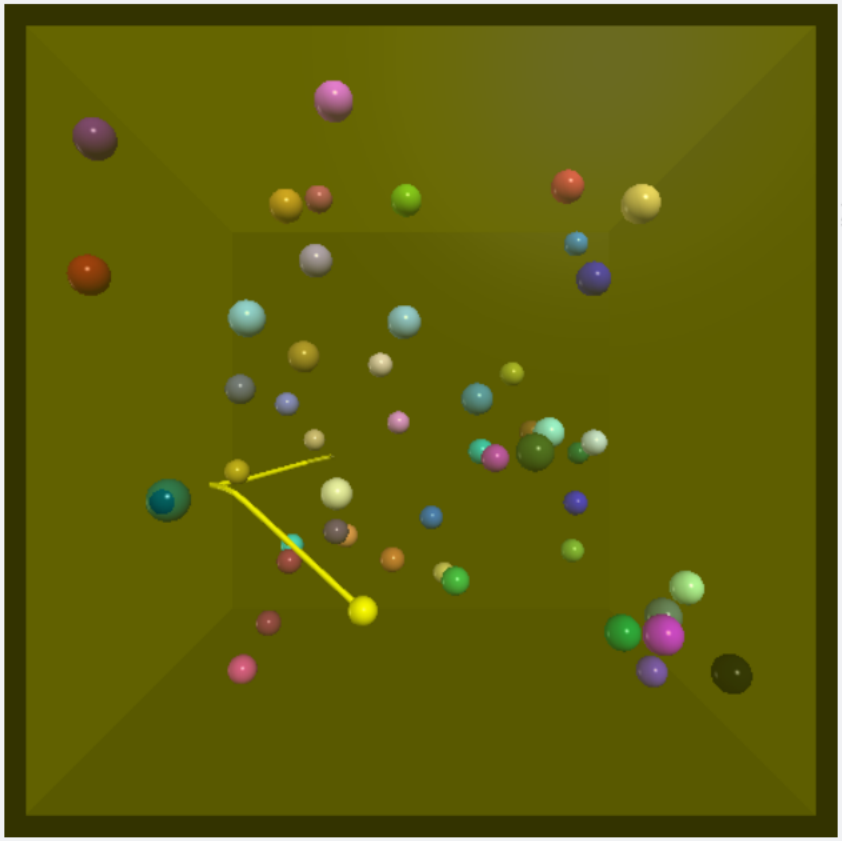


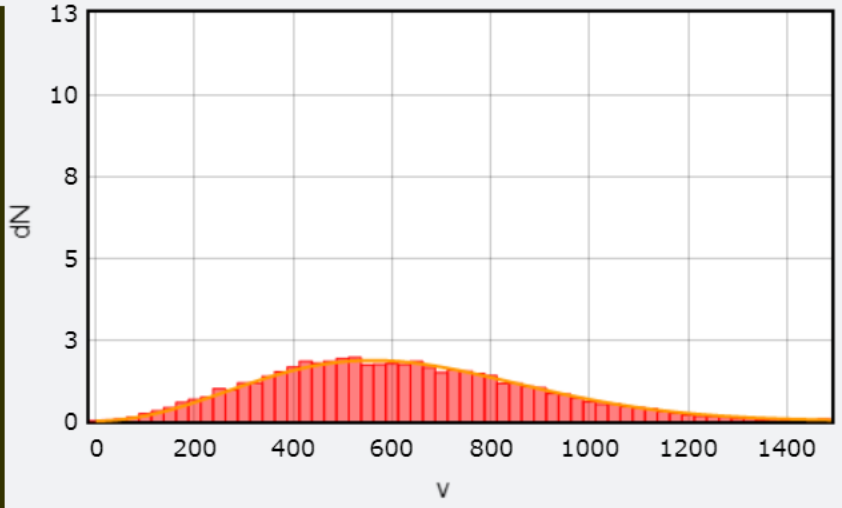
模擬方法

```
if distance > 5*sigma:
        continue
    if distance < 2*sigma:
        continue
    force = (force_on_particle(p_a[i],p_a[j]))
    a_a[i] += force/m
    a_a[j] += -1*force/m #反作用力
```

模擬方法

```
#算kk次
  for i in range(N-1):
     for j in range(i+1,N):
        distance = sum((p_a[i]-p_a[j])**2)**0.5
        if distance <= sigma: ##(2**(1/6))*
           pass
           ## why pass?
        elif distance <= 2*sigma:
```




13
10
8
5
3
0
Np
0
200
400
600
800
1000
1200
1400
v

符合的方程式

- $PV = NkT$ 理想氣體

- $PV = NkT + \frac{1}{3}\left\langle \sum_{i<j}^{N} r_{ij} \cdot f_{ij} \right\rangle$

匯出資料成CSV檔（outputresult.py）

```
#需要import math
        import csv
        import datetime

#使用define 將得到的資料匯出成CSV
def outputresult():

#將開始執行程式的時間定成CSV檔名
x = datetime.datetime.now()
foldername='{0}_{1}{2}_{3}{4}{5}'.format(x.year,x.month,x.day,x.hour,x.minute,x.second)
```

參考資料

- https://en.wikipedia.org/wiki/Lennard-Jones_potential
- http://www.sklogwiki.org/SklogWiki/index.php/Sutherland_potential
- http://personal.rhul.ac.uk/UHAP/027/PH4211/PH4211_files/sutherland.pdf
- http://phys.ubbcluj.ro/~tbeu/MD/C2_for.pdf