## Will

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## 1 Global Swap Algorithm

1. MCS + 1, Time +  $\frac{1}{4L^2 10^6}$ 

- 2. Then we choose two random positions in the system, say i & j. (Since its global swap, they do not have to be neighbors.)
- 3. We then consider whether we will accept this SWAP between i & j, which is based on SWAP rate.
- 4. To Calculate SWAP rate.
  - (a) We set  $\Delta E$  as the change of system energy due to this SWAP (simply meaning SWAP positions i & j).
  - (b) For *i* & *j*, if they are both voids, we set  $\Delta E = 0$ .
  - (c) If not, we consider their surrounding particles Ki, Kj. (Ki represents the surrounding particles of i). Then, say position i has a particle Pi, we make  $\Delta E + \Sigma bond(Pi, Ki) \Sigma bond(Pi, Kj)$ . Similar for Pj.
  - (d)  $\omega_0 = 10^6, E_0 = 1.5$

$$\text{SWAP rate} = \begin{cases} \omega_0 exp(-\frac{E_0}{K_BT}) & \Delta E > 0\\ \omega_0 exp(-\frac{E_0 + \Delta E}{K_BT}) & \Delta E \le 0 \end{cases}$$

- 5. accept the swap with probability  $\frac{\text{SWAP rate}}{10^6}$
- 6. If accepted, we swap the positions of i & j, and change the energy of the system based on  $\Delta E$ .