Lecture 9: Molecular Dynamics Simulation: Ewald Summation

Theories in Statistical Mechanics and Molecular Dynamics Simulations

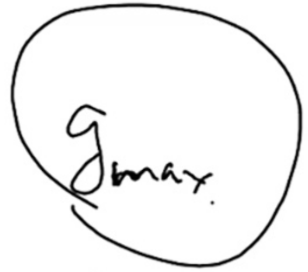
Smooth Particle Mesh Ewald

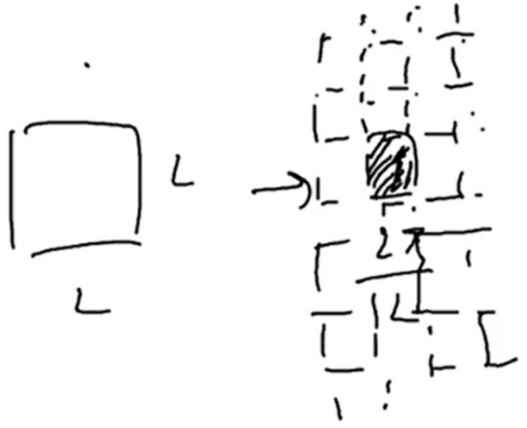
Smooth Particle -Mesh Ewald

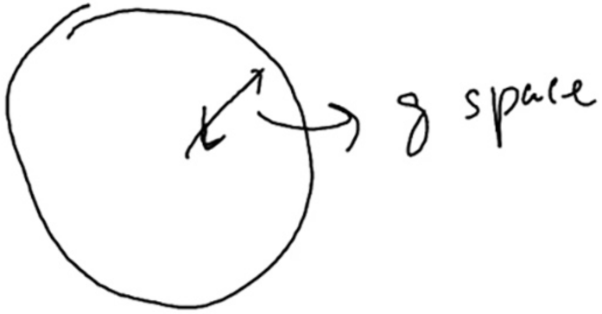
$$U_{long}(\vec{r}_1, \ldots \vec{r}_N) = \frac{1}{V} \sum_{\vec{g} \in S} \frac{4\pi}{|\vec{g}|^2} e^{-|\vec{g}|^2/4\alpha^2} \underline{|S(\vec{g})|^2}$$

$-$ correction

$$S(\vec{g}) = \sum_j q_j e^{i\vec{g}\cdot\vec{r}_i}$$







$O(N^2)$

Fast Fourier Transform

$$S(\vec{g}) = \sum_j q_j e^{i\vec{g}\cdot\vec{r}_j} = \frac{1}{V}\int_V d\vec{r}\, \boxed{\sum_j q_j\, \delta(\vec{r}-\vec{r}_j)}\, e^{i\vec{g}\cdot\vec{r}}$$

Fast Fourier Transform (FFT)

$\vec{x} = (x_1 \cdots\cdots x_N)$

$\vec{y}$: $y_k = \sum_j e^{2\pi i kj/N} x_j$

Fourier Transform

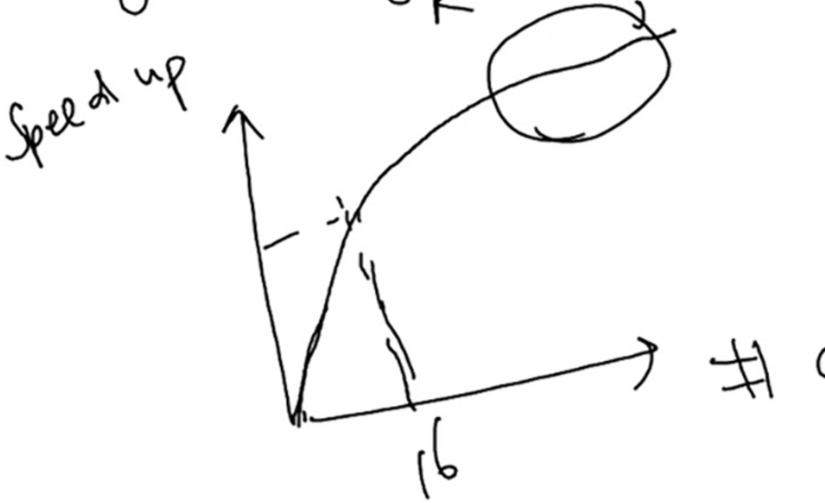
$O(N^2)$

FFT

$O(N \log N)$

$< O(N^{1+\varepsilon})$

for $\forall\, \varepsilon > 0$



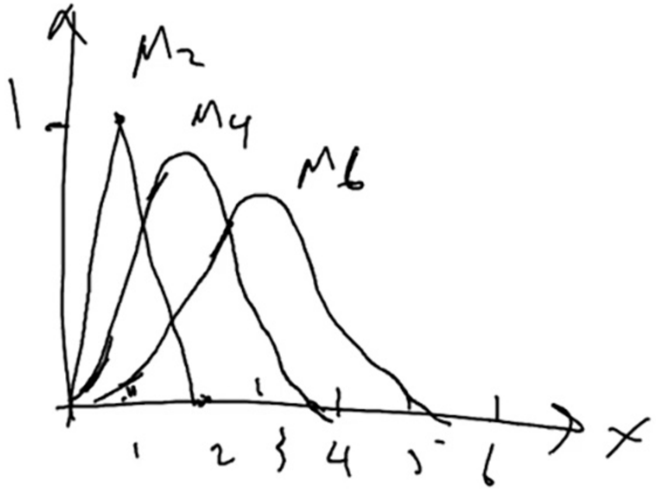
"Smearing" Charge

"Smearing" charge

$M_n(x)$

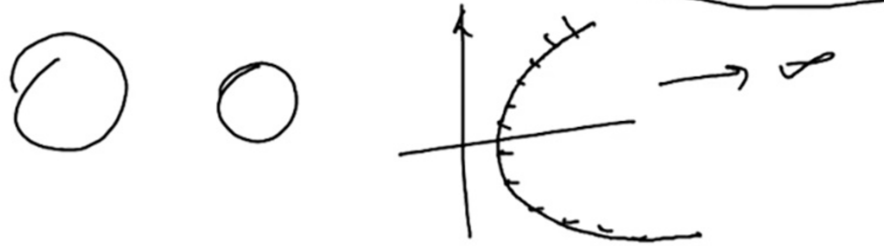
Cardinal B-spline functions

$$M_2(x) = \begin{cases} 1-|x-1| & 0 \le x \le 2 \\ 0 & x<0 \text{ or } x>2 \end{cases}$$



$$M_n(x) = \frac{x}{n-1} M_{n-1}(x) + \frac{n-x}{n-1} M_{n-1}(x-1)$$

① $M_n(x)$ is compact support.



“Smearing” Charge …

② $M_n(x)$ is $n-2$ continues differentiable.

③ $$\frac{dM_n}{dx} = M_{n-1}(x) - M_{n-1}(x-1)$$

④ $$M_n(x) = M_n(n-x)$$

⑤ $$\sum_{j=-\infty}^{+\infty} M_n(x-j) = 1$$

S(n)

$$\vec{s}_j = \vec{r}_j / L \rightarrow e^{i\vec{g}\cdot\vec{r}} = e^{2\pi i \vec{n}\cdot\vec{s}_j}$$

$$\vec{n} = (\vec{n}_a, \vec{n}_b, \vec{n}_c)$$

$$e^{2\pi i \vec{n}\cdot\vec{s}_j} \rightarrow e^{2\pi i \vec{n}\cdot\vec{u}_j / N_e}$$

$$\vec{u}_j = N_e \vec{s}_j \rightarrow$$

$$e^{2\pi i n_a u_{ia}/N_e} = b_n(n_a) \sum_{k=-\infty}^{+\infty} M_n(u_{ia} - k)\, e^{2\pi i n_a k / N_e}$$

$$b_n(\nu) = e^{2\pi i (n-1)\nu / N_e} \sum_{k=0}^{n-2} M_n(k+1)\, e^{2\pi i \nu k / N_e}$$

$$S(\vec{n}) = b_n(n_x)\, b_n(n_y)\, b_n(n_z)\, \tilde{Q}(\vec{n})$$

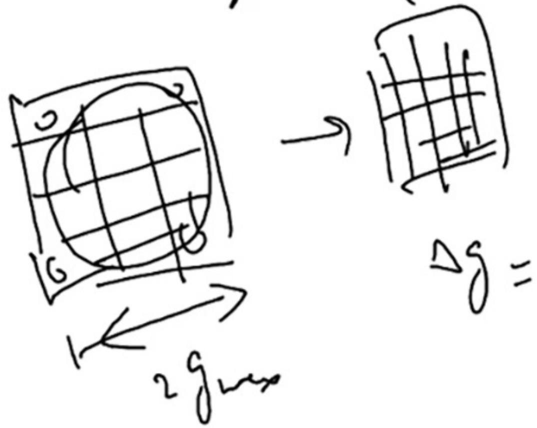
$$\tilde{Q}(\vec{n}) = \sum_{k_x, k_y, k_z = 0}^{N_e - 1} e^{2\pi i n_x k_x / N_e}\, e^{2\pi i n_y k_y / N_e}\, e^{2\pi i n_z k_z / N_e} \times \boxed{Q(\vec{k})}$$

Q(k)

$$Q(\vec{k}) = \sum_{i=1}^{N} q_i \sum_{\hat{j}_1,\hat{j}_2,\hat{j}_3} M_n(u_{x,i} - k_x - \hat{j}_1 N_e) \times$$

$$M_n(u_{y,i} - k_y - \hat{j}_2 N_e) \times$$

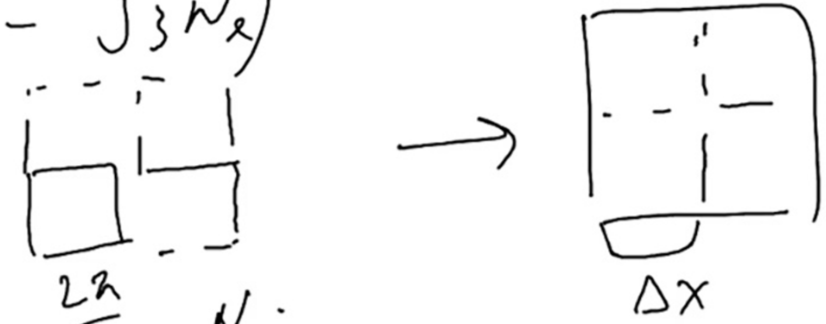
$$M_n(u_{z,i} - k_z - \hat{j}_3 N_e)$$



g_{max}

$$\Delta g = \frac{2\pi}{L}$$

$$N = \frac{g_{max}}{\Delta g} = \frac{g_{max} L}{2\pi}.$$



$$\Delta x = \frac{L}{N} = \frac{L}{g_{max} L / 2\pi} = \frac{2\pi}{g_{max}}$$