

$$E = \frac{1}{4\pi\epsilon_0} \sum_{n_x, n_y, n_z} \sum_{i,j} \frac{q_i q_j}{|r+nL|}$$

E_{real}

$E_{\text{correct.}}$

E_{dipol}

E_{recip}

short ranged
 $\rightarrow \mathcal{O}(N)$

constant

boundary ϵ'
 $\sim (2\epsilon' + 1)^{-1}$

standard Ewald
 $\rightarrow \mathcal{O}(N^{3/2})$

MESH BASED ALGORITHMS

calculation of E_{recip} on a mesh
 $\rightarrow \mathcal{O}(N \log(N))$

PME
 Lagrange interpolation

SMOOTH PME
 smooth Euler B-spline interpolation

P³M
 optimized influence function