

\* Tail Corrections for pair-style lj/expand \*

(1)

$$\text{Interaction Energy: } E_{\text{int}} = 4\epsilon \left[ \left( \frac{\sigma}{r-\Delta} \right)^{12} - \left( \frac{\sigma}{r-\Delta} \right)^6 \right]$$

for  $r < r_c + \Delta$   
————— (1)

$r_c$  is the user-defined cut-off

$r_c + \Delta$  is the actual force cut-off

According to Allen and Tildesley (pg 65), contribution to the energy ( $E_{\text{tail}}$ ) and pressure ( $P_{\text{tail}}$ ) due to cut-off are given by

$$E_{\text{tail}} = 2\pi N \rho \int_{r_c}^{\infty} r^2 E_{\text{int}}(r) dr \quad \text{———— (2)}$$

$$P_{\text{tail}} V = -\frac{2}{3} \pi N \rho \int_{r_c}^{\infty} r^3 \frac{dE_{\text{int}}(r)}{dr} dr \quad \text{———— (3)}$$

From (1) and (2)

$$E_{\text{tail}} = 2\pi N \rho * 4\epsilon * \int_{r_c + \Delta}^{\infty} r^2 \left[ \left( \frac{\sigma}{r-\Delta} \right)^{12} - \left( \frac{\sigma}{r-\Delta} \right)^6 \right] dr$$

Let  $\pi = r - \Delta$   
 $\therefore d\pi = dr$

$$E_{\text{tail}} = 2\pi N \rho * 4\epsilon * \int_{r_c + \Delta - \Delta}^{\infty} (\pi + \Delta)^2 \left[ \left( \frac{\sigma}{\pi} \right)^{12} - \left( \frac{\sigma}{\pi} \right)^6 \right] d\pi$$

(2)

~~On simplification and integration,~~

$$E_{\text{tail}} = 8\pi N\psi \epsilon \sigma^6 \int_{r_c}^{\infty} (\pi^2 + \Delta^2 + 2\pi\Delta) \left[ \sigma^6 \left( \frac{1}{\pi^{12}} \right) - \left( \frac{1}{\pi^6} \right) \right] d\pi$$

On Integration and simplification,

$$E_{\text{tail}} = 8\pi N\psi \epsilon \sigma^6 \left[ \sigma^6 \left( \frac{1}{9r_c^9} + \frac{\Delta}{5r_c^{10}} + \frac{\Delta^2}{11r_c^{11}} \right) - \left( \frac{1}{3r_c^3} + \frac{\Delta}{2r_c^4} + \frac{\Delta^2}{5r_c^5} \right) \right]$$

On comparing this formula to the init-one function on ~~pair-style-lj/expand~~ pair-lj-expand.cpp (line 226), it seems as though

X double shiftcut = shift[i][j] - cut[i][j];  
should be

✓ double shiftcut = -cut[i][j];

where shift[i][j] =  $\Delta_{ij}$   
cut[i][j] =  $r_{cij}$

~~Sim~~ This would also affect P<sub>tail</sub>.

