

$$V_{\text{total}} = \sum_{\substack{i,j \\ i < j}} U_2(i,j) + \sum_{\substack{i,j \\ i < j < k}} U_3(i,j,k)$$

(2)

$$F_{i,x} = - \sum_{j \neq i} \frac{\partial U_2(i,j)}{\partial r_{ix}} - \sum_{\substack{j \neq i, k \neq i \\ j \neq k}} \frac{\partial U_3(i,j,k)}{\partial r_{ix}}$$

$$* \frac{\partial U_2(i,j)}{\partial r_{ix}} = \frac{\partial U_2(i,j)}{\partial r_{ij}} \cdot \frac{\partial r_{ij}}{\partial r_{ix}} = \frac{\partial U_2(i,j)}{\partial r_{ij}} \cdot \frac{(r_{ix} - r_{jx})}{r_{ij}}$$

$$\{ r_{ij} = [(r_{ix} - r_{jx})^2 + (r_{iy} - r_{jy})^2 + (r_{iz} - r_{jz})^2]^{1/2} \}$$

$$\frac{\partial r_{ij}}{\partial r_{ix}} = \frac{1}{2} \frac{2 \cdot (r_{ix} - r_{jx})}{r_{ij}} = \frac{r_{ix} - r_{jx}}{r_{ij}}$$

~~$$\frac{\partial U_3(i,j,k)}{\partial r_{ix}} = \frac{\partial U_3(i,j,k)}{\partial r_{ij}} \frac{\partial r_{ij}}{\partial r_{ix}} + \frac{\partial U_3(i,j,k)}{\partial r_{ik}} \frac{\partial r_{ik}}{\partial r_{ix}}$$~~

$$* \frac{\partial U_3(i,j,k)}{\partial r_{ix}} = \frac{\partial U_3(i,j,k)}{\partial r_{ij}} \frac{\partial r_{ij}}{\partial r_{ix}} + \frac{\partial U_3(i,j,k)}{\partial r_{ik}} \frac{\partial r_{ik}}{\partial r_{ix}}$$

$$= \frac{\partial U_3(i,j,k)}{\partial r_{ij}} \cdot \frac{(r_{ix} - r_{jx})}{r_{ij}} + \frac{\partial U_3(i,j,k)}{\partial r_{ik}} \cdot \frac{(r_{ix} - r_{kx})}{r_{ik}}$$