

PROPAGATORI PER LA DINAMICA MOLECOLARE

simplettici

LEAP-FROG

notazione

$\vec{r}_{i,m}$    
 ↙ indice di peso temporale   
 ↖ indice di atomo

per iniziazione

$$\vec{v}_{i,0+\frac{1}{2}} = \vec{v}_{i,0} + \frac{\vec{f}_i(\{\vec{r}_{i,0}\})}{m_i} \frac{\Delta t}{2} + O(\Delta t^2)$$

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$$\vec{r}_{i,m+1} = \vec{r}_{i,m} + \vec{v}_{i,m+\frac{1}{2}} \Delta t$$

$$\vec{v}_{i,m+\frac{3}{2}} = \vec{v}_{i,m+\frac{1}{2}} + \frac{\vec{f}_i(\{\vec{r}_{i,m+1}\})}{m_i} \Delta t$$

STÖRMER-VERLET

$$\frac{d^2 \vec{r}_{i,m}}{dt^2} = \frac{\vec{r}_{i,m+1} - 2\vec{r}_{i,m} + \vec{r}_{i,m-1}}{\Delta t^2} + O(\Delta t^2) = \frac{\vec{f}_i(\{\vec{r}_{i,m}\})}{m_i}$$

$$\vec{r}_{i,m+1} = 2\vec{r}_{i,m} - \vec{r}_{i,m-1} + \frac{\vec{f}_i(\{\vec{r}_{i,m}\})}{m_i} \Delta t^2 + O(\Delta t^4)$$

Per iniziazione

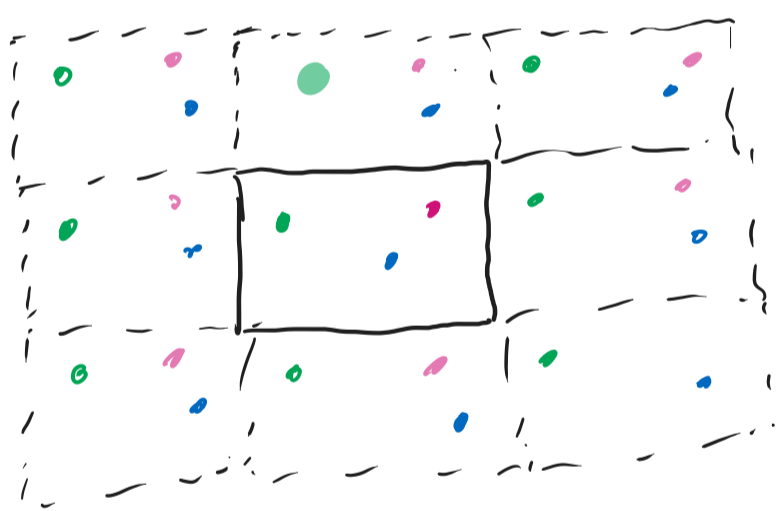
$$\vec{r}_{i,1} = \vec{r}_{i,0} + \vec{v}_{i,0} \Delta t + \frac{1}{2} \frac{\vec{f}_i(\{\vec{r}_{i,0}\})}{m_i} \Delta t^2 + O(\Delta t^3)$$

VELOCITY-VERLET

$$\vec{r}_{i,m+1} = \vec{r}_{i,m} + \vec{v}_{i,m} \Delta t + \frac{1}{2} \frac{\vec{f}_i(\{\vec{r}_{i,m}\})}{m_i} \Delta t^2 + O(\Delta t^3)$$

$$\vec{v}_{i,m+1} = \vec{v}_{i,m} + \frac{1}{2} \left( \frac{\vec{f}_i(\{\vec{r}_{i,m}\})}{m_i} + \frac{\vec{f}_i(\{\vec{r}_{i,m+1}\})}{m_i} \right) \Delta t + O(\Delta t^2)$$

CONDIZIONI AL CONFINAMENTO PERIODICHE



$$\vec{r}_i(i_x, i_y, i_z) = \vec{r}_i + i_x L \hat{x} + i_y L \hat{y} + i_z L \hat{z}$$

$$i_x, i_y, i_z \in \mathbb{Z}$$

Nel metodo LJ trascuro distanze  $> \sim 6\sigma$

TEMPERATURE

Noi simuliamo l'ensemble microcanonico  
o  $N, V, E$

si pone

$$E_{kin} = (3N-3) \frac{1}{2} k_B T$$

$$\sum_{i=1, N} \frac{1}{2} m_i v_i^2 = (3N-3) \frac{1}{2} k_B T$$

$$T = \frac{\sum_i m_i v_i^2}{(3N-3) k_B}$$