

Integração das Equações de Movimento: Métodos Numéricos: Verlet

The Verlet algorithm

$$\mathbf{r}(t + \Delta t) = \mathbf{r}(t) + \mathbf{v}(t)\Delta t + (1/2)\mathbf{a}(t)\Delta t^2 + (1/6)\mathbf{b}(t)\Delta t^3 + O(\Delta t^4)$$

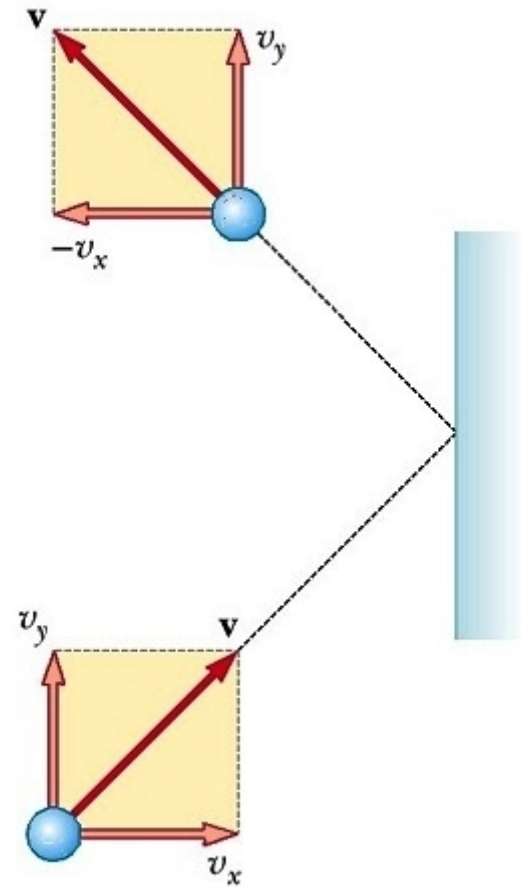
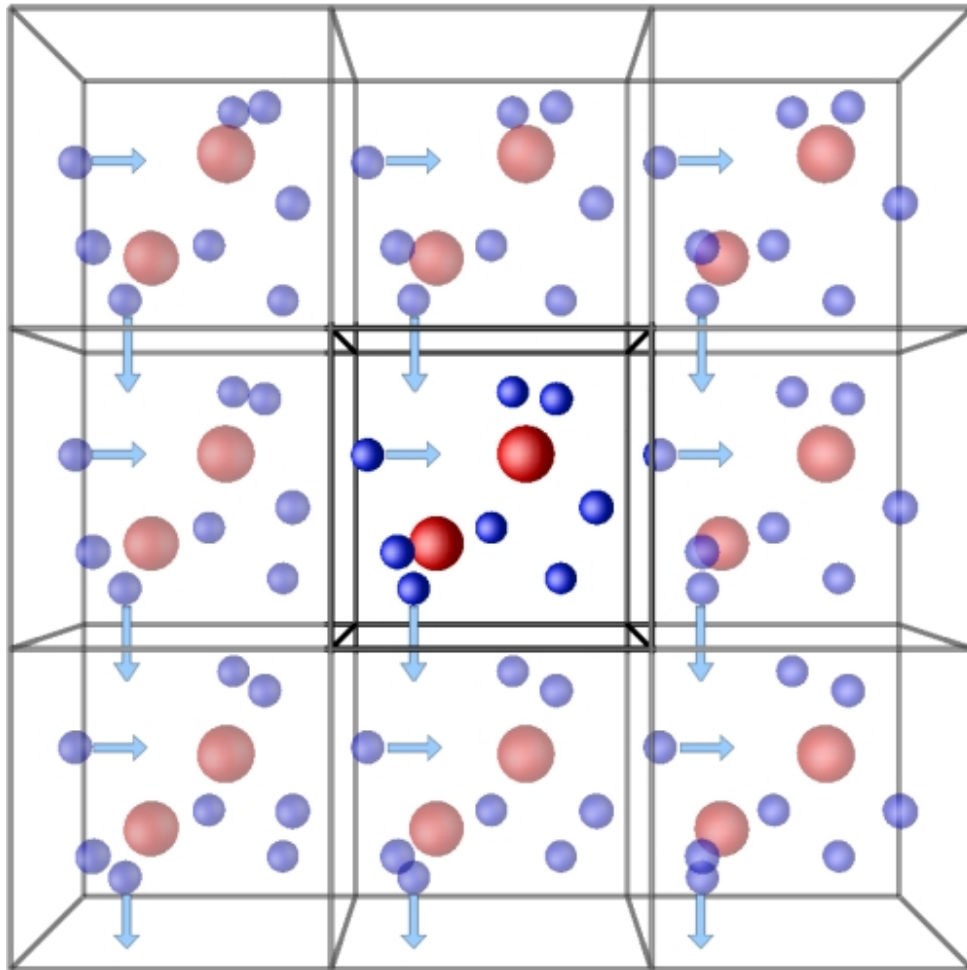
$$\mathbf{r}(t - \Delta t) = \mathbf{r}(t) - \mathbf{v}(t)\Delta t + (1/2)\mathbf{a}(t)\Delta t^2 - (1/6)\mathbf{b}(t)\Delta t^3 + O(\Delta t^4)$$

$$\mathbf{r}(t + \Delta t) = 2\mathbf{r}(t) - \mathbf{r}(t - \Delta t) + \mathbf{a}(t)\Delta t^2 + O(\Delta t^4)$$

$$\mathbf{a}(t) = -(1/m)\nabla V(\mathbf{r}(t))$$

$$\mathbf{v}(t) = \frac{\mathbf{r}(t + \Delta t) - \mathbf{r}(t - \Delta t)}{2\Delta t}$$

Condições Periódicas de Contorno x Reflexões na Parede



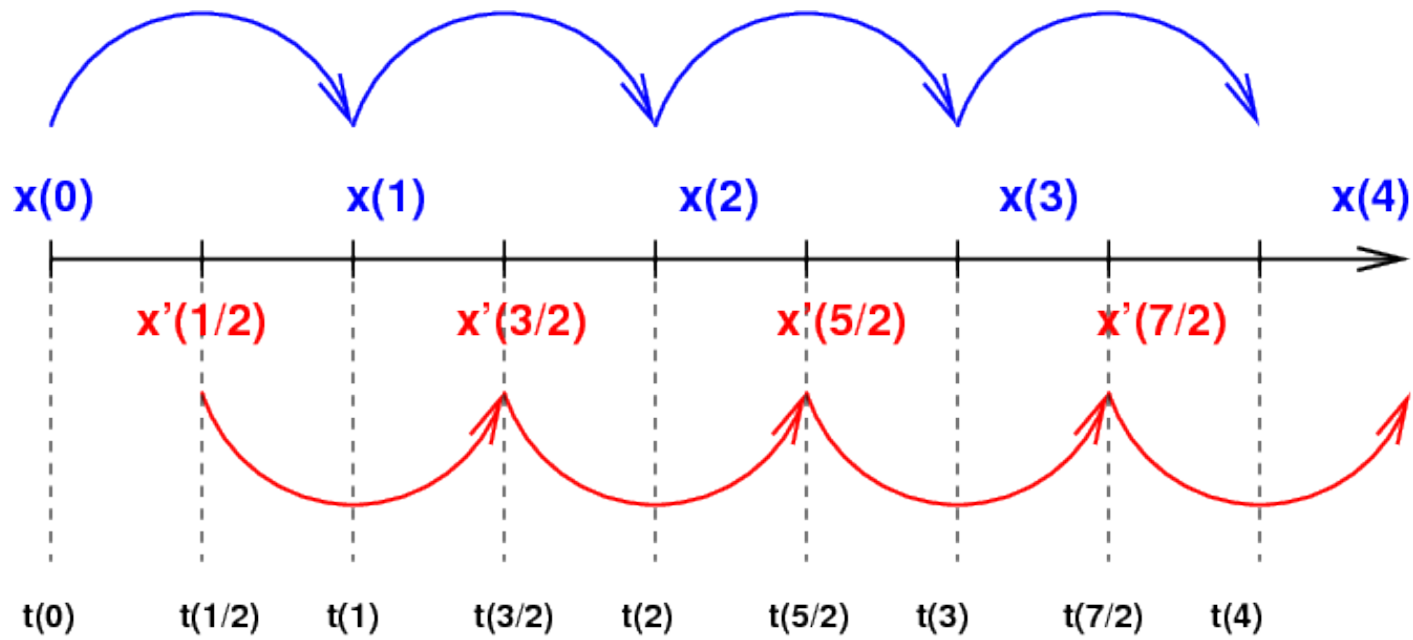
Integração das Equações de Movimento: Métodos Numéricos: Leapfrog

The Leap-frog algorithm

$$r(t + \delta t) = r(t) + v\left(t + \frac{1}{2}\delta t\right)\delta t$$

$$v\left(t + \frac{1}{2}\delta t\right) = v\left(t - \frac{1}{2}\delta t\right) + a(t)\delta t$$

$$v(t) = \frac{1}{2}\left[v\left(t - \frac{1}{2}\delta t\right) + v\left(t + \frac{1}{2}\delta t\right)\right]$$



Integração das Equações de Movimento: Métodos Numéricos: Velocity-Verlet

The Velocity Verlet algorithm

This algorithm yields positions, velocities and accelerations at time t . There is no compromise on precision.

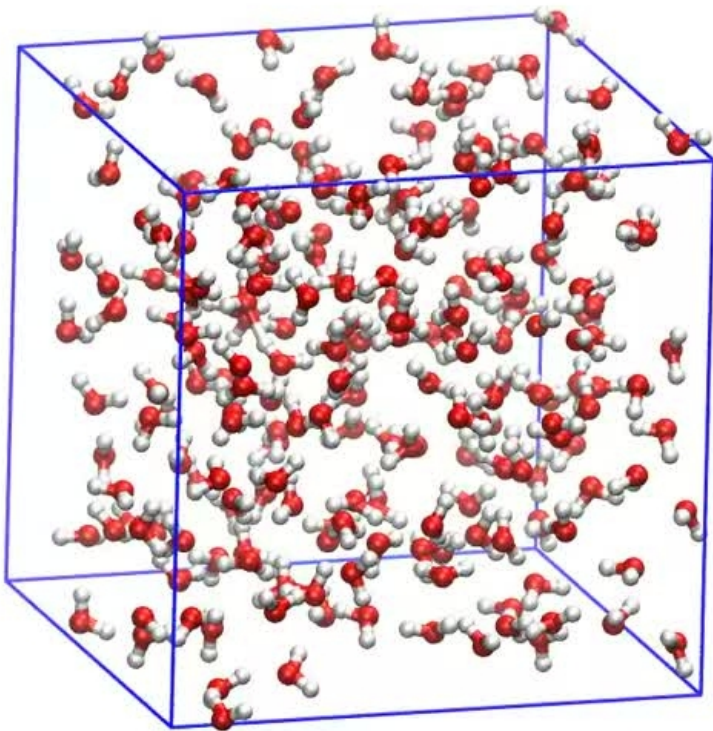
$$r(t + \delta t) = r(t) + v(t)\delta t + \frac{1}{2}a(t)\delta t^2$$

$$v(t + \delta t) = v(t) + \frac{1}{2}[a(t) + a(t + \delta t)]\delta t$$

Dinâmica Molecular Básica:

N átomos numa caixa

$$V(t) = \sum_i \sum_{j>i} \phi(|\mathbf{r}_i(t) - \mathbf{r}_j(t)|)$$



$$K(t) = \frac{1}{2} \sum_i m_i [v_i(t)]^2$$

$$E = K + V$$

$$K = \frac{3}{2} N k_B T$$