Study-Algorithm Anian

Input: Old bond vectors d, unconstrained bond vectors d'
Output: constrained bond vectors d'

while $\frac{|d-d'|}{|d|} >$ tolerance **do**

    for each bond vector i **do**

        $f_i^c \leftarrow \frac{\mu}{2(\Delta t)^2} \frac{d^2 - d'^2}{d' \cdot d} d$

        $\Delta r_{i,0} \leftarrow + \frac{(\Delta t)^2}{m_i} f_i^c$

        $\Delta r_{i,1} \leftarrow - \frac{(\Delta t)^2}{m_i} f_i^c$

        $d_i' \leftarrow d_i' + \Delta r_i$

Running Time: $\Theta(June + July + August)$

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Study-Algorithm Anian (Brute-Force)

Input: Old bond vectors d, unconstrained bond vectors d'
Output: constrained bond vectors d'

while $\frac{|d-d'|}{|d|} >$ tolerance **do**

    for each bond vector i **do**

        $f_i^c \leftarrow \frac{\mu}{2(\Delta t)^2} \frac{d^2 - d'^2}{d' \cdot d} d$

        $\Delta r_{i,0} \leftarrow +\frac{(\Delta t)^2}{m_i} f_i^c$

        $\Delta r_{i,1} \leftarrow -\frac{(\Delta t)^2}{m_i} f_i^c$

        $d_i' \leftarrow d_i' + \Delta r_i$

Running Time: $\Theta(June + July + August)$

$$K_0 = 1750\,\frac{\text{N}}{\text{m}} = 1.05 \cdot 10^6\,\frac{\text{u}}{\text{ps}^2}$$

$$r_0 = 120\,\text{pm}$$

$$\varepsilon_0 = 1.8\,\frac{\text{u}}{\text{ps}^2}$$

$$\sigma = 70\,\text{pm}\ (\text{Atomic radius: Carbon})$$

Tolerance: 10^{-7}(stepwise, relative)