SHAKE Algorithm

After every leapfrog iteration step:

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**
        $f_i^c \leftarrow \frac{\mu}{2(\Delta t)^2} \frac{d^2-d'^2}{d' \cdot d} d$
        $\Delta r_{i,0} \leftarrow +\frac{(\Delta t)^2}{m_i} f_i^c$
        $\Delta r_{i,1} \leftarrow -\frac{(\Delta t)^2}{m_i} f_i^c$
        $d'_i \leftarrow d'_i + \Delta r_i$

Harmonic Potential Parameters

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

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

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

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

SHAKE Algorithm Parameters

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