

# Study-Algorithm Anian

**Input:** Old bond vectors  $d$ , unconstrained bond vectors  $d'$

**Output:** constrained bond vectors  $d'$

```
while  $\frac{|d-d'|}{|d|} > \text{tolerance}$  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:  $\Theta(\text{June} + \text{July} + \text{August})$

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

# Study-Algorithm Anian (Brute-Force)

**Input:** Old bond vectors  $d$ , unconstrained bond vectors  $d'$

**Output:** constrained bond vectors  $d'$

```
while  $\frac{|d-d'|}{|d|} > \text{tolerance}$  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:  $\Theta(\text{June} + \text{July} + \text{August})$

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

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

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