Forces

Notation

Let:

1. r_i be the position of the particle;
2. t time;
3. V the potential of the force field;
4. x^μ the (0-indexed) μth component of vector x;
5. $\partial_n^\mu = \partial/\partial(r_n)^\mu$ – in particular of interest is $(F_n)^\mu = -\partial_n^\mu V$;
6. e_μ the unit vector for μth component;
7. $v_i = r_{i+1} - r_i$;
8. ε_{ijk} the Levi-Civita tensor;
9. $|v|$ the norm, $\|v\| = v/|v|$

Algebra recap

$$\begin{aligned}
\frac{\partial f \cdot g}{\partial x} &= \frac{\partial f}{\partial x} \cdot g + f \cdot \frac{\partial f}{\partial x} \\
\frac{\partial f \times g}{\partial x} &= \frac{\partial f}{\partial x} \times g + f \times \frac{\partial g}{\partial x} \\
(p_0 \times p_1) \cdot p_2 &= e_{ijk}(p_i \times p_j) \cdot p_k \\
v \cdot e_\mu &= v^\mu
\end{aligned}$$

Chirality

$$\begin{aligned}
V &= \frac{1}{2} e_{chi} \sum (C_i - C_i^{nat})^2 \\
C_i &= \frac{(v_{i-1} \times v_i) \cdot v_{i+1}}{d_0^3}
\end{aligned}$$

where d_0 is $|v_{i-1}|$ in the native state, and C_i^{nat} is C_i in the native state.

$$\partial_n^\mu V = e_{chi} \sum (C_i - C_i^{nat}) \partial_n^\mu C_i$$
$$\partial_n^\mu C_i = \frac{1}{d_0^3} \partial_n^\mu (\underbrace{(v_{i-1} \times v_i) \cdot v_{i+1}}_{f_i})$$

with nonzero values:

$$\begin{aligned}
\partial_{i-1}^\mu f_i &= (-\varepsilon^\mu \times v_i) \cdot v_{i+1} \\
&= -(v_i \times v_{i+1})^\mu \\
\partial_i^\mu f_i &= (e^\mu \times v_i - v_{i-1} \times e^\mu) \cdot v_{i+1} \\
&= (v_i \times v_{i+1} + v_{i-1} \times v_{i+1})^\mu \\
\partial_{i+1}^\mu f_i &= (v_{i-1} \times e^\mu) \cdot v_{i+1} + (v_{i-1} \times v_i) \cdot (-e^\mu) \\
&= -(v_{i-1} \times v_{i+1} + v_{i-1} \times v_i)^\mu \\
\partial_{i+2}^\mu f_i &= (v_{i-1} \times v_i)^\mu
\end{aligned}$$

Harmonic tethers

We have:

$$V = \sum \left(\frac{1}{2} k_2 |v_i|^2 + \frac{1}{4} k_4 |v_i|^4 \right)$$
$$\partial_n^\mu V = \sum \left(k_2 |v_i| + k_4 |v_i|^3 \right) \partial_n^\mu |v_i|$$

where

$$\partial_n^\mu |v_i| = \partial_n^\mu \sqrt{v_i \cdot v_i} = \frac{v_i \cdot \partial_n^\mu v_i}{|v_i|}$$
$$\partial_i^\mu |v_i| = \frac{v_i \cdot (-e_\mu)}{|v_i|} = -\|v_i\|^\mu$$
$$\partial_{i+1}^\mu |v_i| = \|v_{i+1}\|^\mu$$

Bond angle

We define θ_i as the bond angle between $i-1, i, i+1$:

$$\cos \theta_i = \frac{v_{i-1} \cdot v_i}{|v_{i-1}||v_i|}$$

We have:

$$\begin{aligned}
\partial_n^\mu \|f\| = \partial_n^\mu \frac{f}{\sqrt{f\cdot f}} &= \frac{\partial_n^\mu f|f| - f\partial_n^\mu \sqrt{f\cdot f}}{f\cdot f} \\
&= \frac{1}{f\cdot f}\left(|f|\partial_n^\mu f - f\frac{1}{\sqrt{f\cdot f}}(f\cdot\partial_n^\mu f)\right) \\
&= \frac{\partial_n^\mu f}{|f|} - \frac{f\cdot\partial_n^\mu f}{|f|^3} \\
\partial_i^\mu \|v_i\| &= -\frac{e_\mu}{|v_i|} + \frac{f^\mu}{|v_i|^3} \\
\partial_{i+1}^\mu \|v_i\| &= \frac{e_\mu}{|v_i|} - \frac{f^\mu}{|v_i|^3}
\end{aligned}$$

and so:

$$\begin{aligned}
\partial_n^\mu \theta_i &= \partial_n^\mu \arccos(\|v_{i-1}\|\cdot\|v_i\|) \\
&= \frac{\partial_n^\mu \|v_{i-1}\|\cdot\|v_i\| + \|v_{i-1}\|\cdot\partial_n^\mu\|v_i\|}{\sqrt{1-(\|v_{i-1}\|\cdot\|v_i\|)^2}}
\end{aligned}$$

with nonzero values:

$$\begin{aligned}
\partial_{i-1}^\mu \theta_i &= \frac{1}{\sqrt{1-(\|v_{i-1}\|\cdot\|v_i\|)^2}}\left(\left(-\frac{e_\mu}{|v_{i-1}|} + \frac{f^\mu}{|v_{i-1}|^3}\right)\cdot\|v_i\|\right) \\
\partial_i^\mu \theta_i &= \frac{1}{\sqrt{1-(\|v_{i-1}\|\cdot\|v_i\|)^2}}\left(\left(-\frac{e_\mu}{|v_i|} + \frac{f^\mu}{|v_i|^3}\right)\cdot\|v_i\| + \|v_{i-1}\|\cdot\left(\frac{e_\mu}{|v_i|} - \frac{f^\mu}{|v_i|^3}\right)\right) \\
\partial_{i+1}^\mu \theta_i &= \frac{1}{\sqrt{1-(\|v_{i-1}\|\cdot\|v_i\|)^2}}\left(\|v_i\|\cdot\left(\frac{e_\mu}{|v_{i+1}|} - \frac{f^\mu}{|v_{i+1}|^3}\right)\right)
\end{aligned}$$

Native bond angle potential is:

$$\begin{aligned}
V &= k_\theta \sum \left(\theta_i - \theta_i^{nat}\right)^2 \\
\partial_n^\mu V &= 2k_\theta \sum \left(\theta_i - \theta_i^{nat}\right)\partial_n^\mu \theta_i
\end{aligned}$$

A heurestic bond angle is a polynomial dependent on residue types in the chain, i.e.

$$\begin{aligned}
V &= \sum_i \sum_{d=0}^{D} a_{i,d}\theta_i^d \\
\partial_n^\mu V &= \sum_i \sum_{d=1}^{D} a_{i,d} d\theta_i^{d-1}\partial_n^\mu \theta_i
\end{aligned}$$

A tabulated bond angle is:

$$\begin{aligned}
V &= \sum f(\theta_i) \\
\partial_n^\mu V &= \sum (\partial_n^\mu f)(\theta_i)\partial_n^\mu \theta_i
\end{aligned}$$

Dihedral angles

Dihedral angle ϕ_i between residues $i-2$, $i-1$, i and $i+1$ is defined as:

$$\cos\phi_i = \frac{(v_{i-1} \times v_i) \cdot (v_i \times v_{i+1})}{|v_{i-1} \times v_i||v_i \times v_{i+1}|}$$