Forcefield

Introduction

Notation:

1. r_i – the position of the particle; $v_i = r_{i+1} - r_i$ is the vector from ith to $(i+1)$th particle;
2. t – time;
3. V – the potential of the force field;
4. v^μ – the μth component of v;
5. D – an arbitrary 1d differential operator, for example $\partial/\partial t$;
6. $\nabla_n^\mu = \partial/\partial(r_n)^\mu$, in particular of interest is $(F_n)^\mu = -\nabla_n^\mu V$;
7. e – the vector of ones;
8. ε_{ijk} – the Levi-Civita tensor;
9. $\delta_{\mu\nu}$ – the Kronecker delta;
10. $|v|$ – the norm, $\|v\| = v/|v|$ – the normalized vector.

Calculus hacks:

$$D|f| = D\sqrt{f \circ f} = \frac{Df \cdot f + f \cdot Df}{2\sqrt{f \cdot f}} = \frac{f \cdot Df}{|f|}$$
$$D\|f\| = D\frac{f}{|f|} = \frac{|f|Df - fD|f|}{|f|^2} = \frac{|f|^2 Df - (f \cdot Df)f}{|f|^3}$$

Vector algebra hacks:

$$D(f \cdot g) = (Df) \cdot g + f \cdot Dg$$
$$D(f \times g) = (Df) \times g + f \times Dg$$
$$(a \times b) \cdot (c \times d) = (a \cdot c)(b \cdot d) - (a \cdot d)(b \cdot c)$$
$$(p_0 \times p_1) \cdot p_2 = \varepsilon_{ijk}(p_i \times p_j) \cdot p_k$$
$$(a \times b) \times c = (a \cdot c)b - (a \cdot b)c$$

Harmonic tethers

The formula for the potential between residues i and j is:

$$
\begin{aligned}
V &= \frac{1}{2}k_2(|v_{ij}| - d_0)^2 + \frac{1}{4}k_4(|v_{ij}| - d_0)^4 \\
DV &= \big(k_2(|v_{ij}| - d_0) + k_4(|v_{ij}| - d_0)^3\big)D|v_{ij}|
\end{aligned}
$$

where k_2 and k_4 are harmonic and anharmonic parts, and

$$
\begin{aligned}
\nabla_i^\mu |v_{ij}| &= \frac{v_{ij} \cdot \nabla_i^\mu v_{ij}}{|v_{ij}|} = -\frac{v_{ij}^\mu}{|v_{ij}|} \\
\nabla_j^\mu |v_{ij}| &= -\nabla_i |v_{ij}|
\end{aligned}
$$

In the original code, k_2 is `H1`, and k_4 is `HH1`.

Bond angle

The bond angle between i, j and k is θ, where:

$$
\begin{aligned}
\cos\theta &= \frac{v_{ji} \cdot v_{jk}}{|v_{ji}||v_{jk}|} \\
\sin\theta &= \frac{|v_{ji} \times v_{jk}|}{|v_{ji}||v_{jk}|}
\end{aligned}
$$

In general,

$$
D\cos\theta = -\sin\theta D\theta \implies D\theta = -\frac{D\cos\theta}{\sin\theta}
$$

Let's start with i:

$$
\begin{aligned}
\nabla_i^\mu \cos\theta &= \nabla_i^\mu (\|v_{ji}\| \cdot \|v_{jk}\|) \\
&= \|v_{jk}\| \cdot \nabla_i^\mu \|v_{ji}\| \\
&= \|v_{jk}\| \cdot \frac{|v_{ji}|^2 e^\mu - v_{ji}^\mu v_{ji}}{|v_{ji}|^3} \\
&= \frac{|v_{ji}|^2 v_{jk}^\mu - (v_{ji} \cdot v_{jk}) v_{ji}^\mu}{|v_{jk}||v_{ji}|^3} \\
\nabla_i \cos\theta &= \frac{v_{ji} \times (v_{ji} \times v_{jk})}{|v_{jk}||v_{ji}|^3}
\end{aligned}
$$

and similarly:

$$
\nabla_k \cos\theta = \frac{v_{jk} \times (v_{jk} \times v_{ji})}{|v_{ji}||v_{jk}|^3}
$$

The derivative for j should be symmetric. Thus:

$$\begin{aligned}
\nabla_i \theta &= -\frac{v_{ji} \times (v_{ji} \times v_{jk})}{|v_{ji}|^2 |v_{ji} \times v_{jk}|} \\
\nabla_j \theta &= -\nabla_i \theta - \nabla_k \theta \\
\nabla_k \theta &= -\frac{v_{jk} \times (v_{jk} \times v_{ji})}{|v_{jk}|^2 |v_{ji} \times v_{jk}|}
\end{aligned}$$

As for the potentials, there are three:

1. from the native structure:

$$\begin{aligned}
V &= k_\theta (\theta - \theta^{nat})^2 \\
DV &= 2k_\theta (\theta - \theta^{nat}) D\theta
\end{aligned}$$

2. heurestic – in the form of a sixth degree polynomial:

$$\begin{aligned}
V &= \sum_{d=0}^{D} \alpha_d \theta^d \\
DV &= \left(\sum_{d=1}^{D} d\alpha_d \theta^{d-1} \right) D\theta
\end{aligned}$$

3. tabulated:

$$\begin{aligned}
V &= f(\theta) \\
DV &= (Df)(\theta) D\theta
\end{aligned}$$

In the original code, θ_i denotes the bond angle between $i-1$, i and $i+1$ (this is important for loading sequence definitions and contact maps). k_θ is `CBA`.

Dihedral angle

The dihedral angle between i, j, k and l is ϕ, where:

$$\begin{aligned}
\cos \phi &= \frac{(v_{ij} \times v_{jk}) \cdot (v_{jk} \times v_{kl})}{|v_{ij} \times v_{jk}||v_{jk} \times v_{kl}|} \\
\sin \phi &= \frac{|v_{jk}| v_{ij} \cdot (v_{jk} \times v_{kl})}{|v_{ij} \times v_{jk}||v_{jk} \times v_{kl}|}
\end{aligned}$$

We have:

$$\begin{aligned}
\nabla_i^\mu \cos \phi &= \|v_{jk} \times v_{kl}\| \cdot \nabla_i^\mu \|v_{ij} \times v_{jk}\| \\
\nabla_i^\mu \|v_{ij} \times v_{jk}\| &= \frac{|v_{ij} \times v_{jk}|^2 \nabla_i^\mu (v_{ij} \times v_{jk}) - (v_{ij} \times v_{jk} \cdot \nabla_i^\mu (v_{ij} \times v_{jk})) v_{ij} \times v_{jk}}{|v_{ij} \times v_{jk}|^3} \\
&= \frac{|v_{ij} \times v_{jk}|^2 (-e^\mu \times v_{jk}) - ((v_{ij} \times v_{jk}) \cdot (-e^\mu \times v_{jk})) v_{ij} \times v_{jk}}{|v_{ij} \times v_{jk}|^3}
\end{aligned}$$