Notes on the force calculation of torsion potential

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The dihedral angle ϕ formed by 4 beads (labeled 1, 2, 3, 4) are defined by

$$\cos\phi = \mathbf{n}_1 \cdot \mathbf{n}_2 \equiv \frac{\mathbf{a}\times\mathbf{b}}{|\mathbf{a}\times\mathbf{b}|} \cdot \frac{\mathbf{b}\times\mathbf{c}}{|\mathbf{b}\times\mathbf{c}|} \tag{1}$$

where $\mathbf{a} \equiv \mathbf{r}_2 - \mathbf{r}_1$, $\mathbf{b} \equiv \mathbf{r}_3 - \mathbf{r}_2$, and $\mathbf{c} \equiv \mathbf{r}_4 - \mathbf{r}_3$ are bond vectors.

Torsion energy is generally a function of ϕ. So to get the forces on beads, it suffices to calculate the derivatives of $\cos\phi$ with respect to $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$. By using the chain rule, the forces on bead are given by

$$\begin{aligned}
\frac{\partial\cos\phi}{\partial\mathbf{r}_1} &= -\frac{\partial\cos\phi}{\partial\mathbf{a}} \\
\frac{\partial\cos\phi}{\partial\mathbf{r}_2} &= \frac{\partial\cos\phi}{\partial\mathbf{a}} - \frac{\partial\cos\phi}{\partial\mathbf{b}} \\
\frac{\partial\cos\phi}{\partial\mathbf{r}_3} &= \frac{\partial\cos\phi}{\partial\mathbf{b}} - \frac{\partial\cos\phi}{\partial\mathbf{c}} \\
\frac{\partial\cos\phi}{\partial\mathbf{r}_4} &= \frac{\partial\cos\phi}{\partial\mathbf{c}}
\end{aligned} \tag{2}$$

Using the identities

$$\frac{\partial}{\partial\mathbf{a}}(\mathbf{a}\times\mathbf{b})\cdot\mathbf{d} = \mathbf{b}\times\mathbf{d} \tag{3}$$

$$\frac{\partial}{\partial\mathbf{a}}|\mathbf{a}\times\mathbf{b}| = \frac{\mathbf{b}\times(\mathbf{a}\times\mathbf{b})}{|\mathbf{a}\times\mathbf{b}|} \tag{4}$$

the derivatives to bond vectors $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$ are found to be

$$\begin{aligned}
\frac{\partial\cos\phi}{\partial\mathbf{a}} &= \frac{\mathbf{b}\times\mathbf{n}_2}{|\mathbf{a}\times\mathbf{b}|} - \cos\phi\frac{\mathbf{b}\times(\mathbf{a}\times\mathbf{b})}{|\mathbf{a}\times\mathbf{b}|^2} = \frac{\mathbf{b}}{|\mathbf{a}\times\mathbf{b}|}\times(\mathbf{n}_2 - \cos\phi\mathbf{n}_1) \\
\frac{\partial\cos\phi}{\partial\mathbf{b}} &== -\frac{\mathbf{a}}{|\mathbf{a}\times\mathbf{b}|}\times(\mathbf{n}_2 - \cos\phi\mathbf{n}_1) + \frac{\mathbf{c}}{|\mathbf{c}\times\mathbf{d}|}\times(\mathbf{n}_1 - \cos\phi\mathbf{n}_2) \\
\frac{\partial\cos\phi}{\partial\mathbf{c}} &== -\frac{\mathbf{b}}{|\mathbf{c}\times\mathbf{d}|}\times(\mathbf{n}_1 - \cos\phi\mathbf{n}_2)
\end{aligned} \tag{5}$$