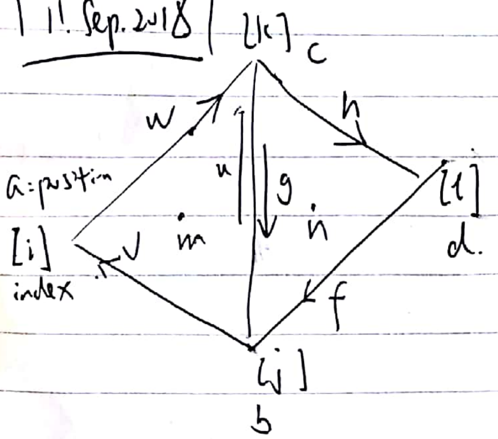
11. Sep. 2018

Important



Kantor and Nelson force

energy $= \hat{\kappa}_b \sum_e 2\,[1-\cos(\theta-\theta_0)]$

loop over ever edge/dihedral angle.

$$E_e = 2\hat{\kappa}_b\,[1-\cos(\theta_e-\theta_0)]$$

$$f_s = -\frac{\partial E_e}{\partial s}$$

$$= -2\hat{\kappa}_b \sin(\theta_e-\theta_0)\frac{\partial \theta_e}{\partial s}$$

We omit the index "e" for clariness.

$$\frac{\partial\theta}{\partial s} = \frac{\partial \arccos(m\cdot n)}{\partial s}$$

$$= -\frac{1}{\sqrt{1-(m\cdot n)^2}}\frac{\partial(m\cdot n)}{\partial s}$$

vectors.

$u = c-b$

$v = a-b$

$w = c-a$

vectors.

$f = b-d$

$g = b-c$

$h = d-c$

$m_m = u\times v$

$m = \frac{m_m}{|m_m|}$

$n_n = g\times h$

$n = \frac{n_n}{|n_n|}$

$A_m = \frac{1}{2}|u\times v|$

$= \frac{1}{2}|m_m|$

area of triangle m

$A_n = \frac{1}{2}|g\times h|$

$= \frac{1}{2}|n_n|$

area of triangle n.

Following the derivation of Timo Krüger 2012 (phD thesis), P149–150.

$n - (m\cdot n)m = n_{mnmn}$ $m - (m\cdot n)n = n_{mnm}$

$$\frac{\partial(m\cdot n)}{\partial a} = \frac{1}{2A_m}\underbrace{(\cancel{b}-c)}_{g}\times n_{mnm}$$

$$\frac{\partial(m\cdot n)}{\partial b} = \frac{1}{2A_n}\underbrace{(d-c)}_{h}\times m_{nmn} + \frac{1}{2A_m}\underbrace{(c-a)}_{w}\times n_{mnm}$$

$$\frac{\partial(m\cdot n)}{\partial c} = \frac{1}{2A_n}\underbrace{(b-d)}_{f}\times m_{nmn} + \frac{1}{2A_m}\underbrace{(a-b)}_{v}\times n_{mnm}$$

$$\frac{\partial(m\cdot n)}{\partial d} = \frac{1}{2A_n}\underbrace{(c-b)}_{u}\, m_{nmn}$$

Since $|m_{nmn}| = |n_{mnm}| = \sqrt{1-(m\cdot n)^2}$. We need to normalize m_{nmn} and n_{mnm}, so that $\sqrt{1-(m\cdot n)^2}$ in $\frac{\partial\theta}{\partial s}$ disappear.