dpotent

The derivatives of the constrained energy functional are calculated.

[called by: knotmin.] [calls: ???.]

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1. An arbitrary curve is given

$$\mathbf{x} \equiv x(\theta)\,\mathbf{i} + y(\theta)\,\mathbf{j} + z(\theta)\,\mathbf{k}, \tag{1}$$

where

$$\begin{array}{rcccccc} x(\theta) & \equiv & x_0 & + & x_m^c\cos(m\theta) & + & x_m^s\sin(m\theta), \\ x'(\theta) & = & & - & m\;x_m^c\sin(m\theta) & + & m\;x_m^s\cos(m\theta), \\ x''(\theta) & = & & - & m^2\,x_m^c\cos(m\theta) & - & m^2\,x_m^s\sin(m\theta), \\ x'''(\theta) & = & & + & m^3\,x_m^c\sin(m\theta) & - & m^3\,x_m^s\cos(m\theta), \end{array} \tag{2}$$

and similarly for $y(\theta)$ and $z(\theta)$. By exploiting "rigid shifts", hereafter we set $x_0 = y_0 = z_0 = 0$. By construction, the curve is closed and infinitely differentiable.

2. The constrained energy functional is given by $\mathcal{F} \equiv \mathcal{F}_1 + \mathcal{F}_2 + \mathcal{F}_3 + \mathcal{F}_4 + \mathcal{F}_5 + \mathcal{F}_6$ where

ifunction = 0

$$\mathcal{F}_1 \equiv \sum_{i,j\neq i} \frac{1}{|\mathbf{x}_i - \mathbf{x}_j|} = \sum_{i,j\neq i} [(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2]^{-1/2} \tag{3}$$

ifunction = 1

$$\mathcal{F}_1 \equiv \int \kappa^2 dl = \int \frac{|\mathbf{x}' \times \mathbf{x}''|^2}{|\mathbf{x}'|^2} d\theta \tag{4}$$

$$\mathcal{F}_2 \equiv \lambda\left(\int \tau\, dl - \mathfrak{t}\right) = \lambda\left(\int \frac{\mathbf{x}' \cdot \mathbf{x}'' \times \mathbf{x}'''}{|\mathbf{x}' \times \mathbf{x}''|^2} d\theta - \mathfrak{t}\right) \tag{5}$$

$$\mathcal{F}_3 \equiv \lambda_x \int y(\theta) z(\theta)\, dl \tag{6}$$

$$\mathcal{F}_4 \equiv \lambda_y y(0) \tag{7}$$

$$\mathcal{F}_5 \equiv \lambda_z z(0) \tag{8}$$

$$\mathcal{F}_6 \equiv \mu_m(\sqrt{x'x' + y'y' + z'z'} - 1)_m, \tag{9}$$

where λ is a Lagrange multiplier used to enforce the integrated torsion constraint, the μ_m are Lagrange multipliers used to enforce the unit speed constraint, and

3. The derivatives with respect to x_m^c are given by

$$\frac{\partial \mathcal{F}_1}{\partial x_m^c} = -\sum_{i,j\neq i} \frac{(x_i - x_j)[\cos(m\theta_i) - \cos(m\theta_j)]}{[(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2]^{3/2}}, \tag{10}$$

$$\frac{\partial \tau}{\partial x_m^c} = \frac{\alpha(y''z''' - y'''z'') + y'(z''\gamma - z'''\beta) + z'(\beta\, y''' - \gamma\, y'') - \tau 2x''\beta}{x''x'' + y''y'' + z''z''} \tag{11}$$

$$\frac{\partial \mathcal{F}_3}{\partial x_m^c} = \frac{x'[-m\sin(m\theta)]}{\sqrt{x'x' + y'y' + z'z'}}, \tag{12}$$

where $\alpha \equiv -m\sin(m\theta)$, $\beta \equiv -m^2\cos(m\theta)$ and $\gamma \equiv m^3\sin(m\theta)$. The derivatives with respect to x_m^s, y_m^c, etc. are similar.