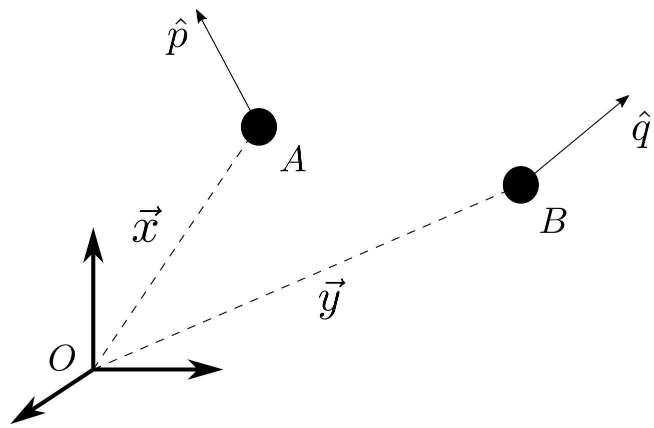

Figure 1: Two oriented particles A and B having position vectors $\vec{\boldsymbol{x}}$ and $\vec{\boldsymbol{y}}$, respectively, with respect to origin O. Their orientations are unit vectors $\hat{\boldsymbol{p}}$ and $\hat{\boldsymbol{q}}$, respectively.

1 Introduction

We will make use of system of particles which have six degrees of freedom per particle. Three degrees of freedom are associated with the position of the particle in space and the remaining three degrees of freedom are associated with the orientation of the particle in space. The energy of such particle systems will be calculated using the work of Szeliski and Tonnesen [2]. We will use rotation vectors to store the orientation of the particles as described in a document by Diebel [1]. A rotation vector represents a 3D rotation about an arbitrary axis passing through the origin. The magnitude of the rotation vector represents the angle of rotation and its direction is the unit vector along the axis.

Consider two oriented particles A and B as shown in Figure 1. Their position vectors are $\vec{\boldsymbol{x}}$ and $\vec{\boldsymbol{y}}$ respectively. Their orientations are represented by unit vectors $\hat{\boldsymbol{p}}$ and $\hat{\boldsymbol{q}}$, respectively. The orientations unit vectors are themselves functions of rotation vectors $\vec{\boldsymbol{u}}$ and $\vec{\boldsymbol{v}}$ respectively. Let

$$\begin{aligned} \vec{\boldsymbol{r}} &= \vec{\boldsymbol{y}} - \vec{\boldsymbol{x}} \\ r &= ||\vec{\boldsymbol{r}}|| \\ \hat{\boldsymbol{r}} &= \frac{\vec{\boldsymbol{r}}}{r} \end{aligned}$$

The energy of oriented particle systems (OPS) is calculated as

$$E = \phi_M(r) + \frac{1}{\gamma}\left(\phi_N(\hat{\boldsymbol{p}}, \hat{\boldsymbol{q}}) + \phi_P(\hat{\boldsymbol{p}}, \hat{\boldsymbol{q}}, \hat{\boldsymbol{r}}) + \phi_C(\hat{\boldsymbol{p}}, \hat{\boldsymbol{q}}, \hat{\boldsymbol{r}})\ \right). \tag{1}$$

ϕ_M is the Morse potential with parameters a and r_e

$$\phi_M = e^{-2a(r-r_e)} - 2e^{-a(r-r_e)}. \tag{2}$$

The co-circularity potential, ϕ_C, is

$$\phi_P = \left(\frac{\hat{\boldsymbol{p}} \cdot \hat{\boldsymbol{r}}}{r}\right)^2. \tag{3}$$

The co-normality potential, ϕ_N, is

$$\phi_N = ||\hat{\boldsymbol{p}} - \hat{\boldsymbol{q}}||^2. \tag{4}$$

The co-circularity potential, ϕ_C, is

$$\phi_C = \left((\hat{\boldsymbol{p}} + \hat{\boldsymbol{q}}) \cdot \frac{\hat{\boldsymbol{r}}}{r} \right)^2. \tag{5}$$

2 Derivatives of Morse Potential

Taking derivatives of equation 2 with respect to x_j and y_j we get

$$\frac{\partial \phi_M}{\partial x_j} = -\frac{2ar_j}{r} \left(e^{-a(r-r_e)} - e^{-2a(r-r_e)} \right) \tag{6}$$

$$\frac{\partial \phi_M}{\partial y_j} = \frac{2ar_j}{r} \left(e^{-a(r-r_e)} - e^{-2a(r-r_e)} \right). \tag{7}$$

3 Derivatives of Orientations

The orientations $\hat{\boldsymbol{p}}$ and $\hat{\boldsymbol{q}}$ can be obtained by rotating the global z-axis $\hat{\boldsymbol{e_z}}$ by rotation vectors $\vec{\boldsymbol{u}}$ and $\vec{\boldsymbol{v}}$ respectively. Let u_i and v_i (with $i = 0, 1, 2$) represent components of the rotation vector and

$$u = ||\vec{\boldsymbol{u}}||$$
$$v = ||\vec{\boldsymbol{v}}||.$$

The angle of rotations are then given by

$$\alpha = \frac{u}{2}$$
$$\beta = \frac{v}{2}.$$

The components of $\hat{\boldsymbol{p}}$ are

$$p_0 = \frac{2\sin\alpha}{u^2} \left(u_1 u \cos\alpha + u_0 u_2 \sin\alpha \right) \tag{8}$$

$$p_1 = \frac{2\sin\alpha}{u^2} \left(-u_0 u \cos\alpha + u_1 u_2 \sin\alpha \right) \tag{9}$$

$$p_2 = \cos^2\alpha + \frac{\sin^2\alpha}{u^2} \left(u_2^2 - u_1^2 - u_0^2 \right). \tag{10}$$

While calculating derivatives of $\hat{\boldsymbol{p}}$ and $\hat{\boldsymbol{q}}$ with respect to components of $\vec{\boldsymbol{u}}$ and $\vec{\boldsymbol{v}}$, care must be taken that α and β are also functions of the components of $\vec{\boldsymbol{u}}$ and $\vec{\boldsymbol{v}}$, respectively.

Let's denote the derivatives of components of orientations with respect to components of rotation vectors as

$$M_{ij} = \frac{\partial p_j}{\partial u_i} \tag{11}$$

$$N_{ij} = \frac{\partial q_j}{\partial v_i}, \tag{12}$$

where $i, j = 0, 1, 2$. The quaternion representing the z-axis is

$$Z = (0, 0, 0, 1)$$

The quaternion representing the rotation by rotation vector $\hat{\boldsymbol{p}}$ is

$$\begin{aligned} Q &= (q_0, q_1, q_2, q_3) \\ &= \left(\cos\alpha, \frac{u_0}{u}\sin\alpha, \frac{u_1}{u}\sin\alpha, \frac{u_2}{u}\sin\alpha\right) \end{aligned}$$

The relationship between $\hat{\boldsymbol{p}}, Q$ and Z is

$$\hat{\boldsymbol{p}} = Q * Z * Q^T$$

where $*$ represents *Hamilton* product. We can calculate M_{ij} as

$$M_{ij} = \frac{\partial p_j}{\partial Q_a}\frac{\partial Q_a}{\partial u_i}$$

where $a = 0, 1, 2, 3$ and $i, j = 1, 2, 3$. Let

$$A_{aj} = \frac{\partial p_j}{\partial Q_a} \qquad B_{ia} = \frac{\partial Q_a}{\partial u_i}$$

where A is a 4×3 matrix and B is a 3×4 matrix. Therefore,

$$M_{ij} = B_{ia}A_{aj}$$

It can be shown that

$$A_{aj} = \frac{\partial p_j}{\partial Q_a} = 2 \times \begin{bmatrix} q_2 & -q_1 & q_0 \\ q_3 & -q_0 & -q_1 \\ q_0 & q_3 & -q_2 \\ q_1 & q_2 & q_3 \end{bmatrix} \tag{13}$$

Now let's look at how to calculate $\frac{\partial Q_a}{\partial u_i}$. First we will differentiate only Q_0. This will give us the first *column* of the 3×4 matrix $\frac{\partial Q_a}{\partial u_i}$.

$$B_{i0} = \frac{\partial Q_0}{\partial u_i} = -\frac{\sin\alpha}{2u}u_i \tag{14}$$

The remaining three components of Q_a give us the remaining 3 *columns*,

$$B_{ij} = \frac{\partial Q_j}{\partial u_i} = \frac{\sin\alpha}{u}\delta_{ij} + \left(\frac{\cos\alpha}{2u^2} - \frac{\sin\alpha}{u^3}\right)u_i u_j \tag{15}$$

This equation will give a 3×3 matrix. We will stack this matrix to the right of the column vector obtained from $\frac{\partial Q_0}{\partial u_i}$ to get the full 3×4 matrix.

4 Derivatives of Co-Planarity Potential

The co-planarity potential (equation 3) can be written in index notation as

$$\phi_p = \left(\frac{p_i r_i}{r}\right)^2, \tag{16}$$

where $r_i = y_i - x_i$. Differentiating with respect to x_j and y_j, we get

$$\frac{\partial \phi_P}{\partial x_j} = \frac{2p_i r_i}{r^4}\left(\left(p_i r_i\right) r_j - r^2 p_j\right) \tag{17}$$

$$\frac{\partial \phi_P}{\partial y_j} = \frac{2p_i r_i}{r^4}\left(r^2 p_j - \left(p_i r_i\right) r_j\right) \tag{18}$$

For derivatives with respect to u_j, we can use chain rule as

$$\frac{\partial \phi_P}{\partial u_i} = \frac{\partial \phi_P}{\partial p_k}\frac{\partial p_k}{\partial u_i} = \frac{2p_j r_j}{r^2} M_{ik} r_k \tag{19}$$

5 Derivatives of Co-Normality Potential

We can write the co-normality potential (equation 4) as

$$\phi_N = p_i p_i + q_i q_i - 2p_i q_i,$$

where $i = 0, 1, 2$ and summation is implied over repeated indices. Therefore, differentiating with respect to p_j and q_j gives,

$$\frac{\partial \phi_N}{\partial p_j} = 2\left(p_j - q_j\right) \tag{20}$$

$$\frac{\partial \phi_N}{\partial q_j} = -2\left(p_j - q_j\right) \tag{21}$$

Therefore, derivatives of ϕ_N with respect to u_i and v_i are

$$\frac{\partial \phi_N}{\partial u_i} = \frac{\partial \phi_N}{\partial p_j}\frac{\partial p_j}{\partial u_i} \tag{22}$$

$$\frac{\partial \phi_N}{\partial v_i} = \frac{\partial \phi_N}{\partial q_j}\frac{\partial q_j}{\partial v_i} \tag{23}$$

If we let $m_j = p_j - q_j$ then we can write the above equations concisely as,

$$\frac{\partial \phi_N}{\partial u_i} = 2M_{ij} m_j \tag{24}$$

$$\frac{\partial \phi_N}{\partial v_i} = -2N_{ij} m_j \tag{25}$$

6 Derivatives of Co-circularity Potential

If we let

$$n_i = p_i + q_i$$
$$r_i = y_i - x_i,$$

then we can write the co-circularity potential (equation 5) as

$$\phi_c = \left(\frac{n_i r_i}{r}\right)^2$$

Differentiating with respect to x_j and y_j, we get

$$\frac{\partial \phi_C}{\partial x_j} = \frac{2 n_i r_i}{r^4} \left((n_i r_i)\, r_j - r^2 n_j \right) \tag{26}$$

$$\frac{\partial \phi_C}{\partial y_j} = \frac{2 n_i r_i}{r^4} \left(r^2 n_j - (n_i r_i)\, r_j \right) \tag{27}$$

To differentiate ϕ_C with respect to p_k and q_k we can write it as

$$\phi_C = \left(\frac{(p_i + q_i)\, r_i}{r}\right)^2$$

Therefore, we get

$$\frac{\partial \phi_C}{\partial p_k} = \frac{\partial \phi_C}{\partial q_k} = \frac{2 n_i r_i}{r^2} r_k \tag{28}$$

We can use chain rule to differentiate ϕ_C with respect to u_i and v_i.

$$\frac{\partial \phi_C}{\partial u_i} = \frac{\partial \phi_C}{\partial p_k} \frac{\partial p_k}{\partial u_i} = \frac{2 n_j r_j}{r^2} M_{ik} r_k \tag{29}$$

$$\frac{\partial \phi_C}{\partial v_i} = \frac{\partial \phi_C}{\partial q_k} \frac{\partial q_k}{\partial v_i} = \frac{2 n_j r_j}{r^2} N_{ik} r_k \tag{30}$$

7 Derivatives of Total Energy

The most crucial part of the code implementation is to calculate the matrices M_{ij} and N_{ij} carefully.

$$\frac{\partial E}{\partial x_j} = \alpha_M \frac{\phi_M}{x_j} + \psi(r) \left(\alpha_P \frac{\partial \phi_P}{\partial x_j} + \alpha_C \frac{\partial \phi_C}{\partial x_j} \right) + \frac{\partial \psi}{\partial x_j} \left(\alpha_P \phi_P + \alpha_N \phi_N + \alpha_C \phi_C \right) \tag{31}$$

$$\frac{\partial E}{\partial y_j} = \alpha_M \frac{\partial \phi_M}{\partial y_j} + \psi(r) \left(\alpha_P \frac{\partial \phi_P}{\partial y_j} + \alpha_C \frac{\partial \phi_C}{\partial y_j} \right) + \frac{\partial \psi}{\partial y_j} \left(\alpha_P \phi_P + \alpha_N \phi_N + \alpha_C \phi_C \right) \tag{32}$$

$$\frac{\partial E}{\partial u_j} = \psi(r) \left(\alpha_P \frac{\partial \phi_P}{\partial u_j} + \alpha_N \frac{\partial \phi_N}{\partial u_j} + \alpha_C \frac{\partial \phi_C}{\partial u_j} \right) \tag{33}$$

$$\frac{\partial E}{\partial v_j} = \psi(r) \left(\alpha_N \frac{\partial \phi_N}{\partial v_j} + \alpha_C \frac{\partial \phi_C}{\partial v_j} \right) \tag{34}$$

References

[1] James Diebel. Representing attitude: Euler angles, unit quaternions, and rotation vectors. *Matrix*, 58:1–35, 2006.

[2] Richard Szeliski and David Tonnesen. Surface Modeling with Oriented Particle Systems. *Siggraph '92*, 26(2):160, 1992.