Appendix A

Differential Geometry

Differential geometry is the mathematical study of intrinsic shape (Kreyszig, 1959; Lord and Wilson, 1984; Koenderink, 1990; Farin, 1992; Gray, 1993). In this appendix we introduce the differential geometry of three dimensional space curves and surfaces embedded in three dimensions.

A.1 The Geometry of Curves

A three dimensional space curve can be thought of as the locus of a point moving through space. The movement can be expressed as a function of a single parameter, such as $\mathbf{x}(t) = (x(t), y(t), z(t))$ where t is a real number, and $x(t)$, $y(t)$, and $z(t)$ are single valued functions. Instead of focusing on the parametrization of the curve we will discuss the shape of the curve, that is the geometric properties of the curve, in terms of the distance traveled along the curve.

A.1.1 Arc Length

The distance traveled in moving along a curve, from say $t = a$ to $t =$b, is given by (Kreyszig, 1959)

$$s = \int_a^b \left\| \frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} \right\| dt = \int_a^b \left(\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} \cdot \frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} \right)^{\frac{1}{2}}$$

which can be written symbolically as

$$ds^2 = d\mathbf{x} \cdot d\mathbf{x}. \tag{A.1}$$

ds is called the *arc element* and s is the *arc length*. Note that arc length is independent of the choice of parametric representation. Thus geometric measures based on the arc length are invariant to parametrization.

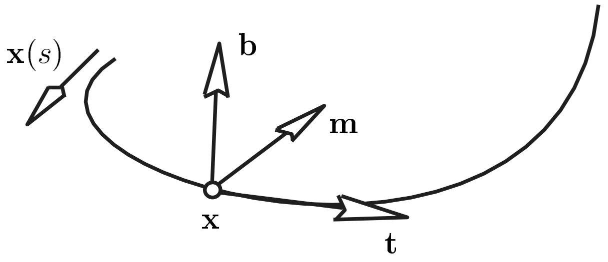

Figure A.1: The Frenet frame.

A.1.2 The Frenet Frame

The first derivative of a curve with respect to arc length defines the unit vector that is tangent to the curve at the point under consideration

$$\dot{\mathbf{x}} = \mathbf{t},$$

where over-struck dot denotes a derivative with respect to s. We call this the *unit tangent vector*. The second derivative with respect to arc length

$$\ddot{\mathbf{x}} = \kappa\mathbf{m}$$

yields a vector with magnitude κ. The unit vector $\mathbf{m}$ is called the *principal normal* and κ the curvature. The tangent and principal normal vectors are orthogonal. Taking the vector product of the tangent and the principal normal yields the unit *bi-normal* vector

$$\mathbf{b} = \mathbf{t} \times \mathbf{m}$$

resulting in a frame at point $\mathbf{x}$, as shown in Figure A.1. This frame, called the *Frenet frame*, describes the local properties of the curve. The first derivative of the bi-normal with respect to arc length

$$\dot{\mathbf{b}} = -\tau\mathbf{m}$$

yields a vector in the direction of the principal normal with magnitude of τ. The scalar τ is the torsion. The curvature, and torsion describe the rotation of the Frenet frame as it moves along the curve in direction s.

A.1.3 The Osculating Circle

The plane spanning the tangent and principal normal vectors is the *osculating plane*. In this plane, there exists a unique circle that is tangent to the curve and with second order continuity matching the curve at $\mathbf{x}(s)$. The circle is named the *osculating circle* and its radius the *radius of curvature*. The fact that it is second order continuous means that the rate of change of the circle's and the curve's tangent vectors, match. This measure of change is the curvature κ and is equal to the inverse of the radius ρ of the circle, that is $\rho = 1/\kappa$. Thus, for straight lines, the curvature is zero and the radius of curvature is infinite. The *osculating circle* is shown in Figure A.2.

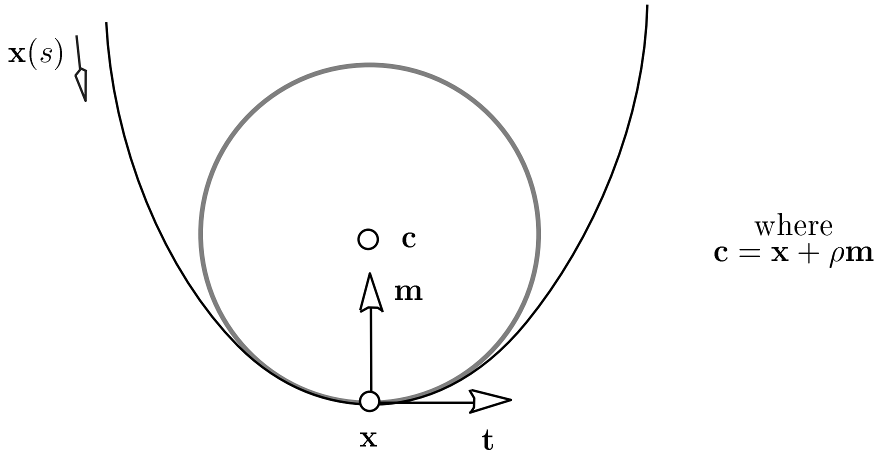

Figure A.2: The osculating circle

As the frame moves along the curve the frame changes position and orientation. One can think of the curvature as the angular velocity (Farin, 1992) of the rotation of the tangent vector, per arc length. The rotation is in the osculating plane, in the direction of the normal vector. The torsion τ is the angular velocity of the bi-normal vector, which twists about the tangent.

A.1.4 The Frenet-Serret formulas

The *Frenet-Serret* formulas (Kreyszig, 1959; Koenderink, 1990; Farin, 1992) describe the changes in the Frenet frame in terms of the frame itself,

$$\begin{bmatrix} \dot{\mathbf{t}} \\ \dot{\mathbf{m}} \\ \dot{\mathbf{b}} \end{bmatrix} = \begin{bmatrix} 0 & \kappa & 0 \\ -k & 0 & \tau \\ 0 & -\tau & 0 \end{bmatrix} \begin{bmatrix} \mathbf{t} \\ \mathbf{m} \\ \mathbf{b} \end{bmatrix}. \tag{A.2}$$

A.2 The Geometry of Surfaces in 3D

A surface may be described by a regular parametrization of position

$$\mathbf{x} = \mathbf{x}(u, v) = \begin{bmatrix} x(u,v) \\ y(u,v) \\ z(u,v) \end{bmatrix},$$

where the coordinates x, y, and z are differentiable functions of the two real variables u and v. To allow a succinct mathematical description of the geometrical properties of the surface, we adopt the notation where subscripts denote partial derivatives with respect to the parameters u and v. For the first partial derivatives we use the notation

$$\mathbf{x}_u = \frac{\partial \mathbf{x}}{\partial u} \qquad \mathbf{x}_v = \frac{\partial \mathbf{x}}{\partial v}.$$

For the second partial derivatives we use the notation

$$\mathbf{x}_{uu} = \frac{\partial^2 \mathbf{x}}{\partial u^2} \qquad \mathbf{x}_{vv} = \frac{\partial^2 \mathbf{x}}{\partial v^2} \qquad \mathbf{x}_{uv} = \frac{\partial \mathbf{x}}{\partial u}\frac{\partial \mathbf{x}}{\partial v} = \frac{\partial^2 \mathbf{x}}{\partial u \partial v} = \frac{\partial^2 \mathbf{x}}{\partial v \partial u} = \mathbf{x}_{vu}.$$

A.2.1 The Arc Element

Given two points on the surface $\mathbf{x}(u, v)$. The vector $d\mathbf{x}$ connecting the two points is given by

$$d\mathbf{x} = \mathbf{x}_u du + \mathbf{x}_v dv.$$

The distance on the surface (Lord and Wilson, 1984) between two such points is

$$ds^2 = d\mathbf{x} \cdot d\mathbf{x} = Edu^2 + 2Fdudv + Gdv^2, \tag{A.3}$$

where

$$E = (\mathbf{x}_u)^2 \qquad F = \mathbf{x}_u \cdot \mathbf{x}_v \qquad G = (\mathbf{x}_v)^2.$$

This is a direct result of equation (A.1). The *arc element*, ds, is a geometric invariant of the surface and thus does not depend on the chosen parametrization, similar to the 3D curve analysis. Equation A.3 for the squared arc element is called the *first fundamental form of the surface* in classical differential geometry.

A.2.2 Tangents and Normal

The vectors tangent to the surface in the directions of the parametrization u and v are given by the partial derivatives $\mathbf{x}_u$ and $\mathbf{x}_v$ respectively. The vector

$$\mathbf{x}_u \times \mathbf{x}_v$$

is orthogonal to the tangent vectors and thus normal to the surface. The magnitude of the normal vector (Kreyszig, 1959) is

$$\|\mathbf{x}_u \times \mathbf{x}_v\| = (\mathbf{x}_u)^2(\mathbf{x}_v)^2 - (\mathbf{x}_u \cdot \mathbf{x}_v)^2 = EG - F^2,$$

so the unit normal is given by

$$\mathbf{n} = \frac{\mathbf{x}_u \times \mathbf{x}_v}{(EG - F^2)^{\frac{1}{2}}}.$$

Figure A.3 shows a local portion of a parametric surface. The dashed lines indicate curves on the surface of constant u and v value. The tangential vectors $\mathbf{x}_u$ and $\mathbf{x}_v$ are the rate of change of the surface along the lines of constant v and u respectively, and the vector $\mathbf{n}$ is normal to the surface.

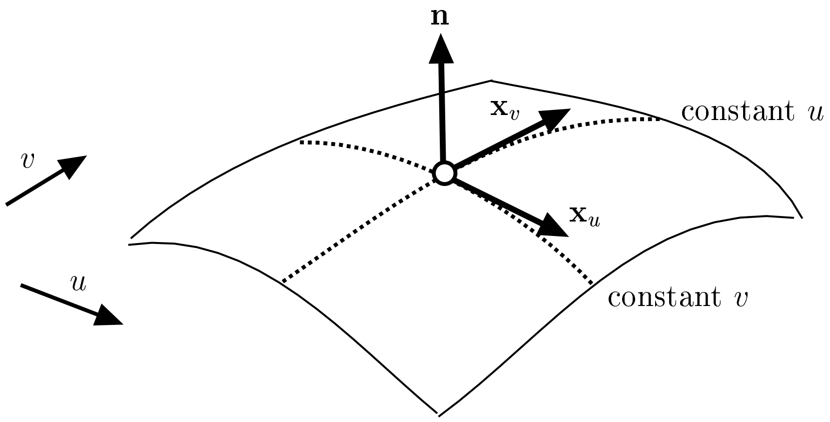

Figure A.3: Surface $\mathbf{x}(u, v)$ with partial derivatives and normal.

A.2.3 The Second Fundamental Form

The first fundamental form (A.3) determines the intrinsic geometrical properties of the surface and is independent of the embedding space. To specify the embedding in Euclidean 3-space requires additional information. That information is the way the *normal* to the surface varies from surface point to surface point. The difference in unit normal at two infinitesimally close points is

$$d\mathbf{n} = \mathbf{n}_u du + \mathbf{n}_v dv.$$

The *second fundamental form* (Kreyszig, 1959; Farin, 1992) is

$$-d\mathbf{n} \cdot d\mathbf{x} = L du^2 + 2M du dv + N dv^2, \tag{A.4}$$

where

$$L = -\mathbf{n}_u \cdot \mathbf{x}_u = +\mathbf{n} \cdot \mathbf{x}_{uu} = \mathbf{n} \cdot \mathbf{x}_{uu} \tag{A.5}$$
$$M = -\mathbf{n}_u \cdot \mathbf{x}_v = -\mathbf{n}_v \cdot \mathbf{x}_u = \mathbf{n} \cdot \mathbf{x}_{uv} \tag{A.6}$$
$$N = -\mathbf{n}_v \cdot \mathbf{x}_v = +\mathbf{n} \cdot \mathbf{x}_{vv} = \mathbf{n} \cdot \mathbf{x}_{vv} \tag{A.7}$$

The equality found in M comes from differentiating the identities $\mathbf{n} \cdot \mathbf{x}_u = 0$ and $\mathbf{n} \cdot \mathbf{x}_v = 0$ with respect to u and v. The first and second fundamental forms together determines the shape of the surface uniquely; however they do not specify global position and orientation.

A.2.4 Normal Curvature

The first and second fundamental forms determine the shape of the surface local to each point on the surface. Consider a 3D space curve on the surface passing through the surface point $\mathbf{x}$. The relation

$$\kappa \cos\theta = \frac{-d\mathbf{n} \cdot d\mathbf{x}}{ds^2} \tag{A.8}$$

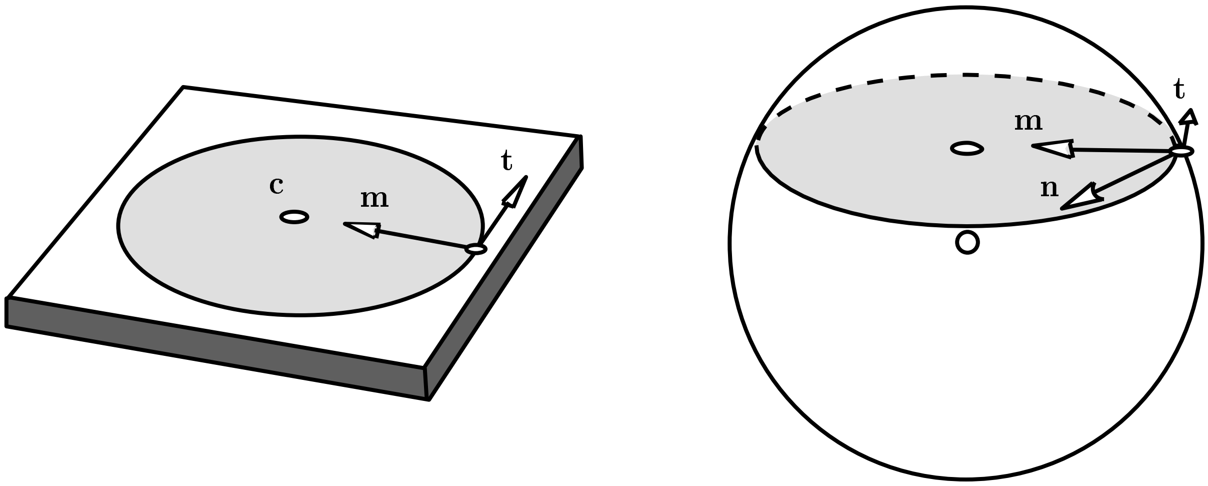

Figure A.4: Curve on sphere where $\mathbf{m} \neq \mathbf{n}$.

relates the curvature κ of the curve to the angle θ between the curve normal $\mathbf{m}$ to the surface normal $\mathbf{n}$. While at first one might expect the normals to match identically one can easily see that this is not necessarily the case, as shown in Figure A.4. Consider a circle as a space curve. The normal $\mathbf{m}$ of the curve is always pointing inward toward the center of the circle. For a curve that is a circle, the osculating circle of the curve is identically the curve. Now consider a sphere where the surface normal $\mathbf{n}$ is always pointing inward to the sphere's center. For circles lying on the sphere, only circles that are great circles of the sphere have normals that match the normals of the sphere. The angle between the curve normal and the surface normal is described by (A.8).

By Meusnier's theorem (Farin, 1992), the osculating circles of all surface curves passing through a point $\mathbf{x}$ and having the same tangent $\mathbf{t}$ form a sphere. This sphere and the surface share a common tangent plane at $\mathbf{x}$, and the sphere has a unique center of curvature, its center. Thus to describe the shape of the surface it is sufficient to study a subset of these curves; namely the curves at $\mathbf{x}$ for which $\mathbf{m} = \mathbf{n}$. There exists one such curve for each tangent vector $\mathbf{t}$. When the osculating plane of a surface curve passing through point $\mathbf{x}$ is perpendicular to the surface tangent plane, then $\theta = 0$ and $\mathbf{m} = \mathbf{n}$. Such curves are called *normal sections* and can be thought of as the intersection of the surface with a plane normal to the surface and which contains the desired tangent vector $\mathbf{t}$, as shown in Figure A.5. The curvature of a normal section at a point $\mathbf{x}$ is the *normal curvature* κ_n and is given by (A.8) with $\theta = 0$

$$\kappa_n = \frac{-d\mathbf{n} \cdot d\mathbf{x}}{ds^2} = \frac{L du^2 + 2M du dv + N dv^2}{E du^2 + 2F du dv + G dv^2}.$$

A.2.5 More Curvature Measures

In differential geometry curvature is measured in a variety of ways. For completeness we will quickly review some of the more common measures.

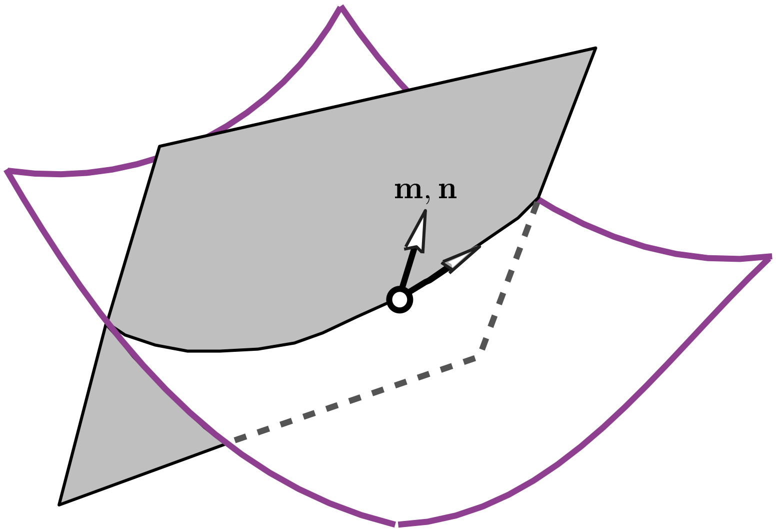

Figure A.5: The normal section.

The extreme values of normal curvature, κ_1 and κ_2, at a given point are called the *principal curvatures*. The unit tangent vectors, $\mathbf{e}_1$ and $\mathbf{e}_2$, for which the extreme values occur are called the *principal vectors*. The corresponding directions are called the *principal directions*. When the principal curvatures are non equal the principal vectors are unique and perpendicular. A *principal frame* (Koenderink, 1990) is defined as a frame with major axes matching the surface normal $\mathbf{n}$ and the principal vectors $\mathbf{e}_1$ and $\mathbf{e}_2$.

The arithmetic mean of the principal curvatures, $H = \frac{1}{2}(\kappa_1+\kappa_2)$, is called the *mean curvature*. The *Gaussian curvature* is the product of the extreme curvatures, $K = \kappa_1\kappa_2$. The measures K and $|H|$ are invariant with respect to coordinate transform (Kreyszig, 1959).

Appendix B

Newtonian Dynamics

This appendix reviews the basic theory of Newtonian dynamics and the mathematics necessary for both un-oriented and oriented particle systems. For completeness we occasionally repeat material presented earlier in the dissertation.

A standard particle is described by its position $\mathbf{x}$ and mass m. An oriented particle is described as a standard particle enhanced with an orientation $\mathbf{R}$ and an inertia tensor $\mathbf{I}$.

B.1 Rotation

Each oriented particle defines both a normal vector $\mathbf{n}_i = z$ and a local tangent plane defined by the local x and y vectors. More formally, we write the state of each particle as $(\mathbf{x}_i, \mathbf{R}_i)$, where $\mathbf{x}_i$ is the particle's position and $\mathbf{R}_i$ is a 3×3 rotation matrix which defines the orientation of its local coordinate frame (relative to the global frame (X, Y, Z)). The third column of $\mathbf{R}_i$ is the local normal vector $\mathbf{n}_i$.

While we use the rotation matrix $\mathbf{R}$ to convert from local coordinates to global coordinates and vice versa, we use a unit quaternion $\mathbf{q}$ as the state to be updated. The unit quaternion

$$\mathbf{q} = (\mathbf{w}, s) \quad \text{with} \quad \begin{array}{rcl} \mathbf{w} & = & \mathbf{n} \sin(\theta/2) \\ s & = & \cos(\theta/2) \end{array}$$

represents a rotation of θ about the unit normal axis $\mathbf{n}$. To update this quaternion, we simply form a new unit quaternion from the current angular velocity $\boldsymbol{\omega}$ and the time step Δt, and use quaternion multiplication (Shoemake, 1985).

B.2 Inertia Tensor

The inertia tensor $\mathbf{I}$ relates the angular momentum vector to the angular velocity vector by a linear transformation. In general $\mathbf{I}$ is represented as a 3x3 matrix,

$$\mathbf{I} = \begin{bmatrix} I_{xx} & I_{xy} & I_{xz} \\ I_{yx} & I_{yy} & I_{yz} \\ I_{zx} & I_{zy} & I_{zz} \end{bmatrix}.$$

The inertia tensor is symmetric; that is, $I_{ij} = I_{ji}$. The diagonal elements, I_{xx}, I_{yy}, and I_{zz}, are called the moments of inertia of the object. The off-diagonal elements are known as the products of inertia.

The inertia tensor is defined with respect to an inertial frame; a set of coordinate axes and an origin about which the object rotates. For any choice of origin, for any body, there always exists a set of coordinate axes which diagonalizes the inertia tensor (Marion, 1970). Thus we can write the inertia tensor as

$$\mathbf{I} = \begin{bmatrix} I_{xx} & 0 & 0 \\ 0 & I_{yy} & 0 \\ 0 & 0 & I_{zz} \end{bmatrix},$$

where the associated moments I_{xx}, I_{yy} and I_{zz} are the principal moments of inertia. These axes are the *principal axes of inertia.*

For oriented particles we are interested in the property of angular momentum, but are not interested in mimicking the inertia of a particular rigid body. Thus we choose the simple inertia tensor of the form

$$\mathbf{I} = c \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \tag{B.1}$$

where c is some scalar constant. We define our inertia tensor about the particle's local origin with respect to the world coordinate axes. Our choice of inertia tensor is equivalent to a spherical object with its centroid at the particle origin. This choice results in a tensor that is constant over change in particle position and orientation. Using principal axes, as we do, allows us to represent the inertia tensor by a triplet (like a vector) encoding the principal moments of inertia. Our choice simplifies the equations of motion as well as the computation of angular momentum and rotational kinetic energy.

B.3 Velocity

Since we are interested in animating a particle system, we must consider how the position and orientation of the particles change over time. Thus, we write the position and orientation as functions of time: $\mathbf{x}(t)$ and $\mathbf{R}(t)$.

The linear velocity is defined as the rate of change of the particle position over time. At time t the velocity of the particle is

$$\mathbf{v}(t) = \frac{\mathrm{d}\mathbf{x}(t)}{\mathrm{d}t}$$

The instantaneous angular velocity is defined as the rate of change of the orientation over time

$$\boldsymbol{\omega}(t) = \frac{\mathrm{d}\mathbf{R}(t)}{\mathrm{d}t}.$$

The vector properties of addition and scalar multiplication hold for instantaneous angular velocities (Hoffmann, 1966). For example, given two instantaneous angular velocities $\boldsymbol{\omega}_1$ and $\boldsymbol{\omega}_2$, the following holds

$$\boldsymbol{\omega}_1 + \boldsymbol{\omega}_2 = \boldsymbol{\omega}_2 + \boldsymbol{\omega}_1.$$

Thus, we can manipulate instantaneous angular velocities as vectors.

We could have derived angular velocity by differentiating the rotation matrix or quaternion but it is simpler to describe it in terms of the rotation $\mathbf{R}(t)$ as shown above. For matrix and quaternion derivations see Baraff (1991). Since we use angular velocity to approximate a rotation over a given time interval, the derivation shown above is ideal for our purposes.

After computing a change in rotation as a vector quantity we then convert it to a quaternion. To update a particle's orientation as a quaternion, we simply form a new unit quaternion $\hat{\boldsymbol{\omega}}$ from the current angular velocity $\boldsymbol{\omega}$ and the time step Δt, and use quaternion multiplication. Details on quaternions can be found in (Shoemake, 1989; Shoemake, 1991).

B.4 Momentum

The linear momentum $\mathbf{p}$ of a particle with mass m and velocity $\mathbf{v}$ is

$$\mathbf{p}(t) = m\mathbf{v}(t).$$

The angular momentum of a particle with inertia $\mathbf{I}$ and angular velocity $\boldsymbol{\omega}$ is

$$\mathbf{L} = \mathbf{I}\boldsymbol{\omega}.$$

The inertia tensor $\mathbf{I}$ relates the angular momentum vector to the angular velocity vector by a linear transformation. The angular momentum simplifies to

$$\mathbf{L} = \begin{bmatrix} I_x\omega_x \\ I_y\omega_y \\ I_z\omega_z \end{bmatrix}$$

when the inertial coordinate frame is aligned with the principal moments. Since we are using the inertia tensor for a spherical object (B.1) the angular momentum simplifies to

$$\mathbf{L} = c\boldsymbol{\omega}$$

for all time values.

B.5 Force and Torque

The force on a particle is the change in momentum which is commonly written in terms of mass and acceleration:

$$\mathbf{f}(t) = \frac{\mathrm{d}\mathbf{p}(t)}{\mathrm{d}t} = \frac{\mathrm{d}m\mathbf{v}(t)}{\mathrm{d}t} = m\frac{\mathrm{d}\mathbf{v}(t)}{\mathrm{d}t} = m\mathbf{a}(t).$$

The torque $\boldsymbol{\tau}$ on a particle is the rate of change in angular momentum and can be written in terms of inertia and angular acceleration:

$$\boldsymbol{\tau}(t) = \frac{\mathrm{d}\mathbf{L}(t)}{\mathrm{d}t} = \frac{\mathrm{d}\mathbf{I}\boldsymbol{\omega}(t)}{\mathrm{d}t} = \frac{\mathrm{d}\mathbf{I}}{\mathrm{d}t}\boldsymbol{\omega}(t) + \mathbf{I}\frac{\mathrm{d}\boldsymbol{\omega}(t)}{\mathrm{d}t} = \boldsymbol{\omega} \times \mathbf{I}\boldsymbol{\omega} + \mathbf{I}\mathbf{b}(t).$$

For our system, the inertia tensor (B.1) is constant over time and thus the torque reduces to

$$\boldsymbol{\tau}(t) = \mathbf{I}\mathbf{b}(t)$$

for all values of time t.

B.6 Potential Energy

We can derive both forces and torques from potential energy functions. This has the advantage of allowing the design of energy functions which exhibit minimal energies at desired particle configurations, and guarantees that the system will not diverge. A force results from the gradient of the potential energy ϕ with respect to a particle's position $\mathbf{x}_i$,

$$f_i = -\nabla_{\mathbf{x}_i}\phi,$$

and a torque results from the gradient of the potential energy with respect to the particle's orientation θ_i,

$$\tau_i = -\nabla_{\theta_i}\phi.$$

As the energy of the system minimizes, the particles migrate to minimal energy configurations.

Appendix C

Gradients of Potential

This appendix presents mathematical background and identities necessary to derive the force and torque vectors from weighted scalar potential fields. The translational force acting on a particle results from the loss in potential energy due to a change in particle position. Likewise, an angular force, or torque, results from the loss in potential energy due to a change in particle orientation. In three dimensions these are written as the negative gradient of the potential energy function with respect to the particle position and orientation, as follows:

$$\mathbf{f}_i = -\nabla_{\mathbf{x}_i} \phi, \tag{C.1}$$

$$\boldsymbol{\tau}_i = -\nabla_{\boldsymbol{\theta}_i} \phi, \tag{C.2}$$

where $\boldsymbol{\theta}_i$ is the infinitesimal change in orientation of particle i.

The six sections discuss fundamental concepts and derive basic identities which can be used to quickly derive the appropriate forces and torques from scalar potentials. Section one presents the multiplication and chain rules of differential calculus applied to the gradient operator. Section two derives the relationship between an infinitesimal rotation and change of the parameters of the potential functions. Section three presents differential identities for the gradient of the Euclidean norm with respect to particle separation and differences in normal vectors. Section four presents differential identities for the gradient of scalar products with respect to combinations of the particle normal and particle separation vectors. Section fives derives the gradient of the weighting function with respect to particle position and orientation. Section six presents identities for deriving the force and torque due to a scalar potential energy function.

C.1 Gradient of Scalar Functions

The derivation of force and torque are based on the application of the multiplication rule and chain rule of differential calculus. If f and g are scalar functions then by the multiplication rule

$$\nabla(fg) = f\nabla g + g\nabla f. \tag{C.3}$$

When f is a function of a scalar variable a then by the chain rule,

$$\nabla f(a) = \frac{\mathrm{d}f}{\mathrm{d}a}\nabla a. \tag{C.4}$$

C.2 Gradient with Respect to Orientation

In this section we derive the gradient with respect to change in infinitesimal orientation of a scalar function, that is $\nabla_{\boldsymbol{\theta}} f$.

Unlike general rotations, infinitesimal rotations behave as vectors. In particular they follow the parallelogram law (addition law) of vectors. Given an infinitesimal rotation about an axis, we can represent the rotation by a vector $\boldsymbol{\theta}$, where the magnitude of the vector represents the angle of rotation, and the direction of the vector $\boldsymbol{\theta}$ points in the direction of the axis of rotation.

C.2.1 The Change in Normal

To understand the relationship between a change in orientation and the corresponding particle normal consider the following. A particle with fixed position and with a vector $\mathbf{n}$ attached, is rotating about its center. As the particle rotates, the vector $\mathbf{n}$ traces a circle about the axis of rotation. The infinitesimal variation in the vector's components may be written, to a first approximation, as the following vector product (Goldstein, 1950)

$$d\mathbf{n} = \mathbf{n} \times d\boldsymbol{\theta}, \tag{C.5}$$

where $d\boldsymbol{\theta}$ is an infinitesimal rotation.

We now introduce matrix-vector notation which allows one to write a vector product as a matrix times a vector. Given two vectors $\mathbf{a}$ and $\mathbf{b}$

$$\mathbf{a} \times \mathbf{b} = \mathbf{A}^\star \mathbf{b}$$

where $\mathbf{A}^\star$ is given by

$$\begin{bmatrix} 0 & -\mathbf{a}_3 & \mathbf{a}_2 \\ \mathbf{a}_3 & 0 & -\mathbf{a}_1 \\ -\mathbf{a}_2 & \mathbf{a}_1 & 0 \end{bmatrix}.$$

Note that $\mathbf{b} \times \mathbf{a}$ equals $(\mathbf{A}^\star)^T\mathbf{b}$, but *does not* equal $\mathbf{b}\mathbf{A}^\star$.

Rewriting (C.5) in matrix-vector notation we have

$$d\mathbf{n} = \mathbf{n} \times d\boldsymbol{\theta} = \begin{bmatrix} 0 & -\mathbf{n}_3 & \mathbf{n}_2 \\ \mathbf{n}_3 & 0 & -\mathbf{n}_1 \\ -\mathbf{n}_2 & \mathbf{n}_1 & 0 \end{bmatrix} d\boldsymbol{\theta} = \mathbf{N}^\star d\boldsymbol{\theta}.$$

Thus the change in vector $\mathbf{n}$ due to the infinitesimal rotation $d\boldsymbol{\theta}$ is

$$\frac{\mathrm{d}\mathbf{n}}{\mathrm{d}\boldsymbol{\theta}} = \mathbf{N}^\star. \tag{C.6}$$

C.2.2 Gradient of a Scalar Function

Now let us say we have a scalar function $f(\mathbf{n})$. By the chain rule we can differentiate f with respect to the infinitesimal rotation $d\boldsymbol{\theta}$:

$$\frac{\mathrm{d}f}{\mathrm{d}\boldsymbol{\theta}} = \left(\frac{\mathrm{d}f}{\mathrm{d}\mathbf{n}}\right)\left(\frac{\mathrm{d}\mathbf{n}}{\mathrm{d}\boldsymbol{\theta}}\right). \tag{C.7}$$

In order to replace the second term on the right hand side $\mathbf{N}^{\star}$, we apply the commutative law of multiplication so that

$$\frac{\mathrm{d}f}{\mathrm{d}\boldsymbol{\theta}} = \left(\frac{\mathrm{d}\mathbf{n}}{\mathrm{d}\boldsymbol{\theta}}\right)\left(\frac{\mathrm{d}f}{\mathrm{d}\mathbf{n}}\right). \tag{C.8}$$

We can do this because the multiplication between the various components of the two terms follow scalar product rules. We replace the first term of the product with (C.6)

$$\mathbf{N}^{\star}\left(\frac{\mathrm{d}f}{\mathrm{d}\mathbf{n}}\right).$$

By matrix-vector notation this is equivalent to the cross-product

$$\mathbf{n}\times\left(\frac{\mathrm{d}f}{\mathrm{d}\mathbf{n}}\right).$$

When computing the differential of a scalar function with respect to a vector, the differential due to each component of the vector is computed separately. In three dimensions, this can be written as the gradient of the function with respect to the differentiating vector, such as,

$$\frac{\mathrm{d}f}{\mathrm{d}\mathbf{n}} = \nabla_{\mathbf{n}} f.$$

Thus we can write the change of a scalar potential function f due to rotation of a particle as

$$\nabla_{\boldsymbol{\theta}} f = \mathbf{n}\times\left(\nabla_{\mathbf{n}} f\right), \tag{C.9}$$

where $\mathbf{n}$ is the particle normal. This is a valuable identity that we can use in the derivation of torque due to an inter-particle potential function.

C.2.3 Directional Derivatives

The concise notation in the above derivation has hidden many of the details and may be confusing to follow. We now show how we go from (C.7) to (C.8). The directional derivative (Hay, 1953) of a function $f(\mathbf{n})$ at $\mathbf{x}$ in the direction $\mathbf{b}$ is

$$\frac{\partial f}{\partial s} = \frac{\partial f}{\partial n_x}\frac{\partial n_x}{\partial s} + \frac{\partial f}{\partial n_y}\frac{\partial n_y}{\partial s} + \frac{\partial f}{\partial n_z}\frac{\partial n_z}{\partial s}$$

where $\partial f/\partial s$ is the rate of change of f in the direction $\mathbf{b}$.

We now differentiate the scalar function f with respect to an infinitesimal rotation $\boldsymbol{\theta} = [\theta_x, \theta_x, \theta_x]^T$.

$$\frac{\mathrm{d}f}{\mathrm{d}\boldsymbol{\theta}} = \nabla_{\boldsymbol{\theta}} f = \begin{bmatrix} \frac{\partial f}{\partial \theta_x} \\ \\ \frac{\partial f}{\partial \theta_y} \\ \\ \frac{\partial f}{\partial \theta_z} \end{bmatrix}.$$

Each element of the vector represents a directional derivative. The derivatives are with respect to a change in orientation about the three major axes. Expanding the elements of the vector we have

$$\begin{bmatrix} \frac{\partial f}{\partial n_x}\frac{\partial n_x}{\partial \theta_x} + \frac{\partial f}{\partial n_y}\frac{\partial n_y}{\partial \theta_x} + \frac{\partial f}{\partial n_z}\frac{\partial n_z}{\partial \theta_x} \\ \\ \frac{\partial f}{\partial n_x}\frac{\partial n_x}{\partial \theta_y} + \frac{\partial f}{\partial n_y}\frac{\partial n_y}{\partial \theta_y} + \frac{\partial f}{\partial n_z}\frac{\partial n_z}{\partial \theta_y} \\ \\ \frac{\partial f}{\partial n_x}\frac{\partial n_x}{\partial \theta_z} + \frac{\partial f}{\partial n_y}\frac{\partial n_y}{\partial \theta_z} + \frac{\partial f}{\partial n_z}\frac{\partial n_z}{\partial \theta_z} \end{bmatrix}.$$

Each of the partial derivatives evaluates to a scalar value, thus the order of the product can be interchanged. For example

$$\frac{\partial f}{\partial n_x}\frac{\partial n_x}{\partial \theta_x} = \frac{\partial n_x}{\partial \theta_x}\frac{\partial f}{\partial n_x}.$$

Thus we can write the above vector as the product of a matrix and vector

$$\begin{bmatrix} \frac{\partial n_x}{\partial \theta_x} & \frac{\partial n_y}{\partial \theta_x} & \frac{\partial n_z}{\partial \theta_x} \\ \\ \frac{\partial n_x}{\partial \theta_y} & \frac{\partial n_y}{\partial \theta_y} & \frac{\partial n_z}{\partial \theta_y} \\ \\ \frac{\partial n_x}{\partial \theta_z} & \frac{\partial n_y}{\partial \theta_z} & \frac{\partial n_z}{\partial \theta_z} \end{bmatrix} \begin{bmatrix} \frac{\partial f}{\partial n_x} \\ \\ \frac{\partial f}{\partial n_y} \\ \\ \frac{\partial f}{\partial n_z} \end{bmatrix}.$$

The matrix is equivalent to $d\mathbf{n}/d\boldsymbol{\theta}$, and the vector is equivalent to $df/d\mathbf{n}$, which is the gradient of f with respect to $\mathbf{n}$. Thus

$$\nabla_{\boldsymbol{\theta}} f(\mathbf{n}) = \left(\frac{\mathrm{d}\mathbf{n}}{\mathrm{d}\boldsymbol{\theta}}\right)\left(\frac{\mathrm{d}f}{\mathrm{d}\mathbf{n}}\right) = \mathbf{N}^\star\left(\nabla_{\mathbf{n}} f\right) = \mathbf{n} \times \nabla_{\mathbf{n}} f.$$

C.3 Gradient of the Euclidean Norm

The Euclidean norm of a vector is defined as a measure of the magnitude of the vector, and for any vector $\mathbf{a}$ is defined as

$$\|\mathbf{a}\| = (\mathbf{a}\cdot\mathbf{a})^{\frac{1}{2}} = (\mathbf{a}_x^2 + \mathbf{a}_y^2 + \mathbf{a}_z^2)^{\frac{1}{2}}.$$

A *unit vector* is a vector with Euclidean norm of one. For any vector $\mathbf{a}$, the unit vector $\hat{\mathbf{a}}$ is given by

$$\hat{\mathbf{a}} = \frac{\mathbf{a}}{\|\mathbf{a}\|}.$$

Differential Identities of Euclidean Norm

The gradient of the Euclidean norm of a vector, with respect to the vector of the norm, is the corresponding unit vector,

$$\nabla_{\mathbf{a}}||\mathbf{a}|| = \hat{\mathbf{a}}. \tag{C.10}$$

The proof, which is omitted, involves substituting s for $(\mathbf{a}_x^2 + \mathbf{a}_y^2 + \mathbf{a}_z^2)$, applying the chain rule, and then solving the partial differential of s with respect to each of $\mathbf{a}_x$, $\mathbf{a}_y$, and $\mathbf{a}_z$.

Suppose the vector $\mathbf{a}$ is a vector separating any two points $\mathbf{b}$ and $\mathbf{c}$. What then is the gradient of the Euclidean norm of $\mathbf{a}$, as the end points $\mathbf{b}$ and $\mathbf{c}$ are varied respectively? If we define $\mathbf{a} = \mathbf{c} - \mathbf{b}$, then the gradient of $||\mathbf{a}||$, while varying $\mathbf{c}$'s position and keeping $\mathbf{b}$ constant, is

$$\nabla_{\mathbf{c}}||\mathbf{a}|| = \hat{\mathbf{a}}. \tag{C.11}$$

And the gradient while keeping $\mathbf{c}$ constant and varying $\mathbf{b}$'s position is

$$\nabla_{\mathbf{b}}||\mathbf{a}|| = -\hat{\mathbf{a}}. \tag{C.12}$$

The proofs are similar to the proof of (C.10) except that as each partial derivative is evaluated, then the chain rule is applied a second time. Again, proofs are omitted.

Gradient of Particle Separation Distance

The potential energy functions we use are defined in part as a function of particle separation, so we now derive equations describing the gradient of the separation distance with respect to change in position and to change in orientation. Let us assume we have two particles $\mathbf{x}_i$ and $\mathbf{x}_j$, and a separation distance vector defined as $\mathbf{r}_{ij} = \mathbf{x}_j - \mathbf{x}_i$. Applying the general identities (C.11) and (C.12), we arrive at the following equations for the gradient with respect to the change in positions of $\mathbf{x}_i$ and $\mathbf{x}_j$,

$$\nabla_{\mathbf{x}_i}||\mathbf{r}_{ij}|| = -\hat{\mathbf{r}}_{ij}, \tag{C.13}$$

$$\nabla_{\mathbf{x}_j}||\mathbf{r}_{ij}|| = \hat{\mathbf{r}}_{ij}. \tag{C.14}$$

In deriving the torque equations we will need to evaluate the gradient with respect to the particle normal vectors $\mathbf{n}_i$ and $\mathbf{n}_j$. Since $\mathbf{r}_{ij}$ is not a function of either normal vector, we have,

$$\nabla_{\mathbf{n}_i}||\mathbf{r}_{ij}|| = 0, \tag{C.15}$$

$$\nabla_{\mathbf{n}_j}||\mathbf{r}_{ij}|| = 0. \tag{C.16}$$

Gradient of the Difference of Normal Vectors

For the case of the co-normality potential we consider the gradient of the difference between two normal vectors $\mathbf{n}_i$ and $\mathbf{n}_j$. Applying the identities (C.11) and (C.12) results in the following equations,

$$\nabla_{\mathbf{n}_i} \|\mathbf{n}_i - \mathbf{n}_j\| = \frac{\|\mathbf{n}_i - \mathbf{n}_j\|}{\mathbf{n}_i - \mathbf{n}_j} \quad (C.17)$$

$$\nabla_{\mathbf{n}_j} \|\mathbf{n}_i - \mathbf{n}_j\| = -\frac{\|\mathbf{n}_i - \mathbf{n}_j\|}{\mathbf{n}_i - \mathbf{n}_j}. \quad (C.18)$$

And since the Euclidean norm is constant as the particle positions change,

$$\nabla_{\mathbf{x}_i} \|\mathbf{n}_i - \mathbf{n}_j\| = 0, \quad (C.19)$$

$$\nabla_{\mathbf{x}_j} \|\mathbf{n}_i - \mathbf{n}_j\| = 0. \quad (C.20)$$

C.4 Variations of Scalar Products

The scalar product of any two vectors $\mathbf{a}$ and $\mathbf{b}$ is defined to be

$$\mathbf{a} \cdot \mathbf{b} = \mathbf{a}_x \mathbf{b}_x + \mathbf{a}_y \mathbf{b}_y + \mathbf{a}_z \mathbf{b}_z.$$

Differential Identities of Scalar Products

For any two vectors $\mathbf{a}$ and $\mathbf{b}$, the gradient of their scalar product is

$$\nabla_{\mathbf{a}}(\mathbf{a} \cdot \mathbf{b}) = \mathbf{b} \quad (C.21)$$

with respect to varying $\mathbf{a}$. Given any three independent vectors $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$, by the distributive property of the scalar product and (C.21), we have

$$\nabla_{\mathbf{b}}(\mathbf{a} \cdot (\mathbf{b} - \mathbf{c})) = \mathbf{a}, \quad (C.22)$$

$$\nabla_{\mathbf{c}}(\mathbf{a} \cdot (\mathbf{b} - \mathbf{c})) = -\mathbf{a}. \quad (C.23)$$

Variations of the Scalar Product of the Normal and Separation Vectors

The co-planarity potential and the co-circularity potential functions are functions of the scalar product of normal vectors and particle separation, that is $\nabla(\mathbf{n}_i \cdot \mathbf{r}_{ij})$. To derive the gradient with respect to a particle position we apply identities (C.22) and (C.23). The relevant equations are:

$$\nabla_{\mathbf{x}_i}(\mathbf{n}_i \cdot \mathbf{r}_{ij}) = -\mathbf{n}_i, \quad (C.24)$$

$$\nabla_{\mathbf{x}_i}(\mathbf{n}_j \cdot \mathbf{r}_{ij}) = -\mathbf{n}_j, \quad (C.25)$$

$$\nabla_{\mathbf{x}_j}(\mathbf{n}_i \cdot \mathbf{r}_{ij}) = \mathbf{n}_i, \quad (C.26)$$

$$\nabla_{\mathbf{x}_j}(\mathbf{n}_j \cdot \mathbf{r}_{ij}) = \mathbf{n}_j. \quad (C.27)$$

To derive the gradient of the product with respect to a given particle normal, we apply identity (C.21). The relevant equations are:

$$\nabla_{\mathbf{n}_i}(\mathbf{n}_i \cdot \mathbf{r}_{ij}) = \mathbf{r}_{ij}, \tag{C.28}$$
$$\nabla_{\mathbf{n}_i}(\mathbf{n}_j \cdot \mathbf{r}_{ij}) = 0, \tag{C.29}$$
$$\nabla_{\mathbf{n}_j}(\mathbf{n}_i \cdot \mathbf{r}_{ij}) = 0, \tag{C.30}$$
$$\nabla_{\mathbf{n}_j}(\mathbf{n}_j \cdot \mathbf{r}_{ij}) = \mathbf{r}_{ij}. \tag{C.31}$$

C.5 Variation of the Weighting Function

The scalar weighting function $w(\|\mathbf{r}_{ij}\|)$ is a monotonically decreasing function used to limit the range of inter-particle interactions, where $\mathbf{r}_{ij} = \mathbf{x}_j - \mathbf{x}_i$ is defined as the distance vector between points $\mathbf{x}_i$ and $\mathbf{x}_j$. In evaluating the gradients of the weighting function we apply the chain rule (C.4) and equations (C.13), (C.14), (C.15), and (C.16). Using the following shorthand notation,

$$\begin{aligned} w &= w(\|\mathbf{r}_{ij}\|), \\ w' &= \frac{\mathrm{d}w(\|\mathbf{r}_{ij}\|)}{\mathrm{d}\|\mathbf{r}_{ij}\|} \end{aligned}$$

we have,

$$\nabla_{\mathbf{x}_i} w = w' \nabla_{\mathbf{x}_i} \|\mathbf{r}_{ij}\| = -\hat{\mathbf{r}}_{ij} w', \tag{C.32}$$
$$\nabla_{\mathbf{x}_j} w = w' \nabla_{\mathbf{x}_j} \|\mathbf{r}_{ij}\| = \hat{\mathbf{r}}_{ij} w', \tag{C.33}$$
$$\nabla_{\mathbf{n}_i} w = w' \nabla_{\mathbf{n}_i} \|\mathbf{r}_{ij}\| = 0, \tag{C.34}$$
$$\nabla_{\mathbf{n}_j} w = w' \nabla_{\mathbf{n}_j} \|\mathbf{r}_{ij}\| = 0. \tag{C.35}$$

C.6 Forces and Torques from Weighted Potentials

In this section we use the results from the previous sections to show how to derive force and torque vectors from weighted scalar potential fields.

Force from a Weighted Potential

The gradient of a weighted scalar potential is computed based on the application of the multiplication and chain rules. Assuming we have two particles positioned at $\mathbf{x}_i$ and $\mathbf{x}_j$, the vector $\mathbf{r}_{ij}$ separating the two particles is $(\mathbf{x}_j - \mathbf{x}_i)$ and the separation distance is $r_{ij} = \|\mathbf{r}_{ij}\|$. Given a potential $\phi(r)$ and a weighting $w(r)$, both scalar functions of distance, the gradient of their product is

$$\nabla_{\mathbf{x}}\left(w(r_{ij})\phi(r_{ij})\right) = w(r_{ij})\frac{\mathrm{d}\phi(r_{ij})}{\mathrm{d}r}\nabla_{\mathbf{x}} r_{ij} + \frac{\mathrm{d}w(r_{ij})}{\mathrm{d}r}\phi(r_{ij})\nabla_{\mathbf{x}} r_{ij}.$$

Applying (C.1), (C.13) and (C.14) the resultant force acting on particle i is thus

$$\mathbf{f}_i = -\nabla_{\mathbf{x}_i}\left(w(r)\phi(r)\right) = \hat{\mathbf{r}}_{ij}\left(w(r_{ij})\frac{\mathrm{d}\phi(r_{ij})}{\mathrm{d}r} + \phi(r_{ij})\frac{\mathrm{d}w(r_{ij})}{\mathrm{d}r}\right)$$

and the force acting on particle j is

$$\mathbf{f}_j = -\nabla_{\mathbf{x}_j} \left(w(r)\phi(r) \right) = -\mathbf{f}_i.$$

It should be clear that these equations also hold for potentials that are a function not only of particle separation but also of particle normals.

Torque from a Weighted Potential

Assuming we have two particles as above and with normals given by $\mathbf{n}_i$ and $\mathbf{n}_j$, and given a potential $\phi(r_{ij}, \mathbf{n}_i, \mathbf{n}_j)$ and a weighting $w(r_{ij})$, then the gradient of their product with respect to variation in normal is

$$\nabla_{\mathbf{n}} \left(w(r_{ij})\phi(r_{ij}, \mathbf{n}_i, \mathbf{n}_j) \right) = w(r_{ij})\nabla_{\mathbf{n}}\phi(r_{ij}, \mathbf{n}_i, \mathbf{n}_j) + \phi(r_{ij}, \mathbf{n}_i, \mathbf{n}_j)\nabla_{\mathbf{n}} w(r_{ij}).$$

And since the gradient of the weighting function is zero this reduces to

$$\nabla_{\mathbf{n}} \left(w(r_{ij})\phi(r_{ij}, \mathbf{n}_i, \mathbf{n}_j) \right) = w(r_{ij})\nabla_{\mathbf{n}}\phi(r_{ij}, \mathbf{n}_i, \mathbf{n}_j).$$

By (C.2), (C.9), and (C.6) the torque vector acting on particle i is

$$\boldsymbol{\tau}_i = -\nabla_{\boldsymbol{\theta}} \left(w(r_{ij})\phi(r_{ij}, \mathbf{n}_i, \mathbf{n}_j) \right) = -\mathbf{n}_i \times \left(\nabla_{\mathbf{n}_i}\phi(r_{ij}, \mathbf{n}_i, \mathbf{n}_j) \right) w(r_{ij}).$$

Likewise the torque acting on particle j is

$$\boldsymbol{\tau}_i = -\mathbf{n}_j \times \left(\nabla_{\mathbf{n}_j}\phi(r_{ij}, \mathbf{n}_i, \mathbf{n}_j) \right) w(r_{ij}).$$

Appendix D

Computation of internal forces

Based on the identities and equations of Appendix C, we derive the inter-particle forces and torques for the distance weighted versions of the co-planarity, the co-normality, the co-circularity, and the Lennard-Jones potentials. For a pair of particles i and j we derive the forces and torques with respect to both particle i and particle j.

D.1 The Co-planarity Potential

The spatially weighted co-planarity potential is

$$\phi_{\mathrm{P}} = (\mathbf{n}_i \cdot \mathbf{r}_{ij})^2 w.$$

To derive the forces and torques, we first derive the gradients of the potential function with respect to the variation in particle positions, particle normals, and the infinitesimal change in particle orientations.

Variation in Position

To derive the gradient with respect to the variation in the particle i's position we apply the multiplication rule (C.3) resulting in two parts to differentiate. To the left side we apply equation (C.32), and to the right side we apply the chain rule (C.4) and equation (C.24):

$$\nabla_{\mathbf{x}_i}\phi_{\mathrm{P}} = (\mathbf{n}_i \cdot \mathbf{r}_{ij})^2 \nabla_{\mathbf{x}_i} w + w \nabla_{\mathbf{x}_i} (\mathbf{n}_i \cdot \mathbf{r}_{ij})^2 = (\mathbf{n}_i \cdot \mathbf{r}_{ij})^2 w'(-\hat{\mathbf{r}}_{ij}) + w2(\mathbf{n}_i \cdot \mathbf{r}_{ij})(-\mathbf{n}_i).$$

The derivation of the gradient with respect to particle j's position is similar, except we apply equations (C.33) and (C.26) where appropriate:

$$\nabla_{\mathbf{x}_j}\phi_{\mathrm{P}} = (\mathbf{n}_i \cdot \mathbf{r}_{ij})^2 \nabla_{\mathbf{x}_j} w + w \nabla_{\mathbf{x}_j} (\mathbf{n}_i \cdot \mathbf{r}_{ij})^2 = (\mathbf{n}_i \cdot \mathbf{r}_{ij})^2 w'\hat{\mathbf{r}}_{ij} + w2(\mathbf{n}_i \cdot \mathbf{r}_{ij})\mathbf{n}_i.$$

Variation in Normal

To derive the gradient with respect to the variation in particle i's normal we apply the multiplication rule (C.3), the chain rule (C.4), and equations (C.34) and (C.28):

$$\nabla_{\mathbf{n}_i}\phi_{\mathrm{P}} = (\mathbf{n}_i \cdot \mathbf{r}_{ij})^2 \nabla_{\mathbf{n}_i} w + w \nabla_{\mathbf{n}_i} (\mathbf{n}_i \cdot \mathbf{r}_{ij})^2 = 2w(\mathbf{n}_i \cdot \mathbf{r}_{ij})\mathbf{r}_{ij}.$$

The derivation with respect to particle j's normal is similar, except we apply equations (C.35) and (C.30) where appropriate:

$$\nabla_{\mathbf{n}_j}\phi_{\mathrm{P}} = (\mathbf{n}_i \cdot \mathbf{r}_{ij})^2 \nabla_{\mathbf{n}_j} w + w \nabla_{\mathbf{n}_j} (\mathbf{n}_i \cdot \mathbf{r}_{ij})^2 = 0.$$

Variation in Orientation

To derive the gradient with respect to the infinitesimal change in the particle orientation we apply equation (C.9) and the above results:

$$\nabla_{\boldsymbol{\theta}_i}\phi_{\mathrm{P}} = \mathbf{n}_i \times \nabla_{\mathbf{n}_i}\phi_{\mathrm{P}} = 2w(\mathbf{n}_i \cdot \mathbf{r}_{ij})(\mathbf{n}_i \times \mathbf{r}_{ij})w.$$

The gradient of the potential with respect to the change in orientation of particle j is zero, because the potential is independent of the orientation of particle j:

$$\nabla_{\boldsymbol{\theta}_j}\phi_{\mathrm{P}} = \mathbf{n}_j \times \nabla_{\mathbf{n}_j}\phi_{\mathrm{P}} = \mathbf{n}_j \times 0 = 0.$$

Forces and Torques

The forces and torques follow directly from the above derivations:

$$\begin{aligned}
\mathbf{f}_{\mathrm{P}_i} &= -\nabla_{\mathbf{x}_i}\phi_{\mathrm{P}} = (\mathbf{n}_i \cdot \mathbf{r}_{ij})^2 \hat{\mathbf{r}}_{ij} w' + 2(\mathbf{n}_i \cdot \mathbf{r}_{ij})\mathbf{n}_i w \\
\mathbf{f}_{\mathrm{P}_j} &= -\nabla_{\mathbf{x}_j}\phi_{\mathrm{P}} = -(\mathbf{n}_i \cdot \mathbf{r}_{ij})^2 \hat{\mathbf{r}}_{ij} w' - 2(\mathbf{n}_i \cdot \mathbf{r}_{ij})\mathbf{n}_i w = -\mathbf{f}_{\mathrm{P}_i} \\
\boldsymbol{\tau}_{\mathrm{P}_i} &= -\nabla_{\boldsymbol{\theta}_i}\phi_{\mathrm{P}} = -2(\mathbf{n}_i \cdot \mathbf{r}_{ij})(\mathbf{n}_i \times \mathbf{r}_{ij})w \\
\boldsymbol{\tau}_{\mathrm{P}_j} &= -\nabla_{\boldsymbol{\theta}_j}\phi_{\mathrm{P}} = 0.
\end{aligned}$$

D.2 The Co-normality Potential

The spatially weighted co-normality potential is

$$\phi_{\mathrm{N}} = \|\mathbf{n}_i - \mathbf{n}_j\|^2 w.$$

To derive the forces and torques, we first derive the gradients of the potential function with respect to the variation in particle positions, particle normals, and the infinitesimal change in particle orientations.

Variation in Position

To derive the gradient with respect to the variation in the particle i's position, we apply the multiplication rule (C.3) resulting in a left and right side to differentiate. To the left side we apply equation (C.32), and to the right side we apply the chain rule (C.4) and equation (C.19):

$$\nabla_{\mathbf{x}_i}\phi_{\mathrm{N}} = \|\mathbf{n}_i - \mathbf{n}_j\|^2\nabla_{\mathbf{x}_i} w + w\nabla_{\mathbf{x}_i}\left(\|\mathbf{n}_i - \mathbf{n}_j\|^2\right) = \|\mathbf{n}_i - \mathbf{n}_j\|^2(-\mathbf{r}_{ij})w'.$$

The derivation of the gradient with respect to particle j's position is similar, except we apply equations (C.33) and (C.20) where appropriate:

$$\nabla_{\mathbf{x}_j}\phi_{\mathrm{N}} = \|\mathbf{n}_i - \mathbf{n}_j\|^2\nabla_{\mathbf{x}_j} w + w\nabla_{\mathbf{x}_j}\left(\|\mathbf{n}_i - \mathbf{n}_j\|^2\right) = \|\mathbf{n}_i - \mathbf{n}_j\|^2\mathbf{r}_{ij}w'.$$

Variation in Normal

To derive the gradient with respect to the variation in particle i's normal we apply the multiplication rule (C.3), the chain rule (C.4), and equations (C.34) and (C.17):

$$\nabla_{\mathbf{n}_i}\phi_{\mathrm{N}} = \|\mathbf{n}_i - \mathbf{n}_j\|^2\nabla_{\mathbf{n}_i} w + w\nabla_{\mathbf{n}_i}\left(\|\mathbf{n}_i - \mathbf{n}_j\|^2\right) = w2(\mathbf{n}_i - \mathbf{n}_j).$$

The derivation with respect to particle j's normal is similar, except we apply equations (C.35) and (C.18) where appropriate:

$$\nabla_{\mathbf{n}_j}\phi_{\mathrm{N}} = \|\mathbf{n}_i - \mathbf{n}_j\|^2\nabla_{\mathbf{n}_j} w + w\nabla_{\mathbf{n}_j}\left(\|\mathbf{n}_i - \mathbf{n}_j\|^2\right) = -w2(\mathbf{n}_i - \mathbf{n}_j).$$

Variation in Orientation

To derive the gradient with respect to the infinitesimal change in the particle orientation we apply equation (C.9) and the above results:

$$\nabla_{\boldsymbol{\theta}_i}\phi_{\mathrm{N}} = \mathbf{n}_i \times \nabla_{\mathbf{n}_i}\phi_{\mathrm{N}} = 2w\left(\mathbf{n}_j \times \mathbf{n}_i\right).$$

The gradient with respect to the infinitesimal change in particle j's orientation is derived by a similar process :

$$\nabla_{\boldsymbol{\theta}_j}\phi_{\mathrm{N}} = \mathbf{n}_j \times \nabla_{\mathbf{n}_j}\phi_{\mathrm{N}} = -2w\left(\mathbf{n}_j \times \mathbf{n}_i\right).$$

Forces and Torques

The forces and torques follow directly from the above derivations:

$$\begin{aligned}
\mathbf{f}_{\mathrm{N}_i} &= -\nabla_{\mathbf{x}_i}\phi_{\mathrm{N}} = \|\mathbf{n}_i - \mathbf{n}_j\|^2\mathbf{r}_{ij}w' \\
\mathbf{f}_{\mathrm{N}_j} &= -\nabla_{\mathbf{x}_j}\phi_{\mathrm{N}} = -\|\mathbf{n}_i - \mathbf{n}_j\|^2\mathbf{r}_{ij}w' = -\mathbf{f}_{\mathrm{N}_i} \\
\boldsymbol{\tau}_{\mathrm{N}_i} &= -\nabla_{\boldsymbol{\theta}_i}\phi_{\mathrm{N}} = -2\left(\mathbf{n}_j \times \mathbf{n}_i\right)w \\
\boldsymbol{\tau}_{\mathrm{N}_j} &= -\nabla_{\boldsymbol{\theta}_j}\phi_{\mathrm{N}} = 2\left(\mathbf{n}_j \times \mathbf{n}_i\right)w = -\boldsymbol{\tau}_{\mathrm{N}_i}.
\end{aligned}$$

D.3 The Co-circularity Potential

The spatially weighted co-circularity potential is

$$\phi_{\mathrm{C}} = \left((\mathbf{n}_i + \mathbf{n}_j) \cdot \mathbf{r}_{ij}\right)^2 w.$$

To derive the forces and torques, we first derive the gradients of the potential function with respect to the variation in particle positions, particle normals, and the infinitesimal change in particle orientations.

Variation in Position

To derive the gradient with respect to the variation in the particle i's position, we apply the multiplication rule (C.3) resulting in a left and right side to differentiate. To the left side we apply equation (C.32), while we apply the chain rule (C.4) to the right side:

$$\begin{aligned}
\nabla_{\mathbf{x}_i}\phi_{\mathrm{C}} &= \left((\mathbf{n}_i + \mathbf{n}_j) \cdot \mathbf{r}_{ij}\right)^2 \nabla_{\mathbf{x}_i} w + w \nabla_{\mathbf{x}_i} \left((\mathbf{n}_i + \mathbf{n}_j) \cdot \mathbf{r}_{ij}\right)^2 \\
&= \left((\mathbf{n}_i + \mathbf{n}_j) \cdot \mathbf{r}_{ij}\right)^2 (-\hat{\mathbf{r}}_{ij}) w' + w2 \left((\mathbf{n}_i + \mathbf{n}_j) \cdot \mathbf{r}_{ij}\right) \nabla_{\mathbf{x}_i} \left((\mathbf{n}_i + \mathbf{n}_j) \cdot \mathbf{r}_{ij}\right).
\end{aligned}$$

To solve the gradient on right hand side of the equation we apply the distributive rule of scalar products, the identity $\nabla(\mathbf{a} + \mathbf{b}) = (\nabla \mathbf{a}) + (\nabla \mathbf{b})$, and equations (C.24) and (C.25), thus the gradient is

$$\nabla_{\mathbf{x}_i}\phi_{\mathrm{C}} = \left((\mathbf{n}_i + \mathbf{n}_j) \cdot \mathbf{r}_{ij}\right)^2 (-\hat{\mathbf{r}}_{ij}) w' - w2 \left((\mathbf{n}_i + \mathbf{n}_j) \cdot \mathbf{r}_{ij}\right) (\mathbf{n}_i + \mathbf{n}_j).$$

The derivation of the gradient with respect to particle j's position is similar, except we apply equations (C.33), (C.26), and (C.27) where appropriate:

$$\nabla_{\mathbf{x}_j}\phi_{\mathrm{C}} = \left((\mathbf{n}_i + \mathbf{n}_j) \cdot \mathbf{r}_{ij}\right)^2 \hat{\mathbf{r}}_{ij} w' + w2 \left((\mathbf{n}_i + \mathbf{n}_j) \cdot \mathbf{r}_{ij}\right) (\mathbf{n}_i + \mathbf{n}_j).$$

Variation in Normal

To derive the gradient with respect to the variation in particle i's normal we apply the multiplication rule (C.3), the chain rule (C.4), and equations (C.34), (C.28), and (C.29):

$$\nabla_{\mathbf{n}_i}\phi_{\mathrm{C}} = \left((\mathbf{n}_i + \mathbf{n}_j) \cdot \mathbf{r}_{ij}\right)^2 \nabla_{\mathbf{n}_i} w + w \nabla_{\mathbf{n}_i} \left((\mathbf{n}_i + \mathbf{n}_j) \cdot \mathbf{r}_{ij}\right)^2 = w2 \left((\mathbf{n}_i + \mathbf{n}_j) \cdot \mathbf{r}_{ij}\right) \mathbf{r}_{ij}.$$

The derivation with respect to particle j's normal is similar, except we apply equations (C.35), (C.30), and (C.31) where appropriate:

$$\nabla_{\mathbf{n}_j}\phi_{\mathrm{C}} = \left((\mathbf{n}_i + \mathbf{n}_j) \cdot \mathbf{r}_{ij}\right)^2 \nabla_{\mathbf{n}_j} w + w \nabla_{\mathbf{n}_j} \left((\mathbf{n}_i + \mathbf{n}_j) \cdot \mathbf{r}_{ij}\right)^2 = w2 \left((\mathbf{n}_i + \mathbf{n}_j) \cdot \mathbf{r}_{ij}\right) \mathbf{r}_{ij}.$$

Variation in Orientation

To derive the gradient with respect to the infinitesimal change in the particle orientation we apply equation (C.9) and the above results:

$$\nabla_{\boldsymbol{\theta}_i}\phi_{\mathrm{C}} = \mathbf{n}_i \times \nabla_{\mathbf{n}_i}\phi_{\mathrm{C}} = 2w\left((\mathbf{n}_i + \mathbf{n}_j)\cdot \mathbf{r}_{ij}\right)(\mathbf{n}_i \times \mathbf{r}_{ij})\,.$$

The gradient with respect to the infinitesimal change in particle j's orientation is derived by a similar process:

$$\nabla_{\boldsymbol{\theta}_j}\phi_{\mathrm{C}} = \mathbf{n}_j \times \nabla_{\mathbf{n}_j}\phi_{\mathrm{C}} = 2w\left((\mathbf{n}_i + \mathbf{n}_j)\cdot \mathbf{r}_{ij}\right)(\mathbf{n}_j \times \mathbf{r}_{ij})\,.$$

Forces and Torques

The forces and torques follow directly from the above derivations:

$$\begin{aligned}
\mathbf{f}_{\mathrm{C}_i} &= -\nabla_{\mathbf{x}_i}\phi_{\mathrm{C}} = \left((\mathbf{n}_i + \mathbf{n}_j)\cdot \mathbf{r}_{ij}\right)^2 \hat{\mathbf{r}}_{ij} w' + 2\left((\mathbf{n}_i + \mathbf{n}_j)\cdot \mathbf{r}_{ij}\right)(\mathbf{n}_i + \mathbf{n}_j) w \\
\mathbf{f}_{\mathrm{C}_j} &= -\nabla_{\mathbf{x}_j}\phi_{\mathrm{C}} = -\left((\mathbf{n}_i + \mathbf{n}_j)\cdot \mathbf{r}_{ij}\right)^2 \hat{\mathbf{r}}_{ij} w' - 2\left((\mathbf{n}_i + \mathbf{n}_j)\cdot \mathbf{r}_{ij}\right)(\mathbf{n}_i + \mathbf{n}_j) w = -\mathbf{f}_{\mathrm{C}_i} \\
\boldsymbol{\tau}_{\mathrm{C}_i} &= -\nabla_{\boldsymbol{\theta}_i}\phi_{\mathrm{C}} = -2\left((\mathbf{n}_i + \mathbf{n}_j)\cdot \mathbf{r}_{ij}\right)(\mathbf{n}_i \times \mathbf{r}_{ij})\, w \\
\boldsymbol{\tau}_{\mathrm{C}_j} &= -\nabla_{\boldsymbol{\theta}_j}\phi_{\mathrm{C}} = -2\left((\mathbf{n}_i + \mathbf{n}_j)\cdot \mathbf{r}_{ij}\right)(\mathbf{n}_j \times \mathbf{r}_{ij})\, w
\end{aligned}$$

D.4 The Lennard-Jones Potential

The Lennard-Jones function is a scalar function defined in three-space as a function of particle separation. Similar to the shorthand notation used for the weighting function, we will use

$$\begin{aligned}
\phi_{\mathrm{LJ}} &= \phi_{\mathrm{LJ}}(\|\mathbf{r}_{ij}\|) \\
{\phi_{\mathrm{LJ}}}' &= \frac{\mathrm{d}\phi_{\mathrm{LJ}}}{\mathrm{d}\|\mathbf{r}_{ij}\|}
\end{aligned}$$

in our derivations. To derive the forces and torques, we first derive the gradients with respect to variation in particle positions, particle normals, and the infinitesimal change in particle orientations.

Variation in Position

To derive the gradient with respect to the variation in the particle positions we apply the chain rule (C.4), and equations (C.13) and (C.14):

$$\begin{aligned}
\nabla_{\mathbf{x}_i}\phi_{\mathrm{LJ}} &= {\phi_{\mathrm{LJ}}}'\nabla_{\mathbf{x}_i}\|\mathbf{r}_{ij}\| = -\hat{\mathbf{r}}_{ij}{\phi_{\mathrm{LJ}}}' \\
\nabla_{\mathbf{x}_j}\phi_{\mathrm{LJ}} &= {\phi_{\mathrm{LJ}}}'\nabla_{\mathbf{x}_j}\|\mathbf{r}_{ij}\| = \hat{\mathbf{r}}_{ij}{\phi_{\mathrm{LJ}}}'.
\end{aligned}$$

Variation in Normal

To derive the gradient with respect to the variation in the particle normals we apply the chain rule (C.4), and equations (C.15) and (C.16):

$$\begin{aligned}
\nabla_{\mathbf{n}_i}\phi_{\mathrm{LJ}} &= {\phi_{\mathrm{LJ}}}'\nabla_{\mathbf{n}_i}\|\mathbf{r}_{ij}\| = {\phi_{\mathrm{LJ}}}'(0) = 0\\
\nabla_{\mathbf{n}_j}\phi_{\mathrm{LJ}} &= {\phi_{\mathrm{LJ}}}'\nabla_{\mathbf{n}_j}\|\mathbf{r}_{ij}\| = {\phi_{\mathrm{LJ}}}'(0) = 0.
\end{aligned}$$

Variation in Orientation

To derive the gradient with respect to the infinitesimal change in the particle orientation we apply equation (C.9) and the above results:

$$\begin{aligned}
\nabla_{\boldsymbol{\theta}_i}\phi_{\mathrm{LJ}} &= \mathbf{n}_i \times \nabla_{\mathbf{n}_i}\phi_{\mathrm{LJ}} = \mathbf{n}_i \times 0 = 0\\
\nabla_{\boldsymbol{\theta}_j}\phi_{\mathrm{LJ}} &= \mathbf{n}_j \times \nabla_{\mathbf{n}_j}\phi_{\mathrm{LJ}} = \mathbf{n}_j \times 0 = 0.
\end{aligned}$$

Forces and Torques

The forces and torques follow directly from the above derivations:

$$\begin{aligned}
\mathbf{f}_{\mathrm{LJ}_i} &= -\nabla_{\mathbf{x}_i}\phi_{\mathrm{LJ}} = \hat{\mathbf{r}}_{ij}{\phi_{\mathrm{LJ}}}'\\
\mathbf{f}_{\mathrm{LJ}_j} &= -\nabla_{\mathbf{x}_j}\phi_{\mathrm{LJ}} = -\hat{\mathbf{r}}_{ij}{\phi_{\mathrm{LJ}}}' = -\mathbf{f}_j\\
\boldsymbol{\tau}_{\mathrm{LJ}_i} &= -\nabla_{\boldsymbol{\theta}_i}\phi_{\mathrm{LJ}} = 0\\
\boldsymbol{\tau}_{\mathrm{LJ}_j} &= -\nabla_{\boldsymbol{\theta}_j}\phi_{\mathrm{LJ}} = 0
\end{aligned}$$

Appendix E

Finite Element Analysis of Surface Energies

To derive the local oriented particle interaction potentials, we analyze the deformation energies of a triangular surface patch defined by three neighboring particles. For this analysis, we assume that the particles are in an equilateral configuration with locations $(0,0)$, $(h,0)$ and $(1/2, \sqrt{3}/2)$ in the (x,y) plane. We examine the small-deflection case where the height from the plane, $z = f(x,y)$, describes the local shape of the surface. Both of these assumptions are reasonable for our surfaces, since the Lennard-Jones forces favor locally hexagonal arrangements, and a sufficiently high sampling density will ensure small deflections. For an analysis of the general parametric patch case, see (Celniker and Gossard, 1991). We use a cubic function for $f(x,y)$ since it can be specified by the heights and gradients at the three corners $\{(z_i, p_i, q_i), i = 0 \ldots 2\}$ and the height z_3 of a "bubble" node in the middle of a triangle. We choose the (x,y) plane to pass through the three particles, which gives us a height of 0 at all three corners. To compute the deformation energies, we take integrals of squared derivatives over the triangle. For example, we can compute the area of the triangle from

$$A = \int\int \sqrt{1 + f_x^2 + f_y^2}\, dx\, dy \approx \frac{\sqrt{3}}{4} h^2 + \frac{1}{2} \int\int f_x^2 + f_y^2 \, dx\, dy.$$

We can compute the average Gaussian curvature from

$$C \approx \frac{1}{2} \int\int f_{xx}^2 + 2 f_{xy}^2 + f_{yy}^2 \, dx\, dy$$

and the average variation in curvature from

$$V \approx \frac{1}{2} \int\int f_{xxx}^2 + 3 f_{xxy}^2 + 3 f_{xyy}^2 + f_{yyy}^2 \, dx\, dy.$$

These three integrals can be thought of as corresponding to the stretching, bending, and "undulation" energies of the surface. After some algebraic manipulation, which we performed using Mathematica$^{\mathrm{TM}}$(Wolfram, 1988), we obtain formulas for the above three equations in terms of the corner gradient values $\{(p_i, q_i)\}$ and the bubble height z_3 (the expressions are quadratic in these variables). In our oriented particle system, we desire to have interactions only between pairs of particles. Since we are only interested in the energies involving two particles, say the particles which control (p_0, q_0) and (p_1, q_1), we minimize the quadratic energies with respect to the p_2, q_2, and z_3 variables (this results in lower energies than arbitrarily setting these unknown quantities to 0, which would be the effect of ignoring these other terms). To further simplify the energies, we express them in terms of averages and differences of gradients

$$\begin{array}{rclcrcl} p_+ &=& (p_0+p_1)/2 & \qquad & q_+ &=& (q_0+q_1)/2 \\ p_- &=& (p_0-p_1)/2 & \qquad & q_- &=& (q_0-q_1)/2. \end{array}$$

Again, using Mathematica$^{\mathrm{TM}}$, we obtain

$$V = h^{-2}6\sqrt{3}p_+^2, \tag{E.1}$$

$$C = \frac{\sqrt{3}}{2268}(567p_+^2 + 316p_-^2 + 8\sqrt{3}p_-q_+ + 48q_+^2 + 315q_-^2), \tag{E.2}$$

$$A = h^2\frac{\sqrt{3}}{4}(1 + \frac{6003}{281880}p_+^2 + \cdots). \tag{E.3}$$

To compute these quantities given the state of two particles, i.e., their positions and orientations, we must first write the scalar quantities p_0, p_1, q_0, and q_1 in terms of $\mathbf{n}_i$, $\mathbf{n}_j$ and $\mathbf{r}_{ij}$. We identify $\mathbf{r}_{ij}$ with the x direction in our local plane, and thus compute

$$p_0 \approx -\mathbf{n}_i \cdot \hat{\mathbf{r}}_{\mathbf{ij}} \;\; \text{and} \;\; \mathbf{p_1} \approx -\mathbf{n_j} \cdot \hat{\mathbf{r}}_{\mathbf{ij}}$$

for small values of p_0 and p_1. Choosing the y direction is more difficult if we wish to keep the interactions pairwise, since we cannot use the location of the third point defining the triangle. A simple choice is use the local z direction along the average normal vector $(\mathbf{n}_i + \mathbf{n}_j)/2$, which leads to the equations

$$q_+ = -(\frac{\mathbf{n}_i + \mathbf{n}_j}{2}) \cdot \frac{\widehat{\mathbf{n}_i + \mathbf{n}_j}}{2} \times \hat{\mathbf{r}}_{\mathbf{ij}} = \mathbf{0}, \tag{E.4}$$

$$q_- = -(\frac{\mathbf{n}_i - \mathbf{n}_j}{2}) \cdot \frac{\widehat{\mathbf{n}_i + \mathbf{n}_j}}{2} \times \hat{\mathbf{r}}_{\mathbf{ij}}, \tag{E.5}$$

$$p_-^2 + q_-^2 \approx \frac{1}{4}\|\mathbf{n}_i - \mathbf{n}_j\|^2. \tag{E.6}$$

We are now in a position to relate the finite element based measures for curvature and variation in curvature to the co-planarity, co-normality, and co-circularity measures. The variation in curvature V (E.2) corresponds directly to the co-circularity ϕ_{C} (4.17). The curvature itself C (E.3) can be written as a sum of the co-circularity potential and the co-normality potential ϕ_{N} (4.14). The co-planarity potential is therefore not needed to write a curvature-based energy measure. It is useful, however, when used in isolation, since it corresponds to terms of the form

$$p_0^2 + p_1^2 \propto p_+^2 + p_-^2.$$

While the area-based measure A (E.3) is too complicated to warrant direct implementation, finite rest area behavior is simulated by the Lennard-Jones interaction potential ϕ_{LJ}.