Chapter 4

Particle Surfaces

In this chapter we present a new model of elastic surfaces based on interacting particle systems. Unlike previous surface models, the new model can be used to split, join, or extend surfaces without the need for manual intervention. While particle systems are much more flexible than deformable surface models in arranging themselves into arbitrary shapes and topologies, they do suffer from one major drawback. In the absence of external forces and constraints, 3-D particle systems prefer to arrange themselves into volumes rather than surfaces. This is because traditional particles are point masses with no preferred orientation along which surfaces might form. To overcome this limitation, we introduce a distributed model of surface shape which we call *oriented particles*, in which each particle represents a small surface element (which we could call a "surfel"). In addition to having a position, an oriented particle also has its own local coordinate frame, which adds three new degrees of freedom to each particle's state. The particles we use have long-range attraction forces and short-range repulsion forces and follow Newtonian dynamics, like the models of volumes presented in the previous chapter.

We begin by extending the mathematics of the particle systems presented in Chapter 3 to include oriented particles. Based on concepts from differential geometry, we derive inter-particle potential functions which encourage particles to form smooth surfaces. A review of the relevant geometric concepts is provided in Appendix A.

4.1 Oriented Particle Systems

This section discusses the basic mathematics of oriented particle systems. We extend the definition of a particle system given in Chapter 3 to include the concepts of orientation, angular inertia, angular velocity, and torque. As such, we build upon our previous presentation, redefining the properties of the system, such as the definitions of a particle, the equations of motion, kinetic and potential energies, and the surface density of particles.

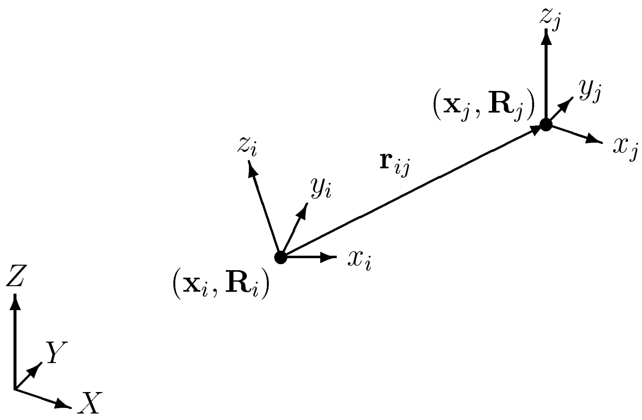

Figure 4.1: Oriented particles in global and local coordinate frames.

The global inter-particle distance $\mathbf{r}_{ij}$ is computed from the global coordinates $\mathbf{x}_i$ and $\mathbf{x}_j$ of particles i and j. The local distance $\mathbf{d}_{ij}$ is computed from $\mathbf{r}_{ij}$ and the rotation matrix $\mathbf{R}_i$.

4.1.1 The Oriented Particle

An oriented particle, like the previously discussed volume based particle, has a position and mass. In addition, each oriented particle has an orientation and inertia tensor. The orientation defines both a normal vector (z in Figure 4.1) and a local tangent plane to the surface (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 define rotation as a matrix for conversion between local and global coordinates and vice versa, we use unit quaternions to store the rotation in practice. The unit quaternion

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

represents a rotation of θ about the unit normal axis $\mathbf{a}$. 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). Our use of rotations is discussed in more detail in Appendix B.

The inertia tensor $\mathbf{I}$ relates the angular momentum to the angular velocity by a linear transformation. The angular velocity of a particle describes the rotation of a particle about the particle's local origin. The inertia tensor is defined about the particle's local origin with respect to the world coordinate axes. Since we are interested in the property of angular momentum but not a particular rigid body we choose a simple inertia tensor, one that is a constant scaling of the identity matrix. This is valid for all positions and orientations of a given particle. We discuss the inertia tensor in more detail in Appendix B.

4.1.2 Equations of Motion

A system of oriented particles is governed by the set of ordinary differential equations of motion: equation (3.1) rewritten here

$$m_i\ddot{\mathbf{x}}_i + \gamma_i\dot{\mathbf{x}}_i + \mathbf{f}_i^{\mathtt{int}} = \mathbf{f}_i^{\mathtt{ext}} \qquad i = 1, \ldots, N$$

and for our choice of inertia tensor, the associated equation for angular motion

$$\mathbf{I}_i\ddot{\mathbf{q}}_i + \xi_i\dot{\mathbf{q}}_i + \boldsymbol{\tau}_i^{int} = \boldsymbol{\tau}_i^{ext} \qquad i = 1, \ldots, N \tag{4.1}$$

where i is the particle index, N is the number of particles in the system, $\ddot{\mathbf{x}}_i$ is the acceleration of a particle, m_i is its mass, $\dot{\mathbf{x}}_i$ is its velocity, γ_i is a translational damping coefficient that controls the rate of dissipation of the particle's translational kinetic energy, $\mathbf{f}_i^{\mathtt{int}}$ is the sum of inter-particle forces, $\mathbf{f}_i^{\mathtt{ext}}$ is the sum of external forces, $\mathbf{q}_i$ is the orientation of particle i in three-space, $\ddot{\mathbf{q}}_i$ is the angular acceleration, $\mathbf{I}_i$ is the angular inertia tensor (B.1), $\dot{\mathbf{q}}_i$ is the angular velocity, ξ_i is an angular damping coefficient that controls the rate of dissipation of the particle's rotational kinetic energy, $\boldsymbol{\tau}_i^{int}$ is the sum of inter-particle torques and $\boldsymbol{\tau}_i^{ext}$ is the sum of external torques.

The inter-particle internal force term (3.2) is redefined

$$\mathbf{f}_i^{\mathtt{int}}(\mathbf{x}_1, \mathbf{q}_1, \mathbf{x}_2, \mathbf{q}_2, \ldots, \mathbf{x}_N, \mathbf{q}_N) \tag{4.2}$$

as a function of position *and orientation.* The external force term (3.3) is redefined as

$$\mathbf{f}_i^{\mathtt{ext}}(\mathbf{x}_i, \mathbf{q}_i, \mathbf{S}) \tag{4.3}$$

a function of particle position, orientation, and and the set $\mathbf{S}$ of external state variables such as gravity and collision objects. The inter-particle torque terms are defined in a similar manner

$$\boldsymbol{\tau}_i^{\mathtt{int}}(\mathbf{x}_1, \mathbf{q}_1, \mathbf{x}_2, \mathbf{q}_2, \ldots, \ldots, \mathbf{x}_N, \mathbf{q}_N). \tag{4.4}$$

External torques are functions of position, orientation, and external state variables

$$\boldsymbol{\tau}_i^{\mathtt{ext}}(\mathbf{x}_i, \mathbf{q}_i, \mathbf{S}). \tag{4.5}$$

4.1.3 Potential Energy

Similar to the use of potential energies for un-oriented particle systems, potential energies provide a convenient description of forces and torques between particles. This formulation also guarantees that the system will not diverge. For a potential function ϕ, the force exerted on particle i with position $\mathbf{x}_i$

$$\mathbf{f}_i = -\nabla_{\mathbf{x}_i}\phi$$

is due to the gradient of the potential energy ϕ with respect to the change in position. The *torque* exerted on particle i with orientation $\mathbf{q}_i$

$$\boldsymbol{\tau}_i = -\nabla_{\theta_i}\phi$$

is due to the gradient of the potential energy with respect to the incremental change in orientation θ_i.

For oriented particle systems we also adopt the pairwise additivity assumption which states that the total potential energy of a particle (3.4) is the sum of the pairwise potential energies between that particle and every other particle. Equation (3.5) describes the total inter-particle forces acting on a particle i due to the inter-particle potential energy functions and

$$\boldsymbol{\tau}_i = -\nabla_{\theta_i}\phi_i = -\sum_{j\neq i}^{N} \nabla_{\theta_i}\phi_{ij} \tag{4.6}$$

describes the total inter-particle torques acting on a particle due to the inter-particle potential energy functions. The equation for the total potential energy of the system (3.6) is the same for oriented particles as for un-oriented particles.

4.1.4 Kinetic Energy

The kinetic energy of an oriented particle is a combination of translational and rotational kinetic energies. The translational kinetic energy K_i of a single oriented particle i is given by equation (3.7). In order to compute the rotational kinetic energy separate from the translational kinetic energy, it is, in general, necessary to choose a inertial coordinate system whose origin is the centroid of the object (Marion, 1970). For a single particle, the rotational kinetic energy of a particle is given by

$$K_{\mathtt{rot}} = \frac{1}{2}\sum_{j,k} \mathbf{I}_{jk}\omega_j\omega_k$$

where the subscripts j and k refer to individual elements of the interia tensor $\mathbf{I}$. Our choice of inertia tensor (B.1) allows us to simplify the rotational kinetic energy to be

$$K_{\mathtt{rot}} = \frac{1}{2}\left(I_{xx}{\boldsymbol{\omega}_x}^2 + I_{yy}{\boldsymbol{\omega}_y}^2 + I_{zz}{\boldsymbol{\omega}_z}^2\right) \tag{4.7}$$

for the principal moments of inertia I_{xx}, I_{yy}, and I_{zz}. For additional details see Appendix B.2.

We write the total kinetic energy of the system as the sum of the individual particle translational (3.7) and rotational kinetic energies (4.7),

$$E_K = \sum_{i}^{N}\left(K_i + K_{\mathtt{rot}i}\right). \tag{4.8}$$

This redefines the system kinetic energy equation (3.8).

4.1.5 System Energy

The total energy of the system, E_S, is simply a summation of the individual particle kinetic and potential energies

$$E_S = E_K + E_P, \tag{4.9}$$

where E_P is given by equation (3.6) and E_K is given by equation (4.8).

4.1.6 Angular Damping

The second term of (4.1) is an angular velocity based damping force, $-\xi_i \dot{\mathbf{q}}_i$. When $\xi_i > 0$ this term accounts for a loss of rotational kinetic energy. This is analogous to the translational damping force $-\gamma_i \dot{\mathbf{x}}_i$. Analogous to the ideal viscous damping unit between neighboring particles is the angular viscous damping unit function

$$-\beta_3 \left(\dot{\mathbf{q}}_i - \dot{\mathbf{q}}_j \right), \tag{4.10}$$

where β_3 is the damping coefficient and $\dot{\mathbf{q}}_i$ and $\dot{\mathbf{q}}_j$ are the angular velocities of particles i and j.

4.1.7 Dynamic Coupling

To compute all inter-particle forces and torques without restrictive assumptions on the potential energies requires N^2 force computations. This is similar to the unoriented particle case. Assuming particles are uniformly distributed as a sampling of a surface, each particle will have at on average a constant number of neighbors, and by ignoring distant particles the inter-particle force calculations for the system are reduced to $O(N)$ computations. Thus we can rewrite the force and energy equations in terms of the set of nearest neighbors. This is a straightforward procedure and since we have already discussed this concept in Chapter 3, we omit deriving the equations for the oriented case.

4.1.8 Weighting Function

In Section 3.2.1 we discussed a weighting function (3.12) which monotonically decreases to zero at the distance of the particle neighborhood range. We have experimented with two other weighting functions. The first one

$$w_2(r) = e^{-r^2/2\sigma_r^2}$$

is based on the Gaussian distribution with $\sigma_r = 1.0$. The second weighting function

$$w_3(x, y, z) = K e^{\left(-\frac{x^2+y^2}{2a^2} - \frac{z^2}{2b^2} \right)} \qquad b \leq a \tag{4.11}$$

generalizes this to favor interactions between particles that lie close to their respective tangent planes. We accomplish this by writing the function in terms of the particle's local coordinates, e.g., by replacing the inter-particle distance $\mathbf{r}_{ij}$ by

$$\mathbf{d}_{ij} = \mathbf{R}_i^{-1} \mathbf{r}_{ij} = \mathbf{R}_i^{-1} (\mathbf{x}_j - \mathbf{x}_i), \tag{4.12}$$

where $\mathbf{d}_{ij} = [x, y, z]^T$, and $\mathbf{R}_i$ is the particle orientation. That is $\mathbf{d}_{ij}$ is the position of particle j in particle i's local coordinate frame.

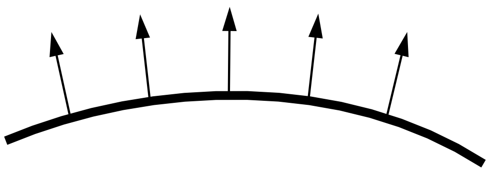

Figure 4.2: Cross sectional view of a of surface

4.1.9 Density

Assuming that a set of particles present a uniform sampling of a surface we can compute the density of particles over the surface. Similar to the volume case we ask the question: "How many particles will it take to fill a given area?" We can approximate the answer by considering the related question: "How many solid equal size circles will it take to fill a given area?" The *area packing factor* is defined as the ratio of the unit-circle to the unit-enclosure (Gasson, 1983). For a given packing, this is equivalent to the ratio of the area of a circle to the associated 2D Voronoi region, where the Voronoi diagram is computed over the center points of the circles. A hexagonal close packing of circles has an area packing factor P_A of

$$P_A = \frac{\pi}{2\sqrt{3}} \approx 0.91.$$

The expected number of circles n in a given area A, is given by

$$n = P_A \frac{A}{A_c} = \frac{A}{4\sqrt{3}r^2},$$

where A_c is the area of the circle with radius r. We can approximate the area of a surface particle A_p

$$A_p = \frac{A_c}{P_A} = \frac{\sqrt{3}}{2}{r_o}^2$$

as the area of a circle, with a radius of one half the Lennard-Jones equilibrium separation r_o, divided by the hexagonal packing factor.

4.2 Surface Potentials

To encourage oriented particles to group themselves into surface-like arrangements, we devise a collection of new inter-particle potential functions. These potential functions can be derived from the deformation energies of local triangular patches using finite element analysis, or from the differential geometry of surfaces. We begin with an intuitive explanation based on analogies with physical surfaces. We follow with an analysis correlating the potential functions to the geometric measures of differential geometry. We defer the details of the finite element analysis to Appendix E.

We derive our potentials by considering an infinitesimally small section of a surface as shown in Figure 4.2. Over a small section one can notice that adjacent points on

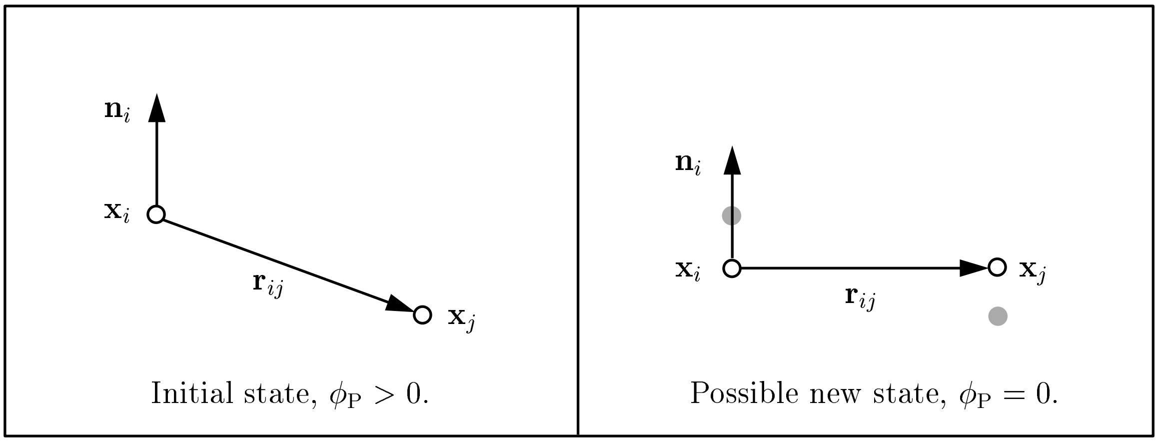

Figure 4.3: Interaction due to co-planarity potential: $\phi_P = (\mathbf{n}_i \cdot \mathbf{r}_{ij})^2$

The original particle positions are drawn in black on left and in gray on right.

the surface have normals that are close to parallel and the points lie near the tangent planes of adjacent points. One can also note that for circular arcs the normals diverge with equal angles. We use these observations to define potential energy functions between adjacent particles which encourage such configurations. We define three potentials: a co-planarity potential to encourage particles to lie in neighboring particle tangent planes, a co-normality potential to encourage particle normals to align, and for surfaces with constant curvature, a co-circularity potential to encourage particle normals to diverge with equal angle.

4.2.1 Co-planarity

For surfaces whose rest (minimum energy) configurations are flat planes, we would expect neighboring particles to lie in each other's tangent planes. We express the *co-planarity* potential as

$$\phi_P(\mathbf{n}_i, \mathbf{r}_{ij}) = (\mathbf{n}_i \cdot \mathbf{r}_{ij})^2 \tag{4.13}$$

The energy is proportional to the scalar product between the surface normal and the vector to the neighboring particle. Recall that two nonzero vectors are perpendicular if and only if their scalar product is zero.

We illustrate this in Figure 4.3. On the left side is a non-zero potential energy state. On the right side the particles have obtained a zero potential energy state, by moving in directions parallel to the normal vector $\mathbf{n}_i$. The forces acting on the two particles are given by the gradient of the potential energy with respect to $\mathbf{x}_i$ and $\mathbf{x}_j$:

$$\begin{aligned}
\mathbf{f}_i &= -\nabla_{\mathbf{x}_i}\phi_P = 2(\mathbf{n}_i \cdot \mathbf{r}_{ij})\mathbf{n}_i \\
\mathbf{f}_j &= -\nabla_{\mathbf{x}_j}\phi_P = -2(\mathbf{n}_i \cdot \mathbf{r}_{ij})\mathbf{n}_i
\end{aligned}$$

For the example given, the product $\mathbf{n}_i \cdot \mathbf{r}_{ij}$ is a negative scalar value. Thus particle i moves in the direction of $-\mathbf{n}_i$ and particle j moves in the direction of $+\mathbf{n}_i$. The torques

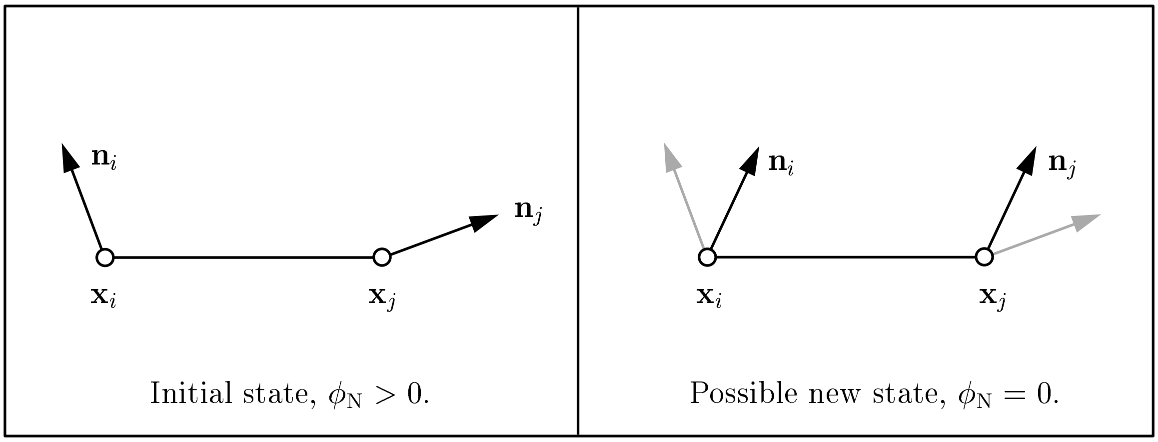

Figure 4.4: Interaction due to co-normality potential: $\phi_{\mathrm{N}} = \|\mathbf{n}_i - \mathbf{n}_j\|^2$

The original particle normals are drawn in black on left and in gray on right.

are given by the gradient of the potential energy with respect to the orientation:

$$\begin{aligned}\boldsymbol{\tau}_i &= -\nabla_{\theta_i}\phi_{\mathrm{P}} = -2(\mathbf{n}_i \cdot \mathbf{r}_{ij})(\mathbf{n}_i \times \mathbf{r}_{ij}) = \mathbf{r}_{ij} \times \mathbf{f}_i \\ \boldsymbol{\tau}_j &= -\nabla_{\theta_j}\phi_{\mathrm{P}} = 0.\end{aligned}$$

For the example given, the torque vector on particle i would be into the page and result in rotating the particle clockwise until $\mathbf{n}_i$ and $\mathbf{r}_{ij}$ form a right angle. There is no torque on particle j because the potential is independent of j's normal. However when we evaluate the potential $\phi_{\mathrm{P}}(\mathbf{n}_j, \mathbf{r}_{ji})$ then the situation reverses, $\boldsymbol{\tau}_i$ will be zero and $\boldsymbol{\tau}_j$ will be non-zero.

4.2.2 Co-normality

The co-planarity potential does not control the "twist" in the surface between two particles. To limit this, we introduce a *co-normality* potential

$$\phi_{\mathrm{N}}(\mathbf{n}_i, \mathbf{n}_j) = \|\mathbf{n}_i - \mathbf{n}_j\|^2 \tag{4.14}$$

which attempts to line up neighboring normals, much like interacting magnetic dipoles.

We illustrate this in Figure 4.4. On the left side the normals are not parallel resulting in a non-zero potential energy state. On the right side the particles have obtained a zero potential energy energy state by rotating until their normals align. The torques acting on the two particles is given by the gradient of the potential energy with respect to orientation:

$$\boldsymbol{\tau}_i = -\nabla_{\theta_i}\phi_{\mathrm{N}} = 2(\mathbf{n}_j \times \mathbf{n}_i) \tag{4.15}$$

$$\boldsymbol{\tau}_j = -\nabla_{\theta_j}\phi_{\mathrm{N}} = -2(\mathbf{n}_j \times \mathbf{n}_i) \tag{4.16}$$

The torque is about an axis orthogonal to $\mathbf{n}_i$ and $\mathbf{n}_j$, applied equally to both particles. For the example given it induces a clockwise rotation on particle i and a counter-clockwise rotation on particle j. This potential is independent of particle positions and

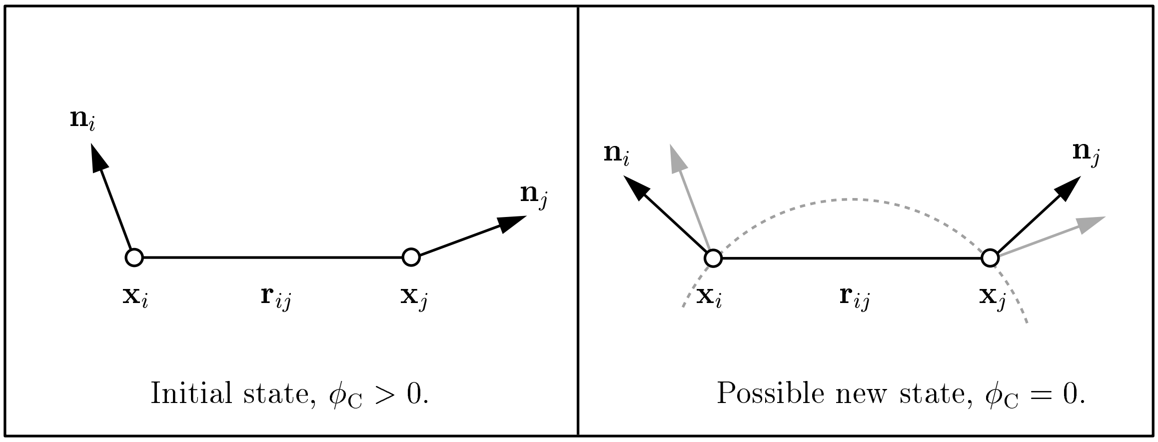

Figure 4.5: Interaction due to co-circularity potential: $\phi_C = ((\mathbf{n}_i + \mathbf{n}_j) \cdot \mathbf{r}_{ij})^2$

The original particle normals are drawn in black on left and in gray on right. The dashed line shows an arc of constant curvature matching the new normals and passing through the particle positions.

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thus the resulting forces are zero. By itself, the co-normality potential is not sufficient to form surfaces as the tangent planes may not align, as seen in this example. However in combination with the co-planarity potential, energy minimization will encourage a set of uniformly spaced particles to arrange into a continuous surface.

4.2.3 Co-circularity

An alternative to surfaces which prefer zero curvature (local planarity) are surfaces which favor constant curvatures. This can be enforced with a *co-circularity* potential

$$\phi_C(\mathbf{n}_i, \mathbf{n}_j, \mathbf{r}_{ij}) = ((\mathbf{n}_i + \mathbf{n}_j) \cdot \mathbf{r}_{ij})^2 \tag{4.17}$$

which is zero when normals are anti-symmetrical with respect to the vector joining the two particles. This is the natural configuration for surface normals on a sphere. That is the energy is zero under the condition that the angle between particle i's normal and the separation vector $\mathbf{r}_{ij}$ is equal to the angle between particle j's normal and the separation vector, or $\mathbf{n}_i \cdot \mathbf{r}_{ij} = \mathbf{r}_{ji} \cdot \mathbf{n}_j$. Since $\mathbf{r}_{ji} = -\mathbf{r}_{ij}$ and the scalar product is distributive we can rewrite the condition $\mathbf{n}_i \cdot \mathbf{r}_{ij} = \mathbf{r}_{ji} \cdot \mathbf{n}_j$ to be $(\mathbf{n}_i + \mathbf{n}_j) \cdot \mathbf{r}_{ij} = 0$.

We illustrate the co-circularity potential in Figure 4.5. On the left side the angles between normals and the separation vector are unequal. On the right side the particles have obtained a zero potential energy state by rotating until their normals are anti-symmetric. The torques acting on the two particles is given by the gradient of the potential energy with respect to orientation

$$\boldsymbol{\tau}_i = -\nabla_{\theta_i} \phi_C = \alpha(\mathbf{n}_i \times \mathbf{r}_{ij}) \tag{4.18}$$
$$\boldsymbol{\tau}_j = -\nabla_{\theta_j} \phi_C = \alpha(\mathbf{n}_j \times \mathbf{r}_{ij}), \tag{4.19}$$

where $\alpha = 2((\mathbf{n}_i + \mathbf{n}_j) \cdot \mathbf{r}_{ij})$ is a scalar. For each particle the torque is about an axis orthogonal to the particle normal and the separation vector. For the example given it

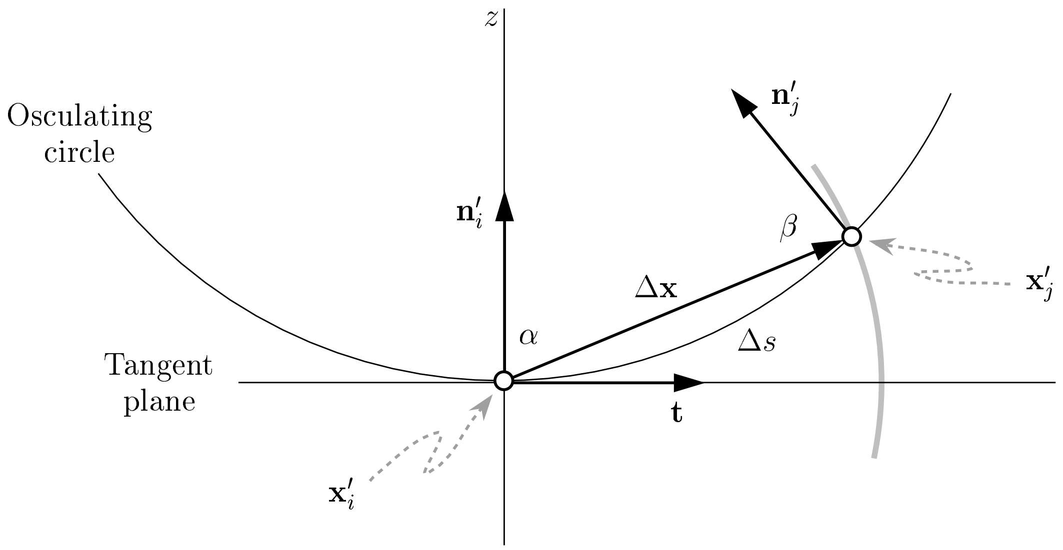

Figure 4.6: The osculating circle in the local coordinate frame of particle i

induces a counter-clockwise rotation on particle i and a clockwise rotation on particle j. The forces resulting from the change in potential are

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

For particle i, the term $((\mathbf{n}_i+\mathbf{n}_j)\cdot\mathbf{r}_{ij})$ is a scalar value that is zero when the particles are anti-symmetric. The force on particle i is in the direction $(\mathbf{n}_i+\mathbf{n}_j)$ and for particle j in the opposite direction. This in effect rotates the line segment $\mathbf{r}_{ij}$ in the plane defined by $\mathbf{r}_{ij}$ and $(\mathbf{n}_i+\mathbf{n}_j)$. For the example given it rotates $\mathbf{r}_{ij}$ clockwise.

4.3 Geometric Interpretation in Local Coordinates

Another viewpoint relating the potentials to the local geometry of the surface may be found by considering the potentials in the context of a particle's local reference frame. This transformation results in simplified equations for the potentials.

We begin by writing the states of particles i and j in the local reference frame of particle i, where $\mathbf{R}_i$ is the particle orientation, and where we denote local coordinates by a prime $'$:

$$\mathbf{x}'_i = \mathbf{R}_i^{-1}(\mathbf{x}_i-\mathbf{x}_i) = [0,0,0]^T \tag{4.20}$$

$$\mathbf{x}'_j = \mathbf{R}_i^{-1}(\mathbf{x}_j-\mathbf{x}_i) = [x_j,y_j,z_j]^T \tag{4.21}$$

$$\mathbf{n}'_i = \mathbf{R}_i^{-1}\mathbf{n}_i = [0,0,1]^T \tag{4.22}$$

$$\mathbf{n}'_j = \mathbf{R}_i^{-1}\mathbf{n}_j = [n_x,n_y,n_z]^T \tag{4.23}$$

$$\mathbf{r}'_{ij} = \Delta\mathbf{x} = \mathbf{x}'_j-\mathbf{x}'_i = [x_j,y_j,z_j]^T \tag{4.24}$$

Figure 4.6 illustrates two particles in local coordinates with $\mathbf{x}'_i$ and $\mathbf{x}'_j$ lying in the osculating plane containing $\mathbf{x}'_i$, $\mathbf{x}'_j$, and $\mathbf{n}'_i$. Note that $\mathbf{x}'_i$ is at the origin, the normal $\mathbf{n}'_i$ is in the direction of the z axis and the tangent vector to the curve is orthogonal to the normal. The osculating circle tangent at $\mathbf{x}'_i$ is also shown. In this example the normal $\mathbf{n}'_j$ lies in the osculating plane, although in other cases it may not. The length of the curve segment from $\mathbf{x}'_i$ to $\mathbf{x}'_j$ is labeled as Δs. The chord of the segment is the difference of positions and is labeled $\Delta\mathbf{x}$. If we assume the particles maintain a constant separation distance, then as the curvature varies the point $\mathbf{x}'_j$ moves along the gray arc. As the curvature goes to zero, $\mathbf{x}'_j$ moves down to the tangent axis, and Δs tends to the chord length $\|\Delta\mathbf{x}\|$.

In local coordinates the co-planarity potential reduces to

$$\phi_{\mathrm{P}} = (\mathbf{n}'_i \cdot \mathbf{r}'_{ij})^2 = (z_j)^2. \tag{4.25}$$

Minimizing the potential, can be interpreted as encouraging particle j to reduce z_j or, in other words, to move to particle i's tangent plane. Since we are in i's local coordinate this can also be accomplished by rotating and/or moving particle i in the world frame. These three possibilities correspond to the three effects (f_i, f_j, and t_i) that were derived in Section 4.2.1.

The co-normality potential reduces to

$$\phi_{\mathrm{N}} = \|\mathbf{n}'_i - \mathbf{n}'_j\|^2 = 2(1 - n_z). \tag{4.26}$$

By noting $\|\mathbf{n}'_j\| = 1$, the minimum is clearly when $n_z = 1$, or in other words when particle j's normal aligns with the z axis.

The co-circularity potential reduces to

$$\phi_{\mathrm{C}} = \Big((\mathbf{n}'_i + \mathbf{n}'_j) \cdot \mathbf{r}'_{ij}\Big)^2 = \Big((\mathbf{n}'_j \cdot \mathbf{r}'_{ij}) + z_j\Big)^2. \tag{4.27}$$

For this case the interpretation is less apparent, yet with a little algebra it becomes clear. Let α be the angle between $\mathbf{n}'_i$ and $\mathbf{r}'_{ij}$ and let β be the angle between $\mathbf{n}'_j$ and $\mathbf{r}'_{ji}$; where $\mathbf{r}'_{ij} = -\mathbf{r}'_{ji}$. The angle α is given by $\mathbf{n}'_i \cdot \mathbf{r}'_{ij} = \|\mathbf{r}'_{ij}\| \cos\alpha = z_j$. The angle β is given by $\mathbf{n}'_j \cdot \mathbf{r}'_{ji} = \|\mathbf{r}'_{ji}\| \cos\beta = -(\mathbf{n}'_j \cdot \mathbf{r}'_{ij})$. The potential (4.27) is obviously at its minimum (zero) when $z_j = -(\mathbf{n}'_j \cdot \mathbf{r}_{ij})$, or in other words when the angles α and β are equal.

4.4 Curvature

In this section we present a definition of discrete curvature for our oriented particle system. We then show that minimizing the potential energy functions is equivalent to minimizing the squared curvature defined for space curves between pairs of particles. We will also prove that we minimize the magnitude of the sum of squared curvature and torsion measures of space curves defined by pairs of particles. These space curves can be thought of as approximating the normal sections embedded in a surface interpolating the particles. Furthermore as the particle separation goes to zero the space

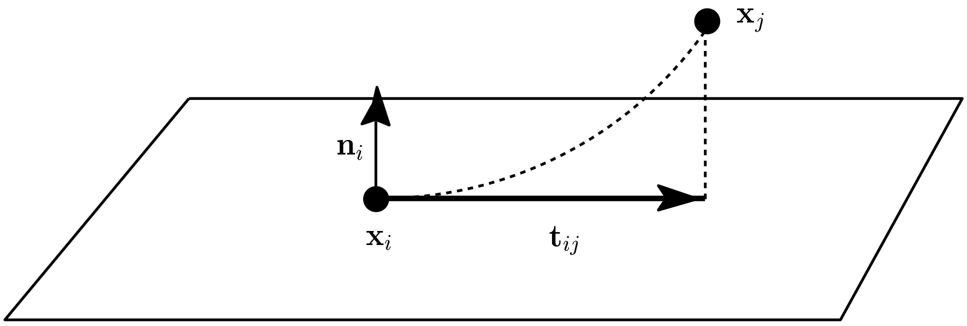

Figure 4.7: Discrete curvature tangent vector

curves between particles become osculating circles of normal sections embedded in the surface. In the limit, we prove that minimizing our potential functions is equivalent to minimizing the squared normal curvature over the surface.

We begin with a review of the basic definitions of normal sections, normal curvature, curvature, and torsion. Given points on a surface and direction tangent to the surface, there exists a unique plane that is defined by the tangent vector and surface normal that includes the given point. The intersection of the plane and the surface defines a space curve embedded in the surface. This curve is called a *normal section*. The curvature of a normal section is the *normal curvature* k_n and is defined as being the curvature of the embedded space curve. The curvature of a space curve is defined as the magnitude of the second derivative of position with respect to arc length, $\kappa = ||\dot{\mathbf{t}}|| = ||\ddot{\mathbf{x}}||$. The torsion of a space curve is defined as the magnitude of the derivative of the bi-normal with respect to arc length, $\tau = ||\dot{\mathbf{b}}||$. We defer a more detailed discussion of differential geometry to Appendix A.

4.4.1 Discrete Curvature

We now define a discrete curvature measure κ_d for our particle system. The discrete curvature is defined for a given position and direction. The position is the position $\mathbf{x}_i$ of a given particle and the direction is in a tangent direction $\mathbf{t}_{ij}$ of an adjacent particle $\mathbf{x}_j$. The tangent direction is the vector formed by $\mathbf{x}_i$ and the projection of $\mathbf{x}_j$ onto particle i's tangent plane, as shown in Figure 4.7.

Without loss of generality, we will work in the the local coordinates of particle i, where $'$ indicates local coordinates as given in Section 4.3. The position of $\mathbf{x}'_i$ is $[0,0,0]^T$, the normal $\mathbf{n}'_i$ is $[0,0,1]^T$, and the position of $\mathbf{x}'_j$ is $[x_j, y_j, z_j]^T$. The unit tangent vector $\hat{\mathbf{t}}_{ij}$ is given by $[x_j/t, y_j/t, 0]^T$ where $t = (x_j^2 + y_j^2)^{1/2}$.

We now determine the circle with normal matching $\mathbf{n}'_i$ at $\mathbf{x}'_i$ and passing through the points $\mathbf{x}'_i$ and $\mathbf{x}'_j$. We do this in a 2D plane where the x axis of this plane aligns with the tangent vector $\hat{\mathbf{t}}_{ij}$ and the y axis aligns with the particle normal $\mathbf{n}'_i$. We pick the three points

$$(x_1, y_1) \quad = \quad (0,0)$$

$$\begin{aligned}(x_2, y_2) &= (t, z_j)\\ (x_3, x_3) &= (-t, z_j)\end{aligned}$$

where (x_3, y_3) is the reflection of $\mathbf{x}'_j$ about particle i's normal. The equation

$$x^2 + y^2 + 2dx + 2ey + f = 0 \tag{4.28}$$

defines a circle of radius $(d^2+e^2-f)^{1/2}$ in the xy plane, when $d^2+e^2 > f$ (Zwillinger, 1995). Three non-collinear points determine a unique circle. For the three such points (x_1, y_1), (x_2, y_2), and (x_3, y_3) the equation

$$\begin{vmatrix} (x^2+y^2) & x & y & 1\\ (x_1^2+y_1^2) & x_1 & y_1 & 1\\ (x_2^2+y_2^2) & x_2 & y_2 & 1\\ (x_3^2+y_3^2) & x_3 & y_3 & 1 \end{vmatrix} = 0 \tag{4.29}$$

defines the unique circle passing through the points. Expanding the determinant gives

$$2z_j(x^2+y^2) - 2(t^2+z_j^2)y = 0.$$

as our equation of the circle. Writing in the form of (4.28)

$$\begin{aligned} d &= 0\\ e &= -\frac{(t^2+z_j^2)}{2z_j}\\ f &= 0 \end{aligned}$$

and thus the radius R is

$$R = \frac{x_j^2+y_j^2+z_j^2}{2z_j}.$$

We define the discrete curvature

$$\kappa_d = \frac{2z_j}{x_j^2+y_j^2+z_j^2}, \tag{4.30}$$

as the curvature of the unique circle passing through $\mathbf{x}'_i$ and $\mathbf{x}'_j$, such that at point $\mathbf{x}'_i$ the tangent and normal of the circle match $\hat{\mathbf{t}}_{ij}$ and $\mathbf{n}'_i$. In the global reference frame the discrete curvature is given as

$$\kappa_d = \frac{2}{\|\mathbf{r}_{ij}\|^2}(\mathbf{n}_i \cdot \mathbf{r}_{ij}). \tag{4.31}$$

4.4.2 Minimizing Discrete Curvature

We show that minimizing the co-planarity potential for a pair of particles, with particle spacing constrained by the Lennard-Jones potential, minimizes the squared discrete curvature measure of that pair.

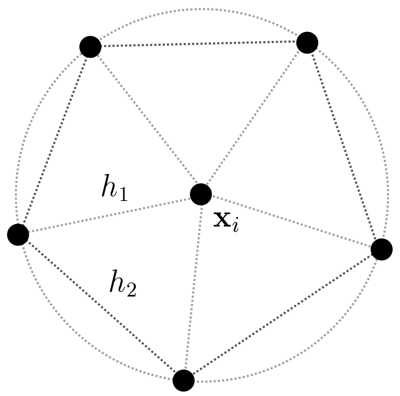

Figure 4.8: Inter-particle spacings h_1 and h_2.

In local coordinates, the co-planarity potential (4.25) is

$$\phi_{\mathrm{P}} = z_j^2$$

and the discrete curvature (4.30) squared is

$$\kappa_d{}^2 = \frac{4z_j^2}{\|\mathbf{r}'_{ij}\|^4}.$$

Since infinite energies are excluded from our simulations, we can assume that

$$0 < r_{\min} \leq \|\mathbf{r}_{ij}\|.$$

If not, the Lennard-Jones potential energy would be infinite. For completeness we mention that $\|\mathbf{r}_{ij}\| = \|\mathbf{r}'_{ij}\|$. The minimum bound $r_{\min}$ on the separation distance bounds the discrete curvature

$$\left(r_{\min}^4 \leq \|\mathbf{r}'_{ij}\|^4.\right) \;\Rightarrow\; \left(\kappa_d^2 \leq \frac{4z_j^2}{r_{\min}^4}\right).$$

Minimizing the co-planarity potential minimizes the squared discrete curvature between particle pairs

$$\begin{aligned} \phi_{\mathrm{P}} \to \min \;\; &\Rightarrow \;\; z_j^2 \to 0 \\ &\Rightarrow \;\; \kappa_d^2 \to 0. \end{aligned}$$

4.4.3 Normal Curvature

We show that our discrete curvature measure is equivalent to the normal curvature of a surface in the limit of infinitesimal particle separation. Let us assume we have a particle i surrounded by a set of symmetrically spaced particles $\mathcal{N} = \{\mathbf{x}_1, \mathbf{x}_2, \ldots \mathbf{x}_N\}$ as shown in Figure 4.8. Let h_1 be the distance between each particle pair $\mathbf{x}_i$ and $\mathbf{x}_j \in \mathcal{N}$. Let h_2 be the distance between adjacent neighboring particles.

As the separating length h_2 approaches zero, N goes ∞, and the particles surrounding $\mathbf{x}_i$ now form a continuous circle. Thus our discrete curvature measure κ_d is defined for all tangent vectors in particle i's tangent plane.

As the separating length h_1 goes to zero, we define the curvature measure

$$\kappa_d^\star = \lim_{h_1 \to 0} \kappa_d.$$

It should be clear that the circle defined between our particle pairs (as in Figure 4.6) becomes the osculating circle of some space curve passing through the two particles. Thus the discrete curvature $\kappa_d^\star$ becomes the curvature κ of the space curve.

We now relate κ to the normal curvature measure. For any smooth surface, a point on the surface, and a tangent direction, there exists a plane that is normal to the surface and which also includes the point and tangent vector. The space curve lying in that plane and embedded in the surface is the normal section with a curvature called the normal curvature κ_n. Since the circle we define lies in the plane normal to particle i, in the limit as h_1 tends to zero, this circle becomes the normal section, and our discrete curvature becomes the normal curvature, that is $\kappa_d^\star = \kappa = \kappa_n$.

4.4.4 Minimizing Torsion

This proof shows that minimizing the co-normality potential, with particle spacing constrained by the Lennard-Jones potential, minimizes the sum of the squared curvature and squared torsion measures of a space curve. We consider a space curve passing through the points $\mathbf{x}_i$ and $\mathbf{x}_j$, such that the unit normal vectors of the curve at $\mathbf{x}_i$ and $\mathbf{x}_j$ match the particle normal vectors $\mathbf{n}_i$ and $\mathbf{n}_j$ respectively.

An equation for the rate of change of the normal per unit arc length of a space curve is given by the Frenet-Serret formulas (A.2)

$$\dot{\mathbf{m}} = -\kappa\mathbf{t} + \tau\mathbf{b}. \tag{4.32}$$

For a discrete system, the change in normal is

$$\dot{\mathbf{m}} = \frac{\mathbf{n}_j - \mathbf{n}_i}{\Delta s}, \tag{4.33}$$

where Δs is the unit arc length. We combine (4.32) and (4.33) to get

$$-\kappa\mathbf{t} + \tau\mathbf{b} = \frac{\mathbf{n}_j - \mathbf{n}_i}{\Delta s}.$$

We now take the scalar product of both sides

$$\kappa^2(\mathbf{t}\cdot\mathbf{t}) - 2\kappa\tau(\mathbf{t}\cdot\mathbf{b}) + \tau^2(\mathbf{b}\cdot\mathbf{b}) = \frac{\|\mathbf{n}_j - \mathbf{n}_i\|^2}{\Delta s^2}. \tag{4.34}$$

The tangent and bi-normal are orthogonal and unit vectors so the following hold

$$\begin{aligned} \mathbf{t}\cdot\mathbf{t} &= 1 \\ \mathbf{b}\cdot\mathbf{b} &= 1 \\ \mathbf{t}\cdot\mathbf{b} &= 0. \end{aligned}$$

Equation (4.34) thus reduces to

$$\kappa^2 + \tau^2 = \frac{\|\mathbf{n}_j - \mathbf{n}_i\|^2}{\Delta s^2}. \tag{4.35}$$

We can now rewrite (4.35) in terms of the co-normality potential (4.14)

$$\phi_{\mathrm{N}} = \|\mathbf{n}_i - \mathbf{n}_j\|^2 = \|\mathbf{n}_j - \mathbf{n}_i\|^2 \tag{4.36}$$

to arrive at the equation

$$\kappa^2 + \tau^2 = \frac{\phi_{\mathrm{N}}}{\Delta s^2}.$$

As in to Section 4.4.2, we can assume

$$0 < r_{\min} \leq \|\mathbf{r}_{ij}\|.$$

Since the $\Delta s > \|\mathbf{r}_{ij}\|$, we have the relation

$$0 < r_{\min} < \Delta s.$$

The bound on the arc length bounds the sum $\kappa^2 + \tau^2$

$$\left(r_{\min}^2 < \Delta s^2\right) \;\Rightarrow\; \left(\kappa^2 + \tau^2 < \frac{\phi_{\mathrm{N}}}{r_{\min}^2}\right).$$

Thus minimizing the co-normality potential minimizes the sum of the squared curvature and squared torsion measures

$$(\phi_{\mathrm{N}} \to \min) \;\Rightarrow\; \left(\kappa^2 + \tau^2 \to 0\right).$$

4.4.5 Discussion

We have shown that a combination of co-planarity and Lennard-Jones minimizes the squared curvature of space curves defined between particle pairs. Likewise, a combination of co-normality and Lennard-Jones minimizes the sum of the squared curvature and squared torsion measures. We did not find a similar proof for the co-circularity potential. The co-circularity potential's goal is to encourage symmetric curvature between particle pairs, but in isolation this does not imply minimum curvature. Smooth surfaces can be constructed using only the co-planarity and co-normality potentials, and in fact many of the examples in the dissertation were created using only these two potentials.

However, in the finite element analysis of Appendix E we show that the co-circularity potential corresponds to an energy measure based on the variation in curvature of a three particle patch. And we also show that an approximation of the Gaussian curvature over the patch can be written as a sum of the co-circularity and co-normality potentials. Thus, this analysis shows that the co-planarity potential is not necessary needed to write a curvature-based energy measure. At first sight, these two different analyses may suggest contradicting results. The observation we draw is that either the co-planarity or the co-circularity potential is required, but not both. In fact the two potentials are closely related. The co-planarity potential is based on the scalar product of particle normal and the separation vector, and the co-circularity potential is based on the scalar product of the separation vector and sum of particle normals. Another point to note is that the different analyses are minimizing different curvature measures.

To summarize, minimizing co-planarity and co-normality minimizes the magnitude of curvature and torsion of curves defined between particle pairs, and minimizing co-circularity and co-normality minimizes the magnitude of the Gaussian curvature integrated over a three particle patch. That is

$$\begin{aligned} \phi_{\mathrm{P}} + \phi_{\mathrm{LJ}} &\Rightarrow \kappa_d^2 \\ \phi_{\mathrm{N}} + \phi_{\mathrm{LJ}} &\Rightarrow \kappa_d^2 + \tau^2 \\ \phi_{\mathrm{C}} + \phi_{\mathrm{N}} + \phi_{\mathrm{LJ}} &\Rightarrow \kappa^2. \end{aligned}$$

4.5 Dynamics

For practical considerations we limit particle interactions between nearest neighbors. To do this we use a distance based weighting function $w(\mathbf{r}_{ij})$ which decays the energy potential to zero at the neighborhood boundary. To control the bending and stiffness characteristics of our deformable surface, we use a scalar weighted sum of potential energies

$$\begin{aligned} E_{ij} &= \alpha_{\mathrm{P}}\phi_{\mathrm{P}}(\mathbf{n}_i, \mathbf{r}_{ij})w(\mathbf{r}_{ij}) + \alpha_{\mathrm{N}}\phi_{\mathrm{N}}(\mathbf{n}_i, \mathbf{n}_j, \mathbf{r}_{ij})w(\mathbf{r}_{ij}) + \alpha_{\mathrm{C}}\phi_{\mathrm{C}}(\mathbf{n}_i, \mathbf{n}_j, \mathbf{r}_{ij})w(\mathbf{r}_{ij}) \\ &\quad + \alpha_{\mathrm{LJ}}\phi_{\mathrm{LJ}}(\mathbf{r}_{ij}). \end{aligned}$$

The first two terms control the surface's resistance to bending, and the third term controls the surface's tendency towards uniform local curvature, and the last term controls the average inter-particle spacing.

Having defined the internal energy associated with our system, we can derive its equations of motion. By weighting our potential functions the corresponding forces and torques are different than those given in Section 4.2. The differences are (1) the weighting of the original potential terms found in Section 4.2, and (2) new force terms based on the gradient of the weighting function. The derivation of the distance weighted inter-particle forces and torques are given in Appendix D and listed below. For convenience we use the short hand notation

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

For the spatially weighted co-planarity potential, $\phi_{\mathrm{P}}(\mathbf{n}_i, \mathbf{r}_{ij})w(\mathbf{r}_{ij})$, we have:

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

For the spatially weighted co-normality potential, $\phi_{\mathrm{N}}(\mathbf{n}_i, \mathbf{n}_j, \mathbf{r}_{ij})w(\mathbf{r}_{ij})$, we have:

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

For the spatially weighted co-circularity potential, $\phi_{\mathrm{C}}(\mathbf{n}_i, \mathbf{n}_j, \mathbf{r}_{ij})w(\mathbf{r}_{ij})$, we have:

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

For the Lennard-Jones potential we have:

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

These forces have the following simple physical interpretations. The co-planarity potential gives rise to a force parallel to the particle normal and proportional to the distance between the neighboring particle and the local tangent plane. The first term in the force, which can often be ignored, arises from the gradient of the spatial weighting function. The cross product of this force with the inter-particle vector produces a torque on the particle. The co-normality potential produces a torque proportional to the cross-product of the two particle normals, which acts to line up the normals. The force term for the co-normality potential arises from the weighting function and can usually be ignored. The co-circularity force is similar to the co-planarity force, except that the local tangent plane is defined from the average of the two normal vectors. The Lennard-Jones force exerts a force parallel to the separation vectors holding the particle system together. It effectively counteracts the forces due to the gradient of the weighting function.

To compute the total inter-particle force and torque from all the potentials, we use the formulas

$$\begin{aligned}
\mathbf{f}_{ij} &= 2\alpha_{\mathrm{LJ}} \mathbf{f}_{\mathrm{LJ}_i}(\mathbf{r}_{ij}) + \alpha_{\mathrm{P}}(\mathbf{f}_{\mathrm{P}_i}(\mathbf{n}_i, \mathbf{r}_{ij}) + \mathbf{f}_{\mathrm{P}_i}(\mathbf{n}_j, \mathbf{r}_{ji})) + 2\alpha_{\mathrm{N}} \mathbf{f}_{\mathrm{N}_i}(\mathbf{n}_i, \mathbf{n}_j, \mathbf{r}_{ij}) + 2\alpha_{\mathrm{C}} \mathbf{f}_{\mathrm{C}_i}(\mathbf{n}_i, \mathbf{n}_j, \mathbf{r}_{ij}) \\
\boldsymbol{\tau}_{ij} &= \alpha_{\mathrm{P}} \boldsymbol{\tau}_{\mathrm{P}_i}(\mathbf{n}_i, \mathbf{r}_{ij}) + 2\alpha_{\mathrm{N}} \boldsymbol{\tau}_{\mathrm{N}_i}(\mathbf{n}_i, \mathbf{n}_j, \mathbf{r}_{ij}) + 2\alpha_{\mathrm{C}} \boldsymbol{\tau}_{\mathrm{C}_i}(\mathbf{n}_i, \mathbf{n}_j, \mathbf{r}_{ij})
\end{aligned}$$

Note that most forces and torques are doubled, i.e., actions generate opposite reactions. The main exception to this is $\mathbf{f}_{\mathrm{P}}$ and $\boldsymbol{\tau}_{\mathrm{P}}$, which arise from an asymmetric potential function. This can easily be changed by defining a new potential

$${\phi_{\mathrm{P}}}^*(\mathbf{n}_i, \mathbf{n}_j, \mathbf{r}_{ij}) = \phi_{\mathrm{P}}(\mathbf{n}_i, \mathbf{r}_{ij}) + \phi_{\mathrm{P}}(\mathbf{n}_j, \mathbf{r}_{ij}),$$

although the results would be the same. The second exception is due to the co-circularity potential which results in torques of equal magnitude but about different axes; $\boldsymbol{\tau}_{\mathrm{P}_i}$ is about the axis $(\mathbf{n}_i \times \mathbf{r}_{ij})$ and $\boldsymbol{\tau}_{\mathrm{P}_j}$ is about the axis $(\mathbf{n}_j \times \mathbf{r}_{ij})$, which may be different. However it does produce the desired result.

These forces and torques can be summed over all interacting particles to obtain

$$\mathbf{f}_i = \sum_{j \in \mathcal{N}_i} \mathbf{f}_{ij} + \mathbf{f}_{\mathrm{ext}}(\mathbf{x}_i) - \beta_0 \mathbf{v}_i - \sum_{j \in \mathcal{N}_i} \beta_1 (\mathbf{v}_j - \mathbf{v}_i) \tag{4.37}$$

$$\boldsymbol{\tau}_i = \sum_{j \in \mathcal{N}_i} \boldsymbol{\tau}_{ij} - \beta_2 \boldsymbol{\omega}_i - \sum_{j \in \mathcal{N}_i} \beta_3 (\boldsymbol{\omega}_j - \boldsymbol{\omega}_i) \tag{4.38}$$

where $\mathcal{N}_i$ are the neighbors of i, $\mathbf{v} = \dot{\mathbf{x}}$ and $\boldsymbol{\omega} = \dot{\mathbf{q}}$. Here, we have lumped all external forces such as gravity, user-defined control forces, and non-linear constraints into $\mathbf{f}_{\mathrm{ext}}$, and added velocity dependent damping forces $\beta_0 \mathbf{v}_i$ and $\beta_2 \boldsymbol{\omega}_i$ and the relative velocity dependent damping forces $\beta_1(\mathbf{v}_j - \mathbf{v}_i)$ and $\beta_3(\boldsymbol{\omega}_j - \boldsymbol{\omega}_i)$. The above force equations are related to the equations of motion (3.1) and (4.1) given in Section 4.1.2. The translational damping coefficient γ_i in (3.1) is a function of β_0 and β_1. The rotational damping coefficient ξ_i in (4.1) is a function of β_2, and β_3.

4.6 Summary

We have presented a new distributed model of surface shape based on particle systems, differential geometry, and physics. We extended the volume based particle model of Chapter 3 to create oriented particles whose minimum energy configurations are sheets of particles rather than tightly packed clusters of particles. Each particle represents a local frame, a combination of position and orientation information. The particle's local XY plane represents the surface tangent plane at the particle's position, and the local Z axis represents the surface normal. Each frame can be thought of as a small surface element or discrete surface sample.

To encourage particles to arrange into surfaces, we introduced three new potential energy functions. The co-planarity potential encourages neighboring particle tangent planes to align. The co-normality potential encourages neighboring particle normals to align, controlling the "twist" in the surface between two particles. The co-circularity potential encourages surfaces of constant curvature, e.g. a sphere, rather than surfaces of zero curvature, e.g. a plane. We have also used differential geometry (Appendix A) to show how these potentials minimize the squared curvature for curves defined between particles. In the limit of zero inter-particle spacing, this is equivalent to minimizing the squared normal curvature over the surface. We also showed the co-normality potential minimize the sum of squared curvature and torsion measures for curves defined between particles. In Appendix E we show how the sum of the co-circularity and co-normality potentials minimizes the Gaussian curvature of a triangular patch defined by three particles.

Forces and torques on the particles are derived from the change in energy with respect to changes in the particle's position and orientation, respectively. In addition the surfaces respond to external forces such as gravity and collisions with other objects. In Chapter 8 we present results from simulations which illustrate the behavior of oriented particles.