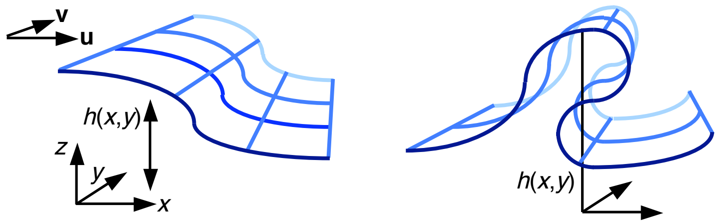
PHYS 4xx Mem 4 - Surface curvature

Polymer curvature is described by the unit tangent vector $\mathbf{t} = \partial\mathbf{r}/\partial s$ and the curvature $C \equiv \mathbf{n}\cdot(\partial\mathbf{t}/\partial s) = \mathbf{n}\cdot(\partial^2\mathbf{r}/\partial s^2)$, where $\mathbf{n}$ is the normal to the curve at position $\mathbf{r}$ and where s is the arc length. Generalize this to a surface through a choice of coordinates and representation: for example, a set of basis vectors $\mathbf{u}$,$\mathbf{v}$ embedded in the surface itself:



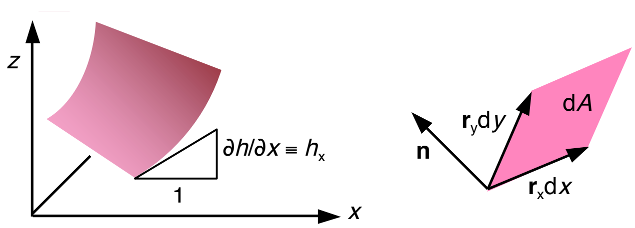
(a) (b)

A common approach in membrane studies employs Cartesian coordinates to write a point $\mathbf{r}$ on the surface as

$$\mathbf{r} = [x,\ y,\ h(x,y)], \tag{1}$$

where h is the "height" away from the xy plane. Unfortunately, $h(x,y)$ may not be single-valued as illustrated by the overhang region panel (b).
The Monge representation is an approximation in which overhangs are forbidden.

Analytical geometry within the Monge Representation



(a) (b)

Construct two tangent vectors by making a unit step in the x and y directions, and a step $\partial h/\partial x \equiv h_x$ in the z-direction:

$$\partial_x\mathbf{r} = (1,\ 0,\ h_x) = (1,\ 0,\ \partial_x h) \qquad \text{(dimensionless)} \tag{2a}$$

$$\partial_y\mathbf{r} = (0,\ 1,\ h_y) = (0,\ 1,\ \partial_y h), \tag{2b}$$

where $\partial_x \equiv \partial/\partial x$ and $h_x = \partial_x h$. Note: $\partial_x\mathbf{r}$ and $\partial_y\mathbf{r}$ are *not* unit vectors, and are *not* generally orthogonal; however, they define the plane tangent to the surface at point $[x,\ y,\ h(x,y)]$, and can generate the unit normal vector $\mathbf{n}$ to the surface *via* the cross product

$$\mathbf{n} \equiv (\partial_x\mathbf{r}) \times (\partial_y\mathbf{r}) \,/\, |(\partial_x\mathbf{r}) \times (\partial_y\mathbf{r})| = (-h_x,\ -h_y,\ 1) \,/\, (1 + h_x^2 + h_y^2)^{1/2}. \tag{3}$$

A segment of length dx along the x-axis corresponds to a vector $(\partial_x\mathbf{r})dx$ along the surface. The cross product of the vectors $(\partial_x\mathbf{r})dx$ and $(\partial_y\mathbf{r})dy$ gives the area element dA

on the surface corresponding to dx dy in the coordinate plane:

$$dA = |(\partial_x \mathbf{r}) \times (\partial_y \mathbf{r})|\, dx\, dy = (1 + h_x^2 + h_y^2)^{1/2}\, dx\, dy, \tag{4}$$

according to Eq. (2). The quantity $(1 + h_x^2 + h_y^2)$ is called the metric g of the surface

$$g \equiv 1 + h_x^2 + h_y^2 = 1 + (\partial_x h)^2 + (\partial_y h)^2, \tag{5}$$

such that $dA = \sqrt{g}\, dx\, dy$.

The curvature of a surface can be obtained from $C \equiv \mathbf{n} \bullet (\partial^2 \mathbf{r} / \partial s^2)$. The curvature is direction-dependent; e.g., the curvature of a cylindrical shell of radius R is zero in a direction parallel to the cylindrical axis, and $1/R$ along a circle perpendicular to the axis.

The extremal values of the curvature as a function of direction are called the principal curvatures, denoted by C_1 and C_2; the combinations $(C_1 + C_2)/2$ and $C_1 \bullet C_2$ are the mean and Gaussian curvatures, respectively.

To determine the curvature $C \equiv \mathbf{n} \bullet (\partial_s^2 \mathbf{r})$, we need Eq. (3) for $\mathbf{n}$, as well as the derivatives $\mathbf{r}' = \partial_s \mathbf{r}$ and $\mathbf{r}'' = \partial_s^2 \mathbf{r}$:

$$\mathbf{r}' = (\partial_x \mathbf{r}) x' + (\partial_y \mathbf{r}) y', \tag{6}$$

$$\mathbf{r}'' = (\partial_x^2 \mathbf{r})(x')^2 + (\partial_y^2 \mathbf{r})(y')^2 + 2(\partial_x \partial_y \mathbf{r}) x' y' + (\partial_x \mathbf{r}) x'' + (\partial_y \mathbf{r}) y'', \tag{7}$$

where $x' \equiv \partial_s x$, $x'' \equiv \partial_s^2 x$ etc. The last two terms in Eq. (7) do not contribute to $\mathbf{n} \bullet (\partial_s^2 \mathbf{r})$, owing to the orthogonality of $\mathbf{n}$ with $\partial_x \mathbf{r}$ and $\partial_y \mathbf{r}$, leaving

$$C = \mathbf{n} \bullet \mathbf{r}'' = b_{xx}(x')^2 + b_{yy}(y')^2 + 2b_{xy} x' y'. \tag{8}$$

The scalar coefficients $b_{\alpha\beta}$ are

$$b_{\alpha\beta} \equiv \mathbf{n} \bullet (\partial_\alpha \partial_\beta \mathbf{r}) \qquad (\alpha, \beta = x, y). \tag{9}$$

Differentiating the orthogonality condition $\mathbf{n} \bullet (\partial_\alpha \mathbf{r}) = 0$ leads to the relation $\partial_\beta [\mathbf{n} \bullet (\partial_\alpha \mathbf{r})] = \mathbf{n} \bullet (\partial_\alpha \partial_\beta \mathbf{r}) + (\partial_\beta \mathbf{n}) \bullet (\partial_\alpha \mathbf{r}) = 0$, or, from the definition (9),

$$b_{\alpha\beta} = -(\partial_\alpha \mathbf{r}) \bullet (\partial_\beta \mathbf{n}) \qquad (\alpha, \beta = x, y). \tag{10}$$

The direction-dependence of the curvature is implicit in Eq. (8) through $\mathbf{r}''$, the second derivative of the position with respect to arc length along a particular direction. After some mathematics to obtain the extremal values

$$(C_1 + C_2)/2 = (g_{xx} b_{yy} + g_{yy} b_{xx} - 2g_{xy} b_{xy}) / 2g \tag{11a}$$

$$C_1 C_2 = (b_{xx} b_{yy} - b_{xy}^2) / g, \tag{11b}$$

The metric is the determinant of the metric tensor $g_{\alpha\beta}$, whose components here are

$$g_{\alpha\beta} = (\partial_\alpha \mathbf{r}) \bullet (\partial_\beta \mathbf{r}) \qquad (\alpha, \beta = x, y). \tag{12}$$

We now determine the mean and Gaussian curvatures in the Monge representation. First, we evaluate $\partial_x \mathbf{n}$ using Eq. (3), finding

$$\partial_x \mathbf{n} = - \{ ([1+h_y^2]h_{xx} - h_x h_y h_{xy}), ([1+h_x^2]h_{xy} - h_x h_y h_{xx}), (h_x h_{xx} + h_y h_{xy}) \} / (1 + h_x^2 + h_y^2)^{3/2}.$$

$$\partial_y \mathbf{n} = - \{ ([1+h_y^2]h_{xy} - h_x h_y h_{yy}), ([1+h_x^2]h_{yy} - h_x h_y h_{xy}), (h_x h_{xy} + h_y h_{yy}) \} / (1 + h_x^2 + h_y^2)^{3/2}. \quad (13)$$

where $h_{xx} = \partial_x \partial_x h$ *etc.*These somewhat intimidating relations can be combined with Eqs. (2) and (10) to yield the simple

$$b_{\alpha\beta} = h_{\alpha\beta} / (1 + h_x^2 + h_y^2)^{1/2} \qquad (\alpha, \beta = x, y). \quad (14)$$

Lastly, Eqs. (12) and (14) can be substituted into (11):

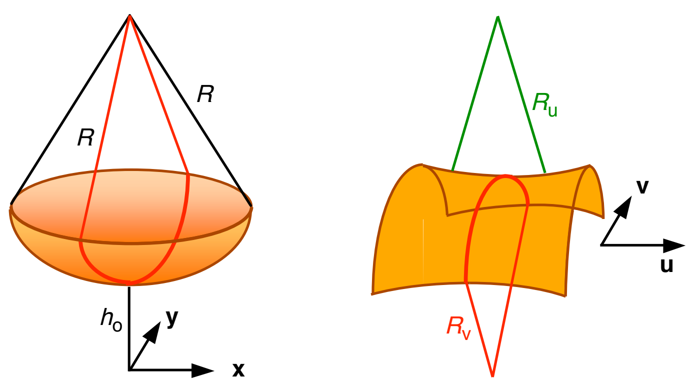
$$(C_1+C_2)/2 = \{(1+h_x^2)h_{yy} + (1+h_y^2)h_{xx} - 2h_x h_y h_{xy}\} / 2(1 + h_x^2 + h_y^2)^{3/2} \quad (15a)$$

$$C_1 C_2 = (h_{xx}h_{yy} - h_{xy}^2) / (1 + h_x^2 + h_y^2)^2. \quad (15b)$$

For many situations of interest, $h(x,y)$ is a slowly-varying function corresponding to gentle undulations, so to leading order

$$(C_1 + C_2)/2 \cong (h_{xx} + h_{yy})/2 \quad (16a)$$

$$C_1 C_2 \cong h_{xx}h_{yy} - h_{xy}^2, \quad (16b)$$



(a) (b)

To confirm the geometrical meaning of Eq. (16) consider the shape of a surface in the region of a minimum or inflection point, as illustrated. Place the minimum directly over the coordinate origin at x=y=0. A Taylor series expansion describes the height of the surface for small regions near the minimum, namely

$$h(x, y) = h_o + h_x x + h_y y + h_{xx}x^2/2 + h_{yy}y^2/2 + h_{xy}xy + ..., \quad (17)$$

where the height at the origin is h_o. For surfaces like a bowl, the derivatives h_x and h_y vanish at the local minimum in height, showing that the surface is quadratic in x and y with coefficients proportional to the local curvature. The curvatures at the saddle point in panel(b) have opposite sign: the normals are canted towards each other in the **u**-direction, but away from each other in the **v**-direction; that is $R_u \cdot R_v < 0$, where R_u and R_v are the radii of curvature in the **u** and **v** directions, respectively.

Membrane bending energy

The simplest form for the energy density of bending deformations is

$$\mathcal{F} = (\kappa_b/2)(C_1 + C_2 - C_0)^2 + \kappa_G C_1 C_2, \quad (18)$$

where κ_b and κ_G are the bending rigidity (or bending modulus) and Gaussian bending rigidity (or saddle-splay modulus) respectively. Introducing the constant term C_0, known as the spontaneous curvature, permits Eq. (18) to describe bilayers that are curved in their equilibrium state because their two (monolayer) leaflets are compositionally inequivalent. The existing measurements are consistent with the rather broad range $0 > \kappa_G/\kappa_b > -2$, with notable exceptions.

Membrane persistence length

At $T > 0$, the membrane fluctuates with local curvatures governed by the membrane bending resistance κ_b (for a closed sphere, the integral of C_1C_2 over the surface is independent of the local fluctuations so the overall energy is insensitive to κ_G).

The larger κ_b/k_BT, the flatter the membrane and the correlation in $\langle \mathbf{n}_1 \cdot \mathbf{n}_2 \rangle$ decays exponentially with a persistence length ξ_p characteristic of the membrane. Determining ξ_p theoretically involves more complicated math than the persistence length of a flexible filament. The proof is performed in *Mechanics of the Cell* for student interested in the details. Here, we simply quote the result:

$$\xi_p \sim b \exp(4\pi\kappa_b / 3k_BT), \quad \text{(Peliti and Leibler)} \quad (19)$$

where b is the elementary legnth scale of the membrane. Computer simulations (Gompper and Kroll, 1995) are consistent with Eq. (19). The exponential dependence of ξ_p on the bending resistance of a surface should be contrasted with the linear dependence of ξ_p on the bending resistance of a polymer.

Put another way, it becomes easier to bend a membrane as the temperature increases, an observation that can be quantified by an effective bending rigidity

$$\kappa(\ell) = \kappa_b - (3k_BT/4\pi)\ln(\ell/b), \quad (20)$$

that depends on the length scale ℓ of the undulations: the surface becomes softer when viewed at longer wavelengths. Numerically, if we set $b \sim 1$ nm, and $\kappa_b \sim 10k_BT$, we expect $\xi_p \sim 10^6$ km. Dramatic as this result is, it does not mean that the membranes of a cell are planar, only that they undulate smoothly on cellular length scales.