

# Biomembranes

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## 1 Differential Geometry for Surface PDE

Codimension-1 surfaces of dimension  $d$  embedded in  $(d + 1)$ -dimensional Euclidean space can be described through parameterizations  $\chi : \mathbb{R}^d \rightarrow \mathbb{R}^{d+1}$ , or through the level set of a function  $b : \mathbb{R}^{d+1} \rightarrow \mathbb{R}$ . In either case the differential geometry of these surfaces should be expressed in terms of the simple formulas of the ambient Euclidean metric space, but this requires some work. The problem is that, unless the surface is completely ‘flat’, any distance along the surface must be translated into a distance in the Euclidean metric space, and vice versa. To express the change in a function value with respect to a change in  $x$ , one must disambiguate the space in which  $x$  is allowed to move. If  $x$  ranges through the familiar Euclidean metric space, then in general it will cover a greater distance along the surface. Likewise, if  $x$  ranges through a distance along the surface, then in general that distance will appear shorter in the direction it moves in Euclidean space. These discrepancies must be accounted for in order to compute derivatives of non-constant quantities on the surface.

### 1.1 Differential Geometry for Parametric Surfaces, $\chi : (\xi_1, \dots, \xi_d) \mapsto \gamma \subset \mathbb{R}^{d+1}$

Let  $\gamma$  be a smooth, closed codimension-one manifold in  $\mathbb{R}^3$

For  $V \subset \mathbb{R}^2$  with  $\xi_1, \xi_2 \in V$ , put  $\chi : (\xi_1, \xi_2) \mapsto (\chi_1(\xi_1, \xi_2), \chi_2(\xi_1, \xi_2), \chi_3(\xi_1, \xi_2)) = x \in \gamma$

Denote the tangent space at  $x \in \gamma$  by  $T_x\gamma := \text{span}\{\lambda^1, \lambda^2\}$  where  $\lambda^1, \lambda^2$  are linearly independent vectors tangent to  $\gamma$  at  $x$ .

$$\text{Write the Jacobian of } \chi \text{ as } D\chi(\xi_1, \xi_2) = (\partial_1\chi, \partial_2\chi) := \begin{pmatrix} \frac{\partial\chi_1}{\partial\xi_1} & \frac{\partial\chi_1}{\partial\xi_2} \\ \frac{\partial\chi_2}{\partial\xi_1} & \frac{\partial\chi_2}{\partial\xi_2} \\ \frac{\partial\chi_3}{\partial\xi_1} & \frac{\partial\chi_3}{\partial\xi_2} \end{pmatrix}$$

**Definition 1.1** (Metric Tensor  $g_{ij} : x \mapsto \mathbb{R}^{2 \times 2}$ , and First Fundamental Form I :  $(x; \lambda^1, \lambda^2) \in T_x\gamma \rightarrow \mathbb{R}$ ).

**Definition 1.2** (Curvature Tensor  $h_{ij} : x \mapsto \mathbb{R}^{2 \times 2}$ , and Second Fundamental Form II :  $(x; \lambda^1, \lambda^2) \in T_x\gamma \rightarrow \mathbb{R}$ ).

unit normal vector  $n$ ,  $g = g_{ij}$ ,  $h = h_{ij}$ , Laplace-Beltrami operator  $\Delta_\gamma$ , surface gradient  $\nabla_\gamma$

**Definition 1.3** (Surface Gradient). *Let  $\chi : V \rightarrow \gamma$  be a smooth parameterization of the surface  $\gamma$  over  $V \subset \mathbb{R}^2$ . For  $v : \gamma \rightarrow \mathbb{R}$  a smooth function, the surface gradient  $\nabla_\gamma v = \nabla_\gamma v(\chi(\xi_1, \xi_2))$  is defined as*

$$\nabla_\gamma v(\chi(\xi_1, \xi_2)) := D\chi g^{-1} \nabla(v \circ \chi)(\xi_1, \xi_2) \quad (1)$$

$$= \begin{pmatrix} \frac{\partial\chi_1}{\partial\xi_1} & \frac{\partial\chi_1}{\partial\xi_2} \\ \frac{\partial\chi_2}{\partial\xi_1} & \frac{\partial\chi_2}{\partial\xi_2} \\ \frac{\partial\chi_3}{\partial\xi_1} & \frac{\partial\chi_3}{\partial\xi_2} \end{pmatrix} \begin{pmatrix} g^{11} & g^{12} \\ g^{21} & g^{22} \end{pmatrix} \begin{pmatrix} \frac{\partial v}{\partial\xi_1} \\ \frac{\partial v}{\partial\xi_2} \end{pmatrix} \quad (2)$$

Notice that this entire computation is made in  $V \subset \mathbb{R}^2$ .

**Definition 1.4** (Tangential Divergence).

**Definition 1.5** (Surface Laplacian, the Laplace Beltrami operator). *Let  $\chi : V \rightarrow \gamma$  be a smooth parameterization of the surface  $\gamma$  over  $V \subset \mathbb{R}^2$ . For  $v : \gamma \rightarrow \mathbb{R}$  a smooth function, the surface Laplacian  $\Delta_\gamma v = \Delta_\gamma v(\chi(\xi_1, \xi_2))$  is defined as*

$$\Delta_\gamma v(\chi(\xi_1, \xi_2)) := \text{div}_\gamma ((\nabla_\gamma v)^T) \quad (3)$$

**Theorem 1.6** (Vector Mean Curvature).  $Hn = -\Delta_\gamma \text{id}_\gamma$

*Proof.* □

## 1.2 Differential Geometry for Surfaces Defined through Level Sets, $\gamma := \{x \in \mathbb{R}^{d+1} : b(x) = 0\}$

## 2 Evolution Equations on Stationary Surfaces

### 2.1 Heat Equation

$$u_t = \kappa \Delta_\gamma u \quad (4)$$

**Weak form:**

**Discretization:** the  $\theta$ -method:

$$\langle \varphi_h, \frac{u_h^{n+1} - u_h^n}{\tau} \rangle = \langle \varphi_h, [(1 - \theta)\Delta_\gamma u_h^n + \theta\Delta_\gamma u_h^{n+1}] \rangle \quad (5)$$

### 2.2 Allen-Cahn

$$u_t = \varepsilon \Delta_\gamma u + \lambda(u - u^3) \quad (6)$$

## 3 Evolving Surfaces

The classical Helfrich model (??) approximates the energy required to hold a phospholipid bilayer in a geometric configuration that deviates from its preferred, or spontaneous, curvature. The model also includes energy penalties  $\lambda$  and  $\mu$  for changes in surface area and enclosed volume. Treating  $\lambda$  and  $\mu$  as Lagrange multipliers capture the fact that surface area and enclosed volume changes happen on a longer timescale than conformational changes.

For  $\Gamma \subset \mathbb{R}^3$ , a closed smooth codimension-one surface

$$E(\gamma) := \kappa(x) \int_\gamma (H(x) - c_0(x))^2 + \lambda + \mu s \cdot n \, dS \quad (7)$$

where  $H(x) = k_1(x) + k_2(x)$ : sum of *principle curvatures*  $k_1$  and  $k_2$ ,  $c_0(x)$ : *spontaneous curvature*, and  $\kappa(x)$ : *bending modulus*.

[?]

## 4 Evolution Equations on Evolving Surfaces

## 5 Numerics

### 5.1 Scalar Finite Elements for Geometric PDE and Evolving Parametric Surfaces

### 5.2 Vector Finite Elements for Geometric PDE and Evolving Parametric Surfaces

**Example 5.1** (Weakly Enforcing an Identity: computing the vector mean curvature on a parametric surface). **Numerical Approximation of vector mean curvature  $Hn$ :**

$$\langle \varphi, Hn \rangle = \langle \nabla_\gamma \varphi, \nabla_\gamma \text{id}_\gamma \rangle$$

The matrix equation  $MH = rhs$ , where  $rhs_i = \sum_{K \in \mathcal{T}} \int_K \nabla_\gamma \varphi_i : \nabla_\gamma \text{id}_\gamma \, dx$ ,  $M_{ij} = \sum_{K \in \mathcal{T}} \int_K \varphi_i : \varphi_j \, dx$

### 5.3 Schur Complement

### 5.4 adaptive time stepping

### 5.5 adaptive mesh refinement/coarsening