# A continuous mechanobiological model of lateral inhomogeneous biological surfaces

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## Abstract

Thin elastic surfaces containing molecules influencing the mechanical properties of the surface itself are wide spreaded structures of different scales in biological systems. Prominent examples are bilayer membranes and cell tissues. In this paper we present a continuous dynamical model of deforming lateral inhomogeneous surfaces, using the example of biological membranes. In agreement with experimental observations the membrane consists of different molecule species undergoing lateral phase separation and influencing the mechanical properties of the membrane. The presented model is based on the minimization of a free energy leading to a coupled nonlinear PDE system of fourth order, related to the Willmore flow and the Cahn-Hilliard equation. First simulations show the development of budding structures from stochastic initial conditions as a result of the gradient flow, which is comparable to experimentally observed structures. In our model mechanical properties are described via macroscopic mechanical moduli. However, the qualitative and quantitative relationships of mechanical moduli and the local composition of the membrane are unkown. Since the exact relationship significantly influences the emerging structures, this study motivates the development of techniques allowing for upscaling from the molecular scale.

*Keywords:* bilayer membrane, lipid bilayer, continuous model, phase separation, Helfrich energy, Cahn-Hilliard energy, gradient flow

## 1. Introduction

Elastic surfaces with long lateral extension but a relatively small diameter are one of the most basal building blocks of a variety of structures in biology: One example are biological membranes, which define a mechanical boundary

of cells as well as of substructures inside cells. These structures usually have a size up to a few micrometers, whereas the diameter of a membrane is only a few nanometers. Another example on larger scales are cell tissues. For example, in early human embryos they display a size of 100 micrometer but a diameter of only a few micrometers. In both, membranes and cell tissues, it has been proven that lateral inhomogeneous distributions of molecules influencing the mechanical properties of the layer are essential for the genesis and maintenance of biological structures: In membranes it has been shown that lateral phase separation of lipid molecules can lead to the budding of vesicles [3]. Furthermore, it has been suggested that lateral organization in membranes is a necessary condition for the biogenesis and maintenance of cellular membrane systems itself [24]. Thus, it is critical for the function of each biological cell. In cell tissues, it has been shown that patterns of certain molecules (called morphogenes) organize tissue morphology in the embryo, indispensable for the development of any organ [27].

With respect to bending, thin lateral homogeneous layers behave elastically and in the linear regime are well described by the plate equation [9], idealizing the layer to a two dimensional (2D) curved surface. This idea was further developed by Helfrich [16] and Willmore [36], describing the evolution of a 2D surface using the steepest descent of the $L^2$-gradient of the classical bending energy

$$F_{\text{Helfrich}} = \int_\Gamma \frac{\kappa}{2}(H - H_0)^2 \, ds + \int_\Gamma \kappa_G K \, ds, \tag{1}$$

without any restrictions on the magnitude of curvatures, e.g., on the first metric tensor. Here, $ds$ depicts the surface measure, $H$ is the mean curvature and $K$ the Gaussian curvature, both depending on the geometry of the surface $\Gamma$ [14]. If $C_1$ and $C_2$ are the two principal curvatures, $H$ is defined as their sum and $K$ as their product (see also FIG 1). $H_0, \kappa, \kappa_G$ are the elastic moduli, which are constant if the surface is lateral homogeneous. $H_0$ is the spontaneous curvature and represents the preferred curvature in the relaxed state. It is non zero if, for example, membrane molecules or cells are wedge-shaped. Parameters $\kappa$ and $\kappa_G$ are the bending rigidity and the Gaussian rigidity, respectively. Both values represent the stiffness of the surface: in tubular structures (were $K$ vanishes; c.f. FIG 1B) $\kappa$ penalises curvatures; in saddle structures (were $H$ vanishes; c.f. FIG 1A) $\kappa_G$ causes a penalty of curvatures. In general structures both moduli contribute to the energy penalty of curved surfaces. Most of the geometries appearing in biological

layers exhibit various intermediate structures of tubes, saddle structures and spheres (FIG 1 A-C). To consider lateral inhomogeneous membranes, we need
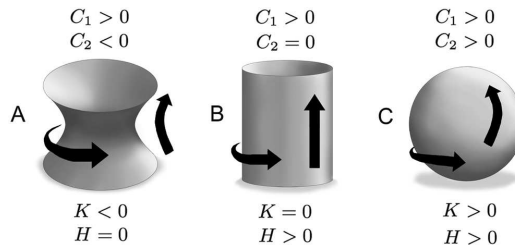


Figure 1: Principle curvatures $C_1, C_2$, mean curvature $H = C_1 + C_2$ and Gaussian curvature $K = C_1 C_2$ for different geometries: (A) Saddle, (B) Tube, (C) Sphere.

to introduce appropriate models for the dynamics of biochemical molecules. In the presented study we focus on the modelling of biological membranes. Experimental membrane models are well established, what principally allows to verify our model with the help of experiments. Other applications of our approach concern thin biological tissues changing their curvature during evagination process. However, the dynamics of morphogenes leading to the evagination process is very versatile and its exact influence on tissue mechanics is mostly unknown. Mathematical models may support experimental studies and provide better understanding of the processes involved in tissue deformation.

In contrast to the elastical behaviour with respect to bending, membrane molecules can move freely in lateral direction of the membrane. Therefore its lateral behaviour can be compared to a two-dimensional (2D) fluid, first described in the 'fluid mosaic' model by Singer [32]. In living cells biological membranes are composed of many different lipids, proteins and other molecules with different functions [1]. For both, lipids [3] and proteins [4] lateral phase separation and clustering have been shown. Mathematically lateral phase separation is well described by the minimization of the Cahn Hilliard energy [5] on a surface

$$F_{\text{Cahn-Hilliard}} = \sigma \int_{\Gamma} \left( \frac{\xi^2}{2} (\nabla^\Gamma \phi)^2 + f(\phi) \right) ds, \tag{2}$$

where $\sigma$ is the line-tension, $\xi$ a transition length, $\nabla^\Gamma$ the surface gradient and $f$ a double well potential.

The first theoretical work in the field of membrane budding considering the interplay of a curvature dependence and phase separation goes back to Lipowsky [22]. Since then a lot of effort has been made studying membrane budding using continuous modeling by minimization of a free energy, conststing of different couplings of the two energy parts (1) and (2). Earlier works have used phenomenological coupling terms [2, 8, 18, 34, 39], whereas more recent works have derived the coupling terms directly from first physical principles [23, 35]. The techniques used to describe the membranes range from parametric representations [18, 34] based on modelling membranes as continuous hypersurfaces to phase field descriptions [23, 35], where membranes with a finite thickness are embedded in a surrounding fluid. However, the advantage of the parametric approach is the relatively low computational cost for simulations, since numerical calculations are performed on a 2D-surface.

According to our knowledge, up to now there have been available no parametric models considering the deformations of the lateral phase separating membranes, in which coupling between the two parts of energies (1) and (2) results directly from first physical principles.

Since the first derivation of the homogeneous layer free energy (1) following a phenomenologigal approach [16], different experimental and theoretical efforts have been made to derive its macroscopical elastic moduli directly from the molecular properties [7, 21, 26, 28, 29, 33, 37]. However, most of these approaches are limited to the impact of selected molecule properties, special surface geometries, small curvatures or the consideration of 1D curves. Furthermore, all of these approaches consider lateral homogeneous surfaces. In contrast, biological surfaces often display lateral inhomogeneties. Up to now, a general approach determining the elastic moduli for an arbitrary curved and inhomogeneous surface directly from the molecular scale does not exist. The dynamics of inhomogeneous membranes depends strongly on the detailed relationship between mechanical moduli and the local composition of the membrane. A rigourous multiscale derivation of this relationship is an open problem and a rewarding field of research in applied mathematics.

In this paper we present a continuous model of deforming inhomogeneous membranes consisting of two components using a parametric description of the membrane. The mechanical model is coupled with a model for the lateral phase separation of the two components. The presented model is not restricted to small curvatures or symmetric geometries. Although the presented model does not result from a rigourous upscaling from the molecular

scale, the coupling between the energies (1) and (2) is based on the first physical principles. It reflects the assumption that different molecules can vary in their shape and stiffness.

Although we restrict us to biological membranes the presented approach can be straight forward modified to describe tissues under the mechanial control of morphogenes. One possibility is reducing the presented model assuming that the lateral inhomogeneity is constant in time, i.e. only small time scales are considered. Another possibility is following the ideas of Cummings [11] coupling surface dynamics and lateral reaction-diffusion equations.

The paper is organised as follows. In Section 2 we formulate the mathematical model in terms of energy functionals and gradient flows. In Section 3 preliminary notions and formulas are presented and in Section 4 main result concerning the form of the mathematical model is formulated. Section 5 includes the derivation of the detailed model based on the calculation of the Frechet derivatives of energy functionals. Finally, in Section 6 we present numerical simulations of the model. All notions and definitions are summarised in the Appendix.
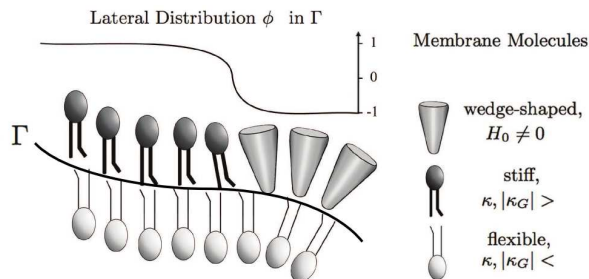
## 2. The mathematical model



Figure 2: Continuous model bilayer membrane: The bilayer is represented by the hypersurface $\Gamma$ and its lateral inhomogenity by the order parameter $\phi$. Mechanical molecule properties are outlined on the right hand side.

The bilayer is represented by a continuous two-dimensional (2D) surface $\Gamma$ depicted by a parametric representation $\vec{X}(u_1, u_2) : U \to \Gamma \subset \mathbb{R}^3$ with $U = [0,1] \times [0,1]$. Here, we consider a membrane composed of two different lipid species or lipids and proteins. The concentration of the two components $A$ and $B$ in $\Gamma$ is described by the order parameter $\phi : U \to [-1, 1]$. That is,

5

if $\phi = 1$ the membrane is locally composed purely of species $A$ and if $\phi = -1$ locally only species $B$ is present. Our model is based on the minimization of a free energy $F = F_1 + F_2 + F_3$ containing both the curvature depending part $F_1 + F_2$ and the Cahn-Hilliard energy $F_3$ [5] inducing lateral phase separation. In detail it reads

$$
\begin{aligned}
F_1 &= \frac{1}{2} \int_\Gamma \kappa(\phi)(H - H_0(\phi))^2 \, ds, \\
F_2 &= \int_\Gamma \kappa_G(\phi) K \, ds, \\
F_3 &= \sigma \int_\Gamma \left( \frac{\xi^2}{2} (\nabla^\Gamma \phi)^2 + f(\phi) \right) \, ds.
\end{aligned}
\tag{3}
$$

Since different components of the membrane may differ in their mechanical properties (such as shape and stiffness), each macroscopic mechanical modulus $h$ ($h \in \{\kappa, \kappa_G, H_0\}$) is taken as a function of the order parameter $\phi$. Each function $h$ is chosen such that $h(1) = h^A$ and $h(-1) = h^B$, where $h^A$ and $h^B$ are the mechanical moduli of the pure components. Furthermore, $\sigma$ is the line-tension, $\xi$ a transition length, $\nabla^\Gamma$ the surface gradient and $f$ a double well potential.

Instead of minimizing $F = F_1 + F_2 + F_3$ directly we adopt a dynamic point of view. Thus, assuming local mass conservation lateral dynamics of the two species $A$ and $B$ is determined by the lateral continuity equation

$$
\partial_t \phi + \nabla^\Gamma \cdot \vec{j} = 0,
$$

where $\nabla^\Gamma \cdot$ is the surface divergence operator [14]. The flux is determined by the lateral gradient of the chemical potential $\mu(u_1, u_2)$ by $\vec{j} = \nabla^\Gamma \mu$. $\mu$ is proportional to the variation of the free energy $F$ with respect to $\phi$, thus $\mu = L_\phi \frac{\delta}{\delta \phi}[F]$; the mobility $L_\phi$ is assumed to be constant. We obtain the following dynamical equation for $\phi$

$$
\partial_t[\phi] = L_\phi \Delta^\Gamma \left[ \frac{\delta}{\delta \phi}[F] \right],
$$

where $\Delta^\Gamma$ is the Laplace-Beltrami operator [14]. Given a certain deformation of the membrane system, it evolves in the direction of the steepest decent of the free bilayer energy. Assuming an overdamped motion, which is a

6

typical assumption for molecular systems, dynamics of the deformation $\vec{X}$ in $U \times [0, T]$ is given by the following $L^2-$gradient flow under the constraint of incompressibility of the membrane layer:

$$\partial_t[\vec{X}] = -L_X \frac{\delta}{\delta \vec{X}} \left[ F + \int_\Gamma \gamma \, ds \right] \tag{4}$$

$$\partial_t[\sqrt{g}] = \nabla^\Gamma \cdot [\partial_t[\vec{X}]] = 0, \tag{5}$$

where $L_X$ is a kinetic coefficient, $\frac{\delta}{\delta \vec{X}}[F]$ denotes the variation of $F$ with respect to $\vec{X}$ and $\gamma$ is a local langrange multiplyer [15]. The gradient flow (4) leads to a minimization of the free energy $F$ under the constraint of incompressibility (5), where $g$ denotes the determinant of the first fundamental tensor matrix.

Although variations of partial parts of $F$ have been derived in separate works, a complete treatment of $F$ including Gaussian curvature contributions can not be found in the literature. Here, we present the detailed calculation of the Frechet derivatives.

## 3. Technical remarks

Before we derive the main results, i.e. the Frechet derivatives of the energies, let us summarize some important technical remarks. Let $\vec{A}(\vec{X}, t) \in \mathbb{R}^3$ be the force acting on the membrane at $\vec{X}$ at time $t$. We assume, that the force is determined by the variation $F'$ in form of the following $L^2$-gradient flow:

$$\int \vec{A} \cdot \vec{\psi} \, d\mu = -\langle F', \vec{\psi} \rangle = -\frac{d}{d\epsilon} [F(\vec{X} + \epsilon \vec{\psi})] \Big|_{\epsilon=0}, \tag{6}$$

where $\vec{\psi} \in C^\infty(\Omega, \mathbb{R}^3)$ is an arbitrary test function. Since (6) holds for all $\vec{\psi}$, especially $(\psi^\perp, \psi^1, \psi^2) = (1, 0, 0)$, $(\psi^\perp, \psi^1, \psi^2) = (0, 1, 0)$ and $(\psi^\perp, \psi^1, \psi^2) = (0, 0, 1)$, let us consider the decomposition in tangential and normal parts $\vec{\psi} = \psi \vec{n} + \sum_k \psi^k \partial_k \vec{X}$ and $\vec{A} = A^\perp \vec{n} + \sum_u A^u \partial_u \vec{X}$. It follows

$$\int \vec{A} \cdot \vec{\psi} \, d\mu = -\int (A^\perp \vec{n} + \sum_u A^u \partial_u \vec{X}) \cdot \psi \vec{n} \, d\mu$$

$$- \int (A^\perp \vec{n} + \sum_u A^u \partial_u \vec{X}) \cdot (\sum_k \psi^k \partial_k \vec{X}) \, d\mu$$

7

$$= -\int A^{\perp} \psi \, d\mu - \sum_{u,k} \int A^u \partial_u \vec{X} \cdot \partial_k \vec{X} \psi^k \, d\mu.$$

as well as

$$\langle F', \vec{\psi} \rangle = \langle F', \psi \vec{n} \rangle + \langle F', \sum_k \psi^k \partial_k \vec{X} \rangle$$

$$= \left. \frac{d}{d\epsilon} F(\vec{X} + \epsilon \psi \vec{n}) \right|_{\epsilon=0} + \left. \frac{d}{d\epsilon} F(\vec{X} + \epsilon \sum_k \psi^k \partial_k \vec{X}) \right|_{\epsilon=0}.$$

In the following $\delta^{\perp}$ and $\delta^k$ depict the variation in normal direction and $k$-tangential direction regarding $\Gamma$, respectively, where $\delta^t = \sum_k \delta^k$. We mention furthermore the following geometric relations derived in [41]

$$\delta^{\perp}[H] = -\Delta^{\Gamma}[\psi] - \psi(H^2 - 2K) \tag{7}$$

and

$$\delta^{\perp}[\sqrt{g}] = \psi H \sqrt{g}, \tag{8}$$

where $g$ is the determinant of the first fundamental tensor [14] (corresponding definitions of geometric operators and quantities are given for convenience in the appendix).

Following [25] it holds that

$$\delta^{\perp}[K] = \widehat{\Delta}^{\Gamma}[\psi] - HK\psi, \tag{9}$$

where $\widehat{\Delta}^{\Gamma}$ is the second surface laplacian (c.f. appendix). Following, [19] it has been shown that

$$\delta^{\perp}[g^{ij}] = -2 \sum_k g^{jk} b_k^i \psi = -2b^{ij}\psi, \tag{10}$$

$$\delta^t[g^{ij}] = -\nabla^i[\psi^j] - \nabla^j[\psi^i], \tag{11}$$

$$\delta^t[g^{ij}] = -\nabla^i[\psi^j] - \nabla^j[\psi^i], \tag{12}$$

where $(g_{ij})$ is the first fundamental tensor, $(b_{ij})$ is the second fundamental tensor, $\nabla_i$ is the covariant derivative and rised indices denote contravariant indices (c.f. appendix). Furthermore, it holds

$$\delta^t[b_{ij}] = \sum_k \left( \nabla_j[\psi^k]b_{ik} + \nabla_i[\psi^k]b_{jk} + \nabla_k[b_{ij}]\psi^k \right) \tag{13}$$

8

according to [6] as well as the Mainardi-Codazzi-equation [10]

$$\nabla_c[b_{ab}] = \nabla_b[b_{ac}]. \tag{14}$$

In addition we will use the results of [17] stating

$$\sum_a \nabla_a[b^a{}_b] = \partial_b[H], \tag{15}$$

and the results of [6] stating

$$\delta^t[b_{ij}] = \sum_k \left(\nabla_k[b_{ij}]\psi^k + b_{ik}\nabla_j[\psi^k] + b_{jk}\nabla_i[\psi^k]\right). \tag{16}$$

We should mention that in some of the publications cited above the mean curvature $\widehat{H}$ differs from the definition used in this study showing the relation $\widehat{H} = -H/2$.

## 4. Statement of the main result

In the following we assume vanishing boundary integrals, which are for example appearing at closed surfaces. Furthermore, we assume that the elastic moduli and the function $f(\phi)$ are given by regular functions, i.e., $\kappa, \kappa_G, H_0, f \in C^\infty([0,1])$.

**Theorem 1.** *The deformation of a lateral phase separating and incompressible membrane is given by the equations*

$$\begin{aligned}
\partial_t \vec{X} &= -L_X \frac{\delta}{\delta \vec{X}} \left[ F + \int_\Gamma \gamma \, ds \right] \\
&= -L_X \left[ A^\perp \vec{n} + \sum_k A^k \partial_k \vec{X} \right]
\end{aligned} \tag{17}$$

*with the constraint*

$$\partial_t[\sqrt{g}] = 0, \tag{18}$$

*where*

$$\begin{aligned}
A^\perp &= -\Delta^\Gamma[\kappa(\phi)](H - H_0(\phi)) \\
&\quad -\kappa(\phi)(\Delta^\Gamma[H - H_0(\phi)] + (H - H_0(\phi))(H^2 - 2K)
\end{aligned}$$

9

$$-\frac{1}{2}(H - H_0(\phi))^2 H)$$

$$+\widehat{\Delta}^\Gamma[\kappa_G(\phi)]$$

$$-\xi^2 \sum_{i,j} b^{ij} \partial_i[\phi]\partial_j[\phi] + H(\frac{\xi^2}{2}(\nabla^\Gamma[\phi])^2 + f(\phi))$$

$$+H\gamma$$

*and*

$$
\begin{aligned}
A^k &= -\frac{1}{2}\partial^k[\kappa(\phi)](H - H_0(\phi))^2 \\
&\quad +\kappa(\phi)(H - H_0(\phi))\partial^k[H_0(\phi)] \\
&\quad -\partial^k[\kappa_G(\phi)]K \\
&\quad +\xi^2 \sum_u \nabla_u[\partial^k\phi\partial^u\phi] - \partial^k[\frac{\xi^2}{2}(\nabla^\Gamma\phi)^2 + f(\phi)] \\
&\quad -\partial^k[\gamma].
\end{aligned}
$$

*Furthermore, lateral dynamics of the order parameter $\phi$ is given by*

$$
\begin{aligned}
\partial_t\phi &= L_\phi\Delta^\Gamma\left[\frac{\delta}{\delta\phi}[F]\right] \\
&= L_\phi\Delta^\Gamma\left[\frac{1}{2}\kappa'(\phi)(H - H_0(\phi))^2 - \kappa(\phi)(H - H_0(\phi))H_0'(\phi) \right. \\
&\qquad\qquad\qquad\left. +\kappa_G'(\phi)K - \xi^2\Delta^\Gamma\phi + f'(\phi)\right].
\end{aligned}
$$

The proof of the theorem will be given in the following section, where each term of the Frechet derivative of energies is calculated separately.

## 5. Proof of the main result

**Lemma 2.**

$$
\begin{aligned}
\frac{\delta^\perp[F_1]}{\delta\vec{X}} &= -\Delta^\Gamma[\kappa(\phi)](H - H_0(\phi)) \\
&\quad -\kappa(\phi)(\Delta^\Gamma[H - H_0(\phi)] + (H - H_0(\phi))(H^2 - 2K) \\
&\qquad\qquad\qquad\qquad -\frac{1}{2}(H - H_0(\phi))^2 H).
\end{aligned}
$$

*Proof:* Using the chain rule and $ds = \sqrt{g}d^2u$ yields

$$
\begin{aligned}
\delta^\perp[F_1] &= \frac{1}{2}\int \delta^\perp\left[\kappa(\phi)(H-H_0(\phi))^2\right]\sqrt{g}\,d^2u \\
&\quad + \frac{1}{2}\int \kappa(\phi)(H-H_0(\phi))^2\delta^\perp[\sqrt{g}]\,d^2u \\
&= \frac{1}{2}\int \kappa(\phi)2(H-H_0(\phi))\delta^\perp[H]\sqrt{g}\,d^2u \\
&\quad + \frac{1}{2}\int \kappa(\phi)(H-H_0(\phi))^2\delta^\perp[\sqrt{g}]\,d^2u
\end{aligned}
$$

and using (7) and (8) it follows that

$$
\begin{aligned}
\delta^\perp[F_1] &= \int \Big\{\kappa(\phi)(H-H_0(\phi))(-\Delta^\Gamma[\psi]-\psi(H^2-2K)) \\
&\quad + \frac{\kappa(\phi)}{2}(H-H_0(\phi))^2\psi H\Big\}\sqrt{g}\,d^2u.
\end{aligned}
$$

Using Green's identities for the first surface laplace operator two times [40] it follows, that

$$
\begin{aligned}
\delta^\perp[F_1] &= \int \Big\{-\Delta^\Gamma[\kappa(\phi)(H-H_0(\phi)]\psi - \kappa(\phi)(H-H_0(\phi))(H^2-2K)\psi \\
&\quad + \frac{\kappa(\phi)}{2}(H-H_0(\phi))^2\psi H\Big\}\sqrt{g}\,d^2u \\
&= \int \Big\{-\Delta^\Gamma[\kappa(\phi)](H-H_0(\phi)) \\
&\quad -\kappa(\phi)\Big(\Delta^\Gamma[H-H_0(\phi)] + (H-H_0(\phi))(H^2-2K) \\
&\quad -\frac{1}{2}(H-H_0(\phi))^2 H\Big)\Big\}\psi\sqrt{g}\,d^2u,
\end{aligned}
$$

leading to the assertion of the lemma. $\qquad\square$

**Lemma 3.**

$$
\frac{\delta^\perp[F_2]}{\delta\vec{X}} = \widehat{\Delta}^\Gamma[\kappa_G(\phi)].
$$

11

*Proof:* Using the product rule, it follows that

$$\delta^{\perp}[F_2] \;=\; \int \delta^{\perp}[\kappa_G(\phi)]K\sqrt{g}\,d^2u + \int \kappa_G(\phi)\delta^{\perp}[K]\sqrt{g}\,d^2u$$
$$+ \int \kappa_G(\phi)K\delta^{\perp}[\sqrt{g}]\,d^2u.$$

and considering (9) we obtain

$$\delta^{\perp}[F_2] \;=\; \int \kappa_G(\phi)(\widehat{\Delta}^{\Gamma}[\psi] - HK\psi)\sqrt{g}\,d^2u + \int \kappa_G(\phi)K\psi H\sqrt{g}\,d^2u$$
$$=\; \int \kappa_G(\phi)\widehat{\Delta}^{\Gamma}[\psi]\sqrt{g}\,d^2u.$$

Green's identities for the second laplacian [40] yield

$$\delta^{\perp}[F_2] \;=\; \int \widehat{\Delta}^{\Gamma}[\kappa_G(\phi)]\psi\sqrt{g}\,d^2u.$$

$\square$

**Lemma 4.**

$$\frac{\delta^{\perp}[F_3]}{\delta\vec{X}} = -\xi^2 \sum_{i,j} b^{ij}\partial_i[\phi]\partial_j[\phi] + H\left(\frac{\xi^2}{2}(\nabla^{\Gamma}[\phi])^2 + f(\phi)\right).$$

*Proof:* Equality (8) and the product rule yield

$$\delta^{\perp}[F_3] \;=\; \int \delta^{\perp}\left[\frac{\xi^2}{2}(\nabla^{\Gamma}[\phi])^2 + f(\phi) + \right]\sqrt{g}\,d^2u$$
$$+ \int \left\{\frac{\xi^2}{2}(\nabla^{\Gamma}[\phi])^2 + f(\phi)\right\}\psi H\sqrt{g}\,d^2u.$$

Using $(\nabla^{\Gamma}[\phi])^2 = \sum_{i,j} g^{ij}\partial_i[\phi]\partial_j[\phi]$ we obtain

$$\delta^{\perp}[F_3] \;=\; \int \frac{\xi^2}{2}\sum_{i,j}\delta^{\perp}[g^{ij}]\partial_i[\phi]\partial_j[\phi]\sqrt{g}\,d^2u$$
$$+ \int \left\{\frac{\xi^2}{2}(\nabla^{\Gamma}[\phi])^2 + f(\phi)\right\}\psi H\sqrt{g}\,d^2u.$$

12

Since (10) holds it follows

$$\delta^{\perp}[F_3] \;=\; \int \{-\xi^2 \sum_{i,j} b^{ij} \partial_i[\phi]\partial_j[\phi] + \frac{\xi^2}{2} H((\nabla^{\Gamma}[\phi])^2 + f(\phi)\} \psi \sqrt{g} \, d^2u,$$

what yields the assertion of the Lemma. $\square$

**Proposition 5.**

$$\delta^k[g_{ij}] = \partial_i[\partial_k \vec{X} \psi^k] \cdot \partial_j \vec{X} + \partial_j[\partial_k \vec{X} \psi^k] \cdot \partial_i \vec{X}$$

*Proof:* It holds

$$\delta^k[g_{ij}] \;=\; \partial_i[\delta^k[\vec{X}]] \cdot \partial_j \vec{X} + \partial_i \vec{X} \cdot \partial_j[\delta^k[\vec{X}]].$$

The claim of the Proposition follows directly from

$$\delta^k[\vec{X}] := \frac{d}{d\epsilon}[\vec{X} + \epsilon \partial_k \vec{X} \psi^k]\Big|_{\epsilon=0} = \partial_k \vec{X} \psi^k$$

$\square$

**Proposition 6.**

$$\delta^t[H] = \sum_{i,j,k} g^{ij} \nabla_k[b_{ij}]\psi^k.$$

*Proof:* It holds

$$\begin{aligned}
\delta^t[H] \;&=\; \delta^t[\sum_i b_i{}^i] = \delta^t[\sum_{i,j} g^{ij} b_{ij}] \\
&=\; \sum_{i,j} \delta^t[g^{ij}]b_{ij} + \sum_{i,j} g^{ij} \delta^t[b_{ij}],
\end{aligned}$$

due to (11) and (13). Since $(b_{ij})_{i,j}$ and $(g^{ij})_{i,j}$ are symmetric, it follows

$$\delta^t[H] \;=\; -2\sum_{i,j} \nabla^i[\psi^j]b_{ij} + 2\sum_{i,j,k} g^{ij}\nabla_i[\psi^k]b_{jk} + \sum_{i,j,k} g^{ij}\nabla_k[b_{ij}]\psi^k.$$

Furthermore, it holds $2\sum_{i,j,k} g^{ij}\nabla_i[\psi^k]b_{jk} = 2\sum_{j,k} \nabla^j[\psi^k]b_{jk} = 2\sum_{i,j} \nabla^i[\psi^j]b_{ij}$, i.e., the first two terms vanish, and the claim holds true. $\square$

13

**Proposition 7.**

$$\int \eta \delta^k[\sqrt{g}]\, d^2u = -\sum_{k,u} \int \partial^u[\eta] g_{uk} \psi^k \sqrt{g}\, d^2u.$$

*Proof:* Applying the chain rule on the determinant it follows

$$\int \eta \delta^k[\sqrt{g}]\, d^2u \;\; = \;\; \int \frac{1}{2} \sum_{i,j} \sqrt{g} g^{ij} \delta^k[g_{ij}] \eta\, d^2u.$$

Using Proposition 5 and Green's formula it follows

$$\int \eta \delta^k[\sqrt{g}]\, d^2u \;\; = \;\; \int \sum_{i,j} \sqrt{g} g^{ij} \partial_i[\partial_k \vec{X} \psi^k] \cdot \partial_j \vec{X} \eta\, d^2u$$

$$= \;\; -\int \sum_{i,j} \partial_i[\eta g^{ij} \sqrt{g} \partial_j \vec{X}] \cdot \partial_k \vec{X} \psi^k\, d^2u.$$

Since $\sum_{i,j} \partial[g^{ij} \sqrt{g} \partial_j \vec{X}] \cdot \partial_k \vec{X} = -\sqrt{g} \Delta^\Gamma \vec{X} \cdot \partial_k \vec{X} = \sqrt{g} H \vec{n} \cdot \partial_k \vec{X} = 0$ it holds

$$\int \eta \delta^k[\sqrt{g}]\, d^2u \;\; = \;\; -\sum_{i,j} \int \partial_i[\eta] g^{ij} \partial_j \vec{X} \cdot \partial_k \vec{X} \psi^k \sqrt{g}\, d^2u$$

$$= \;\; -\sum_{j} \int \partial^j[\eta] \partial_j \vec{X} \cdot \partial_k \vec{X} \psi^k \sqrt{g}\, d^2u$$

$$= \;\; -\sum_{j} \int \partial^j[\eta] g_{jk} \psi^k \sqrt{g}\, d^2u.$$

Since $\delta^t = \sum_k \delta^k$ the claim follows directly. $\qquad \square$

**Lemma 8.**

$$\frac{\delta^k[F_1]}{\delta \vec{X}} = -\frac{1}{2} \partial^k[\kappa(\phi)](H - H_0(\phi))^2 + \kappa(\phi)(H - H_0(\phi)) \partial^k[H_0(\phi)].$$

*Proof:* Using the product rule we obtain

$$\delta^t\left[\frac{1}{2} \int \kappa(\phi)(H - H_0(\phi))^2 \sqrt{g}\, d^2u\right]$$

$$= \;\; \frac{1}{2} \int \kappa(\phi) \delta^t[(H - H_0(\phi))^2] \sqrt{g}\, d^2u + \frac{1}{2} \int \kappa(\phi)(H - H_0(\phi))^2 \delta^t[\sqrt{g}]\, d^2u.$$

14

Propositions 6-7 and the product rule provide

$$\delta^t \left[ \frac{1}{2} \int \kappa(\phi)(H - H_0(\phi))^2 \sqrt{g} \, d^2u \right]$$

$$= \int \kappa(\phi)(H - H_0(\phi)) \sum_{i,j,k} g^{ij} \nabla_k[b_{ij}] \psi^k \sqrt{g} \, d^2u$$

$$- \frac{1}{2} \sum_{k,u} \int \partial^u \left[ \kappa(\phi)(H - H_0(\phi))^2 \right] g_{uk} \psi^k \sqrt{g} \, d^2u$$

$$= \int \kappa(\phi)(H - H_0(\phi)) \sum_{i,j,k} g^{ij} \nabla_k[b_{ij}] \psi^k \sqrt{g} \, d^2u$$

$$- \frac{1}{2} \sum_{k,u} \int \partial^u \left[ \kappa(\phi) \right] (H - H_0(\phi))^2 g_{uk} \psi^k \sqrt{g} \, d^2u$$

$$- \sum_{k,u} \int \kappa(\phi)(H - H_0(\phi)) \partial^u[(H - H_0(\phi))] g_{uk} \psi^k \sqrt{g} \, d^2u$$

$$= \int \kappa(\phi)(H - H_0(\phi)) \sum_{i,j,k} g^{ij} \nabla_k[b_{ij}] \psi^k \sqrt{g} \, d^2u$$

$$- \frac{1}{2} \sum_{k,u} \int \partial^u \left[ \kappa(\phi) \right] (H - H_0(\phi))^2 g_{uk} \psi^k \sqrt{g} \, d^2u$$

$$- \sum_{k,u} \int \kappa(\phi)(H - H_0(\phi)) \partial^u[H] g_{uk} \psi^k \sqrt{g} \, d^2u$$

$$+ \sum_{u,k} \int \kappa(\phi)(H - H_0(\phi)) \partial^u[H_0(\phi)] g_{uk} \psi^k \sqrt{g} \, d^2u.$$

Due to (14) and (15), the covariant derivatives and the first metric tensor commute and it follows

$$\sum_{i,j} g^{ij} \nabla_k[b_{ij}] = \sum_{i,j} g^{ij} \nabla_j[b_{ik}] = \sum_j \nabla_j \left[ \sum_i g^{ij} b_{ik} \right]$$

$$= \sum_j \nabla_j[b^j{}_k] = \partial_k[H] = \sum_u g_{uk} \partial^u[H].$$

Since the first and third term cancel each other, we obtain

$$\delta^t \left[ \frac{1}{2} \int \kappa(\phi)(H - H_0(\phi))^2 \sqrt{g} \, d^2u \right]$$

15

$$= -\frac{1}{2} \sum_{k,u} \int \partial^u [\kappa(\phi)](H - H_0(\phi))^2 g_{uk} \psi^k \sqrt{g}\, d^2 u$$

$$+ \sum_{k,u} \int \kappa(\phi)(H - H_0(\phi)) \partial^u [H_0(\phi)] g_{uk} \psi^k \sqrt{g}\, d^2 u.$$

$\square$

**Proposition 9.**

$$\sum_i \overline{b^i}_j b_{ik} = g_{jk},$$

*where $\overline{b^i}_j$ are components of the inverse of the matrix $(b_i{}^j)$.*

*Proof:* It holds

$$\sum_i \overline{b^i}_j b_{ik} = \sum_i (\overline{\sum_l g^{li} b_{jl}}) b_{ik}$$

and since $(\mathbf{AB})^{-1} = \mathbf{B}^{-1}\mathbf{A}^{-1}$ it follows

$$\sum_i \overline{b^i}_j b_{ik} = \sum_i (\sum_l \overline{g^{lj} b_{il}}) b_{ik}$$

$$= \sum_i (\sum_l g_{lj} \overline{b_{il}}) b_{ik} = \sum_l (\sum_i \overline{b_{il}} b_{ik}) g_{lj} = \sum_l \delta_l^k g_{lj} = g_{kj},$$

which was claimed. $\square$

**Proposition 10.**

$$\delta^t[K] = \sum_{i,j,k} \overline{b^i}_j \nabla_k [b_i{}^j] \psi^k K.$$

*Proof:* It holds

$$\delta^t[K] = \delta^t[\det(b_i{}^j)] = \sum_{i,j} K \overline{b^i}_j \delta^t[b_i{}^j]$$

$$= \sum_{i,j} K \overline{b^i}_j \delta^t[\sum_k g^{kj} b_{ik}] = \sum_{i,j,k} K \overline{b^i}_j \delta^t[g^{kj}] b_{ik} + \sum_{i,j,k} K \overline{b^i}_j g^{kj} \delta^t[b_{ik}].$$

16

Using (15) and (16) it follows

$$
\begin{aligned}
\delta^t[K] \;=\; & -2\sum_{i,j,k} K\overline{b^i{}_j}\nabla^k[\psi^j]b_{ik} \\
& + \sum_{i,j,k} K\overline{b^i{}_j}g^{kj}\sum_u\Big(b_{iu}\nabla_k[\psi^u]+b_{uk}\nabla_i[\psi^u]+\nabla_u[b_{ik}]\psi^u\Big) \\
\;=\; & -2\sum_{i,j,k} K\overline{b^i{}_j}\nabla^k[\psi^j]b_{ik} \\
& +2\sum_{i,j,u,k} K\overline{b^i{}_j}g^{kj}b_{iu}\nabla_k[\psi^u]+\sum_{i,j,k,u} K\overline{b^i{}_j}g^{kj}\nabla_u[b_{ik}]\psi^u \\
\;=\; & -2\sum_{i,j,k} K\overline{b^i{}_j}\nabla^k[\psi^j]b_{ik} \\
& +2\sum_{i,j,u} K\overline{b^i{}_j}b_{iu}\sum_k g^{kj}\nabla_k[\psi^u]+\sum_{i,j,k,u} K\overline{b^i{}_j}g^{kj}\nabla_u[b_{ik}]\psi^u \\
\;=\; & -2\sum_{i,j,k} K\overline{b^i{}_j}\nabla^k[\psi^j]b_{ik} \\
& +2\sum_{i,j,u} K\overline{b^i{}_j}b_{iu}\nabla^j[\psi^u]+\sum_{i,j,k,u} K\overline{b^i{}_j}g^{kj}\nabla_u[b_{ik}]\psi^u \\
\;=\; & -2\sum_{i,j,k} K\overline{b^i{}_j}\nabla^k[\psi^j]b_{ik} \\
& +2\sum_{i,j,k} K\overline{b^i{}_j}b_{ik}\nabla^j[\psi^k]+\sum_{i,j,k,u} K\overline{b^i{}_j}g^{kj}\nabla_u[b_{ik}]\psi^u.
\end{aligned}
$$

Proposition 9 yields

$$
\begin{aligned}
\delta^t[K] \;=\; & -2\sum_{j,k} g_{jk}K\nabla^k[\psi^j]+2\sum_{j,k} Kg_{jk}\nabla^j[\psi^k]+\sum_{i,j,k,u} K\overline{b^i{}_j}g^{kj}\nabla_u[b_{ik}]\psi^u \\
\;=\; & \sum_{i,j,k,u} \overline{b^i{}_j}g^{kj}\nabla_u[b_{ik}]\psi^u K.
\end{aligned}
$$

Since covariant derivatives and the first metric tensor commute, we obtain

$$
\delta^t[K] \;=\; \sum_{i,j,u} \overline{b^i{}_j}\nabla_u[b_i{}^j]\psi^u K,
$$

which is the claim. $\qquad\square$

17

**Lemma 11.**

$$\frac{\delta^k[F_2]}{\delta \vec{X}} = -\partial^k[\kappa_G(\phi)]K.$$

*Proof:* It holds

$$\partial^t[\int \kappa_G(\phi)K\sqrt{g}\,d^2u] = \int \kappa_G(\phi)\partial^t[K]\sqrt{g}\,d^2u + \int \kappa_G(\phi)K\partial^t[\sqrt{g}]\,d^2u.$$

Using Propositions 6 and 10 and the product rule we obtain

$$
\begin{aligned}
\partial^t[\int \kappa_G(\phi)&K\sqrt{g}\,d^2u]\\
&= \sum_{i,j,k}\int \kappa_G(\phi)\overline{b^i}_j\nabla_k[b_i{}^j]K\psi^k\sqrt{g}\,d^2u\\
&\quad - \sum_{u,k}\int \partial^u[\kappa_G(\phi)]Kg_{uk}\psi^k\sqrt{g}\,d^2u - \sum_{k}\int \kappa_G(\phi)\partial_k[K]\psi^k\sqrt{g}\,d^2u.
\end{aligned}
$$

From the definition of the covariant derivative it follows that

$$
\begin{aligned}
\partial^t[\int \kappa_G(\phi)&K\sqrt{g}\,d^2u]\\
&= \sum_{i,j,k}\kappa_G(\phi)\overline{b^i}_j\Big\{\partial_k[b_i{}^j] + \sum_{l}(\Gamma^j_{kl}b_i{}^l - \Gamma^l_{ki}b_l{}^j)\Big\}K\psi^k\sqrt{g}d^2u\\
&\quad - \sum_{u,k}\int \partial^u[\kappa_G(\phi)]Kg_{uk}\psi^k\sqrt{g}\,d^2u - \sum_{k}\int \kappa_G(\phi)\partial_k[K]\psi^k\sqrt{g}\,d^2u.
\end{aligned}
$$

Applying the chain rule to the determinant leads to

$$
\begin{aligned}
\partial^t[\int \kappa_G(\phi)&K\sqrt{g}\,d^2u]\\
&= \sum_{i,j,k}\int \kappa_G(\phi)\overline{b^i}_j\partial_k[b_i{}^j]\psi^kK\sqrt{g}\,d^2u\\
&\quad + \int \kappa_G(\phi)\sum_{i,j,k,l}\overline{b^i}_j\Big\{\Gamma^j_{kl}b_i{}^l - \Gamma^l_{ki}b_l{}^j\Big\}\psi^kK\sqrt{g}\,d^2u\\
&\quad - \sum_{u,k}\int \partial^u[\kappa_G(\phi)]Kg_{uk}\psi^k\sqrt{g}\,d^2u - \sum_{i,j,k}\int \kappa_G(\phi)\overline{b^i}_j\partial_k[b_i{}^j]\psi^kK\sqrt{g}\,d^2u.
\end{aligned}
$$

18

$$= \int \kappa_G(\phi) \Big\{ \sum_{i,j,k,l} \overline{b^i}_j b_i^{\ l} \Gamma_{kl}^j - \sum_{i,j,k,l} \overline{b^i}_j b_l^{\ j} \Gamma_{ki}^l \Big\} \psi^k K \sqrt{g} \, d^2 u$$

$$- \sum_{u,k} \int \partial^u [\kappa_G(\phi)] K g_{uk} \psi^k \sqrt{g} \, d^2 u.$$

Since $\sum_l \overline{b_i^{\ l}} b_l^{\ j} = \delta_i^j$, where $\delta_i^j$ is the Kronecker symbol, it follows

$$\partial^t [\int \kappa_G(\phi) K \sqrt{g} \, d^2 u]$$

$$= \int \kappa_G(\phi) \Big\{ \sum_{j,k,l} \delta_j^l \Gamma_{kl}^j - \sum_{i,k,l} \delta_l^i \Gamma_{ki}^l \Big\} \psi^k K \sqrt{g} \, d^2 u$$

$$- \sum_{u,k} \int \partial^u [\kappa_G(\phi)] K g_{uk} \psi^k \sqrt{g} \, d^2 u$$

$$= \int \kappa_G(\phi) \Big\{ \sum_{k,j} \Gamma_{kj}^j - \sum_{k,i} \Gamma_{ki}^i \Big\} \psi^k K \sqrt{g} \, d^2 u$$

$$- \sum_{u,k} \int \partial^u [\kappa_G(\phi)] K g_{uk} \psi^k \sqrt{g} \, d^2 u$$

$$= - \sum_{u,k} \int \partial^u [\kappa_G(\phi)] K g_{uk} \psi^k \sqrt{g} \, d^2 u,$$

which is the claim. $\qquad \square$

**Proposition 12.**

$$\nabla_a [\psi^z] = \sum_{b,k} g^{zb} \partial_b \vec{X} \cdot \partial_a [\partial_k \vec{X} \psi^k], \tag{19}$$

*Proof:* It holds

$$\sum_{b,k} g^{zb} \partial_b \vec{X} \cdot \partial_a [\partial_k \vec{X} \psi^k]$$

$$= \sum_{b,k} g^{zb} \partial_b \vec{X} \cdot \partial_a [\partial_k \vec{X}] \psi^k + \sum_{b,k} g^{zb} \partial_b \vec{X} \cdot \partial_k \vec{X} \partial_a [\psi^k]$$

$$= \frac{1}{2} \sum_{b,k} g^{zb} \Big\{ 2 \partial_b \vec{X} \cdot \partial_a [\partial_k \vec{X}] + \partial_k [\partial_b \vec{X}] \cdot \partial_a \vec{X} - \partial_b [\partial_k \vec{X}] \cdot \partial_a \vec{X}$$

19

$$+\partial_a[\partial_b\vec{X}]\cdot\partial_k\vec{X} - \partial_b[\partial_a\vec{X}]\cdot\partial_k\vec{X}\Big\}\psi^k + \sum_{b,k} g^{zb}g_{bk}\partial_a[\psi^k]$$

$$= \frac{1}{2}\sum_{b,k} g^{zb}\Big\{\partial_k[\partial_b\vec{X}\cdot\partial_a\vec{X}] + \partial_a[\partial_b\vec{X}\cdot\partial_k\vec{X}] - \partial_b[\partial_a\vec{X}\cdot\partial_k\vec{X}]\Big\}\psi^k$$

$$+ \sum_k \delta_k^z \partial_a \psi^k$$

$$= \sum_k \frac{1}{2}\sum_b g^{zb}\Big\{\partial_k[g_{ba}] + \partial_a[g_{bk}] - \partial_b[g_{ak}]\Big\}\psi^k + \partial_a[\psi^z].$$

With the definition of the Christoffel symbol, it follows

$$\sum_{b,k} g^{zb}\partial_b\vec{X}\cdot\partial_a[\partial_k\vec{X}\psi^k] = \partial_a[\psi^z] + \sum_k \Gamma_{ak}^z\psi^k = \nabla_a[\psi^z],$$

which was the claim. In particularly, we obtain $\sum_b g^{zb}\partial_b\vec{X}\cdot\partial_a[\partial_k\vec{X}] = \Gamma_{ak}^z$.
$\square$

**Proposition 13.**

$$\nabla_b[\psi_a] = \sum_k \partial_a\vec{X}\cdot\partial_b[\partial_k\vec{X}\psi^k]. \tag{20}$$

*Proof:* It holds

$$\nabla_b[\psi_a] = \sum_l g_{la}\nabla_b[\psi^l] = \sum_l g_{la}\sum_{u,k} g^{ul}\partial_u\vec{X}\cdot\partial_b[\partial_k\vec{X}\psi^k]$$

$$= \sum_{u,k}\delta_a^u\partial_u\vec{X}\cdot\partial_b[\partial_k\vec{X}\psi^k] = \sum_k \partial_a\vec{X}\cdot\partial_b[\partial_k\vec{X}\psi^k],$$

which was the claim. $\square$

**Lemma 14.**

$$\frac{\delta^k[F_3]}{\delta\vec{X}} = \xi^2\sum_u \nabla_u[\partial^k[\phi]\partial^u[\phi]] - \frac{\xi^2}{2}\partial^k[(\nabla^\Gamma[\phi])^2 + f(\phi)].$$

*Proof:* Using the chain rule it follows

$$\delta^t\Big[\int\{\frac{\xi^2}{2}(\nabla^\Gamma[\phi])^2 + f(\phi)\}\sqrt{g}\,d^2u\Big]$$

$$\tag{21}$$

$$= \int\{\frac{\xi^2}{2}\delta^t[(\nabla^\Gamma[\phi])^2]\sqrt{g}\,d^2u + \int\{\frac{\xi^2}{2}(\nabla^\Gamma[\phi])^2 + f(\phi)\}\delta^t[\sqrt{g}]\,d^2u.$$

20

Considering the first term of equation (21) it holds

$$\int \frac{\xi^2}{2}\delta^t[(\nabla^\Gamma[\phi])^2]\sqrt{g}\,d^2u \;=\; \frac{\xi^2}{2}\int \delta^t[\sum_{i,j} g^{ij}\partial_i[\phi]\partial_j[\phi]]\sqrt{g}\,d^2u.$$

From Kentaro [19] it follows $\delta^t[g^{ij}] = -\nabla^i[\psi^j] - \nabla^j[\psi^i]$. Thus, it follows:

$$\int \frac{\xi^2}{2}\delta^t[(\nabla^\Gamma[\phi])^2]\sqrt{g}\,d^2u \;=\; -\frac{\xi^2}{2}\sum_{i,j}\int (\nabla^i[\psi^j] + \nabla^j[\psi^i])\partial_i[\phi]\partial_j[\phi]\sqrt{g}\,d^2u$$

$$=\; -\xi^2\sum_{i,j}\int \nabla^i[\psi^j]\partial_i[\phi]\partial_j[\phi]\sqrt{g}\,d^2u$$

$$=\; -\xi^2\sum_{i,j,u}\int g^{iu}\nabla_u[\psi^j]\partial_i[\phi]\partial_j[\phi]\sqrt{g}\,d^2u.$$

Proposition 12 yields

$$\int \frac{\xi^2}{2}\delta^t[(\nabla^\Gamma[\phi])^2]\sqrt{g}\,d^2u$$

$$=\; -\xi^2\sum_{i,j,u}\int g^{iu}\Big(\sum_{b,k} g^{jb}\partial_b\vec{X}\cdot\partial_u[\partial_k\vec{X}\psi^k]\Big)\partial_i[\phi]\partial_j[\phi]\sqrt{g}\,d^2u$$

$$=\; -\xi^2\sum_{u,b,k}\int \partial^u[\phi]\partial^b[\phi]\partial_b\vec{X}\cdot\partial_u[\partial_k\vec{X}\psi^k]\sqrt{g}\,d^2u.$$

Applying Green Formula provides

$$\int \frac{\xi^2}{2}\delta^t[(\nabla^\Gamma[\phi])^2]\sqrt{g}\,d^2u$$

$$=\; \xi^2\sum_{u,b,k}\int \partial_u[\partial^u[\phi]\partial^b[\phi]\partial_b\vec{X}\sqrt{g}]\cdot\partial_k\vec{X}\psi^k\,d^2u$$

$$=\; \xi^2\sum_{u,b,k}\int \Big\{\partial_u[\partial^b[\phi]\partial_b\vec{X}]\cdot\partial_k\vec{X}\partial^u[\phi]\sqrt{g}\psi^k + \partial_u[\sqrt{g}\partial^u[\phi]]g_{bk}\partial^b[\phi]\psi^k\Big\}\,d^2u.$$

Thus, it holds

$$\int \frac{\xi^2}{2}\delta^t[(\nabla^\Gamma[\phi])^2]\sqrt{g}\,d^2u$$

$$(22)$$

$$=\; \xi^2\sum_{u,b,k}\int \Big\{\partial_u[\partial^b[\phi]\partial_b\vec{X}]\cdot\partial_k\vec{X}\partial^u[\phi]\sqrt{g}\psi^k + \partial_u[\sqrt{g}\partial^u[\phi]]g_{bk}\partial^b[\phi]\psi^k\Big\}\,d^2u.$$

Applying Proposition 12 to the first term on the right hand side of equation (22), we obtain

$$\xi^2 \sum_{u,b,k} \int \partial_u[\partial^b[\phi]\partial_b\vec{X}] \cdot \partial_k\vec{X}\partial^u[\phi]\psi^k\sqrt{g}\,d^2u$$

$$= \xi^2 \sum_{u,k} \int \nabla_u[\partial_k\phi]\partial^u[\phi]\psi^2\sqrt{g}\,d^2u$$

$$= \xi^2 \sum_{u,b,k} \int \nabla_u[\partial^b\phi]\partial^u[\phi]g_{bk}\psi^k\sqrt{g}\,d^2u$$

For the second term of (22) it holds

$$\xi^2 \sum_{u,b,k} \int \partial_u[\sqrt{g}\partial^u[\phi]]g_{bk}\partial^b[\phi]\psi^k\,d^2u$$

$$= \xi^2 \sum_{u,b,k} \int \left\{ \partial_u[\partial^u[\phi]]\sqrt{g} + \partial_u[\sqrt{g}]\partial^u[\phi] \right\}\partial^b[\phi]g_{bk}\psi^k\,d^2u.$$

Applying the chain rule on the determinant results in

$$\xi^2 \sum_{u,b,k} \int \partial_u[\partial^b[\phi]\partial_b\vec{X}] \cdot \partial_k\vec{X}\partial^u[\phi]\psi^k\sqrt{g}\,d^2u$$

$$= \xi^2 \sum_{u,b,k} \int \partial_u[\partial^u\phi]\partial^b[\phi]g_{bk}\psi^k\sqrt{g}\,d^2u$$

$$+\xi^2 \sum_{u,b,k,i,j} \int \frac{1}{2}g^{ij}\partial_u[\partial_i\vec{X} \cdot \partial_j\vec{X}]g_{bk}\psi^k\partial^b[\phi]\sqrt{g}\,d^2u$$

$$= \xi^2 \sum_{u,b,k} \int \partial_u[\partial^u\phi]\partial^b[\phi]g_{bk}\psi^k\sqrt{g}\,d^2u$$

$$+\xi^2 \sum_{u,b,k,i,j} \int g^{ij}\partial_u[\partial_i\vec{X}] \cdot \partial_j\vec{X}\partial^b[\phi]g_{bk}\psi^k\sqrt{g}\,d^2u.$$

Using the alternative definition of the Christoffel symbol $\sum_b g^{zb}\partial_b\vec{X}\cdot\partial_a[\partial_k\vec{X}] = \Gamma^z_{ak}$ (see proof Proposition 12), we obtain

$$\xi^2 \sum_{u,b,k} \int \partial_u[\partial^b[\phi]\partial_b\vec{X}] \cdot \partial_k\vec{X}\partial^u[\phi]\psi^k\sqrt{g}\,d^2u$$

$$= \xi^2 \sum_{u,b,k} \int \partial_u[\partial^u\phi]\partial^b[\phi]g_{bk}\psi^k\sqrt{g}\,d^2u$$

$$+\xi^2 \sum_{u,b,k,i} \int \Gamma^i_{ui}\partial^u[\phi]\partial^b[\phi]g_{bk}\psi^k\sqrt{g}\,d^2u.$$

Transposing the indices $(u \leftrightarrow i)$ and using $\Gamma^i_{ui} = \Gamma^i_{iu}$ and the definition of the covariant derivative leads to

$$\xi^2 \sum_{u,b,k} \int \partial_u[\partial^b[\phi]\partial_b\vec{X}]\cdot\partial_k\vec{X}\partial^u[\phi]\psi^k\sqrt{g}\,d^2u$$

$$= \xi^2 \sum_{u,b,k} \int \partial_u[\partial^u\phi]\partial^b[\phi]g_{bk}\psi^k\sqrt{g}\,d^2u$$

$$+\xi^2 \sum_{u,b,k,i} \int \Gamma^u_{ui}\partial^i[\phi]\partial^b[\phi]g_{bk}\psi^k\sqrt{g}\,d^2u$$

$$= \xi^2 \sum_{u,b,k} \left\{ \int \left(\partial_u[\partial^u[\phi]] + \sum_i \Gamma^u_{ui}\partial^i[\phi]\right)\partial^b[\phi]g_{bk}\psi^k\sqrt{g}\,d^2u\right\}$$

$$= \xi^2 \sum_{u,b,k} \int \nabla_u[\partial^u\phi]\partial^b[\phi]g_{bk}\psi^k\sqrt{g}\,d^2u.$$

Using the reformultation of the terms of equation (22) we obtain

$$\int \frac{\xi^2}{2}\partial^t[(\nabla^\Gamma[\phi])^2]\sqrt{g}\,d^2u = \xi^2 \sum_{u,b,k} \int \nabla_u[\partial^b[\phi]]\partial^u[\phi]\psi^k g_{bk}\sqrt{g}\,d^2u$$

$$+\xi^2 \sum_{u,b,k} \int \nabla_u[\partial^u[\phi]]\partial^b[\phi]g_{bk}\psi^k\sqrt{g}\,d^2u. \tag{23}$$

Furthermore, substituting in equation (21) provides

$$\delta^t\left[\int \{\frac{\xi^2}{2}(\nabla^\Gamma[\phi])^2 + f(\phi)\}\sqrt{g}\,d^2u\right]$$

$$= \xi^2 \sum_{u,b,k} \int \left\{\nabla_u[\partial^b[\phi]]\partial^u[\phi] + \nabla_u[\partial^u[\phi]]\partial^b[\phi]\right\}g_{bk}\psi^k\sqrt{g}\,d^2u$$

$$+ \int \{\frac{\xi^2}{2}(\nabla^\Gamma[\phi])^2 + f(\phi)\}\delta^t[\sqrt{g}]\,d^2u.$$

Finally, using the chain rule for covariant derivatives we obtain

$$\delta^t\Big[\int\{\frac{\xi^2}{2}(\nabla^\Gamma[\phi])^2 + f(\phi)\}\sqrt{g}\,d^2u\Big]$$

$$= \xi^2\sum_{u,b,k}\int \nabla_u[\partial^b[\phi]\partial^u[\phi]]g_{bk}\psi^k\sqrt{g}\,d^2u$$

$$-\sum_{u,k}\int \partial^u[\frac{\xi^2}{2}(\nabla^\Gamma[\phi])^2 + f(\phi)]g_{uk}\psi^k\sqrt{g}\,d^2u.$$

$\square$

**Lemma 15.**

$$\partial_t\phi(\vec{u},t) = L_\phi\Delta^\Gamma\Big[\frac{1}{2}\kappa'(\phi)(H - H_0(\phi))^2 + \kappa(\phi)(H - H_0(\phi))H_0'(\phi)$$

$$+\kappa_G(\phi)K - \xi^2\Delta^\Gamma\phi + f'(\phi)\Big]$$

*Proof:*

$$\delta^\phi[F_1] = \frac{1}{2}\int \delta^\phi[\kappa(\phi)](H - H_0(\phi))^2\,d\mu - \int \kappa(\phi)(H - H_0(\phi))\delta^\phi[H_0(\phi)]\,d\mu$$

$$= \frac{1}{2}\int \kappa'(\phi)(H - H_0(\phi))^2\psi\,d\mu + \int \kappa(\phi)(H - H_0(\phi))H_0'(\phi)\psi\,d\mu$$

thus it follows

$$\frac{\delta F_1}{\delta\phi(\vec{u})} = \frac{1}{2}\kappa'(\phi)(H - H_0(\phi))^2 - \kappa(\phi)(H - H_0(\phi))H_0'(\phi).$$

Futhermore, we have

$$\delta^\phi[F_2] = \int \delta^\phi[\kappa_G(\phi)]K\,d\mu = \int \kappa_G'(\phi)K\psi\,d\mu$$

and consequently

$$\frac{\delta[F_2]}{\delta\phi(\vec{u})} = \kappa_G'(\phi)K.$$

The third energy term reads

$$\delta^\phi[F_3] = \xi^2\int (\nabla^\Gamma[\phi])(\nabla^\Gamma[\psi])\,d\mu + \int f'(\phi)\psi\,d\mu.$$

24

Then, using Green Formula we obtain

$$\delta^{\phi}[F_3] \quad = \quad -\xi^2 \int \Delta^{\Gamma}[\phi]\psi \, d\mu + \int f'(\phi)\psi \, d\mu.$$

Finally, it holds

$$\frac{\delta F_3}{\delta \phi(\vec{u})} = -\xi^2 \Delta^{\Gamma}[\phi] + f'(\phi)$$

and we obtain

$$\begin{aligned}
\frac{\delta F}{\delta \phi(\vec{u})} \quad = \quad & \frac{1}{2}\kappa'(\phi)(H - H_0(\phi))^2 - \kappa(\phi)(H - H_0(\phi))H_0'(\phi) \\
& +\kappa_G'(\phi)K - \xi^2 \Delta^{\Gamma}[\phi] + f'(\phi).
\end{aligned}$$

$\square$

## 6. Simulations

Using the outlined macroscopic modelling approach, in this section we investigate dynamics and minimal configurations of lateral sorting and deformation of membranes. We approximate numerically the fourth order partial differential equation system (17)-(19) using a mixed formulation of bilinear finite elements, where the surface of the membrane is discretised using a quadrangular grid. Time discretisation is based on an adaptive semi-implicit Euler scheme. For all simulations shown in this section we assume constant rigidities $\kappa$ and $\kappa_G$ but different spontaneous curvatures $H_0^A$ and $H_0^B$ for the lipid and molecule species $A$ and $B$, reflecting that the two components differ in their shape. If not otherwise stated, $H_0(\phi) \equiv H_0^{lin}$ is chosen as a linear interpolation between the two values $H_0(-1) = H_0^A$ and $H_0(+1) = H_0^B$. Furthermore, we use the double well potential $f(\phi) = \frac{100}{4}(1 - \phi^2)^2$.

*Simulation of a membrane patch*

To validate the model based on the experimental data, we start from the simulations of membrane patches with a slightly curved membrane and stochastically perturbed initial conditions with the average $\langle \phi(t = 0) \rangle = \Phi^0 = -0.85$ (cf. FIG 3 B). We assume $\kappa \equiv 10^2$, $\kappa_G \equiv -10^2$, $H_0^A = -5$, $H_0^B = 5$, $\sigma = 50$, $\xi = 0.3$, $L_X = 0.0005$, $L_\phi = 0.5$, Dirichlet-zero boundary
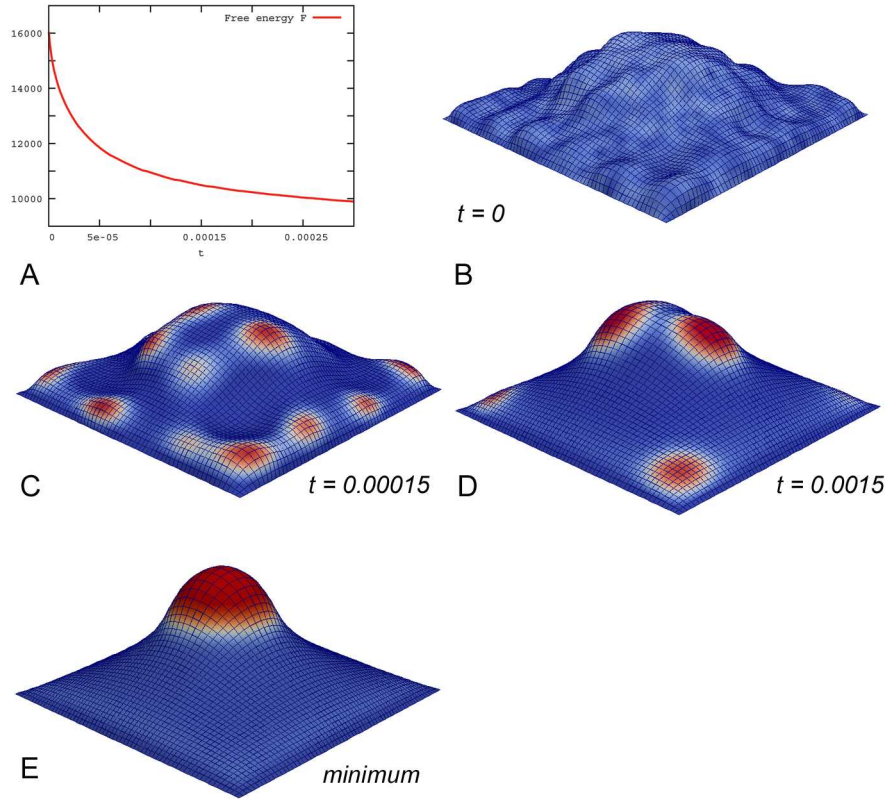
25

Figure 3: Simulation of membrane dynamics (B)-(E) reveals minimum structures (E) comparable to experiments starting from disordered initial conditions (B). (A): Corresponding energy decay. The two colours red and blue correspond to to local high concentrations of membrane species A and species B, respectively.

conditions for the membrane and natural boundary conditions for the order parameter $\phi$.

Simulations show the transition from very heterogeneous initial conditions to the single domain of one component with a budded geometry displaying the minimal configuration (cf. FIG 3 E). This shape and pattern is comparable to stable structures observed in experiments with real membranes. Plotting the energy (3) during the simulation reveals the expected decay in time (cf. FIG 3 A).
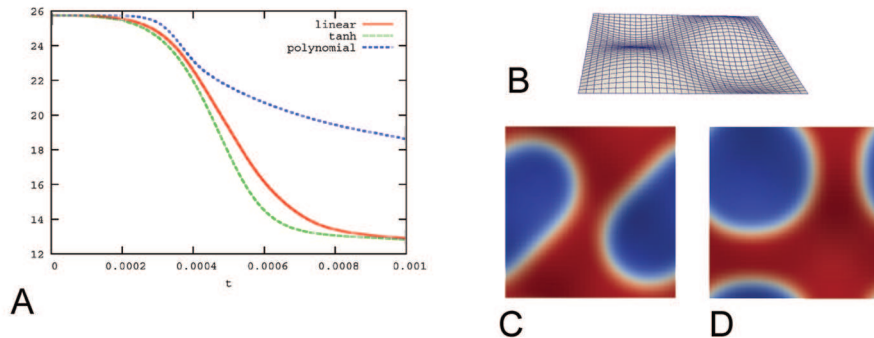
Figure 4: Lateral sorting on a fixed non-planar geometry. (A) The decay of the Cahn-Hilliard energy from instable initial conditions using different functions for the spontaneous curvature $H_0(\phi)$. (B) corresponding membrane geometry. (C)-(D) Various minimum patterns depending on the definition of $H_0(\phi)$.

*Qualitative sensitivity analysis*

To investigate the dependence of lateral dynamics and lateral minimum patterns on the choice of the (unknown) function $H_0(\phi)$, we perform simulations fixing a non planar membrane setting $X^0(U) = 0.06\sin(2\pi u_1)\sin(2\pi u_2)$ (cf. FIG 4 B) and $L_X = 0$ but allowing lateral phase separation, starting with $\langle\phi^0\rangle = \Phi^0 = 0$. Corresponding results are presented in FIG 4. We compare the impact of the three different monotonous functions $H_0^{(1)}(\phi) = a_1 + b_1\phi$, $H_0^{(2)}(\phi) = a_2 + b_2\tanh(-\phi)$ and $H_0^{(3)}(\phi) = a_3 + b_3 x^5$ on the dynamics and minimum patters of lateral sorting. Here, $a_i$ and $b_i$ are chosen so that $H_0^{(i)}(-1) = 0$ and $H_0^{(i)}(1) = -16$ holds for $i \in \{1, 2, 3\}$. Furthermore we set $\kappa \equiv 0.12$, $\kappa_G \equiv -0.12$, $\sigma = 1$, $\xi = 0.4$, $L_\phi = 1.0$ and periodic boundary conditions for the the order parameter $\phi$. We find that different choices of function $H_0(\phi)$ strongly influence the dynamics of the model as well as the minimum patterns. Depending on the choice of $H_0^{(i)}$ the Cahn-Hilliard energy decays at different moments and with different strengths of decay from the instable initial conditions, see FIG 4 A, resulting in the case of $H_0^{(3)}$ in a different minimum pattern, see FIG 4 D, compared to $H^{(1)}$ and $H^{(2)}$, see FIG 4 C.

*Quantitative sensitivity analysis*

To investigate how sensitive is the minimum geometry of the membrane to the choice of an elastic coefficient, we perform simulations with various values of $H_0^A$ but keeping $H_0^B = 0$. The corresponding results are shown in
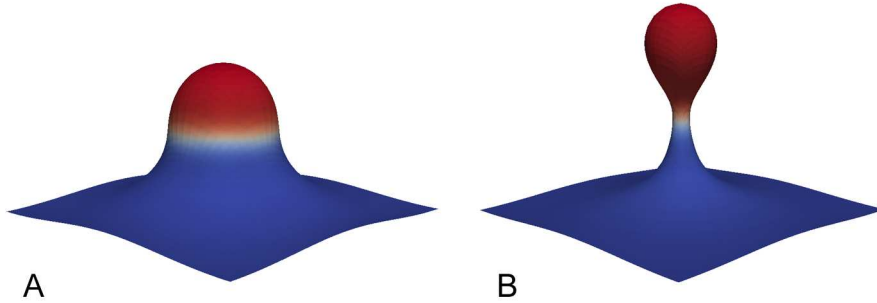
27

Figure 5: $H_0$-induced budding transition: The minimum geometry is sensitive to the choice of elastical coefficient. (A) $H_0^A = -8$, (B) $H_0^B = -8.5$.

FIG 5, with $\sigma = 1$, $\xi = 0.3$, $L_X = 0.0005$, $L_\phi = 0.05$, Dirichlet-zero boundary conditions for the x-y-axis of the membrane and natural boundary conditions for the z-axis and the order parameter $\phi$. Our simulations reveal that an increase of $H_0^A$ from zero to $H_0^A = -8$ results in a minimum shape with an increased budded geometry. However, the geometry does not correspond to the incomplete bud (cf. FIG 5 A). Interestingly, choosing $H_0^A = -8.5$ results in a complete bud. This effect has been previously described as the budding transition by [12]. This example shows that small changes in the parameter value can lead to a very different minimal geometry of the membrane.

*Discussion*

In this paper we developed a mathematical model of membrane deformation governed by the dynamics of biomolecules diffusing on the membrane surface. Using the example of the spontaneous curvature $H_0$, in showed that both, the exact value of the different components of the membrane, $H_0^A$ and $H_0^B$, and the choice of the interpolating function $H_0(\phi)$ can strikingly influence dynamics and the minimal confuiguration of shapes and lateral patterns. These findings emphasize the importance of a rigourous upscaling directly from the molecular scale of the macroscopic moduli depending on $\phi$.

## 7. Acknowledgements

## Appendix A. Notation

*General notation*

| | |
|---|---|
| $a$ | scalar |
| $\vec{a}$ | covariant vector $a_i$, e.g. $(\vec{a})_i = a_i$ |
| $\mathbf{a}$ | matrix with components $a_{ij}$, e.g. $(\mathbf{a})_{ij} = a_{ij}$ |
| $\alpha^i$ | contravariant depiction of a vector or matrix component or a derivative regarding index $i$, e.g. $\alpha^i = \sum_j g^{ij}\alpha_j$ where $(g^{ij})_{i,j}$ is the inverse of the first fundamental tensor and $\alpha \in \{a, a_j, \partial, \nabla\}$ |
| $\vec{a}\mathbf{a}$ | multiplication of a vector with a matrix from the left hand side, e.g. $(\vec{a}\mathbf{a})_i = \sum_j v_j a_{ji}$ |
| $\mathbf{a}\vec{a}$ | multiplication of a vector with a matrix from the right hand side, e.g. $(\mathbf{a}\vec{a})_i = \sum_j a_{ij} v_j$ |
| $\vec{a} \cdot \vec{b}$ | standard vector scalar product, e.g. $(\vec{a} \cdot \vec{b}) = \sum_i a_i b_i$ |
| $\mathbf{a} \cdot \mathbf{b}$ | standard matrix scalar product, e.g. $\vec{a} \cdot \vec{b} = \sum_{ij} a_{ij} b_{ij}$ |
| $\mathbf{ab}$ | standard matrix multiplication, e.g. $(\mathbf{ab})_{ik} = \sum_j a_{ij} b_{jk}$ |
| $\overline{\mathbf{a}}$ | inverse of a matrix, e.g. $(\mathbf{a}^{-1})_{ij} = (\overline{\mathbf{a}})_{ij} = \overline{a^{ij}}$ |
| $\vec{n}$ | outer unit normal |
| $\partial_i \vec{X}$ | basis vector of the tangential space, e.g. $\partial_i \vec{X} = \partial_i[\vec{X}]$ |
| $H$ | Mean curvature |
| $H_0$ | Spontaneous curvature |
| $K$ | Gaussian curvature |

*Differential and integral operators*

| | |
|---|---|
| $\int \dots ds$ | surface integral on a manifold |
| $\partial_t[\mathbf{a}]$ | partial derivative in the direction of $t$, e.g. $\partial_t[\mathbf{a}]$ |
| $\nabla_t[\mathbf{a}]$ | covariant derivative in the direction of $t$ |
| $\nabla^\Gamma[\mathbf{a}]$ | first surface gradient |
| $\nabla^\Gamma \cdot [\mathbf{a}]$ | first surface divergence |
| $\Delta^\Gamma[\mathbf{a}]$ | first surface laplacian |
| $\widehat{\nabla}^\Gamma[\mathbf{a}]$ | second surface gradient |
| $\widehat{\nabla}^\Gamma \cdot [\mathbf{a}]$ | second surface divergence |
| $\widehat{\Delta}^\Gamma[\mathbf{a}]$ | second surface laplacian |
| $\delta^\alpha[F]$ | Frecht-derivative or variation, e.g. $\delta^\alpha[F] = \frac{d}{d\epsilon}[F(\vec{X} + \vec{\psi})]\big|_{\epsilon=0}$, where $F$ is a functional on $\vec{X}$. For |

$\alpha = X$ holds $\vec{\psi} \in C^{\infty}(\Gamma, \mathbb{R}^3)$, for
$\alpha = \perp$ holds $\vec{\psi} = \psi \vec{n}$, $\psi \in C^{\infty}(\Gamma, \mathbb{R})$, for
$\alpha = k$ holds $\vec{\psi} = \partial_k \vec{X} \psi$, $\psi \in C^{\infty}(\Gamma, \mathbb{R})$;
$\vec{\psi}$ and $\psi$ are arbitrary testfunctions. It holds $\delta^t = \sum_k \delta^k$.

$\frac{\delta F}{\delta \vec{X}(\vec{u})}$   strong formulation of $\delta^{\vec{X}}[F]$ in $\vec{X}(\vec{u})$.

## Appendix B. Detailed Definitions

**Definition 1.** *First fundamental tensor*

The components of the first fundamental tensor are defined by [17]

$$g_{ij} = \partial_i \vec{X} \cdot \partial_j \vec{X}; \quad i, j = 1, ..., D,$$

where $g = \det(g_{ij})$ and $\overline{g^{ij}}$ are the component of its inverse. It holds that $\overline{g^{ij}} = g^{ij}$ (c.f. Definition 4). Furthermore $g_{ij} = g_{ji}$.

**Definition 2.** *Second fundamental tensor*

The components of the second fundamental tensor are defined by [17]

$$b_{ij} = -\partial_i \vec{X} \cdot \partial_j \vec{n}; \quad i, j = 1, ..., D,$$

where $b = \det(b_{ij})$ and $\overline{b^{ij}}$ are the component of its inverse. It holds that $b_{ij} = b_{ji}$.

**Definition 3.** *Surface measure*

The surface measure is defined by [13]

$$ds = \sqrt{g} \, d^2 u,$$

where $\int ... ds$ is the surface integral on a manifold.

**Definition 4.** *Rising- and lowering of indices*

A rised index denotes a contravariant index of a tensor component, a lowered index a covariant index. For further details we refer to Klingbeil [20]. With the help of the components of the first fundamental tensor and its inverse one can transform between covariant and contravariant indices by

$$\sum_u g_{ju} T^{ui} = T_j{}^i \text{ and } \sum_u g^{ju} T_{ui} = T_i{}^j.$$

It holds that

$$\sum_u g^{iu} g_{uj} = g_i^j = \delta_i^j,$$

where $\delta_i^j$ depicts the Kronecker symbol. For differential operators we define rised indices analogously, e.g.

$$\partial^k[T_j{}^i] = \sum_u g^{uk} \partial_u[T_j{}^i].$$

**Definition 5.** *Mean curvature and Gaussian curvature*

The mean curvature $H$ and the Gaussian curvature $K$ are defined by (c.f.[31])

$$H = \text{trace}(b_i{}^j)$$

and

$$K = \det(b_i{}^j).$$

**Definition 6.** *Christoffel symbol*

Christoffel symbols are defined by

$$\Gamma^i_{jk} = \frac{1}{2} \sum_l g^{il} \Big( \partial_k[g_{jl}] + \partial_j[g_{lk}] - \partial_l[g_{jk}] \Big),$$

where

$$\Gamma^k_{ij} = \Gamma^k_{ji},$$

(c.f. [13]). Furthermore it holds that (c.f. Prop. 12)

$$\sum_b g^{zb} \partial_b \vec{X} \cdot \partial_a[\partial_k \vec{X}] = \Gamma^z_{ak}.$$

**Definition 7.** *Covariant derivative*

The covariant derivative in the direction of $k$ of the components of a typ- $\left(\frac{P}{Q}\right)$-tensor field is depicted by $\nabla_k$ and defined as follows:

$$\nabla_k[T^{i_1...i_P}_{j_1...j_Q}] = \partial_k[T^{i_1...i_P}_{j_1...j_Q}] + \sum_l \sum_{\alpha=1}^{P} \Gamma^{i_\alpha}_{kl} T^{i_1...i_{\alpha-1}li_{\alpha+1}....i_P}_{j_1.....................j_Q} - \sum_l \sum_{\beta=1}^{Q} \Gamma^l_{kj_\beta} T^{i_1........................i_P}_{j_1...j_{\beta-1}lj_{\beta+1}.....j_Q}.$$

In particular for a scalar function $f$

$$\nabla_k[f] = \partial_k[f],$$

for vectors with contravariant indices

$$\nabla_k[T^i] = \partial_k[T^i] + \sum_l \Gamma^i_{kl} T^l$$

and for mixed matrices

$$\nabla_k[T_j{}^i] = \partial_k[T_j{}^i] + \sum_l \Gamma^i_{kl} T_j{}^l - \sum_l \Gamma^l_{kj} T_l{}^i$$

holds. In general covariant derivatives do not commutate, i.e.

$$\nabla_k \nabla_u \neq \nabla_u \nabla_k$$

and applied to the first fundamental tensor they vanish [13]

$$\nabla_k[g^{ij}] = 0 = \nabla_k[g_{ij}].$$

Since the product rule for covariant derivatives holds

$$\nabla_k[T^{b_1.....b_M}_{a_1.....a_L} U^{d_1.....d_P}_{c_1.....c_N}] = \nabla_k[T^{b_1.....b_M}_{a_1.....a_L}] U^{d_1.....d_P}_{c_1.....c_N} + T^{b_1.....b_M}_{a_1.....a_L} \nabla_k[U^{d_1.....d_P}_{c_1.....c_N}]$$

it follows that covariant derivatives and the first fundamental tensor commutate, e.g.

$$\nabla_k[g_{ij} T^{b_1.....b_M}_{a_1.....a_L}] = g_{ij} \nabla_k[T^{b_1.....b_M}_{a_1.....a_L}],$$
$$\nabla_k[g^{ij} T^{b_1.....b_M}_{a_1.....a_L}] = g^{ij} \nabla_k[T^{b_1.....b_M}_{a_1.....a_L}].$$

For further details to covariant derivatives of tensors we refer to [13, 20].

**Definition 8.** *First surface gradient*

The first surface gradient $\nabla^\Gamma$ for a function $f$ on $\Gamma$ is defined by (c.f. [38])

$$\nabla^\Gamma[f] = \sum_{i,j} g^{ij} \partial_j[f] \partial_i \vec{X}.$$

In particular it holds that $\vec{n} \cdot \nabla^\Gamma f = 0$. Furthermore the first Laplacian (or Laplace-Beltrami operator) is defined by

$$\Delta^\Gamma[f] = \frac{1}{\sqrt{g}} \sum_{i,j} \partial_i \left[ \sqrt{g} g^{ij} \partial_j[f] \right].$$

Following Rusu [30] it holds

$$H\vec{n} = -\Delta^\Gamma[\vec{X}].$$

Furthermore following Taniguchi [34] it holds that

$$\sum_k \nabla_k[\nabla^k[f]] = \sum_k \nabla_k[\partial^k[f]] = \Delta^\Gamma[f].$$

For the corresponding Greens formula and further integral theorems we refer to [40].

**Definition 9.** *Second surface gradient*

The second surface gradient $\widehat{\nabla}^\Gamma$ for a function $f$ on $\Gamma$ is defined by (c.f. [38])

$$\widehat{\nabla}^\Gamma[f] = \sum_{i,j} \overline{b^{ij}} K \partial_j[f] \partial_i \vec{X}.$$

Especially it holds that $\vec{n} \cdot \widehat{\nabla}^\Gamma[f] = 0$. Furthermore the second Laplacian is defined by

$$\widehat{\Delta}^\Gamma[f] = \frac{1}{\sqrt{g}} \sum_{i,j} \partial_i \left[ \sqrt{g} \overline{b^{ij}} K \partial_j[f] \right].$$

For the corresponding Greens formula and further integral theorems we refer to [38].

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