FIRST VARIATION OF THE GENERAL CURVATURE-DEPENDENT SURFACE ENERGY

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ABSTRACT. We consider general surface energies, which are weighted integrals over a closed surface with a weight function depending on the position, the unit normal and the total curvature of the surface. Energies of this form have applications in many areas, such as materials science, biology and image processing. Often one is interested in finding a surface that minimizes such an energy, which entails finding its first variation with respect to perturbations of the surface. We present a concise derivation of the first variation of the general surface energy using tools from shape differential calculus. We first derive a scalar strong form and next a vector weak form of the first variation. The latter reveals the variational structure of the first variation, avoids dealing explicitly with the second fundamental form, and thus can be easily discretized using parametric finite elements. Our results are valid for surfaces in any number of dimensions and unify all previous results derived for specific examples of such surface energies.

Keywords: Surface energy, gradient flow, mean curvature, Willmore functional.

1. INTRODUCTION

We consider the general weighted surface energy

$$(1) \qquad J(\Gamma) = \int_{\Gamma} \gamma(x, \nu, \kappa) \, dS,$$

for a smooth immersed orientable closed $(d-1)$ dimensional surface Γ in $\mathbb{R}^d$. The energy (1) is weighted by a smooth function $\gamma = \gamma(x, \nu, \kappa)$, which depends on the surface point x, the unit normal ν at x, and the total curvature $\kappa = \sum_{i=1}^{d-1} \kappa_i$ given by the sum of the principal curvatures κ_i at x. We derive the first variation of the energy (1) with respect to perturbations of the surface Γ: we first obtain a scalar strong form and next a vector weak form of the first variation. The latter reveals the variational structure of the first variation, avoids dealing explicitly with the second fundamental form, and thus can be easily discretized using parametric finite elements. We exploit further the vector formulation and describe gradient flows for (1) that give descent directions for minimizing (1).

Examples of the surface energy. Energies of the form (1) have attracted attention in various fields, such as materials science, biology and image processing. Setting $\gamma(x, \nu, \kappa)$ equal to specific forms in (1), we obtain many examples that are of practical interest in these fields. The following are some of these examples.

- *Anisotropic surface energy*: By restricting the weight γ in (1) to

$$\gamma = \gamma(x, \nu),$$

  we obtain the general form for anisotropic surface energy that has been the subject of extensive investigation in modeling of crystals [2, 1, 32, 41, 42, 44, 46] in materials science. This form has also found application in the problems of boundary detection [26] and 3d scene reconstruction [25] in image processing.

- *Willmore functional*: The special form of (1)

$$\gamma = \frac{1}{2}\kappa^2,$$

  models the bending energy of membranes and is significant in the study of biological vesicles [21, 23, 36]. We refer to the book [47] for more information. The Willmore functional is also employed as a regularization term in boundary detection problems in image processing [40].

- *Spontaneous curvature*: If the spatially-varying function $\kappa_0(x)$, so-called spontaneous curvature, describes the preferred total curvature of an unconstrained piece of membrane, then [21, 36] proposed the modified bending energy

$$\gamma = \frac{1}{2}\left(\kappa - \kappa_0(x)\right)^2.$$

  It can be used to model the effect of an asymmetry in the membrane [16] or that of an additional field, as in the theory of surfactants [12, 30, 33].

- *Weighted Willmore functional*: The modified form of the Willmore functional

$$\gamma = g(x)\kappa^2,$$

  has been recently proposed as a space-varying regularization term depending on the image [40]. This form is also related to the modeling of biomembranes when the concentration or composition of lipids changes spatially [7, 13, 45].

Other image processing applications that involve various effects of the curvature in the minimization of the energy (1) are in shape matching [31] and in surface restoration [14]. Also a curvature-dependent weight function $\gamma = \gamma(\kappa)$ has been used recently in [18] to achieve higher-order feature-preserving regularization in image segmentation.

Related work and main contributions. Often one is interested in a minimum or a stationary point of these energies. Therefore, the first variation of (1) with respect to deformations of the surface Γ becomes an essential step in this investigation. Although the first variation of (1) has been derived in the special cases $\gamma = \gamma(x, \nu)$ [8, 24, 32, 46, 42], $\gamma = \frac{1}{2}\kappa^2$ [47], $\gamma = g(x)\kappa^2$ [40], $\gamma = \gamma(\kappa)$ [18], a general result for (1) in any number of dimensions, to our knowledge, does not exist. We believe that derivation of the first variation of (1) in its general form is useful to scientists working on the various problems involving surface energies, such as those mentioned above, in that it makes it easier for them to experiment with different forms of $\gamma(x, \nu, \kappa)$ taylored to their applications. Still the analytical formula is only one part of the picture. Typically one would like to compute the configurations predicted by the formulas as well, and this necessitates a discretization of the analytical formula in a way suitable for numerical computations. This constitutes our motivation and leads to the following two major contributions of our work:

- *Scalar form of the first variation of energy* (1)*:* We derive, using shape differential calculus [15, 39], the following expression for the first variation of (1) with respect

to a given velocity $\vec{V}$ for a $(d-1)$ dimensional surface Γ:

$$(2) \qquad dJ(\Gamma; \vec{V}) = \int_\Gamma \left(\mathrm{div}_\Gamma[\gamma_y]_\Gamma - \Delta_\Gamma[\gamma_z] + \gamma\kappa - \gamma_z \sum \kappa_i^2 + \partial_\nu \gamma \right) \vec{V} \cdot \nu \, dS.$$

Hereafter, the weight $\gamma = \gamma(x, y, z)$ is a smooth function of its three arguments, and $\gamma_x, \gamma_y, \gamma_z$ denote its partial derivatives. Moreover, given a function $f = f(x, y, z)$, the symbol $[f]$ indicates the composite function $F(x) = f(x, \nu(x), \kappa(x))$ for $x \in \Gamma$. We refer to Sections 2 and 4 for definitions of the tangential derivatives and other details. This result not only unifies existing work on various forms of the surface energy (1), but it also provides a concise rederivation of them. As expected [15, 39], $dJ(\Gamma; \vec{V})$ in (1) depends solely on the normal velocity $V = \vec{V} \cdot \nu$, so all functions on the right-hand side are scalar. We thus call (2) scalar form. The merit of scalar form (2) is that it clearly delineates how the form of the weight function γ and the geometry of the surface Γ contribute to the first variation and related gradient descent flows. However, numerical discretization of the expression (2) is awkward, because the principal curvatures κ_i need to be approximated numerically. Thus we derive an alternate expression.

- *Vector form of the first variation of energy* (1)*:* We derive a novel weak formulation equivalent to (2), which involves vector quantities as well as first order tangential derivatives and reads as follows:

$$(3) \qquad \begin{aligned} dJ(\Gamma; \vec{\phi}) &= \int_\Gamma (I - (\nabla_\Gamma x + \nabla_\Gamma x^T)) \nabla_\Gamma \vec{\phi} : \nabla_\Gamma \vec{Z} \\ &\quad - \int_\Gamma \nu^T \nabla_\Gamma \vec{\phi} \vec{Y} + \int_\Gamma \gamma \, \mathrm{div}_\Gamma \vec{\phi} + \int_\Gamma \gamma_x \cdot \vec{\phi}, \end{aligned}$$

where $\vec{\phi}$ is the vector perturbation or test function (replacing $\vec{V}$ in (2)) and $\vec{\kappa}, \vec{Z}, \vec{Y}$ are defined by the strong relations

$$\vec{\kappa} = -\Delta_\Gamma x, \qquad \vec{Z} = \gamma_z \nu, \qquad \vec{Y} = \gamma_y,$$

which can also be imposed weakly. Expression (3) reveals the variational structure of the first variation, avoids dealing explicitly with $\sum \kappa_i^2$ which relates to the second fundamental form $\nabla_\Gamma \nu$, and is amenable to direct discretization by C^0 parametric finite element methods. The latter is a key advantage of (3) over (2). Nonetheless, we stress that the expression (3) is derived from (2) (using tensor calculus) and could not be obtained without deriving (2) first (using shape differential calculus). The result (3) is inspired by and extends the works of Rusu [35], Dziuk [19], and Bonito, Nochetto and Pauletti [10]; expression (3) reduces to that in [10] for the Willmore functional. A related expression for the case of $\gamma = \gamma(\kappa)$ was derived by Droske and Bertozzi in [18]. We discuss how to utilize (3) to create a gradient flow for (1).

We should stress that the background required to derive these results are minimal, unlike some related results in literature requiring significant knowledge of certain specialized areas, such as Riemannian geometry. In our case, it suffices that the reader be familiar with basic geometric concepts only, such as the normal and curvature of a surface. Otherwise our paper is mostly self-contained and our derivations rely on multivariable calculus and elementary tensor algebra.

Some critical issues that we do not address in this paper are the existence, uniqueness and regularity of the minimizers of the surface energy (1). The energy (1) is too general (because of the arbitrariness of the weight function $\gamma(x, \nu, \kappa)$) for us to make a comprehensive investigation of these issues. Thus, such an analysis is not in the scope of this paper. There does exist work in literature addressing

these issues in the case of Willmore functional. For these, we refer to the papers [6, 20, 27, 28, 29, 37, 38].

Outline of the paper. The rest of the paper is organized as follows. In Section 2, we introduce the basic tools from shape differential calculus; we refer to [15, 39] for details. These tools form the basis for the computations in later sections. In Section 3, we derive auxiliary results of geometric nature via the distance function to Γ. In Section 4, we use those results to prove (2) and obtain the first variation of specific forms of $\gamma(x, \nu, \kappa)$. In Section 5, we derive (3) upon changing scalar quantities in (2) with vector quantities, and examine the special case $\gamma = g(x)(\kappa - \kappa_0(x))^2$. In Section 6 we formulate gradient flows based on either (2) or (3), the latter giving a novel variational formula for the L^2-gradient flow of (1). In Section 7, we recapitulate our main results.

2. Shape Differential Calculus

We start by defining some of the notation used in the paper. Given $d \times d$ matrices A and B, we define the product $A : B = A_{ij}B_{ij}$. The symbol $\otimes$ denotes the tensor product operation for two vectors and is defined by $(v \otimes w)_{ij} = v_i w_j$. Here we use the Einstein convention, that repeated indices denote summation over those indices.

Given a scalar function $f = f(x, \nu, \kappa)$ defined properly off the $(d-1)$ dimensional surface $\Gamma \subset \mathbb{R}^d$, such that f depends on the surface point $x \in \Gamma$, the unit surface normal $\nu \in S^{d-1}$ at x and the total curvature $\kappa = \sum_{i=1}^{d-1} \kappa_i \in \mathbb{R}$ given by the sum of the principal curvatures κ_i at x, we write the derivatives of f as follows:

- The derivative $f_x (= \nabla f)$ denotes the gradient with respect to *the spatial coordinate x*, namely $f_x = (f_{x_1}, \ldots, f_{x_d})^T$.
- The derivative f_y denotes the gradient with respect to *the normal variable ν* and has the form $f_y = (f_{y_1}, \ldots, f_{y_d})^T$.
- The derivative f_z denotes the derivative with respect to *the curvature variable κ* and is a scalar function.

We define the notation for the second order derivatives by $f_{xx}(= D^2 f)$, f_{yy}, f_{zz}, $f_{xy}, \ldots, f_{zy}$, which are the matrices of the derivatives, for example,

$$(f_{xx})_{ij} = f_{x_i x_j}, \quad i = 1, \ldots, d, \ j = 1, \ldots, d.$$

The Laplacian of f is given by $\Delta f = f_{x_1 x_1} + \ldots + f_{x_d x_d}$.

In contrast we define the *total gradient* by

$$\nabla[f] = (f_{x_i} + f_{y_k} \partial_{x_i} \nu_k + f_z \partial_{x_i} \kappa)_{i=1}^d,$$

where the symbol $[f]$ indicates the composite function $F(x) = f(x, \nu(x), \kappa(x))$, and the normal ν and the curvature κ have been extended properly off the surface Γ.

It is critical to note the difference between ∇f and $\nabla[f]$ to follow the derivations in the paper without any confusion. Similarly we have $\Delta[f] = \mathrm{div}[\nabla[f]]$ acting on all components of f (compare with Δf above).

The notation for the third derivatives of f follows the same conventions. Next we introduce tangential derivatives.

2.1. **Tangential Differentiation.** Let us be given $h \in C^2(\Gamma)$ and a smooth extension $\tilde{h}$ of h, $\tilde{h} \in C^2(U)$ and $\tilde{h}|_\Gamma = h$ on Γ where U is a tubular neighborhood of Γ in $\mathbb{R}^d$ (h does not depend on ν or κ). Then the *tangential gradient* $\nabla_\Gamma h$ of h is defined as follows:

$$\nabla_\Gamma h = \left(\nabla \tilde{h} - \partial_\nu \tilde{h} \, \nu\right)|_\Gamma,$$

where ν denotes the unit normal vector to Γ. For $\vec{W} \in [C^1(\Gamma)]^d$ properly extended to a neighborhood of Γ, we define the *tangential divergence* of $\vec{W}$ by

$$\text{(4)} \qquad \text{div}_\Gamma \vec{W} = \left(\text{div}\vec{W} - \nu \cdot D\vec{W} \cdot \nu\right)|_\Gamma,$$

where $D\vec{W}$ denotes the Jacobian matrix of $\vec{W}$. Finally, the *tangential Laplacian* or *Laplace-Beltrami operator* Δ_Γ on Γ is defined as follows:

$$\text{(5)} \qquad \Delta_\Gamma h = \text{div}_\Gamma(\nabla_\Gamma h) = \left(\Delta \tilde{h} - \nu \cdot D^2 \tilde{h} \cdot \nu - \kappa \, \partial_\nu \tilde{h}\right)|_\Gamma.$$

In Section 3, we will present the formulas for the tangential derivatives of functions that depend on ν and κ.

2.2. The Velocity Method.

We consider now a hold-all domain $\mathcal{D}$, which contains the surface Γ, and a vector field $\vec{V}$ defined on $\mathcal{D}$, which is used to define the continuous sequence of perturbed surfaces $\{\Gamma_t\}_{t \geq 0}$, with $\Gamma_0 := \Gamma$. Each point $x \in \Gamma_0$ is continuously deformed by an ordinary differential equation (ODE) defined by the field $\vec{V}$. The parameter which controls the amplitude of the deformation is denoted by t.

We consider the system of autonomous ODEs

$$\text{(6)} \qquad \frac{dx}{dt} = \vec{V}(x(t)), \quad \forall t \in [0, T], \qquad x(0) = X,$$

where $X \in \Gamma_0 = \Gamma$. This defines the mapping

$$\text{(7)} \qquad x(t, \cdot) : X \in \Gamma \to x(t, X) \in \mathbb{R}^d,$$

and also the perturbed sets

$$\text{(8)} \qquad \Gamma_t = \{x(t, X) : \ X \in \Gamma_0\}.$$

We recall that the family of perturbed sets has its regularity preserved for $\vec{V}$ smooth enough [39]: if Γ_0 is of class C^r, then for any $t \in [0, T]$, Γ_t is also of class C^r.

2.3. Derivative of Shape Functionals.

Let $J(\Gamma)$ be a shape functional. The Eulerian derivative, or *shape derivative*, of the functional $J(\Gamma)$ at Γ, in the direction of the vector field $\vec{V}$ is defined as the limit

$$\text{(9)} \qquad dJ(\Gamma; \vec{V}) = \lim_{t \to 0} \frac{1}{t}\left(J(\Gamma_t) - J(\Gamma)\right).$$

Let B be a Hilbert space of perturbating vector fields. The functional $J(\Gamma)$ is said to be shape differentiable at Γ in B if the shape derivative $dJ(\Gamma; \vec{V})$ exists for all $\vec{V} \in B$ and the mapping $\vec{V} \to dJ(\Gamma; \vec{V})$ is linear and continuous on B.

We now recall a series of results from shape differential calculus in $\mathbb{R}^d$. We start with the shape derivative of surface integrals of functions that do not depend on the geometry.

Lemma 2.1 ([39, Prop. 2.50 and (2.145)]). *Let* $\psi \in W^{2,1}(\mathbb{R}^d)$ *and* Γ *be of class* C^2. *Then the functional* $J(\Gamma) = \int_\Gamma \psi \, dS$ *is shape differentiable and the derivative*

$$\text{(10)} \qquad dJ(\Gamma; \vec{V}) = \int_\Gamma \left(\nabla \psi \cdot \vec{V} + \psi \text{div}_\Gamma \vec{V}\right) dS = \int_\Gamma \left(\partial_\nu \psi + \psi \kappa\right) V \, dS,$$

depends on the normal component $V = \vec{V} \cdot \nu$ *of the velocity* $\vec{V}$.

Let us now consider more general functionals $J(\Gamma)$. We are interested in computing sensitivities for functionals of the form

$$\text{(11)} \qquad J(\Gamma) = \int_\Gamma \varphi(x, \Gamma) \, dS,$$

where the function $\varphi(\cdot, \Gamma) : \Gamma \to \mathbb{R}$ itself depends on the geometric variable Γ. To handle the computation of the sensitivities of such functionals we need to take care

of the derivative of φ with respect to Γ. For this we recall the notions of *material derivative* and *shape derivative*.

Definition 2.1 ([39, Prop.2.71])**.** *The material derivative $\dot{\varphi}(\Gamma; \vec{V})$ of φ at Γ in direction $\vec{V}$ is defined as follows*

$$(12) \qquad \dot{\varphi}(\Gamma; \vec{V}) = \lim_{t \to 0} \frac{1}{t} \big(\varphi(x(t, \cdot), \Gamma_t) - \varphi(\cdot, \Gamma_0) \big),$$

where the mapping $x(t, \cdot)$ is defined as in (7). A similar definition holds for functions $\phi(\cdot, \Omega)$ which depend on domains Ω instead of surfaces Γ.

Definition 2.2 ([39, Def. 2.85, Def 2.88])**.** *The shape derivative $\phi'(\Omega; \vec{V})$ of a domain function $\phi(\Omega) : \Omega \to \mathbb{R}$ at Ω in the direction $\vec{V}$ is defined to be*

$$(13) \qquad \phi'(\Omega; \vec{V}) = \dot{\phi}(\Omega; \vec{V}) - \nabla \phi \cdot \vec{V}.$$

Accordingly, for surface functions $\varphi(\Gamma) : \Gamma \to \mathbb{R}$, the shape derivative is defined as

$$(14) \qquad \varphi'(\Gamma; \vec{V}) = \dot{\varphi}(\Gamma; \vec{V}) - \nabla_\Gamma \varphi \cdot \vec{V}|_\Gamma.$$

Theorem 2.1 ([39, Sect. 2.31, 2.33])**.** *Let $\varphi = \phi(x, \Gamma)$ be given so that the material derivative $\dot{\varphi}(\Gamma; \vec{V})$ and the shape derivative $\varphi'(\Gamma; \vec{V})$ exist. Then, the cost functional $J(\Gamma)$ in (11) is shape differentiable and we have*

$$dJ(\Gamma; \vec{V}) = \int_\Gamma \varphi'(\Gamma; \vec{V}) dS + \int_\Gamma \kappa \varphi V dS,$$

whereas if $\varphi = \psi(\cdot, \Omega)|_\Gamma$ (ψ defined off the surface Γ, as opposed to ϕ defined only on Γ), then we obtain

$$(15) \qquad dJ(\Gamma; \vec{V}) = \int_\Gamma \psi'(\Omega; \vec{V})|_\Gamma dS + \int_\Gamma \big(\partial_\nu \psi + \kappa \psi \big) V dS,$$

where $V = \vec{V} \cdot \nu$ is the normal component of the velocity $\vec{V}$.

3. The Distance Function and Basic Geometry

In this section we employ the distance function to Γ to derive a few geometric results, which are useful later to obtain the first variation of the surface energy (1).

Lemma 3.1 ([22, Sect.3])**.** *The shape derivatives of the normal ν and the total curvature κ of a surface Γ of class C^2 with respect to velocity $\vec{V} \in C^2$ are given by*

$$(16) \qquad \nu' = \nu'(\Gamma; \vec{V}) = -\nabla_\Gamma V,$$

$$(17) \qquad \kappa' = \kappa'(\Gamma; \vec{V}) = -\Delta_\Gamma V,$$

where $V = \vec{V} \cdot \nu$ is the normal component of the velocity.

Proof. The results for ν' and κ' are due to [22]. We repeat the derivations for the sake of completeness. The main idea is to consider the signed distance function $b(x)$ to the surface Γ. It is defined as

$$(18) \qquad b(x) = \begin{cases} \text{dist}(x, \Gamma) & \text{for } x \in \mathbb{R}^d - \Omega \\ 0 & \text{for } x \in \Gamma \\ -\text{dist}(x, \Gamma) & \text{for } x \in \Omega \end{cases}$$

where

$$\text{dist}(x, \Gamma) = \inf_{y \in \Gamma} |y - x|.$$

The signed distance representation of Γ allows us to extend ν and κ smoothly in a tubular neighborhood. We use the fact that

$$(19) \qquad \nu = \nabla b(x)|_\Gamma, \quad \kappa = \Delta b(x)|_\Gamma, \quad \nabla_\Gamma \nu = D^2 b(x)|_\Gamma$$

where $\nabla_\Gamma \nu$ denotes the second fundamental form (see [15, Sect. 8.5]). Once we have the extensions, it is relatively straight-forward to compute ν' and κ'. For this, we use the result [22] that

$$\phi(\cdot, \Omega) \in H^{\frac{3}{2}+\epsilon}(\Omega), \quad \phi(\cdot, \Omega)|_\Gamma = 0,$$

implies existence of $\phi'(\Omega; \vec{V})$ in $H^{\frac{1}{2}+\epsilon}(\Omega)$ and

$$\phi'(\Omega; \vec{V})|_\Gamma = -\partial_\nu \phi\, V|_\Gamma.$$

Noting $b|_\Gamma = 0$, we get

$$b'|_\Gamma = -\partial_\nu b|_\Gamma V = -\nabla b \cdot \nabla b|_\Gamma V = -V.$$

On the other hand

$$0 = (1)' = (\nabla b \cdot \nabla b)' = 2\nabla b' \cdot \nabla b,$$

gives

$$\nu' = \nabla b'|_\Gamma = \nabla_\Gamma b'|_\Gamma + \nabla b'|_\Gamma \cdot \nu\nu = \nabla_\Gamma b'|_\Gamma = -\nabla_\Gamma V.$$

Similarly we compute $\kappa' = \Delta b'|_\Gamma = -\Delta_\Gamma V$, whose derivation we omit. $\square$

Lemma 3.2 ([22, Sect.5]). *The normal derivative of the total curvature of a surface Γ of class C^3 is given by*

(20) $$\partial_\nu \kappa = -\sum_i \kappa_i^2$$

where κ_i denote the principal curvatures of the surface. For a two-dimensional surface in 3d, this is equal to

$$\partial_\nu \kappa = -(\kappa_1^2 + \kappa_2^2) = -(\kappa^2 - 2\kappa_G)$$

where $\kappa_G = \kappa_1 \kappa_2$ denotes the Gauss curvature.

Proof. To prove this result, we will work with the signed distance representation $b(x)$ of Γ, defined by (18). We proceed as follows

$$\begin{aligned} 0 &= \Delta(1) = \Delta(\nabla b \cdot \nabla b) = \partial_{x_i}\partial_{x_i}(\partial_{x_j} b\, \partial_{x_j} b) \\ &= \partial_{x_i}\left(\partial_{x_j x_i} b\, \partial_{x_j} b + \partial_{x_j} b\, \partial_{x_j x_i} b\right) = 2\partial_{x_i}(\partial_{x_j} b\, \partial_{x_j x_i} b) \\ &= 2\left(\partial_{x_j x_i} b\, \partial_{x_j x_i} b + (\partial_{x_j}\partial_{x_i x_i} b)\, \partial_{x_j} b\right) \\ &= 2\left(D^2 b : D^2 b + \nabla(\Delta b) \cdot \nabla b\right). \end{aligned}$$

Then

$$\partial_\nu \kappa = \nabla(\Delta b) \cdot \nabla b|_\Gamma = -|D^2 b|^2|_\Gamma = -|\nabla_\Gamma \nu|^2 = -\sum_i \kappa_i^2,$$

where $|\cdot|$ denotes the Frobenius norm of a matrix. To get this result we used the fact that squared Frobenius norm of a square matrix is equal to the sum of the squares of its eigenvalues, also that the eigenvalues of the second fundamental form $\nabla_\Gamma \nu$ are the principal curvatures κ_i. $\square$

Lemma 3.3. *Let the scalar function $f = f(x, \nu, \kappa)$ and the vector function $\vec{W} = \vec{W}(x, \nu, \kappa)$ on a C^4 surface be given such that $f \in C^2$ and $\vec{W} \in C^1$. Then the explicit formulas for the (total) tangential gradient $\nabla_\Gamma[f]$, the (total) tangential divergence $\mathrm{div}_\Gamma[\vec{W}]$ and the (total) tangential Laplacian $\Delta_\Gamma[f]$ are given by the following*

(21) $$\nabla_\Gamma[f(x, \nu, \kappa)] = \nabla_\Gamma f + \nabla_\Gamma \nu f_y + f_z \nabla_\Gamma \kappa,$$

(22) $$\mathrm{div}_\Gamma[\vec{W}(x, \nu, \kappa)] = \mathrm{div}_\Gamma \vec{W} + \vec{W}_y : \nabla_\Gamma \nu + \vec{W}_z \cdot \nabla_\Gamma \kappa,$$

(23) $$\begin{aligned} \Delta_\Gamma[f(x, \nu, \kappa)] = &\ \Delta_\Gamma f + f_y \cdot (\nabla_\Gamma \kappa + \nu\Sigma\kappa_i^2) + (\nabla_\Gamma \nu f_{yy}) : \nabla_\Gamma \nu^T \\ &+ f_z \Delta_\Gamma \kappa + f_{zz}|\nabla_\Gamma \kappa|^2 + (f_{xy} + f_{yx}^T) : \nabla_\Gamma \nu \\ &+ (f_{xz} + f_{zx}) \cdot \nabla_\Gamma \kappa + (f_{yz} + f_{zy}) \cdot (\nabla_\Gamma \nu \nabla_\Gamma \kappa), \end{aligned}$$

where $\nabla_\Gamma f, \operatorname{div}_\Gamma \vec{W}, \Delta_\Gamma f$ denote the partial derivatives (see Section 2 for the distinction between the partial derivatives $\nabla_\Gamma f, \operatorname{div}_\Gamma \vec{W}, \Delta_\Gamma f$ and the total derivatives $\nabla_\Gamma[f], \operatorname{div}_\Gamma[\vec{W}], \Delta_\Gamma[f]$).

Proof. We work with smooth extensions $\tilde{f}, \tilde{W}$ in a tubular neighborhood of Γ, satisfying

$$f(x,\nu,\kappa) = \tilde{f}(x,\nabla b, \Delta b)|_\Gamma, \qquad \vec{W}(x,\nu,\kappa) = \tilde{W}(x,\nabla b, \Delta b)|_\Gamma.$$

However we will continue to refer to $\tilde{f}, \tilde{W}$ by $f, \vec{W}$ respectively for convenience.

We start by computing the first derivative of f.

$$\tag{24} \partial_{x_i}[f(x,\nabla b, \Delta b)] = f_{x_i} + f_{y_k} b_{x_k x_i} + f_z (\Delta b)_{x_i},$$

or

$$\tag{25} \nabla[f(x,\nabla b, \Delta b)] = \nabla f + D^2 b f_y + f_z \nabla \Delta b,$$

from which we can compute

$$
\begin{aligned}
\nabla[f(x,\nabla b, \Delta b)] &- \nabla[f(x,\nabla b, \Delta b)] \cdot \nabla b \nabla b \\
&= (\nabla f + D^2 b f_y + f_z \nabla \Delta b) - (\nabla f + D^2 b f_y + f_z \nabla \Delta b) \cdot \nabla b \nabla b \\
&= (\nabla f - \nabla f \cdot \nabla b \nabla b) + D^2 b f_y + f_z (\nabla \Delta b - \nabla \Delta b \cdot \nabla b \nabla b).
\end{aligned}
$$

Note that $(D^2 b f_y) \cdot \nabla b \nabla b$ vanishes as $D^2 b \nabla b = 0$. Then we restrict $\nabla[f(x,\nabla b, \Delta b)]$ to Γ and obtain

$$\nabla_\Gamma[f(x,\nu,\kappa)] = \nabla[f(x,\nabla b, \Delta b)]|_\Gamma = \nabla_\Gamma f + \nabla_\Gamma \nu f_y + f_z \nabla_\Gamma \kappa.$$

Now we differentiate (24) once more to compute the second derivative of f

$$
\begin{aligned}
\partial_{x_i x_j}[f(x,\nabla b, \Delta b)] = & f_{x_i x_j} + f_{x_i y_k} b_{x_k x_j} + f_{x_i z} b_{x_k x_k x_j} + f_{y_k x_j} b_{x_k x_i} \\
& + f_{y_k y_l} b_{x_k x_i} b_{x_l x_j} + f_{y_k z} b_{x_l x_l x_j} b_{x_k x_i} + f_{y_k} b_{x_k x_i x_j} + f_{z x_j} b_{x_k x_k x_i} \\
& + f_{z y_l} b_{x_k x_k x_i} b_{x_l x_j} + f_{zz} b_{x_k x_k x_i} b_{x_l x_l x_j} + f_z b_{x_k x_k x_i x_j},
\end{aligned}
$$

or, by reorganizing the terms,

$$
\tag{26}
\begin{aligned}
\partial_{x_i x_j}[f(x,\nabla b, \Delta b)] = & f_{x_i x_j} + f_{y_k} b_{x_k x_i x_j} + f_{y_k y_l} b_{x_k x_i} b_{x_l x_j} \\
& + f_z b_{x_k x_k x_i x_j} + f_{zz} b_{x_k x_k x_i} b_{x_l x_l x_j} \\
& + (f_{x_i y_k} b_{x_k x_j} + f_{y_k x_j} b_{x_k x_i}) \\
& + (f_{x_i z} b_{x_k x_k x_j} + f_{z x_j} b_{x_k x_k x_i}) \\
& + (f_{y_k z} b_{x_l x_l x_j} b_{x_k x_i} + f_{z y_l} b_{x_k x_k x_i} b_{x_l x_j}).
\end{aligned}
$$

From (26), we can compute the Laplacian of f,

$$
\begin{aligned}
\partial_{x_i x_i}[f(x,\nabla b, \Delta b)] = & f_{x_i x_i} + f_{y_k} b_{x_k x_i x_i} + f_{y_k y_l} b_{x_k x_i} b_{x_l x_i} \\
& + f_z b_{x_k x_k x_i x_i} + f_{zz} b_{x_k x_k x_i} b_{x_l x_l x_i} \\
& + (f_{x_i y_k} b_{x_k x_i} + f_{y_k x_i} b_{x_k x_i}) \\
& + (f_{x_i z} b_{x_k x_k x_i} + f_{z x_i} b_{x_k x_k x_i}) \\
& + (f_{y_k z} b_{x_l x_l x_i} b_{x_k x_i} + f_{z y_l} b_{x_k x_k x_i} b_{x_l x_i}),
\end{aligned}
$$

or

$$
\tag{27}
\begin{aligned}
\Delta[f(x,\nabla b, \Delta b)] = & \Delta f + f_y \cdot \nabla \Delta b + D^2 b \cdot f_{yy} \cdot D^2 b \\
& + f_z \Delta \Delta b + f_{zz} \nabla \Delta b \cdot \nabla \Delta b \\
& + (f_{xy} + f_{yx}^T) : D^2 b + (f_{xz} + f_{zx}) \cdot \nabla \Delta b \\
& + (f_{yz} + f_{zy}) \cdot (D^2 b \nabla \Delta b).
\end{aligned}
$$

We intend to compute $\Delta_\Gamma f$ by

$$q\Delta_\Gamma[f(x,\nu,\kappa)] = \big(\Delta[f(x,\nabla b, \Delta b)]$$
$$- \nabla b \cdot D^2[f(x,\nabla b, \Delta b)] \cdot \nabla b - \Delta b \nabla[f(x,\nabla b, \Delta b)] \cdot \nabla b)|_\Gamma.$$

Therefore we also need to compute the normal component of $D^2[f(x,\nabla b, \Delta b)]$ from (26)

$$b_{x_i}\partial_{x_i x_j}[f(x,\nabla b, \Delta b)]b_{x_j} = b_{x_i}f_{x_i x_j}b_{x_j} + f_{y_k}b_{x_i}b_{x_k x_i x_j}b_{x_j} + f_{y_k y_l}b_{x_i}b_{x_k x_i}b_{x_l x_j}b_{x_j}$$
$$+ f_z b_{x_i}b_{x_k x_k x_i x_j}b_{x_j} + f_{zz}b_{x_i}b_{x_k x_k x_i}b_{x_l x_l x_j}b_{x_j}$$
$$+ (b_{x_i}f_{x_i y_k}b_{x_k x_j}b_{x_j} + b_{x_i}f_{y_k x_j}b_{x_k x_i}b_{x_j})$$
$$+ (f_{x_i z}b_{x_i}b_{x_k x_k x_j}b_{x_j} + f_{z x_j}b_{x_i}b_{x_k x_k x_i}b_{x_j})$$
$$+ (f_{y_k z}b_{x_l x_l x_j}b_{x_j}b_{x_k x_i}b_{x_i} + f_{z y_l}b_{x_k x_k x_i}b_{x_i}b_{x_l x_j}b_{x_j}).$$

In this expression, the terms with $b_{x_k x_i}b_{x_i} = 0$ and $b_{x_i}b_{x_k x_i x_j}b_{x_j} = -b_{x_i x_k}b_{x_i x_j}b_{x_j}$ vanish, so that we have

$$b_{x_i}\partial_{x_i x_j}[f(x,\nabla b, \Delta b)]b_{x_j} = b_{x_i}f_{x_i x_j}b_{x_j} + f_z b_{x_i}b_{x_k x_k x_i x_j}b_{x_j} + f_{zz}b_{x_i}b_{x_k x_k x_i}b_{x_l x_l x_j}b_{x_j}$$
$$+ (f_{x_i z}b_{x_i}b_{x_k x_k x_j}b_{x_j} + f_{z x_j}b_{x_i}b_{x_k x_k x_i}b_{x_j}),$$

or

$$\nabla b \cdot D^2[f(x,\nabla b, \Delta b)] \cdot \nabla b = \nabla b D^2 f \nabla b + f_z \nabla b D^2 \Delta b \nabla b$$
$$\text{(28)} \qquad\qquad + f_{zz}\nabla b \cdot \nabla \Delta b \nabla b \cdot \nabla \Delta b$$
$$+ \nabla b \cdot f_{xz}\nabla \Delta b \cdot \nabla b + \nabla b \cdot f_{zx}\nabla \Delta b \cdot \nabla b.$$

Now we can combine (27) and (28) to write

$$\Delta[f(x,\nabla b, \Delta b)] - \nabla b \cdot D^2[f(x,\nabla b, \Delta b)] \cdot \nabla b - \Delta b \nabla[f(x,\nabla b, \Delta b)] \cdot \nabla b$$
$$= \Delta f - \nabla b D^2 f \nabla b - \Delta b f_x \cdot \nabla b$$
$$+ f_z(\Delta \Delta b - \nabla b D^2 \Delta b \nabla b - \Delta b \nabla \Delta b \cdot \nabla b)$$
$$+ f_{zz}(\nabla \Delta b \cdot \nabla \Delta b - \nabla b \cdot \nabla \Delta b \nabla b \cdot \nabla \Delta b)$$
$$+ (f_{xy} + f_{yx}^T) : D^2 b + f_y \cdot \nabla \Delta b + (D^2 b f_{yy}) : D^2 b^T$$
$$+ f_{xz} \cdot (\nabla \Delta b - \nabla \Delta b \cdot \nabla b \nabla b) + f_{zx} \cdot (\nabla \Delta b - \nabla \Delta b \cdot \nabla b \nabla b)$$
$$+ (f_{yz} + f_{zy}) \cdot (\nabla \Delta b D^2 b - \nabla \Delta b \cdot \nabla b D^2 b \nabla b),$$

the restriction of which to Γ yields

$$\Delta_\Gamma[f(x,\nu,\kappa)] = \Delta_\Gamma f + f_y \cdot (\nabla_\Gamma \kappa + \nu \Sigma \kappa_i^2) + (\nabla_\Gamma \nu f_{yy}) : \nabla_\Gamma \nu^T$$
$$+ f_z \Delta_\Gamma \kappa + f_{zz}|\nabla_\Gamma \kappa|^2 + (f_{xy} + f_{yx}^T) : \nabla_\Gamma \nu$$
$$+ (f_{xz} + f_{zx}) \cdot \nabla_\Gamma \kappa + (f_{yz} + f_{zy}) \cdot (\nabla_\Gamma \nu \nabla_\Gamma \kappa).$$

In this derivation, we have replaced $\nabla \Delta b D^2 b$ with $\nabla \Delta b D^2 b - \nabla \Delta b \cdot \nabla b D^2 b \nabla b$ (because $D^2 b \nabla b = 0$) in order to obtain the tangential derivative $\nabla_\Gamma \kappa$ in the final formula for $\Delta_\Gamma f$.

We conclude the proof by deriving the formula for the tangential divergence $\mathrm{div}_\Gamma[\vec{W}(x,\nu,\kappa)]$. For this, we compute the first derivative of the jth component of $\vec{W}(x,\nabla b, \Delta b)$

$$\partial_{x_i}[W^j(x,\nabla b, \Delta b)] = W_{x_i}^j + W_{y_k}^j b_{x_k x_i} + W_z^j (\Delta b)_{x_i},$$

also the divergence of $\vec{W}(x,\nabla b, \Delta b)$

$$\partial_{x_i}[W^i(x,\nabla b, \Delta b)] = W_{x_i}^i + W_{y_k}^i b_{x_k x_i} + W_z^i (\Delta b)_{x_i},$$

and the normal component of $D[\vec{W}(x,\nabla b, \Delta b)]$

$$b_{x_i}\partial_{x_i}[W^j(x,\nabla b, \Delta b)]b_{x_j} = b_{x_i}W_{x_i}^j b_{x_j} + b_{x_i}W_z^j (\Delta b)_{x_i}b_{x_j}.$$

Note $b_{x_k x_i} b_{x_i} = 0$. We can then write the following

$$\partial_{x_i}[W^i(x, \nabla b, \Delta b)] - b_{x_i}\partial_{x_i}[W^j(x, \nabla b, \Delta b)]b_{x_j}$$
$$= W^i_{x_i} - b_{x_i}W^j_{x_i}b_{x_j} + W^i_{y_k}b_{x_k x_i} + W^i_z((\Delta b)_{x_i} - (\Delta b)_{x_j}b_{x_j}b_{x_i}),$$

the restriction of which to Γ results in

$$\operatorname{div}_\Gamma[\vec{W}(x, \nu, \kappa)] = \operatorname{div}_\Gamma\vec{W} + \vec{W}_y : \nabla_\Gamma\nu + \vec{W}_z \cdot \nabla_\Gamma\kappa.$$

This concludes the proof. $\square$

Proposition 3.1 ([15, Sect. 8.5.5, (5.27)]). *For a function $f \in C^1(\Gamma)$ and a vector $\vec{\omega} \in C^1(\Gamma)^d$, we have the following tangential Green's formula*

$$(29) \qquad \int_\Gamma f\operatorname{div}_\Gamma\vec{\omega} + \nabla_\Gamma f \cdot \vec{\omega}dS = \int_\Gamma \kappa f\vec{\omega} \cdot \nu dS.$$

4. First Variation of the Surface Energy: Scalar Form

Now we present the main result of our paper: the first shape derivative of the general weighted surface energy

$$(30) \qquad J(\Gamma) = \int_\Gamma \gamma(x, \nu, \kappa)dS.$$

Theorem 4.1 (scalar form). *The first shape derivative of the general weighted surface energy (30) with $\gamma = \gamma(x, \nu, \kappa)$ at Γ with respect to velocity $\vec{V}$ is given by*

$$(31) \qquad dJ(\Gamma; \vec{V}) = \int_\Gamma -\gamma_y \cdot \nabla_\Gamma V - \gamma_z\Delta_\Gamma V + \left(\gamma\kappa - \gamma_z\sum\kappa_i^2 + \partial_\nu\gamma\right)VdS,$$

or

$$(32) \qquad dJ(\Gamma; \vec{V}) = \int_\Gamma \left(\operatorname{div}_\Gamma[\gamma_y]_\Gamma - \Delta_\Gamma[\gamma_z] + \gamma\kappa - \gamma_z\sum\kappa_i^2 + \partial_\nu\gamma\right)VdS,$$

where $V = \vec{V} \cdot \nu$ and $[\cdot]_\Gamma$ denotes projection to the tangent plane. Also we have

$$(33) \qquad \operatorname{div}_\Gamma[\gamma_y]_\Gamma = \operatorname{div}_\Gamma[\gamma_y] - \kappa\gamma_y \cdot \nu,$$
$$= \operatorname{div}_\Gamma\gamma_y + \gamma_{yy} : \nabla_\Gamma\nu + \gamma_{yz} \cdot \nabla_\Gamma\kappa - \kappa\gamma_y \cdot \nu,$$

and

$$(34) \qquad \Delta_\Gamma[\gamma_z] = \Delta_\Gamma\gamma_z + \gamma_{zy} \cdot (\nabla_\Gamma\kappa + \nu\Sigma\kappa_i^2) + (\nabla_\Gamma\nu\gamma_{zyy}) : \nabla_\Gamma\nu^T$$
$$+ \gamma_{zz}\Delta_\Gamma\kappa + \gamma_{zzz}|\nabla_\Gamma\kappa|^2 + (\gamma_{zxy} + \gamma_{zyx}^T) : \nabla_\Gamma\nu$$
$$+ (\gamma_{zxz} + \gamma_{zzx}) \cdot \nabla_\Gamma\kappa + (\gamma_{zyz} + \gamma_{zzy}) \cdot (\nabla_\Gamma\nu\nabla_\Gamma\kappa).$$

Proof. We use Theorem 2.1 with $\psi = \gamma(x, \nu, \kappa)$. Then we have

$$\psi'(\Gamma; \vec{V}) = \gamma_y \cdot \nu' + \gamma_z\kappa' = -\gamma_y \cdot \nabla_\Gamma V - \gamma_z\Delta_\Gamma V,$$

using (16) and (17). We also compute $\partial_\nu[\gamma(x, \nu, \kappa)]$:

$$\partial_\nu[\gamma(x, \nu, \kappa)] = \partial_\nu\gamma(x, \nu, \kappa) + \gamma_y(x, \nu, \kappa)D\nu\nu + \gamma_z(x, \nu, \kappa)\partial_\nu\kappa$$
$$= \partial_\nu\gamma(x, \nu, \kappa) - \gamma_z(x, \nu, \kappa)\sum\kappa_i^2.$$

The second line follows from Lemma 3.2 and the fact that $D\nu\nu = 0$. Then substituting ψ' and $\partial_\nu\psi$ in (15) we have

$$dJ(\Gamma; \vec{V}) = -\int_\Gamma \gamma_y \cdot \nabla_\Gamma V + \gamma_z\Delta_\Gamma VdS + \int_\Gamma \left(\partial_\nu\gamma - \gamma_z\sum\kappa_i^2 + \gamma\kappa\right)VdS.$$

Integrating the first integral by parts with tangential Green's formula (29), we obtain

$$dJ(\Gamma; \vec{V}) = \int_\Gamma \left(-\operatorname{div}_\Gamma[\gamma_y]_\Gamma - \Delta_\Gamma[\gamma_z] + \partial_\nu\gamma - \gamma_z\sum\kappa_i^2 + \gamma\kappa\right)VdS.$$

Here we have used the fact that $\mathrm{div}_\Gamma(\vec{\omega})_\Gamma = \mathrm{div}_\Gamma\vec{\omega} - \kappa\vec{\omega}\cdot\nu$. We can readily compute $\mathrm{div}_\Gamma[\gamma_z]_\Gamma$ and $\Delta_\Gamma[\gamma_z]$ using Lemma (3.3). $\square$

Remark 4.1. We can compare the results (31) and (32) with the one obtained in [18] for the case of $\gamma = \gamma(\kappa)$. The three terms in the middle of equation (32) are shared. In our case, the dependence of γ on x and ν adds the first and the last terms in the integral (32). More importantly, the simultaneous dependence on x, ν, κ results in much richer structure in the tangential derivatives $\mathrm{div}_\Gamma[\gamma_y]_\Gamma$ and $\Delta_\Gamma[\gamma_z]$ and we elucidate the structure of these terms in detail using Lemma 3.3. In contrast to [18], which requires significant knowledge of Riemannian geometry for its derivations, we make use of shape differential calculus based on signed distance functions representations. This results in a more transparent and self-contained derivation using mostly multivariable calculus, without requiring substantial background in Riemannian geometry.

Given the first shape derivative for the general weighted surface energy (30), we can easily compute the shape derivatives for the special cases mentioned in the introduction.

Anisotropic surface energy. The anisotropic surface energy is given by setting $\gamma = \gamma(x, \nu)$ in (30). Energies of this form, more specifically $\gamma = \gamma(\nu)$, have been used to model anisotropic crystalline surface energy in material science [2, 1, 32, 41, 42, 44, 46]. Such energies have also been used for boundary detection [26] and 3d scene reconstruction [24] problems in image processing. The first variation for $\gamma = \gamma(\nu)$ was given in references [2, 32, 42, 46, 44], of which the latter three made use of a phase-field representation. The result for $\gamma = \gamma(x, \nu)$ was obtained in [8] using tools from Finsler geometry and in [24] for 2d surfaces using a parametric representation. In the following we obtain the first variation in a very concise way as a corollary of Theorem 4.1.

Corollary 4.1. *The first shape derivative of the surface energy* (30) *for* $\gamma = \gamma(x, \nu)$ *(with no curvature dependence) at* Γ *with respect to velocity* $\vec{V}$ *is given by*

$$
\begin{aligned}
dJ(\Gamma; V) \quad &= \int_\Gamma (\kappa\gamma + \partial_\nu\gamma)\, V - \gamma_y \cdot \nabla_\Gamma V \, dS \\
&= \int_\Gamma (\kappa\gamma + \partial_\nu\gamma + \mathrm{div}_\Gamma[\gamma_y]_\Gamma)\, V \, dS,
\end{aligned}
\tag{35}
$$

where $V = \vec{V} \cdot \nu$ *and*

$$
\mathrm{div}_\Gamma[\gamma_y]_\Gamma = \mathrm{div}_\Gamma[\gamma_y] - \kappa\gamma_y \cdot \nu = \mathrm{div}_\Gamma\gamma_y + \gamma_{yy} : \nabla_\Gamma\nu - \kappa\gamma_y \cdot \nu.
$$

Proof. As γ does not depend on κ, we have $\gamma_z = 0$ and $\gamma_{yz} = 0$. Dropping these terms from (32) and (33) respectively, we easily obtain the results for the case $\gamma = \gamma(x, \nu)$. $\square$

Remark 4.2. In the materials science literature [2, 11, 32, 42, 46, 44], one is often interested in anisotropic surface energies of the form

$$
J(\Gamma) = \int_\Gamma \gamma(\nu) dS,
\tag{36}
$$

where $\gamma : S^{d-1} \to \mathbb{R}^+$ is a smooth function, positively homogeneous of degree 1, that is, $\gamma(\lambda y) = |\lambda|\gamma(y)$ for $\lambda \in \mathbb{R}$. Note that the homogeneity assumption implies

$$
\gamma_y(y) \cdot y = \gamma(y).
\tag{37}
$$

To compute the first variation of (36), one defines the Cahn-Hoffman vector [11]

$$
\nu_\gamma = \gamma_y(\nu)
\tag{38}
$$

and the anisotropic mean curvature

(39) $$\kappa_\gamma = \text{div}_\Gamma[\nu_\gamma] = \text{div}_\Gamma[\gamma_y].$$

Then the first variation can be shown to be

$$dJ(\Gamma; \vec{V}) = \int_\Gamma \kappa_\gamma V \, dS.$$

This gives rise to the anisotropic mean curvature motion.

Now we will rederive this result using Corollary 4.1. First note that $\partial_\nu \gamma = 0$ as γ in (36) does not depend on x, also that

(40) $$\text{div}_\Gamma[\gamma_y]_\Gamma = \text{div}_\Gamma[\gamma_y] - \kappa \gamma_y \cdot \nu = \kappa_\gamma - \kappa \gamma,$$

because of the definition (39) and the property (37). If we substitute (40) in (35),

$$dJ(\Gamma; \vec{V}) = \int_\Gamma (\kappa \gamma + \partial_\nu \gamma + \text{div}_\Gamma[\gamma_y]_\Gamma) V \, dS$$

$$= \int_\Gamma (\kappa \gamma + \kappa_\gamma - \kappa \gamma) V \, dS$$

$$= \int_\Gamma \kappa_\gamma V \, dS.$$

Thus we have obtained the same result in a few lines as a special case of Corollary (4.1).

Isotropic energy with curvature. We also consider the case with $\gamma = \gamma(x, \kappa)$, where the weight does not depend on the normal ν. This form generalizes several curvature-dependent surface energy models used in material science, biology and image processing [7, 12, 13, 14, 23, 30, 31, 33, 40, 45]. The first variation for energies of this general form is not given in the literature to the best of our knowledge. However the result follows easily from Theorem 4.1.

Corollary 4.2. *The first shape derivative of the surface energy* (30) *for* $\gamma = \gamma(x, \kappa)$ *(with no normal dependence) at* Γ *with respect to normal velocity* V *is given by*

(41) $$dJ(\Gamma; \vec{V}) = \int_\Gamma \left(-\Delta_\Gamma[\gamma_z] + \gamma \kappa - \gamma_z \sum \kappa_i^2 + \partial_\nu \gamma \right) V \, dS,$$

where $V = \vec{V} \cdot \nu$ *and*

(42) $$\Delta_\Gamma[\gamma_z] = \Delta_\Gamma \gamma_z + \gamma_{zz} \Delta_\Gamma \kappa + \gamma_{zzz} |\nabla_\Gamma \kappa|^2 + (\gamma_{zxz} + \gamma_{zzx}) \cdot \nabla_\Gamma \kappa.$$

Proof. As γ does not depend on ν, we have $\gamma_y = 0$, consequently $\text{div}_\Gamma(\gamma_y)_\Gamma = 0$ in (32). Also we have $\gamma_{zy} = 0$, $\gamma_{zxy} = \gamma_{zyx} = 0$, so that (34) simplifies to (42).   □

Weighted Willmore functional. We can use Corollary 4.2 to compute the shape derivative for a weighted Willmore functional. This functional has been used as a regularization term for boundary detection problems in image processing [40]. It is also useful for modeling of biomembranes when composition or concentration of lipids in the membrane varies spatially [7, 13, 45]. For the weighted Willmore functional, we set $\gamma = \frac{1}{2} g(x) \kappa^2$.

Corollary 4.3. *The first shape derivative of the surface energy* (30) *for* $\gamma = \frac{1}{2} g(x) \kappa^2$ *at* Γ *with respect to velocity* $\vec{V}$ *(with* $V = \vec{V} \cdot \nu$*) is given by*
(43)

$$dJ(\Gamma; \vec{V}) = \int_\Gamma \left(-g \Delta_\Gamma \kappa - 2 g_x \cdot \nabla_\Gamma \kappa + \frac{1}{2} g \kappa^3 - \Delta_\Gamma g \kappa + \frac{1}{2} \partial_\nu g \kappa^2 - g \kappa \sum \kappa_i^2 \right) V \, dS.$$

Proof. To prove this, we use the equations (41) and (42) from Corollary 4.2. We have $\gamma_x = \frac{1}{2} g_x \kappa^2$, $\gamma_z = g\kappa$, $\gamma_{zz} = g$, $\gamma_{zzz} = 0$, $\gamma_{zx} = g_x \kappa$, $\gamma_{zxz} = \gamma_{zzx} = g_x$. Consequently

$$\Delta_\Gamma [\gamma_z] = \Delta_\Gamma g\kappa + g\Delta_\Gamma \kappa + 2g_x \cdot \nabla_\Gamma \kappa,$$

in (42). Substituting this in (41), we obtain the result (43). $\qquad\square$

Willmore functional. Now we compute the shape derivative of the Willmore functional, which is obtained by setting $\gamma = \frac{1}{2}\kappa^2$ in (30). This has been used to model bending energy of membranes [23], also to impose regularity in surface restoration [14] and boundary detection [40] problems in image processing.

Corollary 4.4. *The first shape derivative of the Willmore functional, namely energy (30) with $\gamma = \frac{1}{2}\kappa^2$, at Γ with respect to velocity $\vec{V}$ (with $V = \vec{V} \cdot \nu$) is given by*

$$(44) \qquad dJ(\Gamma; \vec{V}) = \int_\Gamma \left(-\Delta_\Gamma \kappa + \frac{1}{2}\kappa^3 - \kappa \sum \kappa_i^2 \right) V\, dS.$$

For surfaces in 3d, this is equal to

$$(45) \qquad dJ(\Gamma; \vec{V}) = \int_\Gamma \left(-\Delta_\Gamma \kappa - \frac{1}{2}\kappa^3 + 2\kappa\kappa_G \right) V\, dS,$$

where $\kappa_G = \kappa_1 \kappa_2$ is the Gauss curvature.

Proof. The proof follows easily from Corollary 4.3 by setting $g = 1$. To obtain the result for surfaces in 3d, we use Lemma 3.2. $\qquad\square$

Remark 4.3. Given the shape derivative (44) for the Willmore functional $J(\Gamma) = \frac{1}{2} \int_\Gamma \kappa^2 dS$, we can easily obtain the shape derivative in the case of constrained surface area and constrained volume. Namely we would like to impose

$$(46) \qquad \text{Area}(\Gamma) = C_0, \qquad \text{Vol}(\Gamma) = C_1,$$

where $\text{Area}(\Gamma) = \int_\Gamma dS$, $\text{Vol}(\Gamma) = \int_\Omega dx$, and Ω denotes the domain enclosed by Γ. To compute the shape derivative of the Willmore functional $J(\Gamma)$ with these constraints, we consider the Lagrangian

$$\mathcal{L}(\Gamma, \lambda, p) = J(\Gamma) + \lambda \left(\text{Area}(\Gamma) - C_0 \right) + p \left(\text{Vol}(\Gamma) - C_1 \right).$$

and take its shape derivative at Γ with respect to the velocity $\vec{V}$

$$d\mathcal{L}(\Gamma; V) = dJ(\Gamma; V) + \lambda\, d\text{Area}(\Gamma; V) + p\, d\text{Vol}(\Gamma; V),$$

$$= \int_\Gamma \left(-\Delta_\Gamma \kappa + \frac{1}{2}\kappa^3 + (\lambda - \Sigma\kappa_i^2)\kappa + p \right) V\, dS.$$

This result follows from Corollary 4.4 and the shape derivatives of $\text{Area}(\Gamma)$ and $\text{Vol}(\Gamma)$

$$d\text{Area}(\Gamma; V) = \int_\Gamma \kappa V\, dS, \qquad d\text{Vol}(\Gamma; V) = \int_\Gamma V\, dS.$$

Spontaneous curvature. As our final result in this section, we consider $\gamma = \frac{1}{2}(\kappa - \kappa_0(x))^2$, where $\kappa_0(x)$ is the spontaneous curvature and is space-dependent. The spontaneous curvature describes the preferred total curvature of an unconstrained piece of membrane and was proposed in [21, 36] as part of a modified bending energy. It can be used to model the asymmetry in a membrane [16] or the net effect of an additional field, as in the theory of surfactants [12, 30, 33]. In the following we derive the shape derivative in the existence of spontaneous curvature.

Corollary 4.5. *The first shape derivative of the Willmore functional with spontaneous curvature, namely energy (30) with $\gamma = \frac{1}{2}(\kappa - \kappa_0(x))^2$ at Γ with respect to velocity $\vec{V}$ (with $V = \vec{V} \cdot \nu$) is given by*

$$dJ(\Gamma; \vec{V}) = \int_\Gamma \left(-\Delta_\Gamma(\kappa - \kappa_0) + \frac{1}{2}\kappa(\kappa - \kappa_0)^2 - (\kappa - \kappa_0)\left(\sum_{i=1}^{d-1} \kappa_i^2 + \partial_\nu \kappa_0 \right) \right) V \, dS.$$

Proof. This follows from Corollary 4.2. We first compute the derivatives of γ: $\gamma_x = (\kappa_0)_x(\kappa_0 - \kappa)$, $\gamma_z = (\kappa - \kappa_0)$, $\partial_\nu \gamma = (\kappa_0 - \kappa)\partial_\nu \kappa_0$, $\gamma_{zx} = -(\kappa_0)_x$, $\gamma_{zz} = 1$, $\gamma_{zxz} = 0$, $\gamma_{zzx} = 0$, $\gamma_{zzz} = 0$. Thus we have

$$\Delta_\Gamma[\gamma_z] = \Delta_\Gamma \gamma_z + \gamma_{zz}\Delta_\Gamma \kappa = -\Delta_\Gamma \kappa_0 + \Delta_\Gamma \kappa = \Delta_\Gamma(\kappa - \kappa_0).$$

By substituting this in (32), we obtain

$$dJ(\Gamma; \vec{V}) = \int_\Gamma \left(-\Delta_\Gamma(\kappa - \kappa_0) + \frac{1}{2}\kappa(\kappa - \kappa_0)^2 - (\kappa - \kappa_0)\sum_{i=1}^{d-1} \kappa_i^2 - (\kappa - \kappa_0)\partial_\nu \kappa_0 \right) V \, dS,$$

which upon rearrangement yields the result. $\qquad\square$

5. First variation of the Surface Energy: Vector Form

In this section we derive the weak formulation (3) for the general surface energy (1). Expression (3) entails only first tangential derivatives and does not explicitly require computing the second fundamental form $\nabla_\Gamma \nu$, and so $\sum_i \kappa_i^2 = |\nabla_\Gamma \nu|^2$. This is advantageous and will be exploited later in Section 6.

We start by rewriting the shape derivative (32) of (1) at Γ with respect to perturbation $\vec{\phi}$ (with the normal component $\phi = \vec{\phi} \cdot \nu$) upon integrating by parts:

$$(47) \qquad dJ(\Gamma; \vec{\phi}) = \int_\Gamma -\gamma_y \cdot \nabla_\Gamma \phi + \nabla_\Gamma[\gamma_z] \cdot \nabla_\Gamma \phi + \left(\gamma\kappa - \gamma_z|\nabla_\Gamma \nu|^2 + \partial_\nu \gamma \right) \phi \, dS.$$

To obtain the alternate formula (3) we replace scalar quantities in (47) by the corresponding vector quantities. The following lemma is used to convert the first term.

Lemma 5.1. *Given $f, \phi \in H^1(\Gamma)$ and the vector functions $\vec{f}, \vec{\phi}$, related to f, ϕ by $\vec{f} = f\nu$, $\phi = \vec{\phi} \cdot \nu$, we can rewrite the H^1 scalar product of f, ϕ as follows*

$$(48) \qquad \begin{aligned} \int_\Gamma \nabla_\Gamma f \cdot \nabla_\Gamma \phi &= \int_\Gamma \nabla_\Gamma \vec{f} : \nabla_\Gamma \vec{\phi} - \int_\Gamma (\nabla_\Gamma x + \nabla_\Gamma x^T)\nabla_\Gamma \vec{f} : \nabla_\Gamma \vec{\phi} \\ &\quad + \int_\Gamma f|\nabla_\Gamma \nu|^2 \phi - \int_\Gamma f\nabla_\Gamma \kappa \cdot \vec{\phi}. \end{aligned}$$

Proof. First note that $\nabla_\Gamma f$ is equal to

$$(49) \qquad \nabla_\Gamma f = \nabla_\Gamma(\vec{f} \cdot \nu) = \nabla_\Gamma \vec{f}^T \nu + \nabla_\Gamma \nu^T \vec{f} = \nabla_\Gamma \vec{f}^T \nu + f\nabla_\Gamma \nu \nu = \nabla_\Gamma \vec{f}^T \nu$$

because of the symmetry of $\nabla_\Gamma \nu$ and the fact that ∇_Γ is orthogonal to ν. Using (49), we can rewrite $\nabla_\Gamma f \cdot \nabla_\Gamma \phi$,

$$\begin{aligned} \nabla_\Gamma f \cdot \nabla_\Gamma \phi &= \nabla_\Gamma \vec{f}^T \nu \cdot \nabla_\Gamma(\vec{\phi} \cdot \nu) = \nabla_\Gamma \vec{f}^T \nu \cdot (\nabla_\Gamma \vec{\phi}^T \nu + \nabla_\Gamma \nu^T \vec{\phi}) \\ &= (\nabla_\Gamma \vec{f}^T \nu) \cdot (\nabla_\Gamma \vec{\phi}^T \nu) + (\nabla_\Gamma \vec{f}^T \nu) \cdot (\nabla_\Gamma \nu^T \vec{\phi}) \\ &= (\nu \otimes \nu)\nabla_\Gamma \vec{f} : \nabla_\Gamma \vec{\phi} + \nabla_\Gamma f \cdot (\nabla_\Gamma \nu^T \vec{\phi}). \end{aligned}$$

We integrate over the surface Γ,

$$\int_\Gamma \nabla_\Gamma f \cdot \nabla_\Gamma \phi = \int_\Gamma (\nu \otimes \nu)\nabla_\Gamma \vec{f} : \nabla_\Gamma \vec{\phi} + \int_\Gamma \nabla_\Gamma f \cdot (\nabla_\Gamma \nu^T \vec{\phi}).$$

We use the identity $I - \nu \otimes \nu = \frac{1}{2}(\nabla_\Gamma x + \nabla_\Gamma x^T)$ to rewrite the integral

$$(50) \quad \int_\Gamma \nabla_\Gamma f \cdot \nabla_\Gamma \phi = \int_\Gamma (I - \frac{1}{2}(\nabla_\Gamma x + \nabla_\Gamma x^T)) \nabla_\Gamma \vec{f} : \nabla_\Gamma \vec{\phi} + \int_\Gamma \nabla_\Gamma f \cdot (\nabla_\Gamma \nu^T \vec{\phi}).$$

Now we take the second integral on the right hand side of (50) and integrate by parts using tangential Green's formula (29)

$$(51) \quad \int_\Gamma \nabla_\Gamma f \cdot (\nabla_\Gamma \nu^T \vec{\phi}) = -\int_\Gamma f \operatorname{div}_\Gamma (\nabla_\Gamma \nu^T \vec{\phi}) = -\int_\Gamma f \nabla_\Gamma \nu : \nabla_\Gamma \vec{\phi} - \int_\Gamma f \Delta_\Gamma \nu \cdot \vec{\phi}.$$

To obtain (51), we carried out the differentiation with $\operatorname{div}_\Gamma$ and used the symmetry of $\nabla_\Gamma \nu$ and the fact that $\operatorname{div}_\Gamma \nabla_\Gamma \nu = \Delta_\Gamma \nu$. We will rewrite $f \nabla_\Gamma \nu : \nabla_\Gamma \vec{\phi}$ in (51). First we compute

$$\nabla_\Gamma \vec{f} = \nabla_\Gamma(f\nu) = f\nabla_\Gamma \nu + \nu \otimes \nabla_\Gamma f$$
$$= f\nabla_\Gamma \nu + \nu \otimes \nabla_\Gamma \vec{f}^T \nu = f\nabla_\Gamma \nu + (\nu \otimes \nu)\nabla_\Gamma \vec{f},$$

using equation (49), whence we obtain

$$f \nabla_\Gamma \nu : \nabla_\Gamma \vec{\phi} = \left(\nabla_\Gamma \vec{f} - (\nu \otimes \nu)\nabla_\Gamma \vec{f}\right) : \nabla_\Gamma \vec{\phi} = (I - \nu \otimes \nu)\nabla_\Gamma \vec{f} : \nabla_\Gamma \vec{\phi}$$
$$= \frac{1}{2}(\nabla_\Gamma x + \nabla_\Gamma x^T)\nabla_\Gamma \vec{f} : \nabla_\Gamma \vec{\phi},$$

which we subsitute in (51),

$$(52) \quad \int_\Gamma \nabla_\Gamma f \cdot \nabla_\Gamma \nu^T \vec{\phi} = -\int_\Gamma \frac{1}{2}(\nabla_\Gamma x + \nabla_\Gamma x^T)\nabla_\Gamma \vec{f} : \nabla_\Gamma \vec{\phi} - \int_\Gamma f \Delta_\Gamma \nu \cdot \vec{\phi}.$$

We substitute (52) in (50) and obtain

$$(53) \quad \int_\Gamma \nabla_\Gamma f \cdot \nabla_\Gamma \phi = \int_\Gamma \nabla_\Gamma \vec{f} : \nabla_\Gamma \vec{\phi} - \int_\Gamma (\nabla_\Gamma x + \nabla_\Gamma x^T)\nabla_\Gamma \vec{f} : \nabla_\Gamma \vec{\phi} - \int_\Gamma f \Delta_\Gamma \nu \cdot \vec{\phi}.$$

The last integral in (53) can be split into two parts by substituting $\vec{\phi} = \phi\nu + \nabla_\Gamma x \vec{\phi}$. We write

$$f \Delta_\Gamma \nu \cdot \vec{\phi} = f\phi \Delta_\Gamma \nu \cdot \nu + f \Delta_\Gamma \nu \cdot \nabla_\Gamma x \vec{\phi},$$

whence

$$(54) \quad f \Delta_\Gamma \nu \cdot \vec{\phi} = -f\phi|\nabla_\Gamma \nu|^2 + f\nabla_\Gamma \kappa \cdot \vec{\phi}.$$

We have used the fact that $\Delta_\Gamma \nu = -|\nabla_\Gamma \nu|^2 \nu + \nabla_\Gamma \kappa$ [15, Chapter 8]. Finally substituting (54) in (53) yields

$$\int_\Gamma \nabla_\Gamma f \cdot \nabla_\Gamma \phi = \int_\Gamma \nabla_\Gamma \vec{f} : \nabla_\Gamma \vec{\phi} - \int_\Gamma (\nabla_\Gamma x + \nabla_\Gamma x^T)\nabla_\Gamma \vec{f} : \nabla_\Gamma \vec{\phi}$$
$$+ \int_\Gamma f|\nabla_\Gamma \nu|^2 \phi - \int_\Gamma f\nabla_\Gamma \kappa \cdot \vec{\phi}.$$

This concludes the proof. $\qquad \square$

Now, with the following theorem, we introduce the alternate vector form of the shape derivative (47).

Theorem 5.1 (vector form). *Using a vector test function $\vec{\phi}$, with $\phi = \vec{\phi} \cdot \nu$, the shape derivative (47) can be rewritten as*

$$(55) \quad \begin{aligned} dJ(\Gamma; \vec{\phi}) &= \int_\Gamma (I - (\nabla_\Gamma x + \nabla_\Gamma x^T))\nabla_\Gamma \vec{\phi} : \nabla_\Gamma \vec{Z} \\ &\quad - \int_\Gamma \nu^T \nabla_\Gamma \vec{\phi} \vec{Y} + \int_\Gamma \gamma \operatorname{div}_\Gamma \vec{\phi} + \int_\Gamma \gamma_x \cdot \vec{\phi}, \end{aligned}$$

where $\vec{Y}(x) = \gamma_y(x, \nu(x), \vec{\kappa}(x) \cdot \nu(x))$, $\vec{Z}(x) = \gamma_z(x, \nu(x), \vec{\kappa}(x) \cdot \nu(x))\nu(x)$.

Proof. Let us define the quantities

$$\vec{Y}(x) = \gamma_y(x, \nu(x), \vec{\kappa}(x) \cdot \nu(x)), \ Z(x) := \gamma_z(x, \nu(x), \vec{\kappa}(x) \cdot \nu(x)), \ \vec{Z}(x) := Z(x)\nu(x).$$

Then the shape derivative (47) at Γ with respect to ϕ can be written as

$$(56) \ \ dJ(\Gamma; \phi) = -\int_\Gamma \vec{Y} \cdot \nabla_\Gamma \phi + \int_\Gamma \nabla_\Gamma Z \cdot \nabla_\Gamma \phi + \int_\Gamma \gamma \kappa \phi - \int_\Gamma Z |\nabla_\Gamma \nu|^2 \phi + \int_\Gamma \partial_\nu \gamma \phi.$$

We replace the second integral in (56) with the corresponding vector expression using Lemma 5.1.

$$(57)$$
$$dJ(\Gamma; \vec{\phi}) = -\int_\Gamma \vec{Y} \cdot \nabla_\Gamma \phi + \int_\Gamma (I - (\nabla_\Gamma x + \nabla_\Gamma x^T)) \nabla_\Gamma \vec{\phi} : \nabla_\Gamma \vec{Z} + \int_\Gamma Z |\nabla_\Gamma \nu|^2 \phi$$
$$- \int_\Gamma Z \nabla_\Gamma \kappa \cdot \vec{\phi} + \int_\Gamma \gamma \kappa \phi - \int_\Gamma Z |\nabla_\Gamma \nu|^2 \phi + \int_\Gamma \partial_\nu \gamma \phi.$$

Integrals with $|\nabla_\Gamma \nu|^2$ cancel out. We apply tangential Green's formula (29) to the following term

$$\int_\Gamma \kappa \gamma \phi = \int_\Gamma \kappa \gamma \vec{\phi} \cdot \nu = \int_\Gamma \gamma \mathrm{div}_\Gamma \vec{\phi} + \int_\Gamma \nabla_\Gamma[\gamma] \cdot \vec{\phi}$$
$$= \int_\Gamma \gamma \mathrm{div}_\Gamma \vec{\phi} + \int_\Gamma \nabla_\Gamma \gamma \cdot \vec{\phi} + \int_\Gamma \vec{\phi}^T \nabla_\Gamma \nu \vec{Y} + \int_\Gamma Z \nabla_\Gamma \kappa \cdot \vec{\phi},$$

(note that $\nabla_\Gamma[\gamma] = \nabla_\Gamma \gamma + \nabla_\Gamma \nu \gamma_y + \gamma_z \nabla_\Gamma \kappa$ from Lemma 3.3), and substitute the result back in (57),

$$(58)$$
$$dJ(\Gamma; \vec{\phi}) = -\int_\Gamma \vec{Y} \cdot \nabla_\Gamma \phi + \int_\Gamma (I - (\nabla_\Gamma x + \nabla_\Gamma x^T)) \nabla_\Gamma \vec{\phi} : \nabla_\Gamma \vec{Z} - \int_\Gamma Z \nabla_\Gamma \kappa \cdot \vec{\phi}$$
$$+ \int_\Gamma \gamma \mathrm{div}_\Gamma \vec{\phi} + \int_\Gamma \nabla_\Gamma \gamma \cdot \vec{\phi} + \int_\Gamma \vec{\phi}^T \nabla_\Gamma \nu \vec{Y} + \int_\Gamma Z \nabla_\Gamma \kappa \cdot \vec{\phi} + \int_\Gamma \partial_\nu \gamma \phi.$$

The integrals $\int_\Gamma Z \nabla_\Gamma \kappa \cdot \vec{\phi}$ cancel out.

We combine two of the integrals $\int_\Gamma \nabla_\Gamma \gamma \cdot \vec{\phi} + \int_\Gamma \partial_\nu \gamma \phi = \int_\Gamma \gamma_x \cdot \vec{\phi}$.

Also we combine the two integrals involving $\vec{Y}$ by

$$-\nabla_\Gamma \phi + \vec{\phi}^T \nabla_\Gamma \nu = -\nabla_\Gamma(\vec{\phi} \cdot \nu) + \vec{\phi}^T \nabla_\Gamma \nu = -\nu^T \nabla_\Gamma \vec{\phi} - \vec{\phi}^T \nabla_\Gamma \nu + \vec{\phi}^T \nabla_\Gamma \nu = -\nu^T \nabla_\Gamma \vec{\phi}.$$

Thereby we obtain

$$dJ(\Gamma; \vec{\phi}) = \int_\Gamma (I - (\nabla_\Gamma x + \nabla_\Gamma x^T)) \nabla_\Gamma \vec{\phi} : \nabla_\Gamma \vec{Z} - \int_\Gamma \nu^T \nabla_\Gamma \vec{\phi} \vec{Y} + \int_\Gamma \gamma \mathrm{div}_\Gamma \vec{\phi} + \int_\Gamma \nabla \gamma \cdot \vec{\phi},$$

which is the sought result. $\qquad\square$

Remark 5.1. Note that the shape derivative (55) contains only first order tangential derivatives and does not include the second fundamental form $\nabla_\Gamma \nu$. Therefore it can be easily discretized in space using a parametric finite element method with piecewise linear basis functions. We refer to [10], [18], [19], [35] for related work.

In the case of a quadratic energy given by $\gamma(x, \nu, \kappa) = \frac{1}{2} g(x)(\kappa - \kappa_0(x))^2$, the alternate formulation (55) of the shape derivative reduces to a linear form. We derive this in the following theorem. If $g = 1$ and $\kappa_0 = 0$, then the corresponding energy is the Willmore functional and the shape derivative simplifies further and reduces to the linear form proposed in [10]. In contrast, the scheme proposed for $\gamma = \gamma(\kappa)$ in [18] reduces to Rusu's scheme [35], which depends quadratically on the curvature vector and is reported to exhibit undesirable tangential motions close to equilibrium shapes [19, 10]. This seems to be related to geometric inconsistency, a new concept for geometric computations elaborated in [10, 9, 34]. A semi-implicit

implementation of Rusu's scheme (and that in [18]) requires initialization of the curvature vector and special care needs to be taken to ensure that the curvature vector is compatible with the surface. This is not the case for the scheme in [10] (and our scheme for quadratic functionals).

Theorem 5.2 (vector form for quadratic weight function). *For $\gamma(x, \nu, \kappa) = \frac{1}{2}g(x)$ $(\kappa - \kappa_0(x))^2$ with smooth functions g, κ_0 defined off the surface Γ, the shape derivative* (55) *of the energy* (1) *with respect to a vector-valued perturbation $\vec{\phi} \in H^1(\Gamma)$ can be rewritten as a linear functional of $\vec{\kappa}, \vec{Z}$*

$$dJ(\Gamma; \vec{\phi}) = \int_\Gamma (I - (\nabla_\Gamma x + \nabla_\Gamma x^T))\nabla_\Gamma \vec{\phi} : \nabla_\Gamma \vec{Z}$$

(59)
$$+ \frac{1}{2}\int_\Gamma \text{div}_\Gamma \vec{\kappa}\,(g\text{div}_\Gamma \vec{\phi} + \nabla g \cdot \vec{\phi}) - \int_\Gamma \vec{Z} \cdot \nu\,(\kappa_0 \text{div}_\Gamma \vec{\phi} + \nabla \kappa_0 \cdot \vec{\phi})$$

$$- \int_\Gamma \kappa_0 \nabla g \cdot \vec{\phi}\vec{\kappa} \cdot \nu + \frac{1}{2}\int_\Gamma \kappa_0^2(g\text{div}_\Gamma \vec{\phi} + \nabla g \cdot \vec{\phi}),$$

where $\vec{Z}(x) = g(x)(\kappa(x) - \kappa_0(x))\nu(x)$. If $g = 1$ in (59), *then* (59) *reduces to*

$$dJ(\Gamma; \vec{\phi}) = \int_\Gamma (I - (\nabla_\Gamma x + \nabla_\Gamma x^T))\nabla_\Gamma \vec{\phi} : \nabla_\Gamma \vec{Z} + \frac{1}{2}\int_\Gamma \text{div}_\Gamma \vec{\phi}\,\text{div}_\Gamma \vec{\kappa}$$

(60)
$$- \int_\Gamma \vec{Z} \cdot \nu(\kappa_0 \text{div}_\Gamma \vec{\phi} + \nabla \kappa_0 \cdot \vec{\phi}) + \frac{1}{2}\int_\Gamma \kappa_0^2 \text{div}_\Gamma \vec{\phi},$$

which can be further simplified provided $\kappa_0 = 0$

(61)
$$dJ(\Gamma; \vec{\phi}) = \int_\Gamma (I - (\nabla_\Gamma x + \nabla_\Gamma x^T))\nabla_\Gamma \vec{\phi} : \nabla_\Gamma \vec{\kappa} + \frac{1}{2}\int_\Gamma \text{div}_\Gamma \vec{\phi}\,\text{div}_\Gamma \vec{\kappa}.$$

Proof. We first write the explicit values of the weight function γ and its derivatives

$$\gamma = \frac{1}{2}g(\kappa - \kappa_0)^2, \qquad \gamma_x = \frac{\nabla_\Gamma g}{2}(\kappa - \kappa_0)^2 - g\nabla\kappa_0(\kappa - \kappa_0), \qquad \gamma_y = 0, \qquad \gamma_z = g(\kappa - \kappa_0).$$

We can further transform γ and γ_x

$$\gamma = \frac{g}{2}\kappa^2 - g\kappa\kappa_0 + \frac{g}{2}\kappa_0^2 = \frac{1}{2}g\text{div}_\Gamma \vec{\kappa} - \kappa_0 \vec{Z} \cdot \nu - \frac{1}{2}g\kappa_0^2,$$

$$\gamma_x = \frac{1}{2}\nabla g(\kappa^2 - 2\kappa\kappa_0 + \kappa_0^2) - g\nabla\kappa_0(\kappa - \kappa_0)$$

$$= \frac{1}{2}\nabla g\text{div}_\Gamma \vec{\kappa} - \kappa_0 \nabla g\vec{\kappa} \cdot \nu + \frac{1}{2}\nabla g\kappa_0^2 - \nabla\kappa_0 \vec{Z} \cdot \nu$$

Now we substitute γ and its derivatives in (55)

$$dJ(\Gamma; \vec{\phi}) = \int_\Gamma (I - (\nabla_\Gamma x + \nabla_\Gamma x^T))\nabla_\Gamma \vec{\phi} : \nabla_\Gamma \vec{Z}$$

$$+ \int_\Gamma \left(\frac{1}{2}g\text{div}_\Gamma \vec{\kappa} - \kappa_0 \vec{Z} \cdot \nu - \frac{1}{2}g\kappa_0^2\right)\text{div}_\Gamma \vec{\phi}$$

$$+ \int_\Gamma \left(\frac{1}{2}\nabla g\text{div}_\Gamma \vec{\kappa} - \kappa_0 \nabla g\vec{\kappa} \cdot \nu + \frac{1}{2}\nabla g\kappa_0^2 - \nabla\kappa_0 \vec{Z} \cdot \nu\right) \cdot \vec{\phi}.$$

Reorganizing the terms yields the equation (59). The results (60) and (61) follow trivially. □

6. Gradient Flows

An important application of the first variation of the general surface energy (1), is the formulation of gradient descent flows, which are instrumental to computing the minima of (1). The gradient descent flows give rise to deformations of Γ that decrease its energy which, once discretized in space and time, lead to a numerical

method. We present now one such formulation which is suitable for C^0 finite element space discretization. We refer to the articles [1, 2, 3, 4, 43] for more information on gradient flows.

We start by introducing a scalar product $b(\cdot, \cdot)$ on Γ, which induces the Hilbert space $H(\Gamma)$. Then we solve the following equation

$$(62) \qquad \vec{V} \in H(\Gamma): \qquad b(\vec{V}, \vec{\phi}) = -dJ(\Gamma; \vec{\phi}), \quad \forall \vec{\phi} \in H(\Gamma).$$

If $\| \cdot \|_{H(\Gamma)}$ is the norm induced by $b(\cdot, \cdot)$, then it turns out that the velocity $\vec{V}$ computed this way decreases the energy provided $\vec{V} \neq 0$

$$dJ(\Gamma; \vec{V}) = -b(\vec{V}, \vec{V}) = -\|\vec{V}\|_{H(\Gamma)}^2 < 0.$$

The choice of b depends on the problem at hand. A natural choice is the $L^2(\Gamma)$ scalar product $b(\vec{V}, \vec{\phi}) = \int_\Gamma \vec{V} \cdot \vec{\phi}$. Other scalar products, such as H^1 and H^{-1}, are possible and have been illustrated in [17]. The L^2 scalar product, in conjunction with the first variation (2), gives

$$\int_\Gamma \vec{V} \cdot \vec{\phi} = - \int_\Gamma \left(\mathrm{div}_\Gamma[\gamma_y]_\Gamma - \Delta_\Gamma[\gamma_z] + \gamma \kappa - \gamma_z |\nabla_\Gamma \nu|^2 + \partial_\nu \gamma \right) \vec{\phi} \cdot \nu, \quad \forall \vec{\phi} \in L^2(\Gamma),$$

or equivalently the *descent direction*

$$\vec{V} = - \left(\mathrm{div}_\Gamma[\gamma_y]_\Gamma - \Delta_\Gamma[\gamma_z] + \gamma \kappa - \gamma_z |\nabla_\Gamma \nu|^2 + \partial_\nu \gamma \right) \nu.$$

Space discretization of this relation via C^0 finite element methods yields discrete surfaces with discontinuous normals, which makes the notion of second fundamental form $\nabla_\Gamma \nu$ problematic. A fully discrete scheme, which reconstructs a Lipschitz normal ν by local averaging and uses a semi-implicit time discretization, has been proposed in [5].

In contrast, we could resort to (3) for the surface energy (1). Then the weak formulation for the L^2 gradient flow would be given by

$$(63) \qquad \begin{aligned} \int_\Gamma \vec{V} \cdot \vec{\phi} &= \int_\Gamma (I - (\nabla_\Gamma x + \nabla_\Gamma x^T)) \nabla_\Gamma \vec{\phi} : \nabla_\Gamma \vec{Z} \\ &\quad - \int_\Gamma \nu^T \nabla_\Gamma \vec{\phi} \vec{Y} + \int_\Gamma \gamma \, \mathrm{div}_\Gamma \vec{\phi} + \int_\Gamma \gamma_x \cdot \vec{\phi}, \end{aligned}$$

and those for total curvature vector $\vec{\kappa}$ and auxiliary vector variables are $\vec{Y}, \vec{Z}$

$$\int_\Gamma \vec{\kappa} \cdot \vec{\phi} = \int_\Gamma \nabla_\Gamma x : \nabla_\Gamma \vec{\phi}, \qquad \int_\Gamma \vec{Y} \cdot \vec{\phi} = \int_\Gamma \gamma_y \cdot \vec{\phi}, \qquad \int_\Gamma \vec{Z} \cdot \vec{\phi} = \int_\Gamma \gamma_z \vec{\phi} \cdot \nu.$$

Equation (63) is advantageous, because it does not require computing the derivatives of the normal ν.

If we have a quadratic weight function $\gamma = \frac{1}{2} g(\kappa - \kappa_0)^2$, then the weak formulation (63) reduces to an expression that is linear in $\vec{\kappa}, \vec{Z}$ with no cross terms

$$(64) \qquad \begin{aligned} \int_\Gamma \vec{V} \cdot \vec{\phi} &= \int_\Gamma (I - (\nabla_\Gamma x + \nabla_\Gamma x^T)) \nabla_\Gamma \vec{\phi} : \nabla_\Gamma \vec{Z} \\ &\quad + \frac{1}{2} \int_\Gamma \mathrm{div}_\Gamma \vec{\kappa} \, (g \mathrm{div}_\Gamma \vec{\phi} + \nabla g \cdot \vec{\phi}) - \int_\Gamma \vec{Z} \cdot \nu \, (\kappa_0 \mathrm{div}_\Gamma \vec{\phi} + \nabla \kappa_0 \cdot \vec{\phi}) \\ &\quad - \int_\Gamma \kappa_0 \nabla g \cdot \vec{\phi} \vec{\kappa} \cdot \nu + \frac{1}{2} \int_\Gamma \kappa_0^2 (g \mathrm{div}_\Gamma \vec{\phi} + \nabla g \cdot \vec{\phi}). \end{aligned}$$

For the Willmore weight $\gamma = \frac{1}{2} \kappa^2$, we obtain the even simpler system

$$(65) \qquad \begin{aligned} \int_\Gamma \vec{V} \cdot \vec{\phi} &= - \int_\Gamma (I - (\nabla_\Gamma x + \nabla_\Gamma x^T)) \nabla_\Gamma \vec{\phi} : \nabla_\Gamma \vec{\kappa} + \tfrac{1}{2} \int_\Gamma \mathrm{div}_\Gamma \vec{\phi} \, \mathrm{div}_\Gamma \vec{\kappa}, \\[4pt] \int_\Gamma \vec{\kappa} \cdot \vec{\phi} &= \int_\Gamma \nabla_\Gamma x : \nabla_\Gamma \vec{\phi}, \end{aligned}$$

which was introduced by Bonito, Nochetto and Pauletti in [10] and was used to compute evolution of biomembranes. We also mention the related schemes [18, 19, 35].

7. Summary of the Main Results

In this paper, we consider the general surface energy (1), which is in the form of a surface integral with anisotropic curvature-dependent weight function $\gamma = \gamma(x, \nu, \kappa)$. This energy is used as a model in many different areas, such as material science, biology and image processing (see the introduction § 1 for examples).

A critical need in practice is the characterization of minima of (1), as well as the development of numerical methods for their computation. For this purpose, we determine the first variation of (1) with respect to deformations of Γ given by velocity fields $\vec{V}$:

$$(66) \quad dJ(\Gamma; \vec{V}) = \int_\Gamma \left(\operatorname{div}_\Gamma[\gamma_y]_\Gamma - \Delta_\Gamma[\gamma_z] + \gamma\kappa - \gamma_z |\nabla_\Gamma \nu|^2 \int_\Gamma \partial_\nu \gamma \phi + \partial_\nu \gamma \right) \vec{V} \cdot \nu \, dS.$$

We refer to Sections 2 and 4 for definitions of the tangential derivatives and other details. This is the first contribution of our paper.

Our second contribution is the following vector formulation equivalent to (66)

$$(67) \quad \begin{aligned} dJ(\Gamma; \vec{\phi}) &= \int_\Gamma (I - (\nabla_\Gamma x + \nabla_\Gamma x^T)) \nabla_\Gamma \vec{\phi} : \nabla_\Gamma \vec{Z} \\ &\quad - \int_\Gamma \nu^T \nabla_\Gamma \vec{\phi} \vec{Y} + \int_\Gamma \gamma \operatorname{div}_\Gamma \vec{\phi} + \int_\Gamma \gamma_x \cdot \vec{\phi}, \end{aligned}$$

where $\vec{\phi}$ is the vector perturbation or test function and $\vec{\kappa}, \vec{Z}, \vec{Y}$ satisfy the relations

$$\vec{\kappa} = -\Delta_\Gamma x, \qquad \vec{Z} = \gamma_z \nu, \qquad \vec{Y} = \gamma_y,$$

which can also be imposed weakly. The main advantage of (67) over (66) is that it does not include the second fundamental form and is thus suitable for direct spatial discretization by C^0 parametric finite elements. This is instrumental to implement a numerical method computing gradient descent flows for the energy (1). For example, in the case of L^2 gradient flows given by $\int_\Gamma \vec{V} \cdot \vec{\phi} = -dJ(\Gamma, \vec{\phi})$, a semi-implicit time discretization of this equation would linearize the system, and thus require only linear solves at each time step. The full expression for the L^2 gradient flow is given by (63). If we further assume that the weight function γ is isotropic and quadratic in κ, namely $\gamma = \frac{1}{2}g(x)(\kappa - \kappa_0(x))^2$ for some scalar function $g(x)$, then the equation (63) reduces to (64), which is linear in both $\vec{\kappa}$ and $\vec{Z}$ with no cross terms. Finally, for $g(x) = 1, \kappa_0(x) = 0$, i.e. $\gamma = \frac{1}{2}\kappa^2$, the case of Willmore energy, equation (63) further simplifies to (65), which coincides with that obtained by Bonito, Nochetto and Pauletti [10].

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