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Shape Calculus for Shape Energies in Image Processing

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Abstract

Many image processing problems are naturally expressed as energy minimization or shape optimization problems, in which the free variable is a shape, such as a curve in 2d or a surface in 3d. Examples are image segmentation, multiview stereo reconstruction, geometric interpolation from data point clouds. To obtain the solution of such a problem, one usually resorts to an iterative approach, a gradient descent algorithm, which updates a candidate shape gradually deforming it into the optimal shape. Computing the gradient descent updates requires the knowledge of the first variation of the shape energy, or rather the first shape derivative. In addition to the first shape derivative, one can also utilize the second shape derivative and develop a Newton-type method with faster convergence. Unfortunately, the knowledge of shape derivatives for shape energies in image processing is patchy. The second shape derivatives are known for only two of the energies in the image processing literature and many results for the first shape derivative are limiting, in the sense that they are either for curves on planes, or developed for a specific representation of the shape or for a very specific functional form in the shape energy. In this work, these limitations are overcome and the first and second shape derivatives are computed for large classes of shape energies that are representative of the energies found in image processing. Many of the formulas we obtain are new and some generalize previous existing results. These results are valid for general surfaces in any number of dimensions. This work is intended to serve as a cookbook for researchers who deal with shape energies for various applications in image processing and need to develop algorithms to compute the shapes minimizing these energies.

1 Introduction

Many image processing tasks are expressed as energy minimization problems in which the free variable is a shape, such as a curve in 2d or a surface in 3d, because the shape is a geometric representation for the object or the region of interest in the data. Examples of such tasks are image segmentation [5, 13, 16, 15], surface regularization [18, 50], geometric interpolation of data point clouds [62] and multiview stereo reconstruction [28, 34, 37]. In these problems, one defines an appropriate shape energy $J(\Gamma)$ that depends on the shape Γ, and the shape energy is designed such that its minimum corresponds to a solution of the image processing problem at hand. For example, as an image segmentation formulation (to locate distinct objects, regions or their boundaries in images), one can choose to use the Geodesic Active Contour model [13, 14], which is

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a weighted integral over candidate curves or surfaces Γ, as the shape energy,

$$J(\Gamma) = \int_\Gamma g(x) dS, \tag{1}$$

where $g(x)$ is an image-based weight function, or one can choose the following variant of Mumford-Shah functional [15]

$$J(\Gamma) = \frac{1}{2} \sum_{i=1,2} \int_{\Omega_i} (I(x) - c_i)^2 dx + \nu \int_\Gamma dS, \qquad c_i = \frac{1}{|\Omega_i|} \int_{\Omega_i} I(x) dx, \tag{2}$$

where $I(x)$ is the image function and Ω_1, Ω_2 are the inside and outside regions of the curve Γ. Then the curve minimizing the energy is a valid solution of segmentation problem.

The energy minimization formulation comes naturally for many image processing problems, because it gives a straight-forward way to penalize unwanted configurations of the shapes considered and to encourage the good configurations, especially when the problem has a data-fitting component or when the problem is hard to formulate in a direct manner. For example, the energy (2) consists of a data term, which is minimized for curves that separate the image into regions of constant intensity. It also has a geometric penalty term, a length integral, which favors shorter curves over longer curves and acts as a regularizer in noisy images.

In order to find the minimizer Γ^* of a given shape energy, one needs to implement an energy minimization or shape optimization algorithm. The shape optimization algorithms usually work iteratively; they start from an initial shape Γ_0 and deform the shape through several iterations with a velocity field $\vec{V}$ until a minimum of the energy is achieved. Thus, a crucial step to solve the minimization problem is the computation of the gradient descent velocities $\vec{V}$ at each iteration, namely deformation velocities that decrease the energy of the shape Γ. This requires understanding how a deformation of Γ induced by a given velocity $\vec{V}$ changes the energy $J(\Gamma)$. An analytical tool that gives us this information is the shape derivative $dJ(\Gamma; \vec{V})$ [22, 31, 52, 53]. It tells us the change in the energy $J(\Gamma)$ of the shape Γ when Γ is deformed by $\vec{V}$ (see Section 3 for a rigorous definition of the shape derivative). If a given velocity $\vec{V}$ satisfies $dJ(\Gamma; \vec{V}) < 0$, then $\vec{V}$ is a gradient descent velocity. If the shape derivative is zero for all $\vec{V}$, then the shape Γ is a stationary point, possibly a minimal shape. The shape derivative concept enables us to compute gradient descent velocities for a given shape Γ and its energy $J(\Gamma)$ in a straight-forward manner. We review this briefly in Section 5. The gradient descent velocity can be computed in other ways too, but we advocate shape differentiation in this paper as it is a very powerful technique and is widely applicable.

We can differentiate the energy more than once, and obtain the second shape derivative $d^2 J(\Gamma; \vec{V}, \vec{W})$, which is defined with respect to two perturbation velocities $\vec{V}, \vec{W}$ [22, 42, 53]. The second shape derivative gives us second order shape sensitivity information. It can be used to perform stability analysis of a given stationary point [20] and it can tell us whether or not the stationary point is a minimum. Moreover it can be used to design fast Newton-type minimization schemes, which converge in fewer iterations. Only a few such schemes exist in image processing [6, 23, 32, 33] (more examples can be found in other areas of science and engineering [12, 27, 29, 43]). The existence of only a few schemes is due to the fact that the *explicit* formulas for the second shape derivatives of most energies in image processing are not known.

Contributions. In this paper, we use the shape differentiation methodology to derive the shape derivatives of large classes of shape energies. We aim our results to be as comprehensive as possible, so that this work will serve as a cookbook for the researchers who need to analyze shape energies and design algorithms that solve image processing problems using shape energies. In Section 2, we list the classes of shape energies that we consider and give examples of how they are used in the literature. The first shape derivatives or other derivatives of equivalent use have been derived for some of these energies. In some cases, these previous results are specific to a certain dimension, for example, curves in 2d or surfaces in 3d. In some cases, the results are specific to a certain geometric representation, such as a parametric surface. In most cases, the *explicit* formulas for the second shape derivative are not known. In fact, to our knowledge, the second shape derivatives have been computed for only two energies [32, 33] in image processing (explicit formulas for some energies relevant to other application areas can be found in literature [12, 27, 29, 43])). In this work, we derive the first shape derivatives for all the classes of energies that we list in Section 2 and the second shape derivatives except for two of the energies (see Tables 1, 2 for a summary of the results, the new formulas derived that are previously unknown are denoted by ($\star$)). These new formulas are the main contribution of this paper. They are derived and laid out explicitly and are intended to serve researchers in image processing. These results are valid for hypersurfaces in any number dimensions and do not depend on the representation of the shape (parametric, level set or other). The only limitation of these results is that in their basic form, they are valid for closed surfaces or surfaces whose boundaries are on the image domain boundary. Other types of surfaces, such as open surfaces with boundaries inside the image domain or surfaces with junctions, require special consideration that we do not include in this paper.

The emphasis in this paper is on deriving the shape derivatives (assuming as much smoothness as needed of the shapes or the functions). Naturally, the existence of these shape derivative rely on certain differentiability requirements, and these may not be easy to satisfy in some practical situations. This will depend on the application and needs to be addressed on a case-by-case basis; therefore, such questions are not addressed in this paper. Moreover, existence of the shape derivatives does not imply the existence of the minimal shapes. This is a critical question that one must ask before using the shape derivatives to compute the minimum of the shape energies. For more information on existence and uniqueness of minimal shapes in shape optimization, we refer the reader to [10, 9].

Outline. We start with Section 2 explaining the major classes of shape energies used in image processing. Our goal is to compute the shape derivatives for these energies. In Section 3, we introduce some basic differential geometry and some results and definitions from shape differential calculus. In Section 4, we use these results to compute the first and second shape derivatives of the energies introduced in Section 2. These shape derivatives are the main contribution of the paper and are summarized in Tables 1, 2. We conclude the paper with Section 5, where we briefly review how the shape derivatives can be used to compute gradient descent velocities for given shapes and energies.

2 Shape Energies in Image Processing

The search for geometric entities or geometric descriptions for objects based on given images is a main theme in image processing. Thus, researchers in this field are constantly devising new shape energies to address their problems, making it a very fertile field for applications of shape optimization. We find it useful to consider the numerous shape energies in image processing in four main classes: minimal surface energies, energies with integrals, higher-order energies, energies with PDEs (partial differential equations). Hybrids from these classes and exceptions are possible. These shape energy classes are explained below with examples from the literature. They are the starting point for the shape derivative calculations in Section 4.

Minimal surface energies: The first example of a shape energy in image processing was the Geodesic Active Contour Model proposed for image segmentation by Caselles, Kimmel and Sapiro in [13, 14] [1]. The main idea of their work was to try to fit a curve or a surface to the edges of an object in the image. For this, they used an edge indicator function $g(x)$ such that $g \approx 0$ on edges and $g \approx 1$ elsewhere and tried to compute a surface minimizing the following energy

$$J(\Gamma) = \int_\Gamma g(x) dS. \tag{3}$$

One can sometimes add an area or volume integral $\int_\Omega g(x)dx$ to (3) to speed up the computations and to facilitate detection of concavities. Minimal surfaces computed from the energy (3) make very satisfactory segmentations as they give continuous and smooth representations of the boundaries of objects or regions in the given images. Thus, the model (3) is very popular and is widely implemented. The implementation is based on the first shape derivative or the first variation of the energy. Only recently the second shape derivative for (3) was computed by Hintermüller and Ring [32] and was used to devise a second order minimization method resulting in faster convergence.

The energy (3) is isotropic, i.e. it does not depend on the orientation or the normal of surface. In [36], Kimmel and Bruckstein proposed an anisotropic energy that fits the general form

$$J(\Gamma) = \int_\Gamma g(x, n) dS. \tag{4}$$

By setting $g = \langle \nabla I, n \rangle$, they aimed to better align solution curves with object boundaries in images and were able to attain improved segmentations. Before [36], the energy (4) had been used by Faugeras and Keriven for multiview stereo reconstruction [28] (later by Jin et al. in [34] and by Kolev et al. [37]). The first shape derivative of (4) for general n-dimensional surfaces has been known in the literature for geometric flows [7, 21]. We derive the second shape derivative in this paper.

The key feature of the energy (4) is the dependence on the geometry through the normal of the surface. The dependence may be through other geometric properties of the surface as well, such as the mean curvature κ

$$J(\Gamma) = \int_\Gamma g(x, \kappa) dS. \tag{5}$$

The integral (5) is usually used as part of a more involved energy, to impose higher regularity of the surface. Examples are the Willmore functional with $g = \frac{1}{2}\kappa^2$ [18, 61] or $g = \kappa^p$ in [50]. Sundaramoorthi et al. noted in [58] that $g = \frac{1}{2}w(x)\kappa^2$ with an image-based weight $w(x)$ yielded better regularizations for image segmentation. Another more general functional form of $g(\kappa)$ was used in [26] to implement a corner-preserving regularization energy. The first shape derivative for (5) and for the energy with the more general geometric weight $g = g(x, n, \kappa)$ was derived in [25] by Doğan and Nochetto.

Energies with integrals: If one views a surface as the boundary separating different regions in the image from each other (in order to identify distinct regions), a logical approach to designing the shape energy is to incorporate terms that compare the properties of the regions across the boundary and try to find surfaces maximizing the difference between the regions. The characteristics of each region can be quantified by computing the statistics of the image features in the region [19]. The statistics

[1] Although the Snakes model of Kass, Witkin, Terzopoulos [35] can also be viewed as a first example, it is not truly a shape energy, because the value of the energy depends on the parametrization of the curve and it can be different for different parametrizations even though the shape is the same.

computations can often be expressed as various integrals over the regions. This results in shape energies with weight functions that depend on integrals over the regions. An example is the following energy (6) proposed by Chan and Vese in [15]. It aims to find a partitioning of the image domain into a foreground region Ω_1 and a background region Ω_2 (inside and outside Γ respectively), each with distinct averages c_1, c_2 of the image intensity $I(x)$ respectively.

$$J(\Gamma) = \frac{1}{2}\sum_{i=1,2}\int_{\Omega_i}(I(x)-c_i)^2 dx + \nu\int_\Gamma dS, \qquad c_i = \frac{1}{|\Omega_i|}\int_{\Omega_i} I(x)dx. \tag{6}$$

More general approaches to incorporating statistics into the shape optimization formulation are described in [19, 46]. To develop a more general statistical formulation, one can consider a Bayesian interpretation of the estimation problem and try to maximize the a posteriori probability $p(\{\Omega_1,\Omega_2\}|I)$, namely the likelihood of having a certain partitioning $\{\Omega_1,\Omega_2\}$ given the image I (multiple phases or regions $\{\Omega_i\}_{i=1}^m$ are possible, but not considered in this paper to simplify the presentation). We can write $p(\{\Omega_1,\Omega_2\}|I)$ as

$$p(\{\Omega_1,\Omega_2\}|I) \propto p(I|\{\Omega_1,\Omega_2\})\; p(\{\Omega_1,\Omega_2\}), \tag{7}$$

and separate the a priori shape information $p(\{\Omega_1,\Omega_2\})$ from image-based cues encoded in $p(I|\{\Omega_1,\Omega_2\})$. A common example of the a priori shape term would be $p(\{\Omega_1,\Omega_2\}) \propto e^{-\nu|\Gamma|}$. Assuming no correlation between labelings of regions, one can simplify the conditional probability

$$p(I|\{\Omega_1,\Omega_2\}) = p(I|\Omega_1)p(I|\Omega_2) = p_1(I)p_2(I).$$

Maximizing the probability (7) is equivalent to minimizing its negative logarithm. Thus we end up with the following energy

$$J(\Gamma) = -\int_{\Omega_1}\log p_1(I(x))dx - \int_{\Omega_2}\log p_2(I(x))dx + \nu\int_\Gamma dS.$$

If the distributions are modeled as parametric ones, with parameters θ_i for p_i, then the energy can be rewritten as

$$J(\Gamma) = -\int_{\Omega_1}\log p(I(x)|\theta_1)dx - \int_{\Omega_2}\log p(I(x)|\theta_2)dx + \nu\int_\Gamma dS. \tag{8}$$

The parameters θ_i depend on the form of the probability density function and often involve integrals over the regions Ω_i. For example, the Gaussian probability density function has the form $p_i(s) = \frac{1}{\sqrt{2\pi\sigma_i^2}}\exp\left(-\frac{(s-c_i)^2}{2\sigma_i^2}\right)$, where the parameters c_i, σ_i are computed by the integrals $c_i = \frac{1}{|\Omega_i|}\int_{\Omega_i} I(x)dx, \quad \sigma_i^2 = \frac{1}{|\Omega_i|}\int_{\Omega_i}(I(x)-c_i)^2 dx$.
It is not hard to see that we can concoct more complicated statistical formulations where shape energies with integrals play a central role. Thus, shape energies with integral parameters have significant use in image processing. The prototype for energies with integrals is

$$J(\Omega) = \int_\Omega g(x, I_w(\Omega))dx, \qquad I_w(\Omega) = \int_\Omega w(x)dx, \tag{9}$$

or one whose weight function g may depend on multiple integrals

$$J(\Omega) = \int_\Omega g(x, I_{w_1}(\Omega), \dots, I_{w_m}(\Omega))dx, \qquad I_{w_i}(\Omega) = \int_\Omega w_i(x)dx. \tag{10}$$

The first shape derivatives for the energies (9), (10) were computed by Aubert et al. in [5]. The second shape derivatives are computed in Section 4 in this paper, where we also deal with the case of nested integrals. Similar to domain energies with integrals, one can conceive of problems where it is necessary to deal with surface energies with integral parameters:

$$J(\Gamma) = \int_\Gamma g(x, I_w(\Gamma))dS, \qquad I_w(\Gamma) = \int_\Gamma w(x)dS. \tag{11}$$

The first and second shape derivatives for the energy (11) are not available in the literature and are computed in Section 4.

Higher order energies: Some image processing problems require encoding nonlocal interactions between points of a surface or a domain. Shape energies involving such interactions may be written as higher order integrals over the surface or the domain. For example, an energy that encodes the interactions between any two points of a surface or a domain would have the form

$$J(\Gamma) = \int_\Gamma \int_\Gamma g(x, y)dS(x)dS(y), \qquad J(\Omega) = \int_\Omega \int_\Omega g(x, y)dxdy. \tag{12}$$

The weight function $g(x, y)$ describes the nature of the interaction between the points x and y. If we want to account for nonlocal interactions of more points, say three, this can be formulated as a multiple integral with even higher order,
like $\int_\Omega \int_\Omega \int_\Omega g(x, y, z)\ dxdydz$.

Examples of higher order shape energies are not many in image processing, but they have been used successfully in applications such as road network extraction from images [49] and topology control of curves in image segmentation [38, 56]. In [56], Sundaramoorthi and Yezzi used the following shape energy to prevent curves from changing topology by merging or splitting:

$$J(\Gamma) = \int_\Gamma \int_\Gamma \frac{1}{|x - y|^\gamma} dS(x)dS(y), \quad \gamma > 0. \tag{13}$$

They added the energy (13) as an additional term to their segmentation energy. Note that the value of the integral (13) blows up as different parts of curve get close to each other, hence a topological change is prevented. In [38], Le Guyader and Vese accomplished the same goal by using a double integral over the domain Ω, instead of the surface Γ. Rochery et al. proposed higher order active contours in [49], as a general formulation with multiple integrals over curves (but not general surfaces). They derived the first variation of the shape energy and illustrate its use with an application in road network detection. In this paper, the shape energies (12) are considered for general surfaces Γ and domains Ω in $\mathbb{R}^d$ and their first and second shape derivatives are derived for general weight functions $g(x, y)$ (note that the second shape derivatives are not known and first variations are reported for specific $g(x, y)$ in previous work). We also explain how shape derivatives for energies with order higher than two can be derived.

Energies with PDEs: Large classes of images can be modeled as piecewise smooth functions with some discontinuities. For such images, the problems of image segmentation and image regularization can be formulated as finding the discontinuity set K and approximating the image intensity function I with a smooth function u on the remaining parts $D - K$ of the image domain $D \subset \mathbb{R}^d$. Mumford and Shah proposed minimizing the following energy for this purpose [40]

$$J(K, u) = \frac{1}{2} \int_D (I - u)^2 + \frac{\mu}{2} \int_{D-K} |\nabla u|^2 + \nu |K|, \quad \mu, \nu > 0 \tag{14}$$

The set of discontinuities that is included in the formulation (14) is very general and can include cracks and triple junctions. Therefore, a direct numerical realization of the minimization of (14) is not practical. For this reason, Chan and Vese proposed an alternative energy in [16]

$$J(\Gamma) = \frac{1}{2} \sum_{i=1}^{2} \int_{\Omega_i} \left((u_i - I)^2 + \mu |\nabla u_i|^2 \right) dx + \nu \int_{\Gamma} dS, \tag{15}$$

where u_1, u_2 are the smooth approximations to the image I computed by

$$-\mu \Delta u_i + u_i = I \text{ in } \Omega_i, \qquad \frac{\partial u_i}{\partial n_i} = 0 \text{ on } \partial\Omega_i, \tag{16}$$

and Ω_1, Ω_2 are the domains inside and outside the surface Γ respectively. In [16], the surface Γ was represented with a level set function. Thus cracks and triple junctions were excluded (a method to represent cases with junctions was proposed in [60] using multiple level set functions). Chan and Vese implemented a gradient descent method based on the first variation of (15). In [33], Hintermüller and Ring derived the first and second shape derivatives of (15). The second shape derivative was used in [23],[33] to develop fast Newton-type minimization methods for (15). A domain energy of the form $\int_\Omega g(x, u, \nabla u) dx$ with a Neumann PDE like (16) was considered Goto and Fujii in [29], where they derived the first and second shape derivatives.

In [8], Brox and Cremers gave a statistical interpretation of the Mumford-Shah functional. They started from a Bayesian model for segmentation and introduced a local Gaussian probability density function for image intensity in each region Ω_i: $p_i(I(x), x) = \frac{1}{\sqrt{2\pi}\sigma_i(x)} \exp\left(-\frac{(I(x)-c_i(x))^2}{2\sigma_i(x)^2} \right)$ with spatially varying mean $c_i(x)$ and variance $\sigma_i(x)$. Then they obtained the following extended Mumford-Shah functional

$$\begin{aligned} J_{BC}(\Gamma, \{c_i\}, \{\sigma_i\}) = & \sum_i \int_{\Omega_i} \left(\frac{(I(x) - c_i(x))^2}{2\sigma_i(x)^2} + \frac{1}{2} \log(2\pi\sigma_i(x)^2) \right) dx \\ & + \frac{\mu}{2} \sum_i \int_{\Omega_i} \left(|\nabla c_i(x)|^2 + |\nabla \sigma_i(x)|^2 \right) dx + \nu \int_{\Gamma} dS, \end{aligned} \tag{17}$$

by linking their model with the filtering theory of Nielsen et al. [41]. We generalize Brox and Cremer's model and write

$$J_0(\Gamma, \{u_{ki}\}) = \sum_i \int_{\Omega_i} \left(f(x, \{u_{ki}\}) + \frac{\mu}{2} \sum_k |\nabla u_{ki}|^2 \right) dx + \nu \int_{\Gamma} dS, \tag{18}$$

where u_{ki} is the smooth of approximation of a k^{th} data channel or statistical descriptor over region Ω_i, and $f(x, \{u_{ki}\})$ denotes a coupled data term, for example, $f(x, \{u_i, v_i\}) = \frac{(I(x)-u_i)^2}{2v_i^2}$ in the case of (17) or $f(x, \{u_{1i}, u_{2i}, u_{3i}\}) = \Sigma_{k=1}^3 (I_k(x) - u_{ki}(x))^2$ for color image segmentation. We write the optimality condition of (18) with respect to $\{u_{ki}\}$

$$-\Delta u_{ki} + f_{u_{ki}}(x, \{u_{li}\}) = 0 \text{ in } \Omega_i, \qquad \frac{\partial u_{ki}}{\partial n} = 0 \text{ on } \partial\Omega_i, \tag{19}$$

and use the solution of (19) to write the reduced shape energy $J(\Gamma) = J_0(\Gamma, \{u_{ki}(\Gamma)\})$

$$J(\Gamma) = \sum_i \int_{\Omega_i} \left(f(x, \{u_{ki}(\Gamma)\}) + \frac{\mu}{2} \sum_k |\nabla u_{ki}(\Gamma)|^2 \right) dx + \nu \int_{\Gamma} dS. \tag{20}$$

The energy (20) is more general than (15) and (17), and its first and second shape derivatives are not known; they are derived in Section 4.4 in this paper.

In (15), the role of the elliptic PDE was in computing a piecewise smooth approximation u to the image data I on the domains Ω_i. One can as well be interested in finding a smooth approximation to data defined on the surface Γ. This requires using an elliptic PDE defined on the surface Γ. Such a formulation was proposed in [34] by Jin, Yezzi and Soatto for stereoscopic reconstruction of 3d objects and their surface reflectance from 2d projections of the objects. The shape energy they used is essentially the following

$$J(\Gamma) = \frac{1}{2}\int_\Gamma (u(x) - d(x))^2 dS + \frac{\mu}{2}\int_\Gamma |\nabla_\Gamma u|^2 dS + \nu \int_\Gamma dS, \tag{21}$$

where u is computed from the surface PDE, $-\mu\Delta_\Gamma u + u = d$ on Γ (see §3.1 for the definition of the surface gradient ∇_Γ and the surface Laplacian Δ_Γ), and $d(x)$ is some data function based on the 2d images of the 3d scene. Jin, Yezzi and Soatto considered the parametric representation of a 2d surface in 3d in order to derive the first variation of the surface energy. Then they implemented a gradient descent algorithm using the level set method. The first shape derivative of (21) for general surfaces in any number of dimensions, to our knowledge, is not available in literature. We consider the following more general energy

$$J(\Gamma) = \int_\Gamma f(x, \{u_k(\Gamma)\}) dS + \frac{\mu}{2}\sum_k \int_\Gamma |\nabla_\Gamma u_k(\Gamma)|^2 dS + \nu \int_\Gamma dS, \tag{22}$$

where $\{u_k\}_{k=1}^m$ are computed from the optimality PDE: $-\mu\Delta_\Gamma u_k + f_{u_k}(x, \{u_l\}) = 0$. We compute the first shape derivative of (22) in Section 4.4. This result includes the case of (21) as well. Unlike [34], it is not restricted to parameterized surfaces and is valid in any number of dimensions.

3 Shape Differential Calculus

In this section, we will reviews some basic differential geometry that we will refer to throughout the paper. We will prove some useful geometric formulas. Finally we will introduce the shape derivative concept and describe some related results that will enable us to differentiate the model energies from Section 2.

3.1 Review of Differential Geometry

We assume that Γ is a smooth orientable compact $(d-1)$ dimensional surface in $\mathbb{R}^d$ without boundary. 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 $\mathbb{R}^d$. The *tangential gradient* $\nabla_\Gamma h$ of h is defined by:

$$\nabla_\Gamma h = \big(\nabla\tilde{h} - \partial_n \tilde{h}\; n\big)|_\Gamma,$$

where n denotes the unit normal vector to Γ and $\partial_n \tilde{h} = \nabla\tilde{h}\cdot n$ is the normal derivative. Similarly, given $\vec{W} \in [C^1(\Gamma)]^d$ and its smooth extension $\tilde{W} \in C^1(U)$, we define the *tangential divergence* of $\vec{W}$ by

$$\mathrm{div}_\Gamma \vec{W} = \big(\mathrm{div}\tilde{W} - n\cdot D\tilde{W}\cdot n\big)|_\Gamma, \tag{23}$$

where $D\tilde{W}$ denotes the Jacobian matrix of $\tilde{W}$. We also define the tangential gradient $\nabla_\Gamma \vec{W}$ of $\vec{W}$, which is a matrix whose i^{th} row is the tangential gradient $\nabla_\Gamma \vec{W}_i$ of the i^{th}

Summary of results (1)

Minimal surface energies

Geodesic active contour energy: $J(\Gamma) = \int_\Gamma g(x)dS + \gamma \int_\Omega g(x)dx,$

[13, 14, 32]: $dJ(\Omega; V) = \int_\Gamma ((\kappa + \gamma)g(x) + \partial_n g(x))\, V dS,$ ($\partial_n g$: normal derivative)

[32]: $$d^2 J(\Gamma; V, W) = \int_\Gamma g \nabla_\Gamma V \cdot \nabla_\Gamma W dS + \int_\Gamma \Big(\partial_{nn} g + (2\kappa + \gamma)\partial_n g + (\kappa^2 - \sum \kappa_i^2 + 2\gamma\kappa) g\Big) VWdS.$$

Normal-dependent surface energy: $J(\Gamma) = \int_\Gamma g(x, n)dS,$

[7, 21]: $dJ(\Gamma; V) = \int_\Gamma (\kappa g + \partial_n g + \mathrm{div}_\Gamma (g_y)_\Gamma)\, V dS,$ (g_y : gradient w.r.t. 2nd arg.)

($\star$) : $$d^2 J(\Gamma; V, W) = \int_\Gamma \nabla_\Gamma V \cdot ((g - g_y \cdot n)Id + g_{yy}) \cdot \nabla_\Gamma W dS + \int_\Gamma \Big(\partial_{nn} g + 2\kappa \partial_n g + (\kappa^2 - \sum \kappa_i^2) g\Big) VWdS - \int_\Gamma (\kappa g_y + n^T g_{xy}) \cdot (\nabla_\Gamma W\, V + \nabla_\Gamma V\, W) dS.$$

Curvature-dependent surface energy: $J(\Gamma) = \int_\Gamma g(x, \kappa)dS,$

[25]: $dJ(\Gamma; V) = \int_\Gamma \Big(-\Delta_\Gamma(g_z) + g\kappa - g_z \sum \kappa_i^2 + \partial_n g\Big) V dS,$ (g_z : deriv. w.r.t. 2nd arg.)

$$\Delta_\Gamma(g_z) = \Delta_\Gamma g_z + g_{zz} \Delta_\Gamma \kappa + g_{zzz} |\nabla_\Gamma \kappa|^2 + (g_{zxz} + g_{zzx}) \cdot \nabla_\Gamma \kappa.$$

Energies with integral parameters (more results in §4.2)

Energies with domain integrals: $J(\Omega) = \int_\Omega g(x, I_w(\Omega))dx,$ $I_w(\Omega) = \int_\Omega w(x)dx,$

[5]: $dJ(\Omega; V) = \int_\Gamma \big(g(x, I_w(\Omega)) + I_{g_p}(\Omega) w(x)\big) V dS,$ (g_p : deriv. w.r.t. 2nd arg.)

($\star$) : $$d^2 J(\Omega; V, W) = \int_\Gamma \big(\partial_n g + I_{g_p} \partial_n w + \kappa (g + I_{g_p} w)\big) VWdS + \int_\Gamma g_p V dS \int_\Gamma w W dS + \int_\Gamma w V dS \int_\Gamma g_p W dS + I_{g_{pp}} \int_\Gamma w V dS \int_\Gamma w W dS.$$

Energies with surface integrals: $J(\Gamma) \int_\Gamma g(x, I_w(\Gamma))dS,$ $I_w(\Gamma) = \int_\Gamma w(x)dS,$

($\star$) : $dJ(\Gamma; V) = \int_\Gamma \big((g + I_{g_p} w)\kappa + \partial_n g + I_{g_p} \partial_n w\big) V dS,$ (g_p : deriv. w.r.t. 2nd arg.)

($\star$) : $$\begin{aligned} d^2 J(\Gamma; V, W) = &\int_\Gamma (g + I_{g_p} w) \nabla_\Gamma V \cdot \nabla_\Gamma W dS \\ &+ \int_\Gamma \big(\partial_{nn} g + I_{g_p} \partial_{nn} w + 2(\partial_n g + I_{g_p} \partial_n w)\kappa\big) VWdS \\ &+ \int_\Gamma (\partial_n g_p + g_p \kappa)\, V dS \int_\Gamma (\partial_n w + w\kappa)\, W dS \\ &+ \int_\Gamma (\partial_n w + w\kappa)\, V dS \int_\Gamma (\partial_n g_p + g_p \kappa)\, W dS \\ &+ I_{g_{pp}} \int_\Gamma (\partial_n w + w\kappa)\, V dS \int_\Gamma (\partial_n w + w\kappa)\, W dS. \end{aligned}$$

Table 1: See the caption of Table 2 for an explanation of the labels ($\star$),[#].

Summary of results (2)
Higher order energies
Higher order domain energies: $J(\Omega) = \int_\Omega \int_\Omega g(x,y)dydx,$ ($\star$,[38]): $dJ(\Omega;V) = \int_\Gamma \int_\Omega \tilde{g}(x,y)dyVdS, \qquad (\tilde{g}(x,y) = g(x,y) + g(y,x))$ ($\star$) : $d^2J(\Omega;V,W) = \int_\Gamma \int_\Gamma \tilde{g}(x,y)W(y)dS(y)V(x)dS(x) + \int_\Gamma \left(\kappa(x)\int_\Omega \tilde{g}(x,y)dy + n(x)\cdot\int_\Omega \tilde{g}_y(x,y)dy\right)VWdS.$
Higher order surface energies: $J(\Gamma) = \int_\Gamma \int_\Gamma g(x,y)dS(y)dS(x),$ ($\star$,[49]): $dJ(\Gamma;V) = \int_\Gamma \left(\kappa(x)\int_\Gamma \tilde{g}(x,y)dS(y) + n(x)\cdot\int_\Gamma \tilde{g}_x(x,y)dS(y)\right)V(x)dS(x),$ ($\star$) : $d^2J(\Gamma;V,W) = \int_\Gamma G(x,\Gamma)\nabla_\Gamma V\cdot\nabla_\Gamma W dS(x) \qquad \left(G(x,\Gamma) = \int_\Gamma \tilde{g}(x,y)dS(y)\right)$ $+ \int_\Gamma \left(n^T G_{xx}(x,\Gamma)\, n + 2\kappa\, G_x(x,\Gamma)\cdot n + (\kappa^2 - \Sigma\kappa_i^2)G(x,\Gamma)\right) VWdS(x)$ $+ \int_\Gamma \kappa \int_\Gamma \tilde{g}\kappa\, WdS(y)VdS(x) + \int_\Gamma n^T \int_\Gamma \tilde{g}_{xy} n\, WdS(y)VdS(x)$ $+ \int_\Gamma \kappa \int_\Gamma \tilde{g}_y\cdot n\, WdS(y)VdS(x) + \int_\Gamma n\cdot\int_\Gamma \tilde{g}_x\kappa\, WdS(y)VdS(x),$
Energies with PDEs
Energies with domain PDEs : $J(\Omega) = \int_\Omega \left(f(x,\{u_k\}) + \frac{\mu}{2}\sum_k \lvert\nabla u_k\rvert^2\right)dx,$ $-\mu\Delta u_l + f_{u_l} = 0$ in Ω, $\frac{\partial u_l}{\partial n} = 0$ on $\partial\Omega$, $l = 1,\ldots,m,$ ($\star$,[8, 29, 33, 60]): $dJ(\Omega;V) = \int_\Gamma \left(f(x,\{u_k\}) + \frac{\mu}{2}\sum_k \lvert\nabla_\Gamma u_k\rvert^2\right)VdS,$ ($\star$,[29, 33]): $d^2J(\Omega;V,W) = \int_\Gamma \left(f\kappa + \frac{\partial f}{\partial n} + \mu\sum_k \nabla_\Gamma u_k^T\left(\frac{\kappa}{2}Id - \nabla_\Gamma n\right)\nabla_\Gamma u_k\right)VWdS$ $+ \int_\Gamma \sum_k \left(f_{u_k}u'_{k,W} + \mu\nabla_\Gamma u_k\cdot\nabla_\Gamma u'_{k,W}\right)VdS.$
Energies with surface PDEs : $J(\Gamma) = \int_\Gamma \left(f(x,\{u_k\}) + \frac{\mu}{2}\sum_k \lvert\nabla_\Gamma u_k\rvert^2\right)dS,$ $-\mu\Delta_\Gamma u_l + f_{u_l} = 0$ on Γ, $l = 1,\ldots,m,$ ($\star$,[34]): $dJ(\Gamma;V) = \int_\Gamma \left(f\kappa + \frac{\partial f}{\partial n} + \mu\sum_k \nabla_\Gamma u_k^T\left(\frac{\kappa}{2}Id - \nabla_\Gamma n\right)\nabla_\Gamma u_k\right)VdS.$

Table 2: Next to each shape derivative formula is a label specifying whether or not the formula is new and citation to its source if it is not new. The label ($\star$) indicates that it is a new result, not available in the literature in any form. The label [#] indicates that the result can be found in reference [#]. The label ($\star$, [#]) indicates that the result is new for general surfaces or domains in $\mathbb{R}^d$ or for general choices of the weight functions $g(x,\Gamma), g(x,\Omega)$, but formulas for restricted situations can be found in reference [#].

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

$$\Delta_\Gamma h = \operatorname{div}_\Gamma(\nabla_\Gamma h) = \big(\Delta\tilde{h} - n \cdot D^2\tilde{h} \cdot n - \kappa\, \partial_n \tilde{h}\big)|_\Gamma. \tag{24}$$

As seen above, in order to compute the full spatial derivatives of surface functions and geometric quantities, such as the normal n and the mean curvature κ, defined only on the surface Γ, we need to extend them to a tubular neighborhood of Γ. This is accomplished using a signed distance function representation of the surface Γ:

$$b(x,\Gamma) = \begin{cases} \ \ \operatorname{dist}(x,\Gamma) & \text{for } x \in \mathbb{R}^d - \Omega \\ \ \ 0 & \text{for } x \in \Gamma \\ -\operatorname{dist}(x,\Gamma) & \text{for } x \in \Omega \end{cases} \tag{25}$$

where $\operatorname{dist}(x,\Gamma) = \inf_{y\in\Gamma} |y - x|$ and Ω is the domain enclosed by Γ. Using (25) we extend the normal n, the mean curvature κ and the second fundamental form $\nabla_\Gamma n$ as follows [22, Chap. 8]:

$$n = \nabla b(x)|_\Gamma, \quad \kappa = \Delta b(x)|_\Gamma, \quad \nabla_\Gamma n = D^2 b(x)|_\Gamma. \tag{26}$$

The extensions (26) allow us to differentiate $n, \kappa, \nabla_\Gamma n$ in the normal direction in addition to the tangential direction, and the normal derivatives of the normal n and the mean curvature κ are given by

$$\partial_n n = 0, \qquad \partial_n \kappa = -\sum_{i=1}^{d-1} \kappa_i^2, \tag{27}$$

respectively, where κ_i denote the principal curvatures of the surface. It is easy to show, using the extension (26),

$$\partial_n n = \nabla(\nabla b)\nabla b|_\Gamma = D^2 b \nabla b|_\Gamma = 0,$$

because $0 = \nabla(1) = \nabla(\nabla b \cdot \nabla b) = 2D^2 b \nabla b$. The expression for $\partial_n \kappa$ can be computed similarly. The proof can be found in [25].

Note that Equation (27) holds only for parallel surfaces defined by the signed distance function.

Lemma 3.1 *The following identities hold on Γ for a function u of class C^2 defined in (or extended properly to) a tubular neighborhood U of the surface Γ,*

$$\frac{\partial}{\partial n}(\nabla_\Gamma u) = D^2 u n - n^T D^2 u n n \tag{28}$$

$$\nabla_\Gamma \left(\frac{\partial u}{\partial n}\right) = n^T D^2 u + \nabla_\Gamma u^T \nabla_\Gamma n - n^T D^2 u n n. \tag{29}$$

If the function u is constant in the normal direction to Γ, i.e. $\frac{\partial u}{\partial n} = 0$ on Γ,

$$n^T D^2 u = -\nabla_\Gamma u^T \nabla_\Gamma n, \tag{30}$$

$$\nabla_\Gamma \left(\frac{\partial u}{\partial n}\right) = 0, \qquad \frac{\partial}{\partial n}(\nabla_\Gamma u) = -\nabla_\Gamma n \nabla_\Gamma u. \tag{31}$$

Proof. We start by computing the normal derivative of the tangential gradient. For this, we resort to the signed distance function extension (26) of the normal n.

$$
\begin{aligned}
\frac{\partial}{\partial n}(\nabla_\Gamma u) &= \partial_{x_j}(u_{x_i} - u_{x_k} n_k n_i) n_j, \qquad i = 0, \dots, d-1 \\
&= \left(\partial_{x_j}(u_{x_i} - u_{x_k} b_{x_k} b_{x_i}) b_{x_j}\right)|_\Gamma, \qquad i = 0, \dots, d-1 \\
&= \left(u_{x_i x_j} b_{x_j} - u_{x_k x_j} b_{x_k} b_{x_i} b_{x_j} - u_{x_k} b_{x_k x_j} b_{x_i} b_{x_j} - u_{x_k} b_{x_k} b_{x_i x_j} b_{x_j}\right)|_\Gamma \\
&= \left(u_{x_i x_j} b_{x_j} - u_{x_k x_j} b_{x_k} b_{x_i} b_{x_j}\right)|_\Gamma \\
&= D^2 u n - n^T D^2 u n n.
\end{aligned}
$$

Note that $b_{x_i x_j} b_{x_j} = b_{x_j x_i} b_{x_j} = \frac{1}{2}\partial_{x_i}(b_{x_j} b_{x_j}) = 0$ because $|\nabla b|^2 = b_{x_j} b_{x_j} = 1$.
Now we compute the tangential gradient of the normal derivative,

$$
\begin{aligned}
\nabla_\Gamma \left(\frac{\partial u}{\partial n}\right) &= \nabla_\Gamma (\nabla u \cdot n) = \partial_{x_i}(u_{x_k} n_k) - \partial_{x_j}(u_{x_k} n_k) n_j n_i, \qquad i = 0, \dots, d-1 \\
&= \left(\partial_{x_i}(u_{x_k} b_{x_k}) - \partial_{x_j}(u_{x_k} b_{x_k}) b_{x_j} b_{x_i}\right)|_\Gamma, \qquad i = 0, \dots, d-1 \\
&= (u_{x_k x_i} b_{x_k} + u_{x_k} b_{x_k x_i} - u_{x_k x_j} b_{x_k} b_{x_j} b_{x_i} - u_{x_k} \underbrace{b_{x_k x_j} b_{x_j}}_{=0} b_{x_i})\big|_\Gamma \\
&= (u_{x_k x_i} b_{x_k} + (u_{x_k} b_{x_k x_i} - (u_{x_l} b_{x_l}) \underbrace{b_{x_k} b_{x_k x_i}}_{=0}) - u_{x_k x_j} b_{x_k} b_{x_j} b_{x_i})|_\Gamma \\
&= n^T D^2 u + \nabla_\Gamma u^T \nabla_\Gamma n - n^T D^2 u n n.
\end{aligned}
$$

We used the fact that $D^2 b$ is symmetric and $\nabla_\Gamma n = D^2 b|_\Gamma$.
To prove (30), we start with the assumption $\frac{\partial u}{\partial n} = (\nabla u \cdot \nabla b)|_\Gamma = 0$ and differentiate,

$$
\begin{aligned}
0 &= \partial_{x_j}(\nabla u \cdot \nabla b) = \partial_{x_j}(u_{x_i} b_{x_i}) = u_{x_i x_j} b_{x_i} + u_{x_i} b_{x_i x_j} \\
&= u_{x_i x_j} b_{x_i} + b_{x_i x_j} u_{x_i} - u_{x_k} b_{x_k} b_{x_i} b_{x_i x_j} \qquad (b_{x_i} b_{x_i x_j} = 0) \\
&= u_{x_i x_j} b_{x_i} + b_{x_i x_j}(u_{x_i} - u_{x_k} b_{x_k} b_{x_i}) \\
\Rightarrow\ & \nabla b^T D^2 u = -(\nabla u - \nabla u \cdot \nabla b \nabla b)^T D^2 b,
\end{aligned}
$$

which on the surface Γ is equivalent to

$$
n^T D^2 u = -\nabla_\Gamma u^T \nabla_\Gamma n. \tag{32}
$$

The identities (31) follow trivially from (32) substituted in (28), (29). ∎

Proposition 3.1 ([22, 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*

$$
\int_\Gamma f \operatorname{div}_\Gamma \vec{\omega} + \nabla_\Gamma f \cdot \vec{\omega} dS = \int_\Gamma \kappa f \vec{\omega} \cdot \nu dS. \tag{33}
$$

3.2 Shape Differentiation

We would like to understand how a quantity depending on a surface Γ (or a domain Ω) changes when Γ is deformed by a given velocity field. For this, we consider a hold-all domain $\mathcal{D}$ (which may or may not be the image domain), containing the surface Γ, and a smooth vector field $\vec{V}$ defined on $\mathcal{D}$. The vector field $\vec{V}$ is used to define the continuous sequence of perturbed surfaces $\{\Gamma_t\}_{t \geq 0}$, with $\Gamma_0 := \Gamma$. Each point $X \in \Gamma_0$ follows

$$
\frac{dx}{dt} = \vec{V}(x(t)), \quad \forall t \in [0, T], \qquad x(0) = X. \tag{34}
$$

This defines the mapping $x(t,\cdot) : X \in \Gamma \to x(t,X) \in \mathbb{R}^d$ and the perturbed sets $\Gamma_t = \{x(t,X) : \ \ X \in \Gamma_0\}$ (similarly perturbations of domains $\Omega_t = \{x(t,X) : \ \ X \in \Omega_0\}$ for domains $\Omega(=\Omega_0)$ contained by Γ).

Let $J(\Gamma)$ be a shape energy, namely a mapping that associates to surfaces Γ a real number. The Eulerian derivative, or *shape derivative*, of the energy $J(\Gamma)$ at Γ in the direction of the vector field $\vec{V}$, is defined as the limit

$$dJ(\Gamma;\vec{V}) = \lim_{t\to 0} \frac{1}{t}\big(J(\Gamma_t) - J(\Gamma)\big). \tag{35}$$

We define the shape derivatives $dJ(\Omega;\vec{V})$ for domain energies $J(\Omega)$ similarly. For more information on the concept of shape derivatives (including the definition and other properties), we refer to the book [22] by Delfour-Zolesio-01 and Zolésio.

We now recall a series of results from shape differential calculus in $\mathbb{R}^d$.

Lemma 3.2 ([53, Prop.2.45]) *Let $\phi \in W^{1,1}(\mathbb{R}^d)$ and $\Omega \subset \mathbb{R}^d$ be an open and bounded domain with boundary $\Gamma = \partial\Omega$ of class C^1. Then the energy $J(\Omega) = \int_\Omega \phi dx$ is shape differentiable. The shape derivative of $J(\Omega)$ is given by*

$$dJ(\Omega;\vec{V}) = \int_\Gamma \phi V dS, \tag{36}$$

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

Lemma 3.3 ([53, Prop. 2.50 and (2.145)]) *Let $\psi \in W^{2,1}(\mathbb{R}^d)$ and Γ be of class C^2. Then the energy $J(\Gamma) = \int_\Gamma \psi dS$ is shape differentiable and the derivative*

$$dJ(\Gamma;\vec{V}) = \int_\Gamma \big(\nabla\psi\cdot\vec{V} + \psi \mathrm{div}_\Gamma \vec{V}\big)dS = \int_\Gamma \big(\partial_n\psi + \psi\kappa\big)V dS, \tag{37}$$

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

Let us now consider more general energies $J(\Gamma)$. Specifically we are interested in computing shape derivatives for energies of the form

$$J(\Gamma) = \int_\Gamma \varphi(x,\Gamma)dS, \qquad J(\Omega) = \int_\Omega \phi(x,\Omega)dx, \tag{38}$$

in which the weight functions φ,ϕ depend not only on the spatial position x, but also on the shape Γ,Ω. Examples are a weight function $\varphi(x,\Gamma) = \varphi(x,n)$ that depends on the normal of the surface Γ [28, 36], or a weight function $\phi(x,\Omega) = \phi(x,u(\Omega))$ that depends on the solution u of a PDE defined on Ω [16, 23, 33]. To handle the computation of the shape derivatives of such energies we need to take care of the derivative of φ,ϕ with respect to the shape Γ,Ω. For this we recall the notions of *material derivative* and *shape derivative*.

Definition 3.1 ([53, Prop.2.71]) *The material derivative $\dot{\varphi}(\Gamma;\vec{V})$ of $\varphi(\Gamma)$ at Γ in direction $\vec{V}$ is defined as follows*

$$\dot{\varphi}(\Gamma;\vec{V}) = \lim_{t\to 0}\frac{1}{t}\big(\varphi(x(t,\cdot),\Gamma_t) - \varphi(\cdot,\Gamma_0)\big), \tag{39}$$

where the mapping $x(t,\cdot)$ is defined as in (34). A similar definition holds for domain functions $\phi(\Omega)$.

Definition 3.2 ([53, Def. 2.85, Def 2.88]) *The shape derivative $\phi(\Omega)$ at Ω in the direction $\vec{V}$ is defined to be*

$$\phi'(\Omega;\vec{V}) = \dot{\phi}(\Omega;\vec{V}) - \nabla\phi\cdot\vec{V}. \tag{40}$$

Accordingly, for surface functions $\varphi(\Gamma)$, the shape derivative is defined to be

$$\varphi'(\Gamma;\vec{V}) = \dot{\varphi}(\Gamma;\vec{V}) - \nabla_\Gamma\varphi\cdot\vec{V}|_\Gamma. \tag{41}$$

The shape derivative concept enables us to compute the change in the shape dependent quantities, such as the normal n and the mean curvature κ, with respect to deformations of the shape by given velocity fields.

Lemma 3.4 *The shape derivatives of the normal n and the mean curvature κ of a surface Γ of class C^2 with respect to velocity $\vec{V}\in C^2$ are given by*

$$n' = n'(\Gamma;\vec{V}) = -\nabla_\Gamma V, \tag{42}$$

$$\kappa' = \kappa'(\Gamma;\vec{V}) = -\Delta_\Gamma V, \tag{43}$$

where $V = \vec{V}\cdot n$ is the normal component of the velocity. Moreover, the shape derivative of the tangential gradient of a function u of class C^1 defined in (or extended properly to) a tubular neighborhood U of the surface Γ is

$$(\nabla_\Gamma u)' = \nabla_\Gamma u' + \nabla_\Gamma u\cdot\nabla_\Gamma V n + \frac{\partial u}{\partial n}\nabla_\Gamma V. \tag{44}$$

Proof. The derivations for n' and κ' can be found in [32, Sect. 3]. Once we have the result for n', we can proceed with the following

$$\begin{aligned}(\nabla_\Gamma u)' &= (\nabla u - \nabla u\cdot nn)' = \nabla u' - \nabla u'\cdot nn - \nabla u\cdot n'n - \nabla u\cdot nn' \\ &= \nabla_\Gamma u' + \nabla u\cdot\nabla_\Gamma V n + \nabla u\cdot n\nabla_\Gamma V \\ &= \nabla_\Gamma u' + \nabla_\Gamma u\cdot\nabla_\Gamma V n + \frac{\partial u}{\partial n}\nabla_\Gamma V.\end{aligned}$$

■

Now we state the shape derivatives of the general shape energies (38).

Theorem 3.1 ([53, Sect. 2.31, 2.33]) *Let $\phi = \phi(\Omega)$ be given so that the material derivative $\dot{\phi}(\Omega;\vec{V})$ and the shape derivative $\phi'(\Omega;\vec{V})$ exist. Then, the shape energy $J(\Omega)$ in (38) is shape differentiable and we have*

$$dJ(\Omega;\vec{V}) = \int_\Omega \phi'(\Omega;\vec{V})dx + \int_\Gamma \phi V dS. \tag{45}$$

For surface functions $\varphi(\Gamma)$, the shape derivative of $J(\Gamma)$ in (38) is given by

$$dJ(\Gamma;\vec{V}) = \int_\Gamma \varphi'(\Gamma;\vec{V})dS + \int_\Gamma \kappa\varphi V dS, \tag{46}$$

whereas if $\varphi(\cdot,\Gamma) = \psi(\cdot,\Omega)|_\Gamma$, then we obtain

$$dJ(\Gamma;\vec{V}) = \int_\Gamma \psi'(\Omega;\vec{V})|_\Gamma dS + \int_\Gamma \left(\frac{\partial\psi}{\partial n} + \kappa\psi\right) V dS. \tag{47}$$

We conclude this section with a Riesz representation theorem, the Hadamard-Zolésio Theorem.

Theorem 3.2 ([53, Sect 2.11 and Th. 2.27]) *The shape derivative of a surface or domain energy always has a representation of the form*

$$dJ(\Gamma; \vec{V}) = \langle G, V \rangle_\Gamma, \tag{48}$$

where we denote by $\langle \cdot, \cdot \rangle_\Gamma$ *a suitable duality pairing on* Γ*; that is, the shape derivative is concentrated on* Γ*.*

Let us point out that an implication of this theorem is that the shape derivative $dJ(\Gamma; \vec{V})$ depends only on $V = \vec{V} \cdot n$, the normal component of the velocity. *For this reason, we will use* V *in our derivations from now on and assume a normal extension when we need the velocity extended to a neighborhood of the surface. Hence, without loss of generality, we have the following assumptions on* V *and* $\vec{V}$

$$\vec{V} = Vn, \qquad \frac{\partial V}{\partial n} = 0 \quad \text{on } \Gamma. \tag{49}$$

Deriving the first shape derivatives using only scalar velocities V, thus normal velocities (49), may at first appear as a restriction, since one is not always able to work with scalar velocities V and may need to use arbitrary vector velocities $\vec{V}$. Because of Theorem 3.2, this turns out not to be a problem; the first shape derivatives computed with scalar velocities V will be the same as those computed with arbitrary $\vec{V}$ with $V = \vec{V} \cdot n$. Moreover, in the case of second shape derivatives introduced in the next subsection, the formulas obtained with scalar velocities V are the same around critical shapes as those obtained with arbitrary vector velocities $\vec{V}$ (given $V = \vec{V} \cdot n$) [11, 42].

3.3 The Second Shape Derivative

We continue to use the scalar velocity fields V, W (corresponding to vector velocity fields $\vec{V}, \vec{W}$ by (49)) to perturb Γ, Ω and we define the second shape derivative as follows

$$d^2 J(\Gamma; V, W) = d\left(dJ(\Gamma; V)\right)(\Gamma; W), \quad d^2 J(\Omega; V, W) = d\left(dJ(\Omega; V)\right)(\Omega; W). \tag{50}$$

The second shape derivatives of functions $\phi(\Omega)$, $\varphi(\Gamma)$ can be defined similarly based on Definition 3.2. Now we can use this to compute the second shape derivative of the domain and the surface energies. We give these results below.

Lemma 3.5 ([32, Sect. 5]) *Let* $\phi \in W^{2,1}(\mathbb{R}^d)$ *and* Γ *be of class* C^2*. Then the second shape derivative of the energy*

$$J(\Omega) = \int_\Omega \phi dx \tag{51}$$

at Ω *with respect to scalar velocity fields* V*,* W *is given by*

$$d^2 J(\Omega; V, W) = \int_\Gamma \left(\partial_n \phi + \kappa \phi\right) VW dS. \tag{52}$$

Lemma 3.6 ([32, Sect. 5]) *Let* $\psi \in W^{3,1}(\mathbb{R}^d)$ *and* Γ *be of class* C^2*. Then the second shape derivative of the energy*

$$J(\Gamma) = \int_\Gamma \psi dS \tag{53}$$

at Γ *with respect to scalar velocity fields* V*,* W *is given by*

$$d^2 J(\Gamma; V, W) = \int_\Gamma \left(\psi \nabla_\Gamma V \cdot \nabla_\Gamma W + \left(\partial_{nn}\psi + 2\kappa \partial_n \psi + (\kappa^2 - \sum \kappa_i^2)\psi\right) VW\right) dS.$$

We employ Lemmas 3.5 and 3.6 and Definition 3.2 to state the second shape derivative for more general energies (38), in which the weight functions also depend on the shape. The assumptions (49) are crucial to obtaining the following result.

Theorem 3.3 *Let $\phi = \phi(x, \Omega)$ be given so that the first and the second shape derivatives $\phi'(\Omega; V)$, $\phi''(\Omega; V, W)$ exist. Then, the second shape derivative of the domain energies in (38) is given by*

$$d^2 J(\Omega; V, W) = \int_\Omega \phi'' dx + \int_\Gamma (\phi'_W V + \phi'_V W)\, dS + \int_\Gamma (\partial_n \phi + \kappa\phi)\, VW dS \tag{54}$$

where $\phi'_V = \phi'(\Omega; V)$, $\phi'' = \phi''(\Omega; V, W)$. For surface functions $\varphi(\Gamma)$ in (38) with $\varphi(\cdot, \Gamma) = \psi(\cdot, \Omega)|_\Gamma$ we obtain

$$\begin{aligned} d^2 J(\Gamma; V, W) \quad &= \quad \int_\Gamma \psi'' dS + \int_\Gamma ((\partial_n \psi'_W + \kappa\psi'_W)\, V + (\partial_n \psi'_V + \kappa\psi'_V)\, W)\, dS \\ &+ \quad \int_\Gamma \Big(\psi \nabla_\Gamma V \cdot \nabla_\Gamma W + \Big(\partial_{nn}\psi + 2\kappa\partial_n\psi + (\kappa^2 - \sum \kappa_i^2)\psi\Big)\, VW\Big)\, dS. \end{aligned} \tag{55}$$

where $\psi'_V = \psi'(\Gamma; V)|_\Gamma$, $\psi''_{V,W} = \psi''(\Gamma; V, W)|_\Gamma$.

Proof. For $J(\Omega) = \int_\Omega \phi(x, \Omega) dx$, the first shape derivative at Ω in direction V is

$$dJ(\Omega; V) \quad = \quad \underbrace{\int_\Omega \phi'(\Omega; V) dx}_{J_1} \quad + \quad \underbrace{\int_\Gamma \phi V dS}_{J_2}.$$

To obtain the second shape derivative, we take the derivatives of J_1 and J_2.

$$\begin{aligned} dJ_1(\Omega; W) &= \int_\Omega \phi''(\Omega; V, W) dx + \int_\Gamma \phi'(\Omega; V) W dS, \\ dJ_2(\Omega; W) &= \int_\Gamma \phi'(\Omega; W) V dS + \int_\Gamma (\partial_n \phi V + \phi V \kappa) W dS. \end{aligned}$$

Plugging in $d^2 J(\Omega; V, W)$ and reorganizing the terms yields the results. We obtain the second shape derivative for the surface energy similarly. ∎

More details on the structure of the second shape derivative can be found in [11, 22, 42]. We should reemphasize that the use of assumptions (49) has allowed us to derive the simpler forms in Theorem 3.3, compared to these references, which investigate the second shape derivative with more general vector velocities or perturbations. For vector velocities with tangential components, the second shape derivative includes additional terms, but these terms disappear at critical shapes. Thus the formula obtained with scalar velocities is sufficient to characterize the second shape derivative at critical shapes, because in this situation, the second shape derivative depends only on the normal components of the vector velocity [11, 42].

4 Shape Derivatives of the Model Energies

We compute the first and second shape derivatives for each shape energy class introduced in Section 2.

4.1 Minimal Surface Energies

We compute the first and the second shape derivatives of surface energies with weight functions that depend only on the local geometry at each point of the surface. We start with an isotropic energy, the Geodesic Active Contour Model, then consider anisotropic, i.e. normal-dependent energies; we describe the case of a curvature-dependent weight as well.

Isotropic surface energies. The archetype shape energy in image processing is the Geodesic Active Contour model [13, 14]:

$$J(\Gamma) := \int_\Gamma g(x)dS + \gamma \int_\Omega g(x)dx, \tag{56}$$

where Γ is a surface in $\mathbb{R}^d$ and Ω is the domain enclosed by Γ. The first and second shape derivatives directly follow from Lemmas 3.2, 3.3, 3.5, 3.6 and the derivations can be found in [32].

Proposition 4.1 *The first shape derivative of the energy* (56) *at* Γ *with respect to velocity* V *is given by*

$$dJ(\Gamma;V) = \int_\Gamma \Big((\kappa+\gamma)g(x) + \partial_n g(x)\Big)V dS.$$

The second shape derivative of (56) *with respect to velocities* V, W *is given by*

$$d^2J(\Gamma;V,W) = \int_\Gamma \Big(g\nabla_\Gamma V\cdot\nabla_\Gamma W + \Big(\partial_{nn}g + (2\kappa+\gamma)\partial_n g + (\kappa^2 - \sum \kappa_i^2 + 2\gamma\kappa)g\Big)VW\Big)\, dS.$$

Anisotropic surface energies. Now we compute the first and the second shape derivatives of the anisotropic surface energy

$$J(\Gamma) := \int_\Gamma g(x,n)dS. \tag{57}$$

The weight function $g(x,n)$ depends on the orientation of the normal of the surface. We assume the derivatives g_x, g_{xx} with respect to the first argument x and the derivatives g_y, g_{yy} with respect to the second argument n, also the mixed derivatives g_{xy}, g_{yx} are well-defined. Applications of (57) are in image segmentation [36] and in multiview stereo reconstruction [28, 37].

Proposition 4.2 *The first shape derivative of the anisotropic surface energy* (57) *at* Γ *with respect to velocity* V *is given by*

$$dJ(\Gamma;V) = \int_\Gamma (\kappa g + \partial_n g)\, V - g_y\cdot\nabla_\Gamma V dS = \int_\Gamma (\kappa g + \partial_n g + \mathrm{div}_\Gamma (g_y)_\Gamma)\, V dS, \tag{58}$$

where g_y *is the derivative of* $g(x,n)$ *with respect to its second variable.*

Proof. To derive the first derivative, we use Theorem 3.1 with $\psi = g(x,n)$. Then

$$\psi'(\Gamma;V) = g_y\cdot n' = -g_y\cdot\nabla_\Gamma V$$

using (42). We also need to compute the normal derivative of $g(x,n)$. We have $\partial_n\psi = \partial_n(g(x,n)) = \partial_n g + g_y^T\partial_n n = \partial_n g$, because $\partial_n n = 0$ by Equation (27) (assuming extension by signed distance function (25), (26)).
We then substitute ψ' and $\partial_n\psi$ in (47) and obtain

$$dJ(\Gamma;V) = \int_\Gamma (\kappa g + \partial_n g)\, V - g_y\cdot\nabla_\Gamma V dS.$$

We can apply the tangential Green's formula (33) to the last term of the integral, and use the identity $\mathrm{div}_\Gamma(\vec{\omega})_\Gamma = \mathrm{div}_\Gamma(\vec{\omega}) - \kappa\vec{\omega}\cdot n$ [22, Chap. 8] to obtain (58). ∎

Proposition 4.3 *The second shape derivative of the anisotropic surface energy* (57) *at* Γ *with respect to velocities* V, W *is given by*

$$\begin{aligned} d^2J(\Gamma;V,W) = &\int_\Gamma \nabla_\Gamma V \cdot ((g - g_y\cdot n)Id + g_{yy})\cdot \nabla_\Gamma W dS \\ &+ \int_\Gamma \Big(\partial_{nn}g + 2\kappa\partial_n g + (\kappa^2 - \sum \kappa_i^2)g\Big) VW dS \\ &- \int_\Gamma (\kappa g_y - g_y^T\nabla_\Gamma n + n^T g_{xy}^T)\cdot(\nabla_\Gamma W\, V + \nabla_\Gamma V\, W) dS. \end{aligned}$$

where Id *is the* $d\times d$ *identity matrix.*

Proof. Use Theorem 3.3 with $\psi = g(x,n)$. Then $\partial_n\psi = \partial_n g,\ \partial_{nn}\psi = \partial_{nn}g$, and

$$\begin{aligned} \psi'(\Gamma;V) &= -g_y\cdot\nabla_\Gamma V \\ \psi''(\Gamma;V,W) &= -\left(g_y\right)'\cdot\nabla_\Gamma V - g_y\cdot(\nabla_\Gamma V)' \qquad (\text{use}(44),(49)) \\ &= \nabla_\Gamma V\cdot g_{yy}\cdot\nabla_\Gamma W - g_y\cdot n\,\nabla_\Gamma V\cdot\nabla_\Gamma W \\ &= \nabla_\Gamma V\cdot(g_{yy} - g_y\cdot n\, Id)\cdot\nabla_\Gamma W \\ \partial_n\psi'(\Gamma;V) &= -\partial_n g_y\cdot\nabla_\Gamma V - g_y\cdot\partial_n\nabla_\Gamma V \\ &= -(g_{yx}n)\cdot\nabla_\Gamma V - g_y\cdot(-\nabla_\Gamma n\nabla_\Gamma V) \\ &= (g_y^T\nabla_\Gamma n - n^T g_{yx}^T)\nabla_\Gamma V, \end{aligned}$$

since $\partial_n\nabla_\Gamma V = -\nabla_\Gamma n\nabla_\Gamma V$ by Lemma 3.1 and assumptions (49). The function g_{yx} is the Hessian obtained by differentiating with respect to the second variable n, and to the first variable x. Now we substitute the derivatives of ψ in (55) to obtain

$$\begin{aligned} d^2J(\Gamma;V,W) = &\int_\Gamma \nabla_\Gamma V\cdot(g_{yy} - g_y\cdot n\, Id)\cdot\nabla_\Gamma W dS \\ &- \int_\Gamma \big((n^T g_{yx}^T - g_y^T\nabla_\Gamma n)\cdot\nabla_\Gamma W + \kappa g_y\cdot\nabla_\Gamma W\big) V \\ &- \int_\Gamma \big((n^T g_{yx}^T - g_y^T\nabla_\Gamma n)\cdot\nabla_\Gamma V + \kappa g_y\cdot\nabla_\Gamma V\big) W dS \\ &+ \int_\Gamma \Big(g\nabla_\Gamma V\cdot\nabla_\Gamma W + \Big(\partial_{nn}g + 2\kappa\partial_n g + (\kappa^2 - \sum\kappa_i^2)g\Big) VW\Big) dS. \end{aligned}$$

Reorganizing the terms yields the result. ∎

Curvature-dependent Energies. Next we compute the shape derivative of the curvature dependent surface energy

$$J(\Gamma) := \int_\Gamma g(x,\kappa) dS. \tag{59}$$

The weight function $g(x,\kappa)$ depends on the mean curvature of the surface. We assume the derivative g_x with respect to the first argument x and the derivatives g_z, g_{zz}, g_{zzz} with respect to the second argument κ, also the mixed derivatives g_{zxz}, g_{zzx} are well-defined. Variants of the energy (59) have been used to impose regularity of curves or surfaces in shape identification problems [18, 26, 58].

Proposition 4.4 *The first shape derivative of the curvature-dependent surface energy* (59) *with* $g = g(x, \kappa)$ *at* Γ *with respect to velocity* $\vec{V}$ *is given by*

$$\begin{aligned} dJ(\Gamma; V) &= \int_\Gamma -g_z \Delta_\Gamma V + \left(g\kappa - g_z \sum \kappa_i^2 + \partial_n g \right) V dS, \\ &= \int_\Gamma \left(-\Delta_\Gamma (g_z) + g\kappa - g_z \sum \kappa_i^2 + \partial_n g \right) V dS, \end{aligned}$$

where $\Delta_\Gamma(g_z)$ *denotes the total derivative*

$$\Delta_\Gamma(g_z) = \Delta_\Gamma g_z + g_{zz} \Delta_\Gamma \kappa + g_{zzz} |\nabla_\Gamma \kappa|^2 + (g_{zxz} + g_{zzx}) \cdot \nabla_\Gamma \kappa$$

and g_z *is the derivative of* $g(x, \kappa)$ *with respect to its second variable;* $g_{zz}, g_{zxz}, g_{zzx}, g_{zzz}$ *are defined similarly.*

The proof of Proposition 4.4 for the shape derivative of (59) is given by Doğan and Nochetto in [25], where they derive the shape derivative also for the more general surface energy

$$J(\Gamma) = \int_\Gamma g(x, n, \kappa) dS.$$

4.2 Shape Energies with Integrals

We compute the shape derivatives for the domain and surface energies with integrals. These energies are found in applications where we need to aggregate properties over regions or surfaces by integration, for example, to compute statistics of given data [5, 19, 46], and the integrals are used as parameters of the weight function.

Energies with Domain Integrals. We start by computing the shape derivatives for the energy with a weight function that depends on a single domain integral:

$$J(\Omega) = \int_\Omega g(x, I_w(\Omega)) dx, \qquad I_w(\Omega) = \int_\Omega w(x) dx. \tag{60}$$

We then consider an energy with a weight that depends on multiple domain integrals:

$$J(\Omega) = \int_\Omega g(x, I_{w_1}, \dots, I_{w_m}) dx, \qquad I_{w_i} = I_{w_i}(\Omega) = \int_\Omega w_i(x) dx, \ i = 1, \dots, m. \tag{61}$$

We also consider the case in which the dependence on domain integrals is recursive:

$$J(\Omega) = \int_\Omega g_0(x, I_{g_1}) dx, \tag{62}$$

where

$$\begin{aligned} I_{g_k} = I_{g_k}(\Omega) &= \int_\Omega g_k(x, I_{g_{k+1}}) dx, \quad k = 1, \dots, m-1, \\ I_{g_m} = I_{g_m}(\Omega) &= \int_\Omega g_m(x) dx. \end{aligned}$$

The first shape derivatives of (60), (61) and (62) (only for two levels of recursion) were computed in [5]. The second shape derivatives of (60), (61) are computed in this section.

Proposition 4.5 *The first shape derivative of the shape energy* (60) *at* Ω *with respect to velocity* V *is given by*

$$dJ(\Omega; V) = \int_\Gamma \big(g(x, I_w(\Omega)) + I_{g_p}(\Omega) w(x) \big) V dS,$$

The second shape derivative of (60) *with respect to velocities V, W is given by*

$$
\begin{aligned}
d^2 J(\Omega; V, W) = &\int_\Gamma \left(\partial_n g + I_{g_p}\partial_n w + \kappa(g + I_{g_p} w)\right) VW dS \\
&+ \int_\Gamma g_p V dS \int_\Gamma wW dS + \int_\Gamma wV dS \int_\Gamma g_p W dS \\
&+ I_{g_{pp}} \int_\Gamma wV dS \int_\Gamma wW dS,
\end{aligned}
$$

We use the short notation for the functions $g = g(x, I_w(\Omega))$, $w = w(x)$, and g_p, g_{pp} denote the derivatives of $g(x, I_w(\Omega))$ with respect to its second variable. $I_{g_p}, I_{g_{pp}}$ are the integrals of g_p, g_{pp} over the domain Ω.

Proof. Let $\phi(x, \Omega) = g(x, I_w(\Omega))$ in Theorem 3.1, and calculate $\phi'(\Omega; V)$.

$$
\phi'(\Omega; V) = g_p(x, I_w) I'_w = g_p(x, I_w) \int_\Gamma w(y) V dS(y).
$$

We have used the fact that Lemma 3.2 applies to I_w, namely we have $I'_w = dI_w(\Omega; V)$. We substitute $\phi'(\Omega; V)$ in the general form (45)

$$
dJ(\Omega; V) = \int_\Omega g_p(x, I_w) \left(\int_\Gamma w(y) V dS(y) \right) dx + \int_\Gamma g(x, I_w) V dS.
$$

Since $I_{g_p} = \int_\Omega g_p(x, I_w) dx$, we can exchange the order of integration and obtain

$$
dJ(\Omega; V) = \int_\Gamma \left(g(x, I_w) + I_{g_p} w(x) \right) V dS.
$$

To compute the second shape derivative, we use Theorem 3.3. We need $\phi'' = \phi''(\Omega; V, W)$, which we compute by Lemma 3.5

$$
\begin{aligned}
\phi'' &= (g_p)' \int_\Gamma w(y) V dS + g_p \left(\int_\Gamma w(y) V dS \right)' \\
&= g_{pp} \int_\Gamma w(z) V dS(z) \int_\Gamma w(y) W dS(y) + g_p \int_\Omega \left(\partial_n w(y) + \kappa w(y)\right) VW dS.
\end{aligned}
$$

Substitute in (54)

$$
\begin{aligned}
d^2 J(\Omega; V, W) = &\int_\Omega g_{pp} dx \int_\Gamma wV dS \int_\Gamma wW dS + \int_\Gamma g_p dx \int_\Omega \left(\partial_n w + \kappa w\right) VW dS \\
&+ \int_\Gamma g_p V dS \int_\Gamma wW dS + \int_\Gamma g_p W dS \int_\Gamma wV dS \\
&+ \int_\Gamma (\partial_n g + \kappa g) VW dS.
\end{aligned}
$$

Reorganizing the various terms yields the result. ∎

Proposition 4.6 *The first shape derivative of the energy* (61) *at Ω with respect to velocity V is given by*

$$
dJ(\Omega; V) = \int_\Gamma \left(g(x, I_{w_1}, \ldots, I_{w_m}) + \sum_{i=1}^m I_{g_{p_i}} w_i(x) \right) V dS.
$$

The second shape derivative of the energy (61) *at* Ω *with respect to velocity* V, W *is*

$$\begin{aligned} d^2J(\Omega; V, W) = &\int_\Gamma \left(\partial_n g + \sum_{i=1}^m I_{g_{p_i}} \partial_n w_i + \kappa (g + \sum_{i=1}^m I_{g_{p_i}} w_i) \right) VWdS \\ &+ \sum_{i=1}^m \left(\int_\Gamma g_{p_i} VdS \int_\Gamma w_i WdS + \int_\Gamma w_i VdS \int_\Gamma g_{p_i} WdS \right) \\ &+ \sum_{i,j=1}^m I_{g_{p_i p_j}} \int_\Gamma w_i VdS \int_\Gamma w_j WdS, \end{aligned}$$

Proof. The proof is essentially the same as that of Proposition 4.5, except that we need to keep track of indices and corresponding terms $w_i, I_{w_i}, g_{p_i}, I_{g_{p_i}}, g_{p_i p_j}, I_{g_{p_i p_j}}$. ■

Proposition 4.7 *The first shape derivative of the energy* (62) *at* Ω *with respect to velocity* V *is given by*

$$dJ(\Omega; V) = \int_\Gamma \left(g_0(x, I_{g_1}) + \sum_{j=1}^{m-1} g_j(x, I_{g_{j+1}}) \prod_{i=0}^{j} I_{g_{i,p}} \right) VdS,$$

where $g_{i,p}$ *denotes the derivative of* $g_i(x, I_{g_{i+1}})$ *with respect to its second argument.*

Proof. Note that the shape derivative of $I_{g_m} = I_{g_m}(\Omega)$ is given by

$$I'_{g_m} = \int_\Gamma g_m(x) VdS.$$

Now we compute the shape derivative of $I_{g_k} = I_{g_k}(\Omega)$.

$$\begin{aligned} I'_{g_k} = &\int_\Omega g_{k,p}(x, I_{g_{k+1}}) I'_{g_{k+1}} dx + \int_\Gamma g_k(x, I_{g_{k+1}}) VdS = I_{g_{k,p}} I'_{g_{k+1}} + \int_\Gamma g_k VdS \\ =& I_{g_{k,p}} \left(I_{g_{k+1,p}} I'_{g_{k+2}} + \int_\Gamma g_{k+1} VdS \right) + \int_\Gamma g_k VdS \\ =& I_{g_{k,p}} I_{g_{k+1,p}} I'_{g_{k+2}} + I_{g_{k,p}} \int_\Gamma g_{k+1} VdS + \int_\Gamma g_k VdS \\ =& I_{g_{k,p}} I_{g_{k+1,p}} \dots I'_{g_m} + I_{g_{k,p}} \dots I_{g_{m-2,p}} \int_\Gamma g_{m-1} VdS + \dots \\ &+ I_{g_{k,p}} \int_\Gamma g_{k+1} VdS + \int_\Gamma g_k VdS \\ =& I_{g_{k,p}} \dots I_{g_{m-1,p}} \int_\Gamma g_m VdS + I_{g_{k,p}} \dots I_{g_{m-2,p}} \int_\Gamma g_{m-1} VdS + \dots \\ &+ I_{g_{k,p}} \int_\Gamma g_{k+1} VdS + \int_\Gamma g_k VdS. \end{aligned}$$

More concisely,

$$I'_{g_k} = \int_\Gamma g_k VdS + \sum_{j=k+1}^{m} \prod_{i=k}^{j-1} I_{g_{i,p}} \int_\Gamma g_j VdS = \int_\Gamma \left(g_k + \sum_{j=k+1}^{m} \prod_{i=k}^{j-1} I_{g_{i,p}} g_j \right) VdS.$$

Then the first shape derivative of energy (62) is given by $dJ(\Gamma; V) = I'_{g_0}$. ■

Energies with Surface Integrals. Similar to the case with domain integrals, we compute the shape derivatives for energies with weight functions that depend on surface integrals

$$J(\Gamma) = \int_\Gamma g(x, I_w(\Gamma))dS, \qquad I_w(\Gamma) = \int_\Gamma w(x)dS. \tag{63}$$

The cases of multiple integral parameters and nested integrals in the weight function g are straight-forward and are not included in this paper.

Proposition 4.8 *The first shape derivative of the energy* (63) *at* Γ *with respect to velocity* V *is given by*

$$dJ(\Gamma;V) = \int_\Gamma \big((g(x,I_w(\Gamma)) + I_{g_p} w(x))\kappa + \partial_n g(x, I_w(\Gamma)) + I_{g_p}\partial_n w(x)\big)\, V dS.$$

The second shape derivative of (63) *at* Γ *with respect to velocities* V, W *is given by*

$$\begin{aligned} d^2 J(\Gamma; V, W) = &\int_\Gamma (g + I_{g_p} w)\nabla_\Gamma V \cdot \nabla_\Gamma W dS \\ &+ \int_\Gamma \big(\partial_{nn} g + I_{g_p}\partial_{nn} w + 2(\partial_n g + I_{g_p}\partial_n w)\kappa + (\kappa^2 - \Sigma\kappa_i^2)(g + I_{g_p} w)\big)\, VW dS \\ &+ \int_\Gamma (\partial_n g_p + g_p\kappa)\, V dS \int_\Gamma (\partial_n w + w\kappa)\, W dS \\ &+ \int_\Gamma (\partial_n w + w\kappa)\, V dS \int_\Gamma (\partial_n g_p + g_p\kappa)\, W dS \\ &+ I_{g_{pp}} \int_\Gamma (\partial_n w + w\kappa)\, V dS \int_\Gamma (\partial_n w + w\kappa)\, W dS. \end{aligned}$$

We use the short notation for the functions $g = g(x, I_w(\Gamma))$*,* $w = w(x)$*, and* g_p, g_{pp} *denote the derivatives of* $g(x, I_w(\Gamma))$ *with respect to its second variable.* $I_{g_p}, I_{g_{pp}}$ *are the integrals of* g_p, g_{pp} *over the surface* Γ*.*

Proof. Let $\psi(x,\Gamma) = g(x, I_w(\Gamma))$ in Theorem 3.1. By Lemma 3.3, we have

$$\psi' = \psi'(\Gamma; V) = g_p(x, I_w) I_w' = g_p \int_\Gamma (\partial_n w + w\kappa) V dS$$

Substitute in the general form (45)

$$dJ(\Gamma;V) = \int_\Gamma g_p dS \int_\Gamma (\partial_n w + w\kappa) V dS + \int_\Gamma (\partial_n g + g\kappa) V dS.$$

We let $I_{g_p} = \int_\Gamma g_p(x, I_w)dS$, reorganize the terms, thus obtain the first shape derivative. Now we use Theorem 3.3 and compute $\partial_n \psi = \partial_n g$, $\partial_{nn}\psi = \partial_{nn} g$, and

$$\begin{aligned} \psi_V' = \psi'(\Gamma;V) = &g_p \int_\Gamma (\partial_n w + w\kappa) V dS, \;\; \partial_n \psi_V' = \partial_n g_p \int_\Gamma (\partial_n w + w\kappa) V dS, \\ \psi'' = \psi''(\Gamma; V, W) = &(g_p)' \int_\Gamma (\partial_n w + w\kappa) V dS + g_p \left(\int_\Gamma (\partial_n w + w\kappa) V dS\right)' \\ = &g_{pp}(x, I_w) \int_\Gamma (\partial_n w + w\kappa) V dS \int_\Gamma (\partial_n w + w\kappa) W dS \\ &+ g_p(x, I_w) \int_\Gamma w \nabla_\Gamma V \cdot \nabla_\Gamma W dS \\ &+ g_p(x, I_w) \int_\Gamma \Big(\partial_{nn} w + 2\kappa\partial_n w + (\kappa^2 - \sum \kappa_i^2) w\Big)\, VW dS, \end{aligned}$$

using Lemma 3.6. We substitute the derivatives of ψ in (55) and obtain

$$
\begin{aligned}
d^2J(\Gamma;V,W) = &\int_\Gamma g_{pp} dS \int_\Gamma (\partial_n w + w\kappa) V dS \int_\Gamma (\partial_n w + w\kappa) W dS \\
&+ \int_\Gamma g_p dS \int_\Gamma w \nabla_\Gamma V \cdot \nabla_\Gamma W dS \\
&+ \int_\Gamma g_p dS \int_\Gamma \left(\partial_{nn} w + 2\kappa \partial_n w + (\kappa^2 - \sum \kappa_i^2) w\right) VW dS \\
&+ \int_\Gamma (\partial_n g_p + g_p \kappa) W dS \int_\Gamma (\partial_n w + w\kappa) V dS \\
&+ \int_\Gamma (\partial_n g_p + g_p \kappa) V dS \int_\Gamma (\partial_n w + w\kappa) W dS \\
&+ \int_\Gamma \left(g \nabla_\Gamma V \cdot \nabla_\Gamma W + \left(\partial_{nn} g + 2\kappa \partial_n g + (\kappa^2 - \sum \kappa_i^2) g\right) VW \right) dS.
\end{aligned}
$$

Reorganizing the various terms yields the result. ∎

4.3 Higher-Order Energies

In this section, we consider energies that have the form of a double integral with a weight function $g(x,y) : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$. These energies are used to model nonlocal interactions between two separate spatial locations x, y. Applications are found in road network detection [49] and topology control of curves for image segmentation [38, 48, 55].

We introduce some notation that will simplify our derivations of the shape derivatives. We denote by $\tilde{g}(x,y)$ the symmetricization of the function $g(x,y)$:

$$\tilde{g}(x,y) = g(x,y) + g(y,x). \tag{64}$$

The derivatives of $\tilde{g}(x,y)$ are then given by

$$
\begin{gathered}
\tilde{g}_x(x,y) = g_x(x,y) + g_y(y,x), \qquad \tilde{g}_y(x,y) = g_y(x,y) + g_x(y,x), \\
\tilde{g}_{xy}(x,y) = g_{xy}(x,y) + g_{yx}(y,x), \quad \ldots, \text{ and so on.}
\end{gathered} \tag{65}
$$

We also introduce the domain integral of $\tilde{g}(x,y)$ and its derivative

$$G(x,\Omega) = \int_\Omega \tilde{g}(x,y) dy, \qquad G_x(x,\Omega) = \int_\Omega \tilde{g}_x(x,y) dy, \tag{66}$$

also the surface integral and its derivatives

$$
\begin{gathered}
G(x,\Gamma) = \int_\Gamma \tilde{g}(x,y) dS(y), \qquad G_x(x,\Gamma) = \int_\Gamma \tilde{g}_x(x,y) dS(y), \\
G_{xx}(x,\Gamma) = \int_\Gamma \tilde{g}_{xx}(x,y) dS(y).
\end{gathered} \tag{67}
$$

Higher-Order Domain Energies. We consider the following higher-order domain energy

$$J(\Omega) = \int_\Omega \int_\Omega g(x,y) \, dy dx, \tag{68}$$

and compute its first and the second shape derivatives.

Proposition 4.9 *The first shape derivative of the higher-order domain energy* (68) *at* Ω *with respect to velocity* V *is*

$$dJ(\Omega;V) = \int_\Gamma G(x,\Omega) V dS = \int_\Gamma \int_\Omega \tilde{g}(x,y) dy V dS, \tag{69}$$

where $\tilde{g}(x,y)$ *is defined by* (64).

Proof. We define $\phi(x,\Omega) = \int_\Omega g(x,y)dy$, so that we work with a more concise form of the energy (68)

$$J(\Omega) = \int_\Omega \phi(x,\Omega)dx. \tag{70}$$

and use Theorem 3.1. We start by writing the shape derivative of ϕ

$$\phi'(\Omega;V)(x) = \int_\Gamma g(x,y)V(y)dS(y),$$

We substitute $\phi'(\Omega;V)$ in the shape derivative of (70),

$$\begin{aligned}
dJ(\Omega;V) &= \int_\Omega \phi'(\Omega;V)dx + \int_\Gamma \phi(x)V(x)dS(x) \\
&= \int_\Omega \int_\Gamma g(x,y)V(y)dS(y)dx + \int_\Gamma \int_\Omega g(x,y)dyV(x)dS(x) \\
&= \int_\Omega \int_\Gamma g(y,x)V(x)dS(x)dy + \int_\Gamma \int_\Omega g(x,y)dyV(x)dS(x) \\
&= \int_\Omega \left(\int_\Gamma (g(x,y) + g(y,x))dy \right) V(x)dS(x).
\end{aligned}$$

and we let $\tilde{g}(x,y) = g(x,y) + g(y,x)$ to obtain the result (69). ∎

Remark 4.1 *Using the same strategy as in the proof of Proposition 4.9, we can write the shape derivatives of even higher-order energies, for example,*

$$J(\Omega) = \int_\Omega \int_\Omega \int_\Omega g(x,y,z)dzdydx.$$

We set $\phi(x,\Omega) = \int_\Omega \int_\Omega g(x,y,z)dzdy$ *and compute its shape derivative*

$$\phi'(\Omega;V)(x) = \int_\Gamma \left(\int_\Gamma (g(x,y,z) + g(x,z,y)dz \right) V(y)dS(y),$$

using Proposition 69. Again we use the formula for the domain shape derivative in Theorem 3.1 and substitute the current values of $\phi(x,\Omega)$ *and* $\phi'(V;\Omega)$*:*

$$\begin{aligned}
dJ(\Omega;V) &= \int_\Gamma \left(\int_\Omega \int_\Omega (g(x,y,z) + g(x,z,y))dzdx \right) V(y)dS(y) \\
&\quad + \int_\Gamma \int_\Omega \int_\Omega g(x,y,z)dzdyV(x)dS(x) \\
&= \int_\Gamma \left(\int_\Omega \int_\Omega (g(x,y,z) + g(y,x,z) + g(y,z,x))dzdy \right) V(x)dS(x).
\end{aligned}$$

Proposition 4.10 *The second shape derivative of the higher-order domain energy* (68) *at* Ω *with respect to velocities* V, W *is*

$$\begin{aligned}
d^2J(\Omega;V,W) &= \int_\Gamma \int_\Gamma \tilde{g}(x,y)W(y)dS(y)V(x)dS(x) \\
&\quad + \int_\Gamma \left(\kappa(x) \int_\Omega \tilde{g}(x,y)dy + n(x) \cdot \int_\Omega \tilde{g}_x(x,y)dy \right) VWdS, \\
&= \int_\Gamma \int_\Gamma \tilde{g}(x,y)W(y)dS(y)V(x)dS(x) \\
&\quad + \int_\Gamma \left(\kappa(x)G(x,\Omega) + n(x) \cdot G_x(x,\Omega)\right) VWdS,
\end{aligned} \tag{71}$$

where $\tilde{g}(x,y), \tilde{g}_x(x,y), G(x,\Omega), G_x(x,\Omega)$ *are defined by* (64), (65), (66).

Proof. The second shape derivative is computed using Theorem 3.3. We define $\phi(x,\Omega) = \int_\Omega g(x,y)dy$, compute the derivatives $\phi'(\Omega;V), \phi''(\Omega;V,W), \partial_n\phi$ and substitute in formula (54). We have $\partial_n \phi(x,\Omega) = n(x)\cdot\int_\Gamma g_x(x,y)\,dy$, also

$$\begin{aligned}
\phi'(x) &= \phi'(\Omega;V)(x) = \int_\Gamma g(x,y)V(y)dS(y),\\
\phi''(x) &= \phi''(\Omega;V,W)(x) = \int_\Gamma \left(\kappa g(x,y)V(y) + \partial_n\cdot(g(x,y)V(y))\right)W(y)dS(y)\\
&= \int_\Gamma \left(\kappa(y)g(x,y) + n(y)\cdot g_y(x,y)\right)VWdS(y). \quad (\partial_n V = 0 \text{ by eqn (49)})
\end{aligned}$$

Then the second shape derivative is given by

$$\begin{aligned}
d^2J(\Omega;V,W) &= \int_\Omega \phi'' dx + \int_\Gamma (\kappa\phi + \partial_n\phi)\,VWdS + \int_\Gamma (\phi'_W V + \phi'_V W)\,dS\\
&= \int_\Omega\int_\Gamma \left(g(x,y)\kappa(y) + n(y)\cdot g_y(x,y)\right)VWdS(y)dx\\
&\quad + \int_\Gamma \left(\kappa(x)\int_\Omega g(x,y)dy + n(x)\cdot\int_\Omega g_x(x,y)dy\right)VWdS(x)\\
&\quad + \int_\Gamma \left(\int_\Gamma g(x,y)W(y)dS(y)V(x) + \int_\Gamma g(x,y)V(y)dS(y)W(x)\right)dS(x).
\end{aligned}$$

We change variables in the integrals, for example we let

$$\int_\Omega\int_\Gamma g(x,y)K(y)V(y)W(y)dS(y)dx = \int_\Gamma \kappa(x)\int_\Omega g(y,x)dyV(x)W(x)dS(x),$$

and reorganize the terms in $d^2J(\Omega;V,W)$ and obtain

$$\begin{aligned}
d^2J(\Gamma;V,W) &= \int_\Gamma \left(\kappa\int_\Omega (g(x,y)+g(y,x))dy + n\cdot\int_\Omega (g_x(x,y)+g_y(y,x))dy\right)VWdS(x)\\
&\quad + \int_\Gamma\int_\Gamma (g(x,y)+g(y,x))W(y)dS(y)V(x)dS(x)\\
&= \int_\Gamma \left(\kappa(x)\int_\Omega \tilde g(x,y)dy + n(x)\cdot\int_\Omega \tilde g_x(x,y)\right)V(x)W(x)dS(x).
\end{aligned}$$

We substitute $G(x,\Omega), G_x(x,\Omega)$ for the integrals of $\tilde g(x,y), \tilde g_x(x,y)$ respectively and obtain the second shape derivative. ∎

Higher-Order Surface Energies. We consider the higher-order surface energy

$$J(\Gamma) = \int_\Gamma\int_\Gamma g(x,y)dS(y)dS(x), \tag{72}$$

and derive its first and second shape derivatives.

Proposition 4.11 *The first shape derivative of the higher order surface energy $J(\Gamma)$ (73) at Γ with respect to velocity V is*

$$\begin{aligned}
dJ(\Gamma;V) &= \int_\Gamma \left(\kappa(x)\int_\Gamma \tilde g(x,y)dS(y) + n(x)\cdot\int_\Gamma \tilde g_x(x,y)dS(y)\right)V(x)dS(x),\\
&= \int_\Gamma \left(\kappa(x)G(x,\Gamma) + n(x)\cdot G_x(x,\Gamma)\right)V(x)dS(x),
\end{aligned} \tag{73}$$

where $\tilde g(x,y), \tilde g_x(x,y)$ are defined by (64), (65) *and $G(x,\Gamma), G_x(x,\Gamma)$ by* (67).

Proof. We will use Theorem 3.1 to calculate the first shape derivative of the energy (72). We define $\psi(x,\Gamma) = \int_\Gamma g(x,y)dS(y)$ (so that $J(\Gamma) = \int_\Gamma \psi(x,\Gamma)dS(x)$) and calculate its derivatives of ψ are

$$\partial_n\psi = n(x)\cdot\int_\Gamma g_x(x,y)dS(y), \qquad \psi'(\Gamma;V) = \int_\Gamma (g(x,y)\kappa(y) + g_y(x,y)\cdot n(y))VdS(y).$$

to be substituted in the formula (47) for the first shape derivative:

$$\begin{aligned}
dJ(\Gamma;V) &= \int_\Gamma \psi'(\Gamma;V)dS(x) + \int_\Gamma (\psi\kappa + \partial_n\psi_x)VdS(x)\\
&= \int_\Gamma\int_\Gamma (g(x,y)\kappa(y) + g_y(x,y)\cdot n(y))\,V(y)dS(y)dS(x)\\
&\quad + \int_\Gamma \left(\kappa(x)\int_\Gamma g(x,y)dS(y) + n(x)\cdot\int_\Gamma g_x(x,y)dS(y)\right)V(x)dS(x).
\end{aligned}$$

We exchange the variables in the first integral,

$$\begin{aligned}
dJ(\Gamma;V) &= \int_\Gamma\int_\Gamma (g(y,x)\kappa(x) + n(x)\cdot g_y(y,x))\,V(x)dS(x)dS(y)\\
&\quad + \int_\Gamma \left(\kappa(x)\int_\Gamma g(x,y)dS(y) + n(x)\cdot\int_\Gamma g_x(x,y)dS(y)\right)V(x)dS(x)\\
&= \int_\Gamma \left(\kappa(x)\int_\Gamma (g(x,y)+g(y,x))dS(y)\right.\\
&\qquad \left. + n(x)\cdot\int_\Gamma (g_x(x,y)+g_y(y,x))dS(y)\right)V(x)dS(x)\\
&= \int_\Gamma \left(\kappa(x)\int_\Gamma \tilde{g}(x,y)dS(y) + n(x)\cdot\int_\Gamma \tilde{g}_x(x,y)dS(y)\right)V(x)dS(x).
\end{aligned}$$

We also replace the integrals of $\tilde{g}(x,y), \tilde{g}_x(x,y)$ by $G(x,\Gamma), G_x(x,\Gamma)$ respectively. ∎

Proposition 4.12 *The second shape derivative of the higher order surface energy $J(\Gamma)$ (73) at Γ with respect to velocities V, W is*

$$\begin{aligned}
d^2J(\Gamma;V,W) &= \int_\Gamma G(x,\Gamma)\nabla_\Gamma V\cdot\nabla_\Gamma W dS(x)\\
&\quad + \int_\Gamma \left(n^T G_{xx}(x,\Gamma)\,n + 2\kappa\,G_x(x,\Gamma)\cdot n + (\kappa^2 - \Sigma\kappa_i^2)G(x,\Gamma)\right)VWdS(x)\\
&\quad + \int_\Gamma \kappa\int_\Gamma \tilde{g}\kappa\,WdS(y)VdS(x) + \int_\Gamma n^T\int_\Gamma \tilde{g}_{xy}n\,WdS(y)VdS(x)\\
&\quad + \int_\Gamma \kappa\int_\Gamma \tilde{g}_y\cdot n\,WdS(y)VdS(x) + \int_\Gamma n\cdot\int_\Gamma \tilde{g}_x\kappa\,WdS(y)VdS(x),
\end{aligned}$$

where $\tilde{g}(x,y), \tilde{g}_x(x,y), \tilde{g}_y(x,y), \tilde{g}_{xy}(x,y), G(x,\Gamma), G_x(x,\Gamma), G_{xx}(x,\Gamma)$ are defined by the formulas (64),(65), (67).

Proof. We define $\psi(x,\Gamma) = \int_\Gamma g(x,y)dS(y)$ and compute its normal derivatives $\partial_n\psi,\ \partial_{nn}\psi$ and its shape derivatives $\psi'_V = \psi'(\Gamma;V),\ \psi'' = \psi''(\Gamma;V,W),\ \partial_n\psi'_V$:

$$\begin{aligned}
\partial_n\psi &= n(x)\cdot\int_\Gamma g_x(x,y)dS(y), \quad \partial_{nn}\psi = n(x)^T\left(\int_\Gamma g_x(x,y)dS(y)\right)n(x),\\
\psi'_V &= \int_\Gamma (g\kappa(y) + g_y\cdot n(y))VdS(y), \quad \partial_n\psi'_V = n\cdot\int_\Gamma (g_x\kappa(y) + g_{yx}^T n(y))VdS(y),\\
\psi'' &= \int_\Gamma g\nabla_\Gamma V\cdot\nabla_\Gamma WdS(y) + \int_\Gamma \left(n^T g_{yy}n + 2\kappa g_y\cdot n + (\kappa^2 - \Sigma\kappa_i^2)g\right)VWdS(y),
\end{aligned}$$

which we subsitute in the general formula (55) for the second shape derivative

$$
\begin{aligned}
d^2J(\Gamma;V,W) &= \int_\Gamma \psi'' dS + \int_\Gamma \left((\partial_n\psi'_W + \kappa\psi'_W)\,V + (\partial_n\psi'_V + \kappa\psi'_V)\,W\right) dS \\
&\quad + \int_\Gamma \left(\psi\nabla_\Gamma V\cdot\nabla_\Gamma W + \left(\partial_{nn}\psi + 2\kappa\partial_n\psi + (\kappa^2 - \Sigma\kappa_i^2)\psi\right) VW\right) dS.
\end{aligned}
$$

and obtain

$$
\begin{aligned}
d^2J(\Gamma;V,W) = &\int_\Gamma\int_\Gamma g\nabla_\Gamma V(y)\cdot\nabla_\Gamma W(y)dS(y)dS(x) \\
&+ \int_\Gamma\int_\Gamma \big(n(y)^T g_{yy} n(y) + 2\kappa(y) g_y\cdot n(y) \\
&\qquad + (\kappa(y)^2 - \Sigma\kappa_i(y)^2)g\big)\,V(y)W(y)dS(y)dS(x) \\
&+ \int_\Gamma \bigg(n(x)\cdot\int_\Gamma (g_x\kappa(y) + g_{yx}^T n(y))W(y)dS(y) \\
&\qquad + \kappa(x)\int_\Gamma (g\kappa(y) + g_y\cdot n(y))W(y)dS(y)\bigg)\,V(x)dS(x) \\
&+ \int_\Gamma \bigg(n(x)\cdot\int_\Gamma (g_x\kappa(y) + g_{yx}^T n(y))V(y)dS(y) \\
&\qquad + \kappa(x)\int_\Gamma (g\kappa(y) + g_y\cdot n(y))V(y)dS(y)\bigg)\,W(x)dS(x) \\
&+ \int_\Gamma\int_\Gamma g dS(y)\nabla_\Gamma V(x)\cdot\nabla_\Gamma W(x)dS(x) \\
&+ \int_\Gamma \bigg(n(x)^T\int_\Gamma g_{xx}dS(y)n(x) + 2\kappa(x)n(x)\cdot\int_\Gamma g_x dS(y) \\
&\qquad + (\kappa(x)^2 - \Sigma\kappa_i(x)^2)\int_\Gamma g dS(y)\bigg)\,V(x)W(x)dS(x).
\end{aligned}
$$

We exchange variables $x\leftrightarrow y$ in the integrals that contain $V(y)$ and reorganize,

$$
\begin{aligned}
d^2J(\Gamma;V,W) = &\int_\Gamma\left(\int_\Gamma (g(x,y)+g(y,x))dS(y)\right)\nabla_\Gamma V\cdot\nabla_\Gamma W dS(x) \\
&+ \int_\Gamma\bigg\{n(x)^T\left(\int_\Gamma (g_{xx}(x,y)+g_{yy}(y,x))dS(y)\right)n(x) \\
&\qquad + 2\kappa(x)n(x)\cdot\left(\int_\Gamma (g_x(x,y)+g_y(y,x))dS(y)\right) \\
&\qquad + (\kappa(x)^2 - \Sigma\kappa_i(x)^2)\int_\Gamma (g(x,y)+g(y,x))dS(y)\bigg\}VW dS(x) \\
&+ \int_\Gamma \kappa(x)\left(\int_\Gamma (g(x,y)+g(y,x))\kappa(y)W(y)dS(y)\right)V(x)dS(x) \\
&+ \int_\Gamma n(x)\cdot\left(\int_\Gamma (g_{xy}(x,y)+g_{yx}(y,x))n(y)W(y)dS(y)\right)V(x)dS(x) \\
&+ \int_\Gamma \kappa(x)\left(\int_\Gamma (g_y(x,y)+g_x(y,x))\cdot n(y)W(y)dS(y)\right)V(x)dS(x) \\
&+ \int_\Gamma n(x)\cdot\left(\int_\Gamma (g_x(x,y)+g_y(y,x))\kappa(y)W(y)dS(y)\right)V(x)dS(x).
\end{aligned}
$$

We replace instances of $g(x,y)$ and its derivatives by $\tilde g(x,y)$ and its derivatives, as defined by (64). We also replace the integrals of $\tilde g, \tilde g_x, \tilde g_{xx}$ by $G(x,\Gamma), G_x(x,\Gamma), G_{xy}(x,\Gamma)$ respectively. ∎

4.4 Shape Energies with PDEs

In some problems, the shape energy may include a function u that is obtained by solving a PDE on the surface Γ or in the domain Ω enclosed by the surface Γ, namely, we consider energies of the form

$$J(\Gamma) = J_0(\Gamma, u(\Gamma)), \quad \mathcal{A}_\Gamma(u) = f \text{ on } \Gamma, \quad \text{or} \quad J(\Omega) = J_0(\Omega, u(\Omega)), \quad \mathcal{A}_\Omega(u) = f \text{ in } \Omega,$$

where $\mathcal{A}_\Gamma, \mathcal{A}_\Omega$ denote some differential operators. The PDEs represented by $\mathcal{A}_\Gamma, \mathcal{A}_\Omega$ might be in various forms and do not seem to be of interest in image processing except for a few specific cases relating to the Mumford-Shah functional [8, 16, 23, 33, 34] (see Section 2). We will consider these cases below. For other examples of shape energies with PDEs in areas outside image processing, we refer to the books [22, 30, 39, 47].

Energies with domain PDEs. We consider the generalization (20) of the Mumford-Shah energy introduced in Section 2 and compute the first and second shape derivatives of the PDE-dependent part, namely the following domain energy,

$$J(\Omega) = \int_\Omega f(x, \{u_k\}) dx + \frac{\mu}{2} \sum_{k=1}^{m} \int_\Omega |\nabla u_k|^2 dx, \tag{74}$$

where the smooth approximation functions $\{u_k\}_{k=1}^m$ are computed from the PDEs

$$-\Delta u_l + f_{u_l}(x, \{u_k\}) = 0 \text{ in } \Omega, \quad \frac{\partial u_l}{\partial n} = 0 \text{ on } \Gamma = \partial\Omega, \quad l = 1, \ldots, m. \tag{75}$$

In (75), f_{u_l} denotes the derivative of the coupled data function $f(x, \{u_k\})$ with respect to the argument u_l and we assume f is given such that unique solutions of (75) and (78) exist in $H^1(\Omega)$. The shape derivations for (74) follow those of Hintermüller and Ring [33] for the Mumford-Shah energy (15) [16].

Proposition 4.13 *The first shape derivative of the energy* (74) *at* Ω *with respect to velocity* V *is*

$$dJ(\Omega; V) = \int_\Gamma \left(f(x, \{u_k\}) + \frac{\mu}{2} \sum_k |\nabla_\Gamma u_k|^2 \right) V dS. \tag{76}$$

The second shape derivative of (74) *with respect to velocities* V, W *is*

$$\begin{aligned} d^2 J(\Omega; V, W) = &\int_\Gamma \left(f\kappa + \frac{\partial f}{\partial n} + \mu \sum_k \nabla_\Gamma u_k^T \left(\frac{\kappa}{2} Id - \nabla_\Gamma n \right) \nabla_\Gamma u_k \right) V W dS \\ &+ \sum_k \int_\Gamma \left(f_{u_k} u'_{k,W} + \mu \nabla_\Gamma u_k \cdot \nabla_\Gamma u'_{k,W} \right) V dS, \end{aligned} \tag{77}$$

where $u'_{k,W} = u'_k(\Omega; W)$ *is the shape derivative of* u_k *at* Ω *with respect to* W *computed from the PDEs*

$$-\mu \Delta u'_k + \sum_l f_{u_k u_l} u'_{l,W} = 0 \text{ in } \Omega, \quad \frac{\partial u'_{k,W}}{\partial n} = \mathrm{div}_\Gamma (V \nabla_\Gamma u_k) - \frac{1}{\mu} f_{u_k} V \text{ on } \Gamma. \tag{78}$$

Proof. We use Theorem 3.1 and let $\phi(x, \Omega) = f(x, \{u_k\}) + \frac{\mu}{2} \sum_k |\nabla u_k|^2$ so that

$$\phi'(\Omega; V) = \sum_k f_{u_k}(x, \{u_l\}) u'_k + \mu \sum_k \nabla u_k \cdot \nabla u'_k,$$

where $u_k' = u_k'(\Omega; V)$. From Theorem 3.1 it follows that

$$dJ(\Omega; V) = \int_\Omega \sum_k (f_{u_k} u_k' + \mu \nabla u_k \cdot \nabla u_k')\, dx + \int_\Gamma \left(f + \frac{\mu}{2} \sum_k |\nabla_\Gamma u_k|^2 \right) V dS. \tag{79}$$

Note that $\nabla u_k = \nabla_\Gamma u_k$ on Γ since $\frac{\partial u_k}{\partial n} = 0$ on Γ.
Now we investigate $u_k'(\Omega; V)$. Consider the weak form of (75)

$$\int_\Omega (\mu \nabla u_l \cdot \nabla \varphi + f_{u_l} \varphi) dx = 0, \qquad \forall \varphi \in H^1(\Omega) \tag{80}$$

and take the shape derivative (φ is shape-independent)

$$\int_\Omega \left(\mu \nabla u_l' \cdot \nabla \varphi + \sum_k f_{u_l u_k} u_k' \varphi \right) dx + \int_\Gamma (\mu \nabla u_l \cdot \nabla \varphi + f_{u_l} \varphi) V dS = 0.$$

Again recall that $\frac{\partial u_l}{\partial n} = 0$ and substitute $\nabla u|_\Gamma = \nabla_\Gamma u$,

$$\int_\Omega \left(\mu \nabla u_l' \cdot \nabla \varphi + \sum_k f_{u_l u_k} u_k' \varphi \right) dx = - \int_\Gamma (\mu \nabla_\Gamma u_l \nabla_\Gamma \varphi + f_{u_l} \varphi) V dS. \tag{81}$$

This equation has a unique solution $u_l' \in H^1(\Omega)$ and we use it as a test function in (80). In this way we see that the first integral in (79) vanishes, which leaves us with the expression for the first shape derivative.
We also write the strong form of the PDE for the shape derivative u_l'. For this, we first integrate the left hand side of (81) by parts with tangential Green's formula (33)

$$\int_\Omega \left(\mu \nabla u_l' \cdot \nabla \varphi + \sum_k f_{u_l u_k} u_k' \varphi \right) dx = \int_\Gamma \Big(\mu \mathrm{div}_\Gamma (V \nabla_\Gamma u_l) - f_{u_l} V \Big) \varphi dS.$$

Then we have the following PDE for u_l'

$$-\mu \Delta u_l' + \sum_k f_{u_l u_k} u_k' = 0 \text{ in } \Omega, \quad \frac{\partial u_l'}{\partial n} = \mathrm{div}_\Gamma (V \nabla_\Gamma u_l) - \frac{1}{\mu} f_{u_l} V \text{ on } \Gamma.$$

To compute the second shape derivative, we now let $\psi(x, \Gamma) = \big(f(x, \{u_k\}) + \frac{\mu}{2} \sum_k |\nabla_\Gamma u_k|^2 \big) V$ and apply Theorem 3.1. We compute the derivatives $\frac{\partial \psi}{\partial n}$ and $\psi'(\Gamma; W)$.

$$\frac{\partial \psi}{\partial n} = \left(\frac{\partial f}{\partial n} + \sum_k f_{u_k} \frac{\partial u_k}{\partial n} + \frac{\mu}{2} \sum_k \frac{\partial}{\partial n} |\nabla_\Gamma u_k|^2 \right) V + \Big(\dots \Big) \frac{\partial V}{\partial n}.$$

Recall that $\frac{\partial u_k}{\partial n} = 0$ on Γ and $\frac{\partial V}{\partial n} = 0$ by the assumptions (49). Also we have $\frac{\partial}{\partial n}(\nabla_\Gamma u) = -\nabla_\Gamma n \nabla_\Gamma u$ by Lemma 3.1. Therefore

$$\frac{\partial \psi}{\partial n} = \left(\frac{\partial f}{\partial n} - \mu \sum_k \nabla_\Gamma u_k^T \nabla_\Gamma n \nabla_\Gamma u_k \right) V.$$

We compute the shape derivative $\psi' = \psi'(\Gamma; W)$,

$$\psi' = \left(\sum_k f_{u_k} u_{k,W}' + \mu \sum_k \nabla_\Gamma u_k \cdot (\nabla_\Gamma u_k)_W' \right) V + \Big(\dots \Big) V'.$$

By Lemma 3.4 and $\frac{\partial u_k}{\partial n}=0$, we have $(\nabla_\Gamma u_k)' = \nabla_\Gamma u'_{k,W} + \nabla_\Gamma u_k \cdot \nabla_\Gamma W n$ and one can trivially see $V' = (\vec{V}\cdot n)' = \vec{V}\cdot(-\nabla_\Gamma W) = -Vn\cdot\nabla_\Gamma W = 0$. Therefore

$$\begin{aligned}\psi' &= \left(\sum_k f_{u_k} u'_{k,W} + \mu \sum_k \left(\nabla_\Gamma u_k \cdot \nabla_\Gamma u'_{k,W} + \nabla_\Gamma u_k \cdot n \nabla_\Gamma u_k \cdot \nabla_\Gamma W\right)\right) V \\ &= \sum_k \left(f_{u_k} u'_{k,W} + \mu \nabla_\Gamma u_k \cdot \nabla_\Gamma u'_{k,W}\right) V. \qquad (\nabla_\Gamma u_k \cdot n = 0)\end{aligned}$$

The second shape deriative is obtained by plugging ψ, $\frac{\partial \psi}{\partial n}$, ψ' in

$$d^2 J(\Omega; V, W) = \int_\Gamma \psi'(\Gamma; W) dS + \int_\Gamma \left(\psi\kappa + \frac{\partial \psi}{\partial n}\right) W dS.$$

∎

Energies with Surface PDEs. In this section we derive the first shape derivative of the PDE-dependent surface energy

$$J(\Gamma) = \frac{1}{2}\int_\Gamma \left(f(x,\{u_k\}) + \frac{\mu}{2}\sum_k |\nabla_\Gamma u_k|^2\right) dS, \tag{82}$$

where the smooth surface functions $\{u_k\}_{k=1}^m$ are computed from the PDE

$$-\mu\Delta_\Gamma u_l + f_{u_l}(x,\{u_k\}) = 0 \text{ on } \Gamma, \quad l = 1,\dots,m. \tag{83}$$

In (83), f_{u_l} denotes the derivative of the coupled data function $f(x,\{u_k\})$ with respect to the argument u_l and we assume f is given such that unique solutions of the PDEs (83), (88) exist in $H^1(\Gamma)$. The shape energy (82) can be used for shape identification problems, in which smooth approximations $\{u_k\}$ of data channels or descriptors on the surface Γ need to be estimated in addition to the surface Γ itself (e.g. stereoscopic segmentation [34]).

Proposition 4.14 *The first shape derivative of the energy* (82) *at* Γ *with respect to velocity* V *is given by*

$$dJ(\Gamma; V) = \int_\Gamma \left(f\kappa + \frac{\partial f}{\partial n} + \mu \sum_k \nabla_\Gamma u_k^T \left(\frac{\kappa}{2} Id - \nabla_\Gamma n\right)\nabla_\Gamma u_k\right) V dS.$$

Proof. We take the first shape derivative using Theorem 3.1:

$$\begin{aligned}dJ(\Gamma;V) &= \int_\Gamma \left(\sum_k f_{u_k} u'_k + \mu \sum_k \nabla_\Gamma u_k \cdot (\nabla_\Gamma u_k)'\right) dS \\ &\quad + \int_\Gamma \kappa \left(f(x,\{u_k\}) + \frac{\mu}{2}\sum_k |\nabla_\Gamma u_k|^2\right) V dS \\ &\quad + \int_\Gamma \frac{\partial}{\partial n}\left(f(x,\{u_k\}) + \frac{\mu}{2}\sum_k |\nabla_\Gamma u_k|^2\right) V dS.\end{aligned} \tag{84}$$

Meaningful interpretation of the expression (84) requires the functions $\{u_k\}$ to be defined off the surface Γ, because we need to be able to compute their full spatial gradient and the normal derivatives. But $\{u_k\}$ are computed with the PDE (83) and are defined only on Γ. To be able to proceed with the derivations, we work with smooth extensions $\{\tilde{u}_k\}$

of $\{u_k\}$ in a tubular neighborhood U of the surface Γ. We define the extension $\tilde{u}_k$ such that it is constant in the normal direction, i.e. $\frac{\partial \tilde{u}_k}{\partial n} = 0$. To keep notation simple, we will continue to refer to the extended function as u_k.

Using $\frac{\partial u_k}{\partial n} = 0$ and identity (31), we find

$$\frac{1}{2}\frac{\partial}{\partial n}|\nabla_\Gamma u_k|^2 = -\nabla_\Gamma u_k^T \nabla_\Gamma n \nabla_\Gamma u_k, \qquad \frac{\partial}{\partial n}\left(f(x,\{u_k\})\right) = \frac{\partial f}{\partial n}.$$

Then using equation (44) and noting $\nabla_\Gamma u_k \cdot n = 0$ and $\frac{\partial u_k}{\partial n} = 0$, we write

$$\nabla_\Gamma u_k \cdot (\nabla_\Gamma u_k)' = \nabla_\Gamma u_k \cdot \left(\nabla_\Gamma u_k' + \nabla_\Gamma u_k \cdot \nabla_\Gamma V n + \frac{\partial u_k}{\partial n}\nabla_\Gamma V\right) = \nabla_\Gamma u_k \cdot \nabla_\Gamma u_k'.$$

Now we can rewrite the shape derivative

$$\begin{aligned} dJ(\Gamma;V) = &\int_\Gamma \left(\sum_k f_{u_k} u_k' + \mu \sum_k \nabla_\Gamma u_k \cdot \nabla_\Gamma u_k'\right) dS \\ &+ \int_\Gamma \kappa \left(f + \frac{\mu}{2}\sum_k |\nabla_\Gamma u_k|^2\right) V dS + \int_\Gamma \left(\frac{\partial f}{\partial n} - \mu \nabla_\Gamma u^T \nabla_\Gamma n \nabla_\Gamma u\right) V dS, \end{aligned} \tag{85}$$

in which the terms containing the shape derivatives u' will vanish as we will see below. To show this, we start with the weak form of the surface PDE (83)

$$\int_\Gamma \left(\mu \nabla_\Gamma u_l \cdot \nabla_\Gamma \varphi + f_{u_l}\varphi\right) dS = 0, \qquad \forall \varphi \in H^1(\Gamma), \tag{86}$$

also using normal extensions $\tilde{\varphi}$ of the test functions φ with $\frac{\partial \tilde{\varphi}}{\partial n} = 0$ (which we continue to refer to as φ). We differentiate the two terms in (86). Start with the second term,

$$\left(\int_\Gamma f_{u_l}\varphi dS\right)' = \int_\Gamma \sum_k f_{u_l u_k} u_k' \varphi dS + \int_\Gamma \left(\kappa f_{u_l} + \frac{\partial f_{u_l}}{\partial n}\right)\varphi V dS.$$

Then the first term,

$$\begin{aligned} \left(\int_\Gamma \mu \nabla_\Gamma u_l \cdot \nabla_\Gamma \varphi dS\right)' = &\int_\Gamma \left(\mu (\nabla_\Gamma u_l)' \cdot \nabla_\Gamma \varphi + \mu \nabla_\Gamma u_l \cdot (\nabla_\Gamma \varphi)'\right) dS \\ &+ \int_\Gamma \kappa \mu \nabla_\Gamma u_l \cdot \nabla_\Gamma \varphi V dS + \int_\Gamma \frac{\partial}{\partial n}(\mu \nabla_\Gamma u_l \cdot \nabla_\Gamma \varphi) V dS. \end{aligned} \tag{87}$$

We use Lemmas 3.1, 3.4 to rewrite the following terms

$$(\nabla_\Gamma u_l)' \cdot \nabla_\Gamma \varphi = \nabla_\Gamma u_l' \cdot \nabla_\Gamma \varphi + \nabla_\Gamma u_l \cdot \nabla_\Gamma V \nabla_\Gamma \varphi \cdot n + \frac{\partial u_l}{\partial n}\nabla_\Gamma \varphi \cdot \nabla_\Gamma V = \nabla_\Gamma u_l' \cdot \nabla_\Gamma \varphi,$$

$$\nabla_\Gamma u_l \cdot (\nabla_\Gamma \varphi)' = \nabla_\Gamma u_l \cdot \nabla_\Gamma \varphi' = 0, \qquad (\text{note}: \nabla_\Gamma \varphi \cdot n = 0,\ \frac{\partial u_l}{\partial n} = 0)$$

$$\frac{\partial}{\partial n}(\nabla_\Gamma u_l \cdot \nabla_\Gamma \varphi) = -\nabla_\Gamma \varphi^T \nabla_\Gamma n \nabla_\Gamma u_l - \nabla_\Gamma u_l^T \nabla_\Gamma n \nabla_\Gamma \varphi = -2\nabla_\Gamma u_l^T \nabla_\Gamma n \nabla_\Gamma \varphi,$$

and substitute back in (87). Then the shape derivative of weak form (86) is

$$\begin{aligned} &\int_\Gamma \left(\mu \nabla_\Gamma u_l' \cdot \nabla_\Gamma \varphi + \sum_k f_{u_l u_k} u_k' \varphi\right) dS \\ &\qquad = \int_\Gamma \left(\kappa f_{u_l}\varphi + \frac{\partial f_{u_l}}{\partial n}\varphi + \mu \nabla_\Gamma u_l^T (\kappa - 2\nabla_\Gamma n)\nabla_\Gamma \varphi\right) V dS. \end{aligned} \tag{88}$$

The function f is given such that these coupled PDEs have a unique solution $\{u_l'\}$ in $H^1(\Omega)$. We plug in the solutions $\{u_l'\}$ as test functions in (86) and find that

$$\int_\Gamma (\mu \nabla_\Gamma u_l \cdot \nabla_\Gamma u_l' + f_{u_l} u_l')\, dS = 0.$$

This removes the first term in the shape derivative (85). ∎

5 Gradient Descent Flows

The main motivation for deriving the shape derivatives $dJ(\Gamma;V), d^2J(\Gamma;V,W)$ of a given shape energy $J(\Gamma)$ is to design algorithms for minimization of the energy $J(\Gamma)$ and for computing the optimal shape Γ^*. In this section, we briefly review how to develop gradient descent flows, namely energy-decreasing evolutions of the shapes, using shape derivatives for this purpose. We refer to [1, 2, 3, 4, 24, 59] for more information on this topic.

We note, in Theorem 3.2, that the shape derivative has the following form

$$dJ(\Gamma;V) = \int_\Gamma G(\Gamma) V \, dS,$$

where $G(\Gamma)$ (or alternatively $G(\Omega)$) is the shape gradient depending on the shape energy. It is easy to see that, formally by setting $V = -G(\Gamma)$, we obtain a gradient descent velocity

$$dJ(\Gamma;V) = -\int_\Gamma G^2 dS \leqslant 0. \tag{89}$$

The velocity $V = -G(\Gamma)$ is the most commonly used gradient descent velocity for shape optimization problems in image processing. Given a method to compute the gradient descent velocity V, we can now perform the minimization by starting from an initial surface Γ_0 and updating it iteratively, recomputing the velocity for the new shape Γ_{k+1} at each step:

$$\vec{X}_{k+1} = \vec{X}_k + \tau_k \vec{V}_k, \qquad \forall \vec{X} \in \Gamma_k, \tag{90}$$

where $\tau_k > 0$ is a step size parameter that can be fixed or chosen by a line search algorithm. The vector velocity $\vec{V}$ can be computed from the normal velocity V; for a surface Γ with normal n, a natural choice is $\vec{V} = Vn$ as the tangential component of the velocity $\vec{V}$ does not change the shape of the surface. An alternative to the explicit update (90) is to embed the surface in a Eulerian representation, such as a level set function φ, extend the velocity V off the surface, and compute the level set evolution solving the following PDE: $\frac{\partial \varphi}{\partial t} = V|\nabla\varphi|$ [44, 45, 51].

Other gradient descent velocities than $V = -G(\Gamma)$ are possible [4, 17, 24, 57, 58, 59]. We can introduce a scalar product $b(\cdot,\cdot)$ associated with a Hilbert space $B(\Gamma)$ on the surface Γ and use it to compute a different gradient flow by solving the following equation

$$b(V,W) = -\int_\Gamma G(\Gamma) W \, dS, \qquad \forall W \in B(\Gamma). \tag{91}$$

It is easy to verify that the solution V of equation (91) is a gradient descent velocity; we substitute it in the shape derivative and see that $dJ(\Gamma;V) = -b(V,V) \leqslant 0$ (as the scalar product $b(\cdot,\cdot)$ is positive definite).

The velocity $V = -G(\Gamma)$ mentioned above is actually the L^2 gradient descent velocity obtained by setting the scalar product equal to the L^2 scalar product, $b(V,W) = \int_\Gamma VW dS$, in (91). We can take advantage of other scalar products $b(\cdot,\cdot)$ in order to obtain velocities that improve the descent process in various ways [17, 24, 57, 58]. For example, an H^1 scalar product,

$$b(V,W) = \int_\Gamma \alpha(x)\nabla_\Gamma V \cdot \nabla_\Gamma W + \beta(x) V W dS, \quad (\alpha(x), \beta(x) > 0),$$

results in smoother velocities that are advantageous in applications of segmentation and tracking [54, 58].

Another option is to use the second shape derivative as the basis of the scalar product, for example, set

$$b(V,W) = d^2 J(\Gamma; V, W), \tag{92}$$

This choice results in a Newton's method for shape optimization. It can yield quadratic convergence in the neighborhood of the solution. However, direct use of the scalar product (92) may not always be possible, because the second shape derivative $d^2 J(\Gamma; \vec{V}, \vec{W})$ may not always satisfy the properties of a scalar product, for example, it may not be positive definite. In this case, one can still design a scalar product $b(\cdot,\cdot)$ based on the second shape derivative and retain partially the favorable convergence properties. This was pursued successfully in [23, 32, 33] and used to achieve a significant reduction in the number iterations needed for convergence to the optimal shape.

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