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Finite Element-Based Level Set Methods for Higher Order Flows

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Abstract In this paper we shall discuss the numerical simulation of geometric flows by level set methods. Main examples under considerations are higher order flows, such as surface diffusion and Willmore flow as well as variants of them with more complicated surface energies. Such problems find various applications, e.g. in materials science (thin film growth, grain boundary motion), biophysics (membrane shapes), and computer graphics (surface smoothing and restoration).

We shall use spatial discretizations by finite element methods and semi-implicit time stepping based on local variational principles, which allows to maintain dissipation properties of the flows by the discretization. In order to compensate for the missing maximum principle, which is indeed a major hurdle for the application of level set methods to higher order flows, we employ frequent redistancing of the level set function.

Finally we also discuss the solution of the arising discretized linear systems in each time step and some particular advantages of the finite element approach such as the variational formulation which allows to handle the higher order and various anisotropies efficiently and the possibility of local adaptivity around the zero level set.

Keywords Level set methods · Higher-order geometric flows · Finite element methods · Semi-implicit time stepping · Energy dissipation

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1 Introduction

Higher order geometric flows received growing attention in the recent years due to emerging applications in various fields, where higher order typically means higher than second order intrinsic derivatives of the surface appearing in the evolution equations. Significant advances have been made in the modelling and understanding of certain flows, while the rigorous mathematical analysis and the construction of flexible computational schemes still lack behind. In particular the use of level set methods, which became popular for lower order flows in the last decade, is not yet well understood. Major obstacles for level set methods in higher order flows are the absence of maximum and comparison principles, which excludes global level set approaches, and the stiffness of the problems, which excludes explicit time stepping to a large extent.

In this paper we develop level set methods for the simulation of higher-order flows based on finite element discretizations in space and semi-implicit time discretizations. The issue of the missing maximum principle is resolved by frequent redistancing. This corresponds to a paradigm for local level set formulations in the continuous setting: a level set solution to a higher-order flow would be an evolving signed distance function that satisfies the geometric evolution equation on the interface (the zero level set) only.

The basis of our approach is a variational formulation of the geometric flows as metric gradient flows (cf. [1, 2, 10]). This means that the computation of an evolving (embedded) curve or surface $\Gamma(t)$ is determined by an energy E (defined on a class of shapes) and a metric structure on a manifold of curves and surfaces. The evolution is determined via the normal velocity v_n, which satisfies an equation of the form

$$\langle v_n, \psi \rangle_{M(\Gamma(t))} = -e'[\Gamma(t)]\psi, \tag{1}$$

for all suitable test velocities ψ, where the scalar product is determined by the metric structure $M(\Gamma(t))$. The right-hand side $e'[\Gamma(t)]\psi$ denotes the variation of the energy functionals with respect to infinitesimal perturbations of the shape with a vector field ψn (which can also be interpreted as a shape derivative, cf. [17]), where n denotes the unit outward normal. Under suitable conditions the shape derivative $e'[\Gamma(t)]$ is a continuous linear functional on the space of test velocities. The most important choices of scalar product in this context are the L^2 and H^{-1} scalar product. In the case of $M(\Gamma(t))$ denoting the L^2-scalar product on $\Gamma(t)$, we obtain

$$\int_{\Gamma(t)} v_n \psi \, d\sigma = -e'[\Gamma(t)]\psi \quad \forall \psi \in L^2(\Gamma(t)).$$

Hence, the normal velocity is just the L^2-representation of the linear functional $e'[\Gamma(t)]$. In the case of e being the area functional, i.e.

$$e[\Gamma(t)] = \int_{\Gamma(t)} 1 \, d\sigma,$$

the variation is computed via the mean curvature h of the surface as

$$e'[\Gamma(t)]\psi = \int_{\Gamma(t)} h\psi \, d\sigma.$$

Thus, one sees that the associated L^2-gradient flow yields the mean curvature flow $v_n = -h$.

In the case of the H^{-1}-scalar product we have

$$\langle v_n, \psi \rangle_{M(\Gamma(t))} = \int_{\Gamma(t)} \nabla_\sigma W_{v_n} \cdot \nabla_\sigma W_\psi \, d\sigma, \tag{2}$$

with the tangential gradient ∇_σ and W_ψ defined by the Laplace-Beltrami equation

$$-\nabla_\sigma \cdot (\nabla_\sigma W_\psi) = \psi, \quad \text{on } \Gamma(t) \tag{3}$$

with the additional normalization condition $\int_{\Gamma(t)} W_\psi \, d\sigma = 0$. In the case of the area functional the equation for the normal velocity becomes

$$\int_{\Gamma(t)} W_{v_n} \psi \, d\sigma = -\int_{\Gamma(t)} W_{v_n} \nabla_\sigma \cdot (\nabla_\sigma \psi) \, d\sigma = \int_{\Gamma(t)} \nabla_\sigma W_{v_n} \cdot \nabla_\sigma W_\psi \, d\sigma = -\int_{\Gamma(t)} h\psi \, d\sigma$$

and hence, $W_{v_n} = -h$. An application of the Laplace-Beltrami operator finally yields $v_n = \nabla_\sigma \cdot (\nabla_\sigma h)$, i.e. motion by the Surface-Laplacian of curvature, which is the simplest form of a surface diffusion law (cf. [27]). Thus, we see that the choice of the H^{-1} scalar product automatically leads to higher order flows, in the above example to a fourth order one.

Another source for higher order geometric flows are simply higher order terms in the surface energy, such as curvatures or even intrinsic derivatives of curvatures. A simple and well-known example is the so-called *Willmore energy*

$$e[\Gamma] = \frac{1}{2} \int_{\Gamma(t)} h^2 \, d\sigma. \tag{4}$$

Since the energy includes second order derivatives via the mean curvature h, its variation (more precisely the L^2 representation) corresponds to a fourth order differential operator. Thus, in the L^2 scalar product one obtains a fourth order flow, the so-called *Willmore flow*, and by analogy to the above computation we even obtain a sixth order flow in the H^{-1} scalar product.

The paper is organized as follows: In Sect. 2 we derive level set formulations for the geometric evolution laws, directly from the metric gradient flow formulation. In Sect. 3 we introduce the finite element formulation for spatial discretization, which is indeed straightforward. As a consequence of the gradient flow formulation, we construct local-in-time variational problems corresponding to implicit time discretizations, and by further quadratic approximations of the energy functional we obtain semi-implicit schemes in Sect. 4. In Sect. 5 we discuss some aspects of redistancing on triangular finite element grids in two and three spatial dimensions. Details about implementation and numerical results are presented in Sect. 6.

Most of the derived discretizations can be considered as special cases of the more complicated evolution laws considered by the authors in [9] or other approaches for surface diffusion and Willmore flow, see [16, 19], respectively. A direct derivation of the energy dissipative discretization schemes from the underlying gradient flow however is not considered in these papers. Moreover, we provide a unified concept for the derivation of (weak) level set formulations, their discretization, and for stability studies. This concept can be applied in a straight-forward way to various higher-order flows such as some almost classical examples considered in the remainder of this paper.

2 Level Set Formulation of the Models

In this section we discuss the level set formulation of the higher order flows distinguishing two cases, namely lower order energies such as the area functional or classical surface energies appearing in materials science, and higher order energies such as the Willmore energy. This distinction is due to the fact that we try to split the higher-order flows into second order systems by the introduction of new variables such as the mean curvature (and constraints defining the new variables in terms of the level set function). In the case of low order energies these variables have to be introduced only in order to approximate the metric, which happens in a very natural way, whereas in the case of higher order energies additional variables are needed in dependence on the metric. In both cases, the constraints can be modeled by using associated Lagrange functionals, the Lagrangian variables will turn out to obey very simple relations in several cases and sometimes also provide interesting new quantities as we shall see below.

2.1 Basic Notations and Level Set Formulations

We start with some basic notations for level set formulations, avoiding a too detailed discussion of level set methods at this point (cf. [28, 29] for further detail). We assume $\Gamma(t) \subset \Omega \subset \mathbb{R}^d$ to be the union of evolving curves or surfaces, which are embedded, i.e.

$$\Gamma(t) = \partial\Theta(t), \quad \overline{\Theta(t)} \subset \Omega^\circ.$$

The level set approach chooses a function $\phi : \Omega \times \mathbb{R} \to \mathbb{R}$ such that

$$\Gamma(t) = \{\phi(.,t) = 0\}, \qquad \Theta(t) = \{\phi(.,t) < 0\}.$$

It is well known (cf. e.g. [28]) that the unit outward normal vector n (pointing into $\Omega \setminus \Theta(t)$), the normal velocity v, and the mean curvature h of the evolving surface can be represented as

$$n = \frac{\nabla\phi}{|\nabla\phi|}|_{\Gamma(t)}, \qquad v_n = -\frac{\partial_t\phi}{|\nabla\phi|}|_{\Gamma(t)}, \qquad h = \nabla\cdot\left(\frac{\nabla\phi}{|\nabla\phi|}\right)|_{\Gamma(t)}, \tag{5}$$

where we assume that $\nabla\phi \neq 0$. Note that with this sign convention a closed sphere with outer normal n has positive mean curvature $h > 0$. For simplicity we impose in the following natural boundary conditions for ϕ (and other variables) on the boundary of the computational domain $\partial\Omega$. These natural boundary conditions will be inherent in the weak formulations (no boundary integrals appearing, no Dirichlet values constrained) and depend on the specific metric and energy functional. They will be detailed in the examples below.

2.2 Level Set Formulation I: Low Order Energies

We start with low order energies, i.e., energy functionals of the form

$$e[\Gamma] = \int_\Theta f(x) + \int_\Gamma g(x,n)\,d\sigma, \tag{6}$$

where n denotes the outward unit normal. In many cases f and also parts of g arise through nonlocal interactions, usually modelled via partial differential equations with boundaries or coefficients dependent on Γ. However, such situations can be incorporated via Lagrange functionals, so that the effective functional to be minimized or differentiated with respect to the shape variable always ends up in the form (6).

In the level set context we average the energy over all level sets of ϕ, which yields a new energy on all level sets, respectively on the level set function ϕ directly. For the sake of simplicity we assume that extensions $F : \Omega \to \mathbb{R}$ and $G : \Omega \times R^d \to \mathbb{R}$ of f and g are known (with G being one-homogeneous in the second variable), if not the extensions can be computed in a rather standard way (e.g. constant in normal direction, cf. [28]). Then we obtain the energy from the layer-cake and co-area formula as

$$\begin{aligned} E[\phi] &= \int_{-\infty}^{\phi_{\max}} \int_{\{\phi=\alpha\}\cap\Omega} G\left(x, \frac{\nabla\phi}{|\nabla\phi|}\right) d\sigma\, d\alpha + \int_{-\infty}^{\phi_{\max}} \int_{\{\phi<\alpha\}\cap\Omega} F(x)\, dx\, d\alpha \\ &= \int_\Omega G(x, \nabla\phi)\, dx + \int_\Omega F(x)(\phi_{\max} - \phi(x))\, dx, \end{aligned}$$

where $\phi_{\max}$ is greater than the maximal value of ϕ appearing in Ω. Since constant terms do not matter for the minimization and variations with respect to ϕ we define the averaged energy as

$$E[\phi] = \int_\Omega G(x, \nabla\phi)\, dx - \int_\Omega F(x)\phi(x)\, dx. \tag{7}$$

In order to compute variations in normal directions we recall the basic level set equation

$$\partial_t \phi = -V_n |\nabla\phi|,$$

for V_n being an extension of the normal velocity v_n. Hence, we compute variations of ϕ only for directions of the form $-V_n|\nabla\phi|$. It is easy to see that the identity

$$E'[\phi](-V_n|\nabla\phi|) = \int_{-\infty}^{\phi_{\max}} e'[\{\phi=\alpha\}] V_n\, d\alpha \tag{8}$$

holds for such variations.

In a similar way we can average the scalar products used in the definitions of the geometric flows. The L^2 scalar product can be averaged with the co-area formula as

$$\int_{-\infty}^{\phi_{\max}} \int_{\{\phi=\alpha\}} \psi_1\psi_2\, d\sigma\, d\alpha = \int_\Omega \psi_1\psi_2|\nabla\phi|\, dx = \langle\psi_1, \psi_2\rangle_\phi. \tag{9}$$

For the H^{-1} scalar product we use the weak formulation of the Laplace-Beltrami Operator and the simple relation

$$\nabla_\sigma W = \mathbf{P}\nabla W, \qquad \mathbf{P} = \mathbf{I} - n\otimes n = \mathbf{I} - \frac{\nabla\phi}{|\nabla\phi|}\otimes\frac{\nabla\phi}{|\nabla\phi|}$$

for the tangential derivative to obtain the scalar product $\langle\psi_1, \psi_2\rangle_\phi$ as

$$\int_{-\infty}^{\phi_{\max}} \int_{\{\phi=\alpha\}} \nabla_\sigma W_{\psi_1} \cdot \nabla_\sigma W_{\psi_2}\, d\sigma\, d\alpha = \int_\Omega (\mathbf{P}\nabla W_{\psi_1})\cdot(\mathbf{P}\nabla W_{\psi_2})|\nabla\phi|\, dx, \tag{10}$$

where a function W_ψ is defined as a weak solution of the (averaged) Laplace-Beltrami equation, i.e.

$$\int_\Omega (\mathbf{P}\nabla W_\psi)\cdot(\mathbf{P}\nabla\eta)|\nabla\phi|\, dx = \int_\Omega \psi\eta|\nabla\phi|\, dx \tag{11}$$

for all suitable test functions η.

Now we can simply reformulate the geometric gradient flow as a metric gradient flow on the level set functions via (note that for a variation ψ, the function $-\frac{\psi}{|\nabla\phi|}$ is an extended normal variation)

$$\left\langle V_n, -\frac{\psi}{|\nabla\phi|}\right\rangle_\phi = -\left\langle \frac{\partial_t\phi}{|\nabla\phi|}, -\frac{\psi}{|\nabla\phi|}\right\rangle_\phi = -E'[\phi](\psi),$$

or, equivalently

$$\left\langle \frac{\partial_t\phi}{|\nabla\phi|}, \frac{\psi}{|\nabla\phi|}\right\rangle_\phi = -E'[\phi](\psi). \tag{12}$$

In the case of the area functional ($F \equiv 0$, $G \equiv 1$) and the L^2 scalar product we thus obtain the well-known (weak) level set formulation of the mean curvature flow

$$\int_\Omega \frac{\partial_t\phi\psi}{|\nabla\phi|}\,dx = -\int_\Omega \frac{\nabla\phi\cdot\nabla\psi}{|\nabla\phi|}\,dx = \int_\Omega H\psi\,dx, \tag{13}$$

for all suitable test functions ψ, where $H = \nabla\cdot(\frac{\nabla\phi}{|\nabla\phi|})$ is the extended mean curvature. For the H^{-1} scalar product we use the variable $W := W_{V_n}$ and the identity

$$\int_\Omega (\mathbf{P}\nabla W)\cdot(\mathbf{P}\nabla W_{-\frac{\psi}{|\nabla\phi|}})|\nabla\phi|\,dx = -\int_\Omega W\psi\,dx$$

to obtain in an analogous way the (weak) level set formulation of the simple surface diffusion law, i.e.,

$$\int_\Omega W\psi\,dx = \int_\Omega \frac{\nabla\phi\cdot\nabla\psi}{|\nabla\phi|}\,dx \tag{14}$$

$$\int_\Omega (\mathbf{P}\nabla W)\cdot(\mathbf{P}\nabla\eta)|\nabla\phi|\,dx = -\int_\Omega \partial_t\phi\eta\,dx \tag{15}$$

for suitable test functions ψ and η. One observes that we have automatically split the problem into a system of second order equations incorporating the new variable W, which actually equals the extended mean curvature H.

We mention that the derivation of the level set formulations could (and have been, see [9, 16, 19]) also be made by directly rewriting the evolution law in terms of the level set function. For complicated energies, this procedure is rather tedious since one needs to compute the shape derivative first (which can be a hard task for itself) and then one has to compute transformations of higher derivatives to the level set form. This can be avoided in the above approach, one can directly convert the energy to level set form and then compute classical variations in a function setting. Clearly the above derivation also provides a natural weak level set formulation, which directly leads to finite element discretizations of the equations. Our approach thus provides a general way to derive (weak) level set formulations no matter how complicated the free energy or the metric structure might be.

For more general metrics we can formulate the above procedure as rewriting the metric via a Lagrange-functional of the form

$$\left\langle \frac{\partial_t\phi}{|\nabla\phi|}, \frac{\psi}{|\nabla\phi|}\right\rangle_\phi = \partial_\phi L[\partial_t\phi, W, Q; \phi]\psi, \tag{16}$$

where W is the collection of $m_W \in \mathbb{N}_0$ new variables introduced to rewrite the metric and Q are the m_W Lagrange multipliers (dual variables) associated to the new constraints defining W. These variables are defined via the conditions

$$\partial_W L[\partial_t\phi, W, Q; \phi] = 0, \qquad \partial_Q L[\partial_t\phi, W, Q; \phi] = 0.$$

In the case of the H^{-1} scalar product above we have

$$L[\psi, W, Q; \phi] = \frac{1}{2}\int_\Omega |\mathbf{P}\nabla W|^2\,dx + \int_\Omega ((\mathbf{P}\nabla W)(\mathbf{P}\nabla Q) + \psi Q)\,dx.$$

It is easy to see from the specific form of the functional that the condition $\partial_W L[\partial_t\phi, W, Q; \phi] = 0$ implies $Q = -W$. Moreover, $\partial_Q L[\partial_t\phi, W, Q; \phi] = 0$ yields (15). Finally, inserting $Q = -W$ in (16) and (12) yields (14).

The natural boundary condition on $\partial\Omega$ for the level set function ϕ is solely determined by the energy functional, we obtain

$$\partial_{\nabla\phi} G(x, \nabla\phi) \cdot n_{\partial\Omega} = 0.$$

Further boundary conditions for auxiliary variables may arise from the specific metric, e.g. we obtain

$$(\mathbf{P}\nabla W) \cdot n_{\partial\Omega} = 0.$$

We shall assume in the following that L depends at most quadratically on $\partial_t\phi$ and W and linearly on Q. The assumptions on $\partial_t\phi$ and W are easy to achieve due to the bilinear nature of the scalar product, and the linearity with respect to the dual variable Q is a natural property of Lagrange functionals. The only nonlinear dependence in L thus appears with respect to the level set function ϕ itself, which can be taken care of easily in the time discretization.

2.3 Level Set Formulation II: Higher Order Energies

The second case we consider are higher-order energies such as the Willmore functional. Then we have to introduce m_U ($m_U \in \mathbb{N}_0$) further variables U for the splitting and another Lagrangian functional Λ in order to take care of the constraints defining the new variables, and m_U associated Lagrangian or dual variables R. Hence, we shall write

$$E[\phi] = \Lambda[\phi, U, R], \tag{17}$$

with U and R being defined via

$$\partial_U \Lambda[\phi, U, R] = 0, \qquad \partial_R \Lambda[\phi, U, R] = 0. \tag{18}$$

Consequently, with the scalar product defined through a Lagrange functional L we equivalently rewrite (12) as

$$\partial_\psi L[\partial_t\phi, W, Q; \phi] = -\partial_\phi \Lambda(\phi, W, Q). \tag{19}$$

We illustrate the procedure for the L^2 gradient flow of the Willmore functional in level set form

$$E[\phi] = \frac{1}{2}\int_\Omega H^2 |\nabla\phi|\,dx = \int_{-\infty}^{\phi_{\max}} \int_{\{\phi=\alpha\}} h^2\,d\sigma\,d\alpha.$$

Here we can simply introduce the variable $U = H$ and the Lagrange functional

$$\Lambda[\phi, U, R] = \frac{1}{2}\int_\Omega U^2|\nabla\phi|\,dx + \int_\Omega \left(-UR + \frac{\nabla\phi\cdot\nabla R}{|\nabla\phi|}\right)dx.$$

Note that $\partial_R\Lambda[\phi, U, R] = 0$ yields exactly the weak formulation of the equation $U = \nabla\cdot(\frac{\nabla\phi}{|\nabla\phi|})$, which defines mean curvature. Moreover, from $\partial_U\Lambda[\phi, U, R] = 0$ we conclude $R = U|\nabla\phi|$. Thus, the dual variable is exactly the *curvature concentration* introduced for the level set formulation of the Willmore flow directly in [19]. One could now use this identity to eliminate U in favour of R as in [19] and one observes that in the general approach above it does not matter which variable we choose for splitting. If we would choose $U = H|\nabla\phi|$ directly as the curvature concentration, then we would obtain the mean curvature as the dual variable.

Natural boundary conditions for the level set functions are inherited already in the formulation via the Lagrange functional. For the Willmore energy we obtain

$$\nabla\phi\cdot n_{\partial\Omega} = \nabla R\cdot n_{\partial\Omega} = 0.$$

2.4 Energy Dissipation for the Level Set Formulation

In the following we verify the energy dissipation for (19). Using the test functions $\partial_t\phi$, we get

$$\begin{aligned}\langle\partial_t\phi, \partial_t\phi\rangle_\phi &= \partial_\psi L[\partial_t\phi, W, Q; \phi]\partial_t\phi\\ &= -\partial_\phi\Lambda[\phi, U, R]\partial_t\phi\\ &= -E'[\phi]\partial_t\phi = -\frac{d}{dt}E[\phi],\end{aligned}$$

or in other words,

$$\frac{d}{dt}E[\phi] = -\langle\partial_t\phi, \partial_t\phi\rangle_\phi = -\|\partial_t\phi\|_\phi^2. \tag{20}$$

The energy dissipation property will play a central role in the later time discretization of the flows.

3 Spatial Discretization

In the following we discuss the spatial discretization of the higher order flows or more precisely their level set formulation (19) introduced above. We assume that the new splitting variables have been introduced such that the highest arising differential operators are of second order, which means that only up to first derivatives of all variables appear in the Lagrange functionals L and Λ. Consequently, and also due to the dissipative nature of the flows, it is natural to use finite element methods for the spatial semi-discretization, which we shall briefly discuss in this section.

We choose appropriate finite element subspaces $\mathcal{V}^h \subset \mathcal{V}$ and look for weak solutions satisfying the variational problems in a product of this subspace. Here we shall use $\mathcal{V} = H^1(\Omega)$ and the standard piecewise linear elements

$$\mathcal{V}^h = \{v \in C(\Omega) \mid v|_T \text{ is linear polynomial for } T \in \mathcal{T}\}, \tag{21}$$

where $\mathcal{T}$ is a decomposition of the polygonal domain Ω into triangles (2D) or tetrahedra (3D). Moreover we assume natural boundary conditions for all variables on the boundary $\partial\Omega$. For the sake of simplicity we assume here that all variables can be discretized robustly by the same kind of elements, i.e., we look for

$$(\phi^h, W^h, U^h, Q^h, R^h) \in \mathcal{P}^h = \mathcal{V}^h \times (\mathcal{V}^h)^{m_U} \times (\mathcal{V}^h)^{m_W} \times (\mathcal{V}^h)^{m_U} \times (\mathcal{V}^h)^{m_W}.$$

This assumption roughly means that our splitting variables do not include flux-type variables (like $\nabla\phi$ or the normal $\frac{\nabla\phi}{|\nabla\phi|}$). The justification of this assumption can be made through appropriate inf-sup conditions on the Lagrange functionals in the above subspaces (as standard in mixed finite element discretizations, cf. [6]), at least after linearization of the system. We do not go into detail at this point for the sake of brevity, but just mention that these conditions are indeed satisfied for all the examples of flows and splitting variables we use here.

The finite element semi-discretization of the geometric flow defined via (19) is then given by the Galerkin discretization

$$\begin{aligned}
&\partial_\psi L[\partial_t\phi^h, W^h, Q^h; \phi^h]\eta_1 + \\
&\qquad \partial_\phi \Lambda(\phi^h, U^h, R^h)\eta_1 = 0 \quad \forall \eta_1 \in \mathcal{V}^h && (22)\\
&\partial_W L[\partial_t\phi^h, W^h, Q^h; \phi^h]\eta_2 = 0 \quad \forall \eta_2 \in (\mathcal{V}^h)^{m_W} && (23)\\
&\partial_Q L[\partial_t\phi^h, W^h, Q^h; \phi^h]\eta_3 = 0 \quad \forall \eta_3 \in (\mathcal{V}^h)^{m_W} && (24)\\
&\partial_U \Lambda(\phi^h, U^h, R^h)\eta_4 = 0 \quad \forall \eta_4 \in (\mathcal{V}^h)^{m_U} && (25)\\
&\partial_R \Lambda(\phi^h, U^h, R^h)\eta_5 = 0 \quad \forall \eta_5 \in (\mathcal{V}^h)^{m_U}. && (26)
\end{aligned}$$

It is easy to see that the discretized problem (22)–(26) still satisfies an energy dissipation property. For this sake we choose $\eta_1 = \partial_t\phi$ and obtain

$$\partial_\psi L[\partial_t\phi^h, W^h, Q^h; \phi^h]\partial_t\phi^h = -\partial_\phi \Lambda(\phi^h, U^h, R^h)\partial_t\phi^h.$$

Using (25) und (26) we deduce

$$\begin{aligned}
\frac{d}{dt}\Lambda(\phi^h, U^h, R^h) &= \partial_\phi \Lambda(\phi^h, U^h, R^h)\partial_t\phi^h + \partial_U \Lambda(\phi^h, U^h, R^h)\partial_t U^h \\
&\quad + \partial_R \Lambda(\phi^h, U^h, R^h)\partial_t R^h \\
&= \partial_\phi \Lambda(\phi^h, U^h, R^h)\partial_t\phi^h.
\end{aligned}$$

Now we define the discrete energy functional

$$E_h[\varphi^h] = \Lambda(\phi^h, U^h, R^h) \tag{27}$$

with U^h and R^h determined by (25) and (26), and a discrete scalar product

$$\langle \psi_1^h, \psi_2^h \rangle_{\phi,h} = \partial_\psi L[\psi_1^h\phi^h, W^h, Q^h; \phi^h]\psi_2^h.$$

Then the semi-discrete energy dissipation becomes

$$\frac{d}{dt}E_h[\phi^h] = \frac{d}{dt}\Lambda(\phi^h, U^h, R^h) = -\langle \partial_t\phi^h, \partial_t\phi^h \rangle_{\phi,h}.$$

We finally mention that in the case of lower order energies, where we need not apply any approximation of E by a Lagrange functional, we indeed obtain $E = E_h$, i.e., energy dissipation with respect to the original energy E.

4 Time Discretization

In the following we discuss the implicit and semi-implicit time discretization of the geometric flows (19), respectively the semi-discrete problems (22)–(23). We mention again that due to the missing maximum principle these discretizations have to be interpreted in a local way, i.e., after computing one (sufficiently small) time step of the level set equation we require a redistancing step, with the details of redistancing to be discussed in the next section.

The time discretization will be carried out at the time steps $0 = t_0 < t_1 < \cdots < t_N = T$, with local time step $\tau_k = t_{k+1} - t_k < \tau$. We shall denote the discrete solution by $\phi_k^{h,\tau} = \phi^{h,\tau}(t_k) \in \mathcal{V}^h$ (with analogous notation for the other variables).

4.1 Implicit Time Stepping

In order to gain further insight into the time discretization based on the Lagrange functionals introduced in the previous session we start with a simple implicit time discretization at least with respect to the energy functional. This means we approximate the scalar product at the previous time step, more precisely we approximate all terms depending on $\phi^{h,\tau}$ in L by values at the previous time step, and we use the backward Euler approximation

$$\partial_t \phi^{h,\tau}(t_{k+1}) \approx \frac{1}{\tau_k}(\phi_{k+1}^{h,\tau} - \phi_k^{h,\tau}).$$

These decisions yield the implicit scheme

$$\frac{1}{\tau_k}\langle \phi_{k+1}^{h,\tau} - \phi_k^{h,\tau}, \eta_1\rangle_k = -\partial_\phi E_h[\phi_{k+1}^{h,\tau}]\eta_1 = -\partial_\phi \Lambda[\phi_{k+1}^{h,\tau}, U_{k+1}^{h,\tau}, R_{k+1}^{h,\tau}]\eta_1$$

for all $\eta_1 \in \mathcal{V}^h$, where we use the short-hand notation

$$\langle \psi_1, \psi_2\rangle_k := \langle \psi_1, \psi_2\rangle_{\phi_k^{h,\tau}} = \partial_\psi L[\psi_1, W_1, Q_1; \phi_k^{h,\tau}].$$

In terms of the Lagrange functionals we can write down the fully discrete implicit scheme as the solution

$$\frac{1}{\tau_k}\partial_\phi L[\phi_{k+1}^{h,\tau} - \phi_k^{h,\tau}, W_{k+1}^{h,\tau}, Q_{k+1}^{h,\tau}; \phi_k^{h,\tau}]\eta_1 + \partial_\phi \Lambda(\phi_{k+1}^{h,\tau}, U_{k+1}^{h,\tau}, R_{k+1}^{h,\tau})\eta_1 = 0 \tag{28}$$

$$\partial_W L[\phi_{k+1}^{h,\tau} - \phi_k^{h,\tau}, W_{k+1}^{h,\tau}, Q_{k+1}^{h,\tau}; \phi_k^{h,\tau}]\eta_2 = 0 \tag{29}$$

$$\partial_Q L[\phi_{k+1}^{h,\tau} - \phi_k^{h,\tau}, W_{k+1}^{h,\tau}, Q_{k+1}^{h,\tau}; \phi_k^{h,\tau}]\eta_3 = 0 \tag{30}$$

$$\partial_U \Lambda(\phi_{k+1}^{h,\tau}, U_{k+1}^{h,\tau}, R_{k+1}^{h,\tau})\eta_4 = 0 \tag{31}$$

$$\partial_R \Lambda(\phi_{k+1}^{h,\tau}, U_{k+1}^{h,\tau}, R_{k+1}^{h,\tau})\eta_5 = 0 \tag{32}$$

for all $(\eta_1, \ldots, \eta_5) \in \mathcal{P}^h$. with respect to

$$(\phi_{k+1}^{h,\tau}, W_{k+1}^{h,\tau}, U_{k+1}^{h,\tau}, Q_{k+1}^{h,\tau}, R_{k+1}^{h,\tau}) \in \mathcal{P}^h.$$

One observes that after time discretization all variations of Lagrange functionals are taken with respect to $\phi_{k+1}^{h,\tau}$ using the fixed previous time value $\phi_k^{h,\tau}$. Hence, the first equation (28) can also be reformulated as a minimization with respect to $\phi_{k+1}^{h,\tau}$. Also the other equations are optimality conditions of an optimization problem, and taking into account the usual convention for Lagrangian's (minimization with respect to primal and maximiza-

tion with respect to dual variables) we actually compute the variables at the next time step $(\phi_{k+1}^{h,\tau}, W_{k+1}^{h,\tau}, U_{k+1}^{h,\tau}, Q_{k+1}^{h,\tau}, R_{k+1}^{h,\tau})$ as a solution of the saddle point problem

$$\inf_{\phi,W,U} \sup_{Q,R} \left(\frac{1}{2\tau} L[\phi - \phi_k^{h,\tau}, W, Q] + \Lambda[\phi, W, Q] \right) \tag{33}$$

over the discrete subspaces. We can also rewrite the discrete problem in the form of minimizing movements for a gradient flow (cf. [2])

$$\phi_{k+1}^{h,\tau} \in \arg\min_{\phi} \left(\frac{1}{2\tau} \|\phi - \phi_k^{h,\tau}\|_k^2 + E_h[\phi] \right),$$

with the squared norm

$$\|\phi - \phi_k^{h,\tau}\|_k^2 := \inf_W \sup_Q L[\phi - \phi_k^{h,\tau}, W, Q]$$

and

$$E_h[\phi] := \inf_U \sup_R \Lambda[\phi, U, R].$$

For illustration purpose we mention the implicit schemes for mean curvature flow

$$\int_\Omega \frac{(\phi_{k+1}^{h,\tau} - \phi_k^{h,\tau})\eta}{\tau |\phi_k^{h,\tau}|}\, dx + \int_\Omega \frac{\nabla \phi_{k+1}^{h,\tau} \cdot \nabla \eta}{|\phi_{k+1}^{h,\tau}|} = 0, \tag{34}$$

with η an appropriate test function. The implicit scheme for surface diffusion reads

$$\int_\Omega Q_{k+1}^{h,\tau} \eta_1 \; + \int_\Omega \frac{\nabla \phi_{k+1}^{h,\tau} \cdot \nabla \eta_1}{|\phi_{k+1}^{h,\tau}|}\, dx = 0$$

$$\int_\Omega (\mathbf{P}_k \nabla (W_{k+1}^{h,\tau} + Q_{k+1}^{h,\tau})) \cdot (\mathbf{P}_k \nabla \eta_2)\, dx = 0$$

$$\frac{1}{\tau} \int_\Omega (\phi_{k+1}^{h,\tau} - \phi_k^{h,\tau}) \eta_3\, dx + \int_\Omega (\mathbf{P}_k \nabla Q_{k+1}^{h,\tau}) \cdot (\mathbf{P}_k \nabla \eta_3)\, dx = 0,$$

with $\mathbf{P}_k = \mathbf{I} - \frac{\nabla \phi_k^{h,\tau}}{|\nabla \phi_k^{h,\tau}|} \otimes \frac{\nabla \phi_k^{h,\tau}}{|\nabla \phi_k^{h,\tau}|}$ and η, η_1, η_2 and η_3 being appropriate test functions. As in the continuous setting we can still deduce $Q_{k+1}^{h,\tau} = -W_{k+1}^{h,\tau}$ from the second equation and eliminate the dual variable in order to obtain an analogous form to (14), (15). For the Willmore flow with $U = H$ we obtain

$$\int_\Omega \left[\frac{(\phi_{k+1}^{h,\tau} - \phi_k^{h,\tau})\eta_1}{\tau |\phi_k^{h,\tau}|} + \frac{1}{2} U_{k+1}^{h,\tau} \frac{\phi_{k+1}^{h,\tau} \cdot \nabla \eta_1}{|\phi_{k+1}^{h,\tau}|} + \frac{\mathbf{P}_{k+1} \nabla \eta_4 \cdot \mathbf{P}_{k+1} \nabla \eta_1}{\tau |\phi_{k+1}^{h,\tau}|} \right] dx = 0$$

$$\int_\Omega (U_{k+1}^{h,\tau} |\phi_{k+1}^{h,\tau}| - R_{k+1}^{h,\tau}) \eta_4\, dx = 0$$

$$\int_\Omega \left(-U_{k+1}^{h,\tau} \eta_5 + \frac{\nabla \phi_{k+1}^{h,\tau} \cdot \nabla \eta_5}{|\phi_{k+1}^{h,\tau}|} \right) dx = 0$$

with $\mathbf{P}_{k+1} = \mathbf{I} - \frac{\nabla \phi_{k+1}^{h,\tau}}{|\nabla \phi_{k+1}^{h,\tau}|} \otimes \frac{\nabla \phi_{k+1}^{h,\tau}}{|\nabla \phi_{k+1}^{h,\tau}|}$ and η_1, η_4 and η_5 being appropriate test functions.

4.2 Semi-Implicit Time Stepping

As one observes from the previous examples, the implicit schemes require the solution of strongly nonlinear systems in each time steps, which is a rather undesirable property and can be an issue with respect to computational efficiency. Indeed, the only implicit scheme in this context is the one by Chambolle (cf. [11]) for mean curvature flow, which is exactly (34) with an intermediate redistancing step. In order to overcome the difficulties with nonlinearities we consider semi-implicit time stepping, which has developed almost as a standard for numerical simulations of higher-order geometric flows, either for parametric (cf. [4, 15, 22–24, 31]), level set (cf. [19, 32]), or diffuse (cf. [5, 21]) representations of the surfaces.

In order to obtain a semi-implicit scheme with linear systems to be solved in each time step we need to construct a quadratic approximation of the energy, respectively the Lagrange functional Λ. This means we replace Λ in each iteration step by a functional $\tilde{\Lambda}^k$ quadratic with respect to ϕ and U, and linear with respect to R. The corresponding discrete energy functional is given by

$$\tilde{E}_h^k[\phi] = \inf_U \sup_R \tilde{\Lambda}^k[\phi, U, R].$$

In order to obtain a consistent approximation of the flow, the condition

$$(\tilde{E}_h^k)'(\phi_k^{h,\tau}) = E_h'(\phi_k^{h,\tau})$$

is needed, which can be translated into a condition on the Lagrange functional as

$$\begin{aligned}
\partial_\phi \Lambda(\phi_k^{h,\tau}, U_k^{h,\tau}, R_k^{h,\tau}) &= \partial_\phi \tilde{\Lambda}^k(\phi_k^{h,\tau}, \tilde{U}_k^{h,\tau}, \tilde{R}_k^{h,\tau}) \\
\partial_U \Lambda(\phi_k^{h,\tau}, U_k^{h,\tau}, R_k^{h,\tau}) &= \partial_U \tilde{\Lambda}^k(\phi_k^{h,\tau}, \tilde{U}_k^{h,\tau}, \tilde{R}_k^{h,\tau}) = 0 \\
\partial_R \Lambda(\phi_k^{h,\tau}, U_k^{h,\tau}, R_k^{h,\tau}) &= \partial_R \tilde{\Lambda}^k(\phi_k^{h,\tau}, \tilde{U}_k^{h,\tau}, \tilde{R}_k^{h,\tau}) = 0.
\end{aligned}$$

Note that this condition includes the primal and dual variables ($U_k^{h,\tau}$ and $R_k^{h,\tau}$), which can be computed given $\phi_k^{h,\tau}$ through the Lagrangian Λ. These may differ from the approximating ones ($\tilde{U}_k^{h,\tau}$ and $\tilde{R}_k^{h,\tau}$), which would usually be computed from the last time step of the scheme. Hence, the derivation of a consistent scheme (and also a stable one, see below), could enforce additional computations for the computation of quadratic approximations (such as Taylor expansions). E.g., for Willmore flow one would have to compute the mean curvature variable from

$$\int_\Omega U_k^{h,\tau} \psi \, dx = -\int_\Omega \frac{\nabla \phi_k^{h,\tau} \cdot \nabla \psi}{|\nabla \phi_k^{h,\tau}|} \, dx \quad \forall \psi \in \mathcal{V}^h.$$

The next time step in a semi-implicit time scheme is then given by

$$\phi_{k+1}^{h,\tau} \in \arg\min_\phi \left(\frac{1}{2\tau} \|\phi - \phi_k^{h,\tau}\|_k^2 + \tilde{E}_h^k[\phi] \right), \tag{35}$$

i.e., as the minimizer of a quadratic optimization problem, and consequently as the solution of a linear system (the first-order optimality condition). If $\tilde{E}_h^k$ is convex, or τ is sufficiently small, then the resulting quadratic functional is strictly convex and thus, the level set function in the next time step is unique.

For lower order energies, the construction of an approximation is again straight-forward, the approximating energy is of the form

$$\tilde{E}_h^k[\phi] = E_h[\phi_k^{h,\tau}] + E_h'[\phi_k^{h,\tau}](\phi - \phi_k^{h,\tau}) + F_h^k[\phi - \phi_k^{h,\tau}], \tag{36}$$

with a quadratic energy F_h^k. A natural choice for the quadratic term might be the second variation $F_h^k[\psi] = \frac{1}{2}E_h''[\phi_k^{h,\tau}](\psi,\psi)$, so that E_h^k would become the second-order Taylor expansion of E around the last time step. However, this choice is not essential for deriving a consistent scheme, one can instead use the appropriate quadratic functionals for increasing the stability of the scheme as we shall argue below.

For higher-order energies we construct an approximation of the Lagrangian via

$$\begin{aligned}\tilde{\Lambda}^k[\phi, U, R] = {} & \Lambda[\phi_k^{h,\tau}, U_k^{h,\tau}, R_k^{h,\tau}] \\ & + \Lambda'[\phi_k^{h,\tau}, U_k^{h,\tau}, R_k^{h,\tau}](\phi - \phi_k^{h,\tau}, U - U_k^{h,\tau}, R - R_k^{h,\tau}) \\ & + \frac{\partial^2}{\partial\phi\partial R}\Lambda[\phi_k^{h,\tau}, U_k^{h,\tau}, R_k^{h,\tau}](\phi - \phi_k^{h,\tau}, R - R_k^{h,\tau}) \\ & + \frac{\partial^2}{\partial U\partial R}\Lambda[\phi_k^{h,\tau}, U_k^{h,\tau}, R_k^{h,\tau}](U - U_k^{h,\tau}, R - R_k^{h,\tau}) \\ & + F_h^k[\phi - \phi_k^{h,\tau}] + G_h^k[U - U_k^{h,\tau}] - \Psi_h^k[R - R_k^{h,\tau}]\end{aligned}$$

with convex quadratic functionals F_h^k, G_h^k, and Ψ_h^k. Note that for appropriate choices of this functionals we obtain that the inf-sup (over U and R) of the approximate Lagrange functional $\tilde{\Lambda}^k$ at $\phi = \phi_k^{h,\tau}$ is attained at $\tilde{U}_k^{h,\tau} = U_k^{h,\tau} = \tilde{R}_k^{h,\tau} = R_k^{h,\tau}$, and the consistency is a direct consequence.

4.3 Stability and Energy Dissipation

Ideally we would like to obtain semi-implicit schemes that yield energy dissipation as the original geometric flows. A sufficient condition on $\tilde{E}_h^k$ yielding energy dissipation is

$$\tilde{E}_h^k[\phi^{h,\tau}] = E_h[\phi^{h,\tau}], \qquad \tilde{E}_h^k[\phi] \geq E_h[\phi] \quad \forall\phi \in \mathcal{V}^h. \tag{37}$$

Together with the definition of $\phi_{k+1}^{h,\tau}$ as a minimizer of (35) we conclude

$$\begin{aligned}\frac{1}{2\tau}\|\phi_{k+1}^{h,\tau} - \phi_k^{h,\tau}\|_k^2 + E_h[\phi_{k+1}^{h,\tau}] &\leq \frac{1}{2\tau}\|\phi_{k+1}^{h,\tau} - \phi_k^{h,\tau}\|_k^2 + \tilde{E}_h^k[\phi_{k+1}^{h,\tau}] \\ &\leq \tilde{E}_h^k[\phi_k^{h,\tau}] = E_h[\phi_k^{h,\tau}].\end{aligned}$$

We mention that (37) can be relaxed to

$$\frac{c}{2\tau}\|\phi_{k+1}^{h,\tau} - \phi_k^{h,\tau}\|_k^2 + \tilde{E}_h^k(\phi) \geq E_h[\phi] \quad \forall\phi \in \mathcal{V}^h, \tag{38}$$

for some $c < 1$, which implies by an analogous argument

$$\frac{1-c}{2\tau}\|\phi_{k+1}^{h,\tau} - \phi_k^{h,\tau}\|_k^2 + E_h[\phi_{k+1}^{h,\tau}] \leq E_h[\phi_k^{h,\tau}].$$

For a higher-order energy approximated by a Lagrangian, the first property in (37) is achieved if

$$\inf_U \sup_R \tilde{\Lambda}^k[\phi_k^{h,\tau}, U, R] = \inf_U \sup_R \Lambda[\phi_k^{h,\tau}, U, R], \tag{39}$$

which is automatic for the approximation derived in the previous section. The second (majorization) property is achieved if

$$\inf_U \sup_R \tilde{\Lambda}^k[\phi, U, R] \geq \inf_U \sup_R \Lambda[\phi, U, R] \quad \forall \phi \in \mathcal{V}^h, \tag{40}$$

whose verifications turns out to be very hard for energies like the Willmore functional.

4.4 Examples for Higher-Order Flows

In the following we provide some examples of semi-implicit schemes constructed in the above manner for some higher-order flows of particular interest:

Example 1: Mean Curvature Flow As a first example we consider the (averaged) area functional

$$E_h[\phi] = E[\phi] = \int_\Omega |\nabla \phi| \, dx.$$

We look for a quadratic approximation as above with an energy of the form

$$F_h^k[\psi] = \frac{1}{2} \int_\Omega a_k |\nabla \psi|^2 \, dx.$$

Then the consistency and the first property of (37) are automatically satisfied. The majorization property can be rewritten as

$$\begin{aligned} \int_\Omega |\nabla \phi| \, dx &\leq \int_\Omega \left(|\nabla \phi_k^{h,\tau}| + \frac{\nabla \phi_k^{h,\tau} \cdot (\nabla \phi - \nabla \phi_k^{h,\tau})}{|\nabla \phi_k^{h,\tau}|} + \frac{a_k}{2} |\nabla \phi - \nabla \phi_k^{h,\tau}|^2 \right) dx \\ &= \int_\Omega \left(\frac{\nabla \phi_k^{h,\tau} \cdot \nabla \phi}{|\nabla \phi_k^{h,\tau}|} + \frac{a_k}{2} |\nabla \phi - \nabla \phi_k^{h,\tau}|^2 \right) dx. \end{aligned}$$

Thus, the majorization property is achieved if

$$2|\nabla \phi| \, |\nabla \phi_k^{h,\tau}| + 2(b_k - 1) \nabla \phi_k^{h,\tau} \cdot \nabla \phi \leq b_k |\nabla \phi|^2 + b_k |\nabla \phi_k^{h,\tau}|^2,$$

for all admissible ϕ, where we have used the notation $b_k = a_k |\nabla \phi_k^{h,\tau}|$. For $b_k \geq 1$ we obtain by the geometric-arithmetic mean inequality that

$$\begin{aligned} 2|\nabla \phi| \, |\nabla \phi_k^{h,\tau}| + 2(b_k - 1) \nabla \phi_k^{h,\tau} \cdot \nabla \phi &\leq 2 b_k |\nabla \phi| \, |\nabla \phi_k^{h,\tau}| \\ &\leq b_k |\nabla \phi|^2 + b_k |\nabla \phi_k^{h,\tau}|^2, \end{aligned}$$

hence the majorization property holds. On the other hand, for $b_k < 1$ one can immediately see a violation via the choice $\phi = -\phi_k^{h,\tau}$. Hence $b_k = 1$ yields the minimal energy of the above form that satisfies the majorization property (and consequently yields stability). The resulting energy for $b_k = 1$ can be written as

$$\tilde{E}_h^k[\phi] = \frac{1}{2} \int_\Omega \frac{|\nabla \phi_k^{h,\tau}|^2 + |\nabla \phi|^2}{|\nabla \phi_k^{h,\tau}|},$$

and the resulting semi-implicit scheme for mean-curvature flow is

$$\int_\Omega \frac{(\phi_{k+1}^{h,\tau} - \phi_k^{h,\tau})\eta}{\tau|\phi_k^{h,\tau}|}\,dx + \int_\Omega \frac{\nabla\phi_{k+1}^{h,\tau}\cdot\nabla\eta}{|\phi_k^{h,\tau}|} = 0,$$

which is exactly the one used in [13]. Also the schemes used in [14] for weighted area functionals can be derived from analogous arguments on energy approximation.

Example 2: Isotropic Surface Diffusion As a second example we consider the surface diffusion flow with the energy equal to the area functional. We therefore use the same approximation of the energy as in the previous example

$$\tilde{E}_h^k[\phi] = \frac{1}{2}\int_\Omega \frac{|\nabla\phi_k^{h,\tau}|^2 + |\nabla\phi|^2}{|\nabla\phi_k^{h,\tau}|},$$

which yields unconditional stability. Together with the approximation of the H^{-1}-metric described above we arrive at the semi-implicit scheme

$$\begin{aligned}
\int_\Omega Q_{k+1}^{h,\tau}\eta_1\,dx \; + \int_\Omega \frac{\nabla\phi_{k+1}^{h,\tau}\cdot\nabla\eta_1}{|\phi_k^{h,\tau}|}\,dx &= 0\\
\int_\Omega (\mathbf{P}_k\nabla(W_{k+1}^{h,\tau} + Q_{k+1}^{h,\tau}))\cdot(\mathbf{P}_k\nabla\eta_2)\,dx &= 0\\
\frac{1}{\tau}\int_\Omega (\phi_{k+1}^{h,\tau} - \phi_k^{h,\tau})\eta_3\,dx - \int_\Omega (\mathbf{P}_k\nabla W_{k+1}^{h,\tau})\cdot(\mathbf{P}_k\nabla\eta_3)\,dx &= 0,
\end{aligned}$$

which is a level set analogue of the scheme used in [15] for graph representations.

Example 3: Willmore Flow As an example with an higher-order energy we consider the Willmore flow, characterized by the L^2-metric and the energy and average energy functional, respectively,

$$e[\Gamma] = \frac{1}{2}\int_\Gamma h^2\,dx \qquad E[\phi] = \frac{1}{2}\int_\Omega H^2|\nabla\phi|\,dx$$

with the mean curvature h and its averaged version H. Obviously we use the same approximation of the L^2-metric as in the case of the mean curvature flow, so that it only remains to derive an energy approximation.

As noticed in Sect. 2, the energy functional can be calculated from the Lagrangian

$$\Lambda[\phi, U, R] = \frac{1}{2}\int_\Omega U^2|\nabla\phi|\,dx + \int_\Omega \left(-UR + \frac{\nabla\phi\cdot\nabla R}{|\nabla\phi|}\right)dx.$$

We can then compute the variations

$$\begin{aligned}
\partial_\phi\Lambda[\phi, U, R]\eta_1 &= \int_\Omega \left(\frac{U^2}{2}\frac{\nabla\phi\cdot\nabla\eta_1}{|\nabla\phi|} + \frac{(\mathbf{P}\nabla\eta_1)\cdot\nabla R}{|\nabla\phi|}\right)dx\\
\partial_U\Lambda[\phi, U, R]\eta_2 &= \int_\Omega (U|\nabla\phi| - R)\eta_2\,dx\\
\partial_R\Lambda[\phi, U, R]\eta_3 &= \int_\Omega \left(-U\eta_3 + \frac{\nabla\phi\cdot\nabla\eta_3}{|\nabla\phi|}\right)dx
\end{aligned}$$

$$\partial^2_{\phi,R}\Lambda[\phi,U,R](\eta_1,\eta_3)=\int_\Omega \frac{(\mathbf{P}\nabla\eta_1)\cdot\nabla\eta_3}{|\nabla\phi|}\,dx$$

$$\partial^2_{U,R}\Lambda[\phi,U,R](\eta_2,\eta_3)=-\int_\Omega \eta_2\eta_3.$$

In order to complete the derivation of the semi-implicit scheme with the above quadratic form of an approximate Lagrangian $\tilde{\Lambda}^k$ it remains to specify the functionals F_h^k, G_h^k and Ψ_h^k. We shall highlight one possibility in the following, which actually yields a similar scheme as used in [19]. The idea of the choice is to look at the energy term (the first integral in Λ) for fixed U and fixed ϕ, respectively. For fixed U we obtain a weighted area functional and consequently use an analogous approximation as for area functionals above, namely

$$F_h^k[\phi]=\frac{1}{4}\int_\Omega (U_k^{h,\tau})^2\frac{|\nabla\phi-\nabla\phi_k^{h,\tau}|^2}{|\nabla\phi_k^{h,\tau}|}\,dx.$$

For fixed ϕ the functional of U is already quadratic, so it seems natural to use the second-order term in the Taylor expansion

$$G_h^k[U]=\frac{1}{2}\int_\Omega (U-U_k^{h,\tau})^2|\nabla\phi_k^{h,\tau}|\,dx.$$

Altogether, this yields the approximate Lagrangian

$$\tilde{\Lambda}^k[\phi,U,R]=\frac{1}{2}\int_\Omega\left(U^2|\nabla\phi_k^{h,\tau}|+(U_k^{h,\tau})^2\frac{|\nabla\phi|^2-|\nabla\phi_k^{h,\tau}|^2}{2|\nabla\phi_k^{h,\tau}|}\right)dx$$
$$+\int_\Omega\left(-UR+\frac{(\mathbf{P_k}\nabla\phi+(\mathbf{I}-\mathbf{P_k})\nabla\phi_k^{h,\tau})\cdot\nabla R}{|\nabla\phi_k^{h,\tau}|}\right)dx.$$

The resulting semi-implicit scheme is

$$\int_\Omega\left(\frac{(\phi_{k+1}^{h,\tau}-\phi_k^{h,\tau})\eta_1}{\tau|\nabla\phi_k^{h,\tau}|}+(U_k^{h,\tau})^2\frac{\nabla\phi_{k+1}^{h,\tau}\cdot\nabla\eta_1}{|\nabla\phi_k^{h,\tau}|}+\frac{(\mathbf{P_k}\nabla R_{k+1}^{h,\tau})\cdot\nabla\eta_1}{|\nabla\phi_k^{h,\tau}|}\right)dx=0$$

$$\int_\Omega (U_{k+1}^{h,\tau}|\nabla\phi_k^{h,\tau}|-R_{k+1}^{h,\tau})\eta_2\,dx=0$$

$$\int_\Omega\left(-U_{k+1}^{h,\tau}\eta_3+\frac{(\mathbf{P_k}\nabla\phi_{k+1}^{h,\tau}+(\mathbf{I}-\mathbf{P_k})\nabla\phi_k^{h,\tau})\cdot\nabla\eta_3}{|\nabla\phi_k^{h,\tau}|}\right)dx=0.$$

for all test functions $\eta_i\in\mathcal{V}^h$.

Example 4: Regularized Anisotropic Motion Laws As a final example we consider the curvature regularization of an anisotropic surface energy, i.e.

$$e[\Gamma]=\int_\Gamma\left(\gamma(n)+\frac{\epsilon^2}{2}h^2\right)d\sigma,$$

which is of particular interest when γ (respectively its one-homogeneous extension to $\mathbb{R}^d$) is not convex. The averaged version of the energy is given by

$$E[\phi] = \int_\Omega \left(\gamma(\nabla\phi) + \frac{\epsilon^2}{2} H^2 |\nabla\phi| \right) dx.$$

In this case it is of practical interest to consider both the mean-curvature type flow (L^2-metric) and the surface diffusion flow (H^{-1}-metric) for this energy (cf. [8, 9, 12, 25])

For the approximations of the L^2-metric or H^{-1}-metric we can use exactly the same schemes as for the mean curvature or for the surface diffusion flow, respectively. Moreover, we can use the same approximation of the curvature dependent term as for the Willmore flow. Thus, we only provide an approximation of the first term in the energy

$$E_1[\phi] = \int_\Omega \gamma(\nabla\phi)\, dx.$$

A simple approximation with isotropic higher-order part is given by

$$\tilde{E}_1^k[\phi] = \int_\Omega \left(\gamma(\nabla\phi) + (\nabla\gamma)(\nabla\phi)(\nabla\phi - \nabla\phi_k^{h,\tau}) + \frac{\lambda}{2} \frac{(\nabla\phi - \nabla\phi_k^{h,\tau})}{|\nabla\phi_k^{h,\tau}|} \right) dx.$$

If λ is chosen large enough it is easy to see that $\tilde{E}_1^k$ actually majorizes E_1. A detailed discussion of semi-implicit schemes for regularized anisotropic motions can be found in [9].

5 Redistancing

It is worth noticing that for energy functionals depending on higher than first derivatives, the "global" level set approach is not well-defined. In this case the resulting evolution equation is a partial differential equation of higher than second order, and therefore does not satisfy a comparison principle. Consequently, even if a solution to the equation for the level set function ϕ exists, one cannot guarantee that ϕ is continuous and that its level sets are still the boundary of the sublevel sets (due to possible intersection and annihilation of level sets). This means that the level set approach can only be interpreted in a local sense, i.e., the level set function only satisfies the partial differential equations at the zero level set. Since one is not really interested in the other level sets of ϕ, one can use an arbitrary extension such as the signed distance function. In a theoretical approach this means one looks for a solution ϕ, which satisfies the partial differential equation only on the implicitly defined set $\{\phi = 0\}$, and is a signed distance function in the remaining part of Ω. In a practical approach one first computes one small time-step of the partial differential equation (i.e., one violates the constraint of being a signed-distance function) and then performs a redistancing step (i.e., one computes a suitable projection to the constraint set of signed-distance functions).

As any redistancing slightly changes the interface, it should only be done if necessary. In our implementation we check the norm of the gradient of the level set function ϕ in a band around the zero level set which is about the grid size. If the norm differs too much from one (e.g. by 10 percent), redistancing is carried out.

Our redistancing algorithm is an approach for unstructured grids based on a local Hopf-Lax formula which was introduced in [7] and given in detail for two dimensions therein. In [34] it was extended to three dimensions, and a detailed description for this dimension can be found in [33].

It should be noted that the approach updates the distance function with 2nd order accuracy. We further mention that the redistancing algorithm does not account for imposed boundary conditions, that means the natural boundary conditions for ϕ may be violated. But we emphasize that this has no effect on the evolution of the zero level set, $\{\phi = 0\}$, in which we are interested only.

6 Implementation and Results

The derived numerical schemes are implemented in the adaptive finite element toolbox AMDiS [3]. The toolbox provides a framework for the efficient solution of systems of partial differential equations by adaptive finite elements on unstructured grids. For details on the software we refer to [34–37].

In order to reduce the computational overhead associated with the level set method we use adaptive mesh refinement and coarsening. Thus only within a small neighborhood (narrow band) around $\Gamma(t) = \{\phi(\cdot, t) = 0\}$ we allow for a fine resolution of the grid. Whereas away from the zero level set the grid is coarsened. The signed distance function serves as an indicator for refinement and coarsening.

In all simulations we use piecewise linear finite elements and solve the resulting linear system using a Schur complement and a GMRES solver. We typically need about 10–15 iterations to reach the error tolerance of 10^{-8}.

As examples we consider variants of the H^{-1}-gradient flow of the energies

$$e_1[\Gamma] = \int_\Gamma \gamma \, d\sigma \quad \text{and} \quad e_2[\Gamma] = \int_\Gamma h^2 \, d\sigma,$$

with $\gamma = \gamma(n)$. Figure 1 shows the evolution of a cube to a sphere by surface diffusion ($e_1[\Gamma] = \int_\Gamma 1 \, d\sigma$ and $e_2[\Gamma] = 0$). It is an example for an isotropic fourth order equation. The discretization is described in detail in Sect. 4.

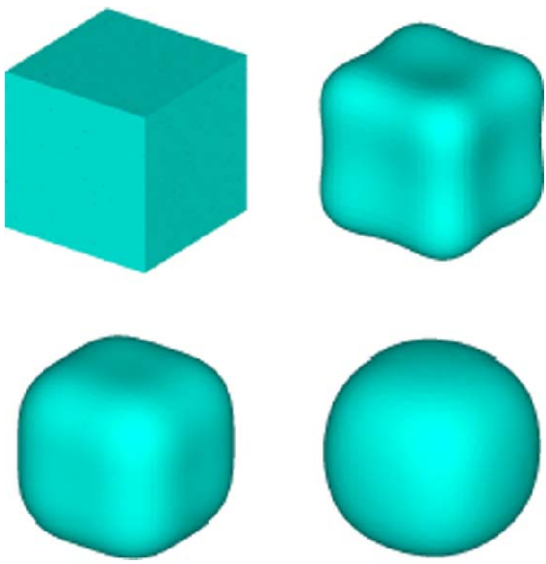

Fig. 1 Evolution by surface diffusion (isotropic evolution). Simulation parameters: $[0, 4] \times [0, 4] \times [0, 4]$ grid, grid size at the interface $h = 0.05$, timestep $\Delta t = 10^{-5}$. From *top left* to *bottom right*: $t = 0.0$, 0.001, 0.005, 0.01

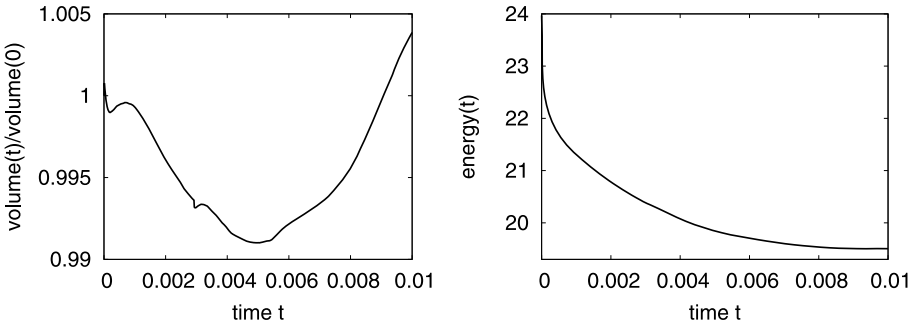

Fig. 2 Change of volume (*left*) and energy dissipation (*right*) in evolution under isotropic surface diffusion

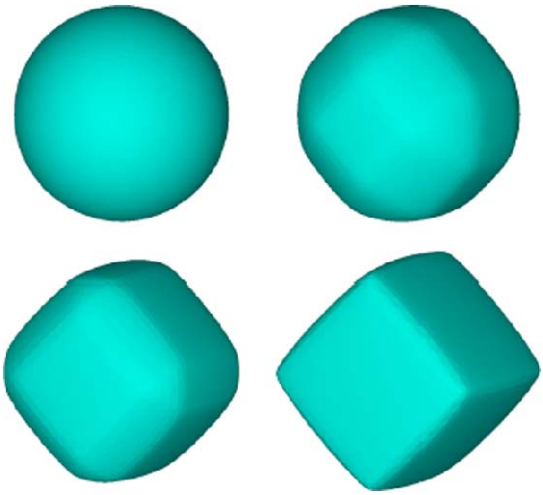

Fig. 3 Evolution by surface diffusion (anisotropic evolution). Simulation parameters: $[0,4]\times[0,4]\times[0,4]$ grid, grid size at the interface $h=0.05$, timestep $\Delta t=10^{-5}$. Stabilization parameter $\lambda=20$. From *top left* to *bottom right*: $t=0.0, 0.0005, 0.002, 0.008$

As a check for correctness of our computations, we control the volume conservation and energy dissipation, see Fig. 2. More detailed comparisons can be found in [33].

Figure 3 shows the evolution of a sphere to a cube-like Wulff-shape by surface diffusion ($(e_1[\Gamma]=\int_\Gamma \gamma\, d\sigma$ and $e_2[\Gamma]=0$, with $\gamma(p)=\gamma_0(R_{\pi/4}(p))$, $R_{\pi/4}$ the clockwise rotation about the angle $\pi/4$, and $\gamma_0(p)=\sum_{1=1}^{3}(0.01|p|^2+p_i^2)^{1/2}$. It is an example for an anisotropic fourth order equation with a convex anisotropy function. The discretization is described in detail in Sect. 4.

As a check for correctness of our computations, we again control the volume conservation and energy dissipation, see Fig. 4.

As an example of a sixth order equation we use a combination of the energies e_1 and e_2

$$e_3[\Gamma]=\int_\Gamma \gamma+\frac{\epsilon^2}{2}h^2\,d\sigma,$$

with ϵ a small parameter. Such energies arise in materials science with γ being non-convex [18, 20, 26, 30], e.g. $\gamma(p)=|p|+\sum_{i=1}^{3}\frac{p_i^4}{|p|^3}$. Thus the curvature term can be viewed as a regularization. For an approach to discretize the equations resulting from the anisotropic term we refer to [9]. The discretization of the remaining terms is described in detail in

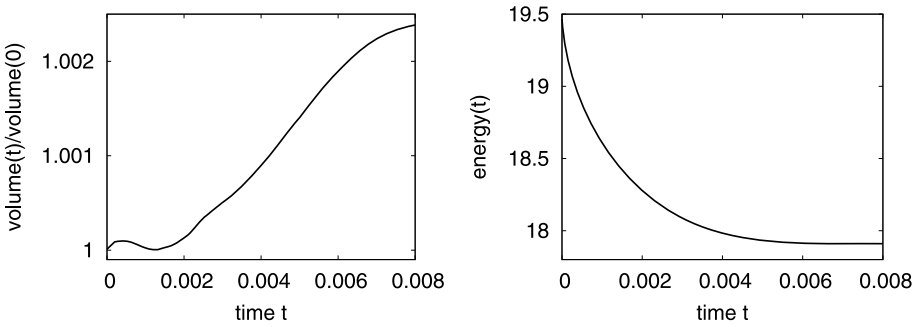

Fig. 4 Change of volume (*left*) and energy dissipation (*right*) in evolution under anisotropic surface diffusion

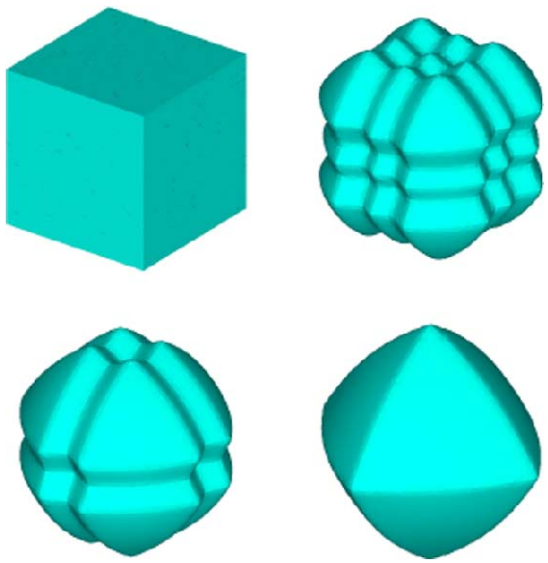

Fig. 5 Evolution by curvature regularized surface diffusion (anisotropic evolution). Simulation parameters: $[0, 4] \times [0, 4] \times [0, 4]$ grid, grid size at the interface $h = 0.05$, timestep $\triangle t = 10^{-6}$. Stabilization parameter $\lambda = 20$. Length scale $\epsilon = 0.02$. From *top left* to *bottom right*: $t = 0.0$, 0.001, 0.005, 0.01

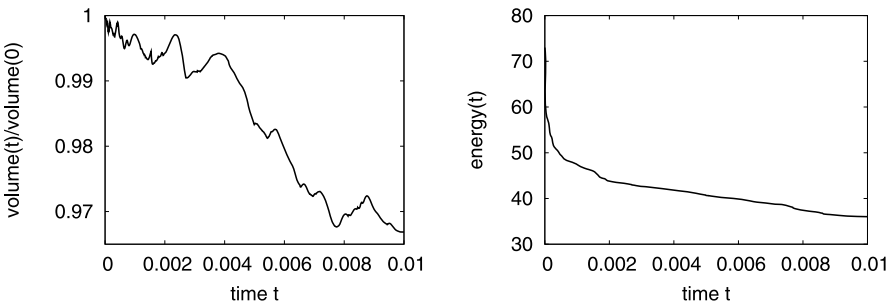

Fig. 6 Change of volume (*left*) and energy dissipation (*right*) in evolution under curvature regularized surface diffusion

Sect. 4. Figure 5 shows the evolution of a cube to the Wulff shape by curvature regularized anisotropic surface diffusion.

Again we check the computation by controling volume conservation and energy dissipation, see Fig. 6.

More detailed comparisons, e.g. the dependency on the grid size can be found in [33].

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