Numerical Analysis of Partial Differential Equations on Evolving Surfaces

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Zusammenfassung auf Deutsch

Diese Dissertation beschäftigt sich mit der numerischen Untersuchung vollständiger Diskretisierungen von parabolischen sowie Wellengleichungen auf bewegten Oberflächen. Dabei ist es uns gelungen, zum ersten Mal optimale Fehlerabschätzungen in Raum und Zeit für Zeitintegratoren der Ordnung zwei und höher herzuleiten. Aufgrund ihrer Allgemeinheit sollten sich die hierbei entwickelten und in dieser Arbeit präsentierten Techniken auch auf nichtlineare partielle Differentialgleichungen übertragen lassen. Somit ist zu hoffen, dass diese Dissertation Anlass zu weiteren wissenschaftlichen Untersuchungen partieller Differentialgleichungen auf beweglichen Oberflächen gibt.

Im ersten Teil der Arbeit wird die volle Diskretisierung für eine lineare parabolische Gleichung auf bewegten Oberflächen untersucht. Die räumliche Diskretisierung wird dabei durch die sogenannte “evolving surface finite element” Methode (ESFEM) realisiert, welche zu einem System gewöhnlicher Differentialgleichungen mit zeitabhängigen Masse- und Steifigkeitsmatrizen führt. Für diese Matrizen werden grundlegende, aber dennoch wichtige Abschätzungen bewiesen, mit derer Hilfe sich die Stabilität der Zeitdiskretisierungsverfahren in einem abstrakten Rahmen analysieren lässt. Zur Lösung der sich ergebenden gewöhnlichen Differentialgleichungen werden zwei verschiedene Methoden betrachtet – die impliziten Runge–Kutta Verfahren sowie die sogenannten "backward difference formulas", kurz BDF Verfahren. Wir zeigen, dass algebraisch stabile, für steife Gleichungen konzipierte Runge-Kutta Methoden, wie beispielsweise Radau IIA, angewendet auf das hier betrachtete Problem uneingeschränkt stabil sind. Danach werden wir Ergebnisse der Dahlquist G–Stabilitätstheorie und Nevanlinna–Odeh Multiplikatorentechnik mit Eigenschaften der räumlichen Semidiskretisierung verknüpfen, um für die BDF Verfahren uneingeschränkte Stabilität bis zur Ordnung fünf nachzuweisen. Kombiniert mit einer entsprechend gewählten Ritz Projektion sowie Abschätzungen, welche aus der Approximation der zugrunde liegenden Geometrie resultieren, liefern die gezeigten Stabilitätseigenschaften dann optimale Fehlerschranken für die vollen Diskretisierungen. Diese theoretischen Ergebnisse werden im Anschluss anhand numerischer Experimente bestätigt.

Im zweiten Teil wird zunächst mit Hilfe des Hamilton’schen Prinzips der stationären Wirkung eine lineare Wellengleichung auf bewegten Oberflächen hergeleitet. In einem ersten Schritt wird dieses Variationsprinzip durch stückweise lineare, bewegte Finite Elemente im Raum diskretisiert. Für die Zeitdiskretisierung werden dann zwei unterschiedliche Variationsintegratoren betrachtet – eine Version des Leapfrog oder Störmer–Verlet Verfahrens sowie Gauß–Runge–Kutta (GRK) Integratoren. Unter derselben Courant–Friedrichs–Lewy

(CFL) Bedingung, wie sie für eine feste Oberfläche erforderlich wäre, werden Stäbilitätsabschätzungen in der aus der Raumdiskretisierung resultierenden Matrix- Vektor Formulierung hergeleitet. Durch geschickte Kombination der algebraischen Stabilität und der Koerzivitätseigenschaft des Verfahrens mit einigen Abschätzungen für die zeitabhängigen Masse- und Steifigkeitsmatrizen können wir die uneingeschränkte Stabilität der GRK Verfahren nachweisen. Wie auch im ersten Teil, sind diese Stabilitätsabschätzungen für die Zeitdiskretisierung hinreichend stark, um daraus auf die Konvergenz des vollständig diskretisierten Verfahrens in den natürlichen zeitabhängigen Normen schließen zu können. Es sei erwähnt, dass die hier im Beweis der optimalen Ordnungsschranken verwendete Ritz Projektion nicht mit der aus dem ersten Teil der Dissertation übereinstimmt. Um auch die im zweiten Teil hergeleiteten Resultate zu veranschaulichen, schließen wir hier ebenfalls mit numerischen Simulationen.

Abstract

This dissertation addresses the numerical study of full discretization methods for linear parabolic equations as well as wave equations on evolving surfaces. It is the first work able to give rigorous proofs concerning error bounds for numerical schemes on evolving surfaces with time integrators of order two and higher. We believe that the developed analytical tools and achieved results in this thesis can be applied or extended to more complicated linear or nonlinear partial differential equations on or of surfaces.

In the first part of this thesis, two fully discrete schemes for a linear parabolic equation on evolving surfaces are studied. The spatial discretization is realized with the evolving surface finite element method. This leads to a system of ordinary differential equations involving time dependent mass and stiffness matrices. For these matrices, basic but nevertheless important estimates are proven in order to study the stability of the time discretization schemes in an abstract framework. Two different methods are considered, namely, the implicit Runge–Kutta method, and the backward difference formulas (BDF). For algebraically stable and stiffly accurate implicit Runge–Kutta methods such as Radau IIA, the unconditional stability in the matrix-vector formulation is proven. In the same framework, using results from Dahlquist's G-stability theory and Nevanlinna–Odeh's multiplier technique together with the properties of the spatial semi-discretization, unconditional stability for the BDF methods up to order five is shown. These stability results, combined with an appropriately chosen Ritz projection and estimates arising from the approximation of the geometry, enable us to derive optimal-order error estimates for the fully discrete schemes. Numerical experiments are presented to confirm the theoretical results.

In the second part, a linear wave equation on evolving surfaces is derived by using Hamilton's principle of stationary action. This variational principle is first discretized in space by piecewise linear evolving surface finite elements. For the time discretization, two variational integrators – a version of the leapfrog or Störmer-Verlet method and Gauß–Runge–Kutta (GRK) methods – are studied. Working on the matrix-vector level, stability estimates for the leapfrog scheme are shown under the same Courant–Friedrichs–Lewy (CFL) condition which would be required for a fixed surface. Concerning the GRK method, its algebraic stability and coercivity property are joined with basic estimates for the evolving mass and stiffness matrices in order to prove unconditional stability for this time discretization scheme. As in the first part, the thus obtained stability results are strong enough to yield convergence of the fully discrete methods in the natural time-dependent norms. It is worth noticing that in order to obtain optimal-order error estimates, the Ritz projection needed for the wave equation is different from the one considered in the parabolic case. Numerous simulations illustrate the optimality of the convergence results.

Contents

Introduction

The analytical and numerical study of partial differential equations (PDEs) on fixed and moving surfaces is a very active research area and has attracted considerable attention over the last years. These equations appear in many applications such as: fluid dynamics [30], material science [8], image processing [41], physiology [28], etc. For PDEs on evolving surfaces, an understanding of linear problems is expected to play a role as crucial as it does for PDEs on fixed domains. The main goal of this thesis is the rigorous theoretical justification of the surface finite element method coupled with time discretization schemes of arbitrary high order when applied to model problems such as linear parabolic equations as well as wave equations on evolving surfaces.

Research motivation and related results

There is a great amount of literature concerning the numerical approximation of PDEs on fixed and moving surfaces. Many of these works are notable such as: the introductory paper on the surface finite element method for solving the Poisson problem for the Laplace-Beltrami operator on a fixed surface [13], where the convergence of the scheme is also analyzed; the recent works using the extension of this surface finite element method and various time discretization schemes to solve parabolic equations on a time-dependent surface [14, 19, 38, 15, 16]; the papers on solving partial differential equations on evolving surfaces by the finite volume method [32], by a grid-based particle method [33], and by level set methods [1, 48]; the study of conservation laws on time-dependent surfaces [18]; and the works [37, 39] for full discretizations of wave equations on evolving surfaces. Additional references can be found in the review article by G. Dziuk & C. Elliott [17]. Many of the aforementioned works will be further referenced in the following.

This work is motivated by the paper of G. Dziuk & C. Elliott [14], where an evolving surface finite element method (ESFEM) was introduced to solve parabolic equations on evolving surfaces. The method is elegant and simple, based on moving triangulated surfaces and it needs only knowledge of the position of the vertices which sit on the smooth surface for all time. Consequently, only the triangulation of the initial surface is needed, then, by moving the vertices with the given velocity, the moving mesh is easily constructed. In [14], the authors proved optimal error estimates in the energy norm for the spatial semi-discretization problem without providing an analysis of the time discretization. Thus, studying the time discretization of the system of ordinary differential equations (ODEs) resulting from the ESFEM method arose as a natural task. In particular, the following general question came up:

For a given time discretization scheme which is known to have some stability and accuracy properties when applied to a parabolic equation on a fixed domain, do these properties remain valid when the same scheme is applied to the parabolic equation on evolving surfaces?

In order to investigate this question, the two well-known and most frequently used time discretization schemes for the classical parabolic equation, namely, the algebraically stable and stiffly accurate implicit Runge–Kutta method Radau IIA and the backward difference formulas (BDF) have been considered. G. Dziuk, C. Lubich & D. Mansour [19] proved stability and optimal error bounds for the ODE system arising from ESFEM approximation for algebraically stable implicit Runge-Kutta methods, in particular Radau IIA collocation methods of arbitrary high order. C. Lubich, D. Mansour & Ch. Venkataraman [38], using results from Dahlquist's G-Stability theory and Nevanlinna-Odeh's multiplier technique as well as the properties of the spatial semi-discretization, proved stability of the full discretization in the natural time-dependent norms for the BDF methods up to order five, and derived optimal-order error estimates in the energy norm.

In view of the above results, our objective is to give a complete theory of the ESFEM method combined with the aforementioned time discretization schemes as applied to the linear parabolic equation in analogy to the classical results. In particular, we provide optimal error bounds for the full discretization in the energy as well as in the L^2- norm. For the sake of completeness, we mention that, after the work [19], G. Dziuk & C. Elliott [15] proved optimal error estimates in the L^2-norm for the spatial semi-discrete problem. Based on the latter Work, they showed optimal error estimates of the fully discrete method with the backward Euler time discretization in [16]. We consider the work [15] a decisive contribution to build upon, particularly the introduction of the Ritz projection. Nevertheless, in extending the results from [16] to the implicit Runge–Kutta method and to the backward difference method up to order five, we do not make use of the techniques introduced in [16], because in our opinion our approach is straightforward and simpler.

Having successfully developed a rigorous and complete theory for the linear parabolic equation on evolving surfaces, we approached the wave equation on evolving surfaces. As expected, the treatment of the time discretization schemes when applied to the resulting ODE system arising from the ESFEM method required different techniques than the ones used for the parabolic case. Unexpectedly, it turned out that the Ritz projection considered for the parabolic case yielded only suboptimal order error bounds for the full discretization of the wave equation. This led to the construction of a modified Ritz projection that not only allowed to show optimal-order error estimates, but is also potentially useful in a much wider context than the particular bilinear forms we considered.

Main challenges

In order to derive optimal order error estimates for full discretization schemes based on the ESFEM method, there are four main problems which have to be investigated:

1. Geometric approximation: The numerical solution and the exact solution live on different surfaces. Thus, a use of a lifting operator in order to compare both functions is necessary. This process causes geometric perturbation errors that must be examined.

2. Material derivative approximation: Beside the given smooth velocity of the smooth surface and its interpolation which is the velocity of the discrete surface, there is a third velocity of the smooth surface determined by the lifting operator. This leads one to analyze the difference between two different material derivatives for functions defined on the smooth surface.

3. Stability analysis for the time discretization: The mass and stiffness matrices are both time-dependent. Therefore, estimates for these matrices are important in order to be able to study the time discretization of the ODE system arising form the ESFEM method. These estimates have then to be cleverly combined with the properties of the time marching method in order to achieve optimal stability estimates.

4. Ritz projection: The lifting process should also be thought about when defining a Ritz projection. The time dependency of the smooth surface as well as of the discrete surface yields to the fact that the material derivative and the Ritz operator do not commute, thus error analysis for the material derivative of the Ritz projection is also needed.

Contributions

The present work is a contribution to the numerical analysis of linear PDEs on evolving surfaces and parts of it have already been published [19, 38] or submitted [37, 39]. We briefly summarize its main results.

- Theorem 8.2: Optimal-order error estimates in the natural time-dependent norms for the evolving surface finite element method in combination with an algebraically stable and stiffly accurate implicit Runge–Kutta method for the parabolic equation on evolving surfaces.

- Theorem 8.3: Optimal-order error estimates in the natural time-dependent norms for the evolving surface finite element method in combination with the backward difference formula up to order five for the parabolic equation on evolving surfaces.

- Theorem 14.5: Optimal-order error estimates in the natural time-dependent norms of the variational fully discrete scheme (the evolving surface finite element method in combination with a version of the leapfrog or Störmer-Verlet method) for the wave equation on evolving surfaces.

- Theorem 14.6: Optimal-order error estimates in the natural time-dependent norms of the variational fully discrete scheme (the evolving surface finite element method in combination with the Gauß–Runge–Kutta method) for the wave equation on evolving surfaces.

Outline

This thesis is divided into two parts.

In the first part, two fully discrete schemes for a linear parabolic equation on evolving surfaces are studied. For both cases, the evolving surface finite element method is applied as a spatial discretization scheme. As for the time discretization, two different methods are considered, namely, the algebraic stable and stiffly accurate implicit Runge–Kutta method and the BDF method. Stability and convergence of the fully discrete schemes are analyzed and optimal-order error estimates in the natural time-dependent norms are achieved. Numerical experiments confirm some of the theoretical convergence results.

In the second part, a linear wave equation on evolving surfaces is derived by using Hamilton's principle of stationary action. The variational principle is first discretized in space by piecewise linear evolving surface finite elements. The time discretization is done using two different variational integrators, namely, a version of leapfrog or Störmer-Verlet method and the Gauß–Runge–Kutta method. In the same framework as in the first part, the stability and convergence of the fully discrete methods is studied and optimal-order error estimates are achieved. Again, numerical experiments confirm the convergence results.

For the sake of transparency, the architecture of the first part is mirrored in the second. In order to keep both parts independent, some notations and, to much lesser extent, proofs are partly repeated explicitly.

Part I. Full Discretization of Parabolic Equations on Evolving Surfaces

We deal with the numerical solution of the parabolic partial differential equation

$$\partial^\bullet u(x,t) + u(x,t)\ \nabla_{\Gamma(t)} \cdot v(x,t) - \Delta_{\Gamma(t)} u(x,t) = 0 \tag{0.1}$$

on a compact moving hypersurface $\Gamma(t) \subset \mathbb{R}^{m+1}$, $t \in [0,T]$, with a given velocity $v(x,t)$. Here $\partial^\bullet u$ denotes the material derivative of u:

$$\partial^\bullet u = \frac{\partial u}{\partial t} + v \cdot \nabla u.$$

Based on the weak form of the parabolic equation

$$\frac{d}{dt}\int_\Gamma u\varphi + \int_\Gamma \nabla_\Gamma u \cdot \nabla_\Gamma \varphi = \int_\Gamma u \partial^\bullet \varphi, \tag{0.2}$$

where $\varphi : \bigcup_{t\in[0,T]} \Gamma(t) \times \{t\} \to \mathbb{R}$ is an arbitrary test function, we consider a finite element approximation using piecewise linear finite elements on a triangulated surface interpolating $\Gamma(t)$ as described in [14]. This leads to the ODE system

$$\frac{d}{dt}\left(M(t)\alpha(t)\right) + A(t)\alpha(t) = 0, \tag{0.3}$$

where $M(t)$ and $A(t)$ are the evolving mass and stiffness matrices and $\alpha(t)$ is the nodal vector of the spatially discrete solution. In order to construct the fully discrete solution, we consider two different kinds of methods, namely, the implicit Runge–Kutta method and the BDF method, for the time discretization of the ODE system (0.3),.

The main purpose is to derive optimal-order error estimates for the concerned fully discrete schemes; namely, the piecewise linear finite elements in combination with the implicit Runge–Kutta method and the piecewise linear finite elements in combination with the BDF method. The keystone is to show stability estimates in the natural time-dependent norms for the time discretization. This will be achieved by first proving some basic estimates for the evolving mass and stiffness matrices which provide an abstract framework in which we can treat the ODE system (0.3). Based on these estimates, we derive stability estimates in the natural time-dependent norms for algebraically stable and stiffly accurate implicit Runge-Kutta methods such as Radau IIA. Continuing along the same foundation, using results from Dahlquist's G-stability theory [7] and Nevanlinna–Odeh's multiplier technique [42], together with the properties of the spatial semi-discretization, we prove that the fully discrete scheme is unconditionally stable for the BDF methods up to order five. These stability estimates for the implicit Runge–Kutta method, as well as for the BDF method, are the only stability estimates that will be used in combination with an appropriately chosen Ritz projection and geometric approximation estimates in order to prove optimal-order error estimates for the fully discrete schemes.

The first part of this document is organized as follows:

In Chapter 1, we begin with recalling the basic notation for the parabolic partial differential equation on evolving surfaces and derive the weak formulation (0.2) of the problem in order to start our numerical analysis.

In Chapter 2, based on the weak formulation (0.2), we describe the spatial discretization of the parabolic equation by using ESFEM method. This leads to the ODE system (0.3) involving the time dependent mass and stiffness matrices, for which we prove basic estimates.

In Chapter 3, we consider implicit Runge–Kutta methods for the time discretization of the resulting ODE system and prove that the fully discrete method is unconditionally stable.

In Chapter 4, in analogy to the previous chapter, we prove stability estimates for the fully discrete scheme by using BDF method for the time discretization.

In Chapter 5, we study the difference between the fully discrete solution and an arbitrary projection of the exact solution of the parabolic equation to the finite element space.

We show that in order to obtain optimal-order error estimates, one needs only to choose an appropriate projection of the exact solution and to control the error coming from the approximation of the geometry. It will be demonstrated that our Ritz map, presented in Chapter 7, is an optimal choice.

In Chapter 6, we prove a number of estimates due to the approximation of the geometry and to the lifting process. These estimates will additionally be useful in the second part of this thesis.

In Chapter 7, we introduce a general Ritz map for evolving surfaces which can be used for other bilinear forms. A particular form will be considered and its approximation properties will be studied.

In Chapter 8, we combine the results from the previous chapters in order to prove optimal-order error estimates of the fully discrete schemes.

In Chapter 9, we confirm some of our theoretical results with numerical experiments.

Part II. Full Discretization of Wave Equations on Evolving Surfaces

In analogy to the treatment in the first part, we study the numerical solution of the wave equation

$$\partial^\bullet \partial^\bullet u(x,t) + \partial^\bullet u(x,t)\ \nabla_{\Gamma(t)} \cdot v(x,t) - \Delta_{\Gamma(t)} u(x,t) = 0 \tag{0.4}$$

on a compact moving hypersurface $\Gamma(t) \subset \mathbb{R}^{m+1}$, $t \in [0,T]$, with a given velocity $v(x,t)$.

Based on the fact that the solution of (0.4) makes the action integral

$$\mathcal{S}[u] = \int_0^T \left(\frac{1}{2} \int_{\Gamma(t)} |\partial^\bullet u|^2 - \frac{1}{2} \int_{\Gamma(t)} |\nabla_\Gamma u|^2 \right) \mathrm{d}t$$

stationary under all paths with fixed endpoints, we develop and analyze fully discrete variational methods. The variational principle is first discretized by the piecewise linear evolving surface finite elements of Dziuk & Elliott [14]. This leads to the semi-discrete Hamilton principle which requests to minimize the discrete action integral

$$\mathcal{S}_h[q] = \int_0^T \left(\frac{1}{2} \dot{q}(t)^{\mathrm{T}} M(t) \dot{q}(t) - \frac{1}{2} q(t)^{\mathrm{T}} A(t) q(t) \right) \mathrm{d}t \tag{0.5}$$

where $M(t)$ and $A(t)$ are the evolving mass and stiffness matrices and $q(t)$ is the nodal vector of the spatially discrete solution. The minimizer of (0.5) is a solution of the *Euler-Lagrange equation*

$$\frac{d}{dt} \left(M(t) \dot{q}(t) \right) + A(t) q(t) = 0. \tag{0.6}$$

The variational time discretization of this system is done by minimizing an approximation of the discrete action integral in order to obtain a *discrete Euler-Lagrange equations* which serve to compute approximations q_n to $q(t_n)$. We investigate two different variational time integrators, namely, a version of the leapfrog or störmer-Verlet method that is stable under a Courant–Friedrichs–Lewy (CFL) condition; and in order to overcome the time step restriction due the CFL condition on one side while obtaining higher order accuracy in time on the other side, Gauß–Runge–Kutta (GRK) methods.

Our goal is to prove optimal-order error estimates for the fully discrete schemes which correspond with the ones obtained for the classical wave equation. As for the parabolic equation in the first part, the key is to prove stability estimates for the time discretization.

The case of the leapfrog method is studied under the same CFL condition that is required for a fixed surface. Working cleverly with the time-dependent norms which are defined by the evolving mass and stiffness matrices, we prove that the fully discrete variational integrator (ESFEM coupled with the leapfrog method) is stable under the CFL condition.

The algebraic stability and the coercivity property of the GRK method together with the properties of the spatial semi-discretization are the main tools to show stability estimates in the natural time-dependent norms for the GRK method. Our treatment here is inspired by the B-convergence theory which was originally developed to study the convergence of implicit Runge–Kutta methods when applied to stiff systems of ordinary differential equations (cf. [6, 9]). In particular, we prove that the order in time of the fully discrete method is at least the B-convergence order of the s-stage GRK method. This order is equal to 2 for $s = 1$, whereas, for $s \geq 2$, the B-convergence order is only equal to s. Under additional regularity assumptions which we expect to be satisfied for closed smooth surfaces, we show that the order is indeed the full classical order of the GRK methods, i.e., $2s$.

The second part of this thesis is outlined as follows:

In Chapter 10, we start with basic notations needed to derive the wave equation on evolving surfaces from the Hamilton variational principle. We establish the variational formulation of the model and prove existence and uniqueness of the weak solution.

In Chapter 11, we follow the approach of Dziuk & Elliott [14] in order to discretize the variational principle with piecewise linear evolving surface finite elements. This leads to the Euler-Lagrange equation (0.6) which we further reformulate as a Hamiltonian system.

In Chapter 12, we describe the variational time discretization of the resulting Hamiltonian system. Here, we prove three stability estimates. The first one is concerned with the leapfrog method and require a CFL condition. The second one is for the implicit midpoint rule (1-stage GRK method) and is established by taking up an idea of Kraaijevanger [31]. The last stability estimates which is for the general GRK method with $s \geq 2$ is shown by using some properties of the GRK method together with the basic estimates proven for the time dependent mass and stiffness matrices.

In Chapter 13, we prove error bounds for a projection of the exact solution onto the finite element space on the discretized surface which will reduce our problem of bounding the total error to estimate the residual of this projection.

In Chapter 14, based on the results obtained in the previous chapters, we state and prove our main two results of this part; namely, optimal-order convergence of the full discretization in the natural time-dependent norms, one under the CFL condition for the ESFEM in combination with leapfrog method, and another unconditionally for the ESFEM in combination with the s-stage GRK method with $s \geq 1$.

In Chapter 15, we present numerical experiments to illustrate some of our theoretical convergence results for the wave equation on evolving surfaces.

Part I.

Full Discretization of Parabolic Equations on Evolving Surfaces

1. Parabolic Equations on Evolving Surfaces

We begin with recalling some basic definitions and results from elementary differential geometry needed in order to formulate the mathematical model which we will study in the first part of this thesis. The model is a linear partial differential equation (PDE) of parabolic type posed on a given time-dependent surface. We then derive the weak formulation of the problem which will be the starting point of our numerical study of this model. The notations as well as the considered equation are taken from Dziuk & Elliott [14].

1.1. Basic notation

For a time interval $t \in [0,T]$, we consider a smoothly evolving family of smooth m-dimensional compact closed hypersurfaces $\Gamma(t)$ in $\mathbb{R}^{m+1}$ without boundary. The unit outward pointing normal is denoted by ν and depends smoothly on time t. We assume that the velocity of the surface is given, with the interpretation that there exist a vector field v such that material points $x(t)$ on the surface $\Gamma(t)$ move with the *velocity*

$$\dot{x}(t) = v(x(t),t) \quad \text{for} \quad x \in \Gamma(t).$$

We define the space-time surface as

$$G_T = \bigcup_{t\in[0,T]} \Gamma(t) \times \{t\}.$$

Throughout the thesis, we often omit the omnipresent argument t in the surface $\Gamma(t)$ wherever it is clear which surface is considered or whenever the stated relations are valid independently of the time t.

The *tangential gradient* of a smooth function $g : G_T \to \mathbb{R}$ is given by

$$\nabla_\Gamma g = \nabla \bar{g} - \nabla \bar{g} \cdot \nu \, \nu,$$

where $\bar{g}$ is an extension of g to an open neighborhood of Γ, $\nabla \bar{g}$ denotes the usual $(m+1)$-dimensional gradient and $a \cdot b = \sum_{j=1}^{m+1} a_j b_j$ for vectors a and b in $\mathbb{R}^{m+1}$. The tangential gradient only depends on the values of g on the surface Γ and is independent of the choice of the extension. Note that $\nabla_\Gamma g \cdot \nu = 0$.

The *Laplace-Beltrami* operator on Γ is then defined as the tangential divergence of the tangential gradient

$$\Delta_\Gamma g = \nabla_\Gamma \cdot \nabla_\Gamma g = \sum_{j=1}^{m+1} (\nabla_\Gamma)_j (\nabla_\Gamma)_j g,$$

and the Green's formula on $\Gamma(\partial\Gamma = \emptyset)$ reads

$$\int_\Gamma \nabla_\Gamma g \cdot \nabla_\Gamma \varphi = -\int_\Gamma \varphi \Delta_\Gamma g. \tag{1.1}$$

The *material derivative* $\partial^\bullet g$ is given by

$$\partial^\bullet g = \frac{\partial \bar{g}}{\partial t} + v \cdot \nabla \bar{g}, \tag{1.2}$$

which only depends on the values of the function g on the space-time surface G_T and is independent of the choice of the extension. For a more detailed discussion concerning surface gradients and material derivatives, we refer the reader to Gilbarg & Trudinger [21] and Dziuk & Elliott [14].

We work with the Sobolev spaces:

$$H^1(\Gamma) = \left\{ g \in L^2(\Gamma) \,|\, \nabla_\Gamma g \in L^2(\Gamma) \right\},$$
$$H^1(G_T) = \left\{ g \in L^2(G_T) \,|\, \nabla_\Gamma g \in L^2(\Gamma), \partial^\bullet g \in L^2(\Gamma) \right\}.$$

For more informations about Sobolev spaces, we refer to the monographs [2] and [47].

1.2. The mathematical model

The conservation of a scalar quantity $u(x,t)$ with a linear diffusive flux on $\Gamma(t)$ can be modeled by the linear parabolic partial differential equation

$$\begin{cases} \partial^\bullet u(x,t) + u(x,t)\ \nabla_{\Gamma(t)} \cdot v(x,t) - \Delta_{\Gamma(t)} u(x,t) &= f \quad \text{in } G_T \\ u(\cdot,0) &= u_0 \quad \text{on } \Gamma(0) \end{cases} \tag{1.3}$$

with given initial data $u_0 \in H^1(\Gamma(0))$.

More details concerning the derivation of the parabolic equation, well-posedness and regularity results can be found in [14] and the reference therein. For the sake of simplicity, we shall set in all chapters $f = 0$. Note that it is easy and straightforward to extend all of the upcoming results to the inhomogeneous problem. Next, we derive the start point of our numerical analysis, the weak formulation of the mathematical model.

Lemma 1.1 (weak formulation)
The weak formulation of (1.3) *reads: Find* $u \in H^1(G_T)$ *such that:*

- *For almost every* $t \in [0, T]$,

$$\frac{d}{dt}\int_{\Gamma(t)} u\varphi + \int_{\Gamma(t)} \nabla_{\Gamma(t)} u \cdot \nabla_{\Gamma(t)}\varphi = \int_{\Gamma(t)} u\partial^\bullet\varphi \quad \textit{for all } \varphi \in H^1(G_T). \tag{1.4}$$

- $u(\cdot, 0) = u_0$.

Proof
The proof uses the Leibniz formula on surfaces [14, Lemma 2.2]

$$\frac{d}{dt}\int_{\Gamma(t)} g = \int_{\Gamma(t)} \partial^\bullet g + g\nabla_{\Gamma(t)} \cdot v. \tag{1.5}$$

Let $\varphi : G_T \to \mathbb{R}$ be a smooth test function. By multiplying the above equation (1.3) by φ, integrating over Γ, performing integration by parts, and using the formula (1.5), we find

$$\begin{aligned} 0 &= \int_{\Gamma(t)} \partial^\bullet u\,\varphi + u\,\varphi\ \nabla_{\Gamma(t)} \cdot v + \nabla_{\Gamma(t)} u \nabla_{\Gamma(t)}\varphi \\ &= \int_{\Gamma(t)} \partial^\bullet(u\varphi) - u\partial^\bullet\varphi + u\ \nabla_{\Gamma(t)} \cdot v\varphi + \nabla_{\Gamma(t)} u \nabla_{\Gamma(t)}\varphi \\ &= \frac{d}{dt}\int_{\Gamma(t)} u\varphi + \int_{\Gamma(t)} \nabla_{\Gamma(t)} u \cdot \nabla_{\Gamma(t)}\varphi, - \int_{\Gamma(t)} u\partial^\bullet\varphi. \end{aligned}$$

■

2. Spatial Discretization by Evolving Surface Finite Elements

This chapter describes the spatial discretization of the parabolic equation using the evolving surface finite element method (ESFEM) of Dziuk & Elliott [14]. The discretization is based on the weak formulation (1.4) which will lead to a system of ordinary differential equations (ODEs) involving time dependent mass and stiffness matrices. For these matrices, we proof basic estimates which will be the only properties of the ESFEM method used while studying the stability analysis of various time discretization schemes.

2.1. The Evolving surface finite element method

In order to construct a finite element approximation based on the weak form (1.4) of the parabolic equation, we first approximate the smooth surface $\Gamma(t)$ by a triangulated surface $\Gamma_h(t)$. Let the discrete surface

$$\Gamma_h(t) = \bigcup_{E(t)\in\mathcal{T}_h(t)} E(t)$$

be the union of m-dimensional simplices $E(t)$ that is assumed to form an admissible triangulation $\mathcal{T}_h(t)$. The vertices $\{a_i(t)\}_{i=1}^N$ of all simplices $E(t)$ are taken to sit on the surface $\Gamma(t)$ for all time $t \in [0,T]$ and to move with the given velocity $v(a_i(t),t)$. We denote by h the maximum diameter of the whole triangulation.

The surface gradient on $\Gamma_h(t)$ is given by

$$\nabla_{\Gamma_h} g = \nabla g - \nabla g \cdot \nu_h \nu_h,$$

where ν_h denotes the normal to $\Gamma_h(t)$.

We define for each $t \in [0,T]$ the finite element space

$$S_h(t) = \{\phi_h \in C^0(\Gamma_h(t)) \,:\, \phi_h|_E \in \mathbb{P}_1 \text{ for all } E \in \mathcal{T}_h(t)\},$$

where $\mathbb{P}_1$ denotes the space of polynomials of degree at most 1. The moving nodal basis $\{\chi_i\}_{i=1}^N$ of $S_h(t)$ are determined by $\chi_i(a_j(t),t) = \delta_{ij}$ for all j, so they give

$$S_h(t) = \text{span}\{\chi_1(\cdot,t),\dots,\chi_N(\cdot,t)\}.$$

The discrete velocity V_h of the discrete surface $\Gamma_h(t)$ is the piecewise linear interpolant of v, i.e.,

$$V_h(x,t) = \sum_{j=1}^{N} v(a_j(t),t)\chi_j(x,t), \quad x \in \Gamma_h(t). \tag{2.1}$$

The discrete material derivative on $\Gamma_h(t)$ is thus given by

$$\partial_h^\bullet \phi_h = \frac{\partial \phi_h}{\partial t} + V_h \cdot \nabla \phi_h. \tag{2.2}$$

It was shown in [14, Proposition 5.4] that the discrete material derivative of the basis functions satisfies the remarkable *transport property*, namely, it is

$$\partial_h^\bullet \chi_j = 0 \quad \text{for} \quad j = 1, \cdots, N. \tag{2.3}$$

After the discretization of the surface and setting the appropriate definitions on the discrete surface $\Gamma_h(t)$, we now formulate the spatial semi-discretization of the parabolic equation as follows.

Problem 2.1 (The spatial semi-discretization)
Find $U_h(\cdot,t) \in S_h(t)$ such that

- *For all temporally smooth ϕ_h with $\phi_h(\cdot,t) \in S_h(t)$ and for all $t \in (0,T]$,*

$$\frac{d}{dt}\int_{\Gamma_h(t)} U_h\,\phi_h + \int_{\Gamma_h(t)} \nabla_{\Gamma_h(t)} U_h \cdot \nabla_{\Gamma_h(t)} \phi_h = \int_{\Gamma_h(t)} U_h \partial_h^\bullet \phi_h. \tag{2.4}$$

- *$U_h(\cdot,0) = U_h^0$, where $U_h^0 \in S_h(0)$ is an appropriate approximation of u_0.*

Remark 2.2
Under suitable regularity assumptions, an error estimate between the exact solution u of the parabolic equation (1.3) and the lift of the spatially discrete solution $u_h = U_h^l$ was proved in [14]:

$$\sup_{0\le t\le T} \|u(\cdot,t) - u_h(\cdot,t)\|^2_{L^2(\Gamma(t))} + \int_0^T \|\nabla_{\Gamma(t)}(u(\cdot,t) - u_h(\cdot,t))\|^2_{L^2(\Gamma(t))}\,dt \le ch^2.$$

An optimal error estimate in the L^2-norm is derived in [15]:

$$\sup_{0\le t\le T} \|u(\cdot,t) - u_h(\cdot,t)\|_{L^2(\Gamma(t))} \le ch^2.$$

While these error bounds for the spatial semi-discretization are of independent interest, they will not be used in the derivation of the error bounds for the fully discrete method including time discretization.

2.2. The ODE system

We make use of the fact that the discrete solution $U_h(\cdot,t) \in S_h(t)$ and define the vector $\alpha(t) \in \mathbb{R}^N$ as the nodal vector with entries $\alpha_j(t) = U_h(a_j(t),t)$ so that

$$U_h(\cdot,t) = \sum_{j=1}^{N} \alpha_j(t)\chi_j(\cdot,t).$$

We often abbreviate $U_h(t) = U_h(\cdot,t), \chi_j(t) = \chi_j(\cdot,t)$, etc.

Consequently, thanks to the transport property of the basis functions (2.3), we prove the following result.

Theorem 2.3 (ODE system)
Solving the spatial semi-discrete problem (2.4) *is equivalent to solving the system of ordinary differential equations (ODEs)*

$$\begin{cases} \frac{d}{dt}\left(M(t)\alpha(t)\right) + A(t)\alpha(t) &= 0 \\ \alpha(0) &= \alpha_0 = (U_h^0(a_j)), \end{cases} \tag{2.5}$$

where $M(t)$ and $A(t)$ are the evolving mass and stiffness matrices given by

$$M(t)_{ij} = \int_{\Gamma_h(t)} \chi_i(\cdot,t)\chi_j(\cdot,t), \qquad A(t)_{ij} = \int_{\Gamma_h(t)} \nabla_{\Gamma_h(\cdot,t)}\chi_i(\cdot,t) \cdot \nabla_{\Gamma_h(t)}\chi_j(t)$$

for $i,j = 1,\dots,N$.

Proof
To obtain the ODE system, we set $\phi_h = \chi_j$ for $j = 1,\dots,N$ in the weak form (2.4) and use the fact that the material derivatives of the basis functions vanish (2.3). We write $\phi_h(\cdot,t) = \sum_{j=1}^N \gamma_j(t)\chi_j(\cdot,t)$, then again by the transport property (2.3) it follows that $\partial_h^\bullet \phi_h(\cdot,t) = \sum_{j=1}^N \dot\gamma_j(t)\chi_j(\cdot,t) \in S_h(t)$. A simple calculation gives

$$\begin{aligned} &\frac{d}{dt}\int_{\Gamma_h(t)} U_h\phi_h + \int_{\Gamma_h(t)} \nabla_{\Gamma_h(t)}U_h \cdot \nabla_{\Gamma_h(t)}\phi_h \\ &= \frac{d}{dt}\Big(\sum_{j=1}^N \gamma_j \int_{\Gamma_h(t)} U_h\chi_j\Big) + \sum_{j=1}^N \gamma_j \int_{\Gamma_h(t)} \nabla_{\Gamma_h(t)}U_h \cdot \nabla_{\Gamma_h(t)}\chi_j \\ &= \sum_{j=1}^N \gamma_j \underbrace{\Big(\frac{d}{dt}\int_{\Gamma_h(t)} U_h\chi_j + \int_{\Gamma_h(t)} \nabla_{\Gamma_h(t)}U_h \cdot \nabla_{\Gamma_h(t)}\chi_j\Big)}_{=0 \text{ by } (2.5)} + \sum_{j=1}^N \dot\gamma_j \int_{\Gamma_h(t)} U_h\chi_j \\ &= \int_{\Gamma_h(t)} U_h \sum_{j=1}^N \dot\gamma_j\chi_j = \int_{\Gamma_h(t)} U_h\partial_h^\bullet\phi_h, \end{aligned}$$

which completes the proof. ■

We shall make use of the following transport lemma [15, Lemma 4.2].

Lemma 2.4
For $W_h(\cdot,t), Z_h(\cdot,t) \in S_h(t)$ we have:

$$\frac{d}{dt}\int_{\Gamma_h(t)} W_h Z_h = \int_{\Gamma_h(t)} \partial_h^\bullet W_h Z_h + W_h \partial_h^\bullet Z_h + W_h Z_h \nabla_{\Gamma_h(t)} \cdot V_h. \tag{2.6}$$

With the matrix

$$\mathcal{B}_h(V_h)_{ij} = \delta_{ij} \nabla_{\Gamma_h(t)} \cdot V_h - \Big((\nabla_{\Gamma_h(t)})_i V_{hj} + (\nabla_{\Gamma_h(t)})_j V_{hi} \Big), \quad (i,j = 1,\dots,m+1),$$

we have for the derivative of Dirichlet's integral

$$\begin{aligned} &\frac{d}{dt}\int_{\Gamma_h(t)} \nabla_{\Gamma_h(t)} W_h \cdot \nabla_{\Gamma_h(t)} Z_h \\ &= \int_{\Gamma_h(t)} \nabla_{\Gamma_h(t)} \partial_h^\bullet W_h \cdot \nabla_{\Gamma_h(t)} Z_h + \int_{\Gamma_h(t)} \nabla_{\Gamma_h(t)} W_h \cdot \nabla_{\Gamma_h(t)} \partial_h^\bullet Z_h \\ &\qquad + \int_{\Gamma_h(t)} \mathcal{B}_h(V_h) \nabla_{\Gamma_h(t)} W_h \cdot \nabla_{\Gamma_h(t)} Z_h. \end{aligned} \tag{2.7}$$

We denote time derivatives of k-th order by the superscript (k). The notation $\partial_h^{(k)}$ is for the k-th order discrete material derivative which is defined by (2.2). We then discover formulas for higher order Leibniz rules.

Lemma 2.5
Assume that the following quantities exist and set $a = \nabla_{\Gamma_h} \cdot V_h$. Then, there exist polynomials $g_{kl} = g_{kl}(a, \dot{a}, \dots, a^{(l)})$, $l = 1,\dots,k$ so that

$$\frac{d^k}{dt^k}\int_{\Gamma_h(t)} f = \int_{\Gamma_h(t)} \partial_h^{(k)} f + \sum_{l=1}^{k} \int_{\Gamma_h(t)} g_{kl} \partial_h^{(k-l)} f. \tag{2.8}$$

Similarly, there exist polynomials $G_{kl} = G_{kl}(B, \dot{B}, \dots, B^{(l)})$ with the matrix $B = \mathcal{B}_h(V_h)$, so that

$$\begin{aligned} \frac{d^k}{dt^k}\int_{\Gamma_h(t)} \nabla_{\Gamma_h(t)} f \cdot \nabla_{\Gamma_h(t)} \phi_h = &\int_{\Gamma_h(t)} \nabla_{\Gamma_h(t)} \partial_h^{(k)} f \cdot \nabla_{\Gamma_h(t)} \phi_h \\ &+ \sum_{l=1}^{k} G_{kl} \nabla_{\Gamma_h(t)} \partial_h^{(k-l)} f \cdot \nabla_{\Gamma_h(t)} \phi_h, \end{aligned} \tag{2.9}$$

for any function ϕ_h with $\partial_h^\bullet \phi_h = 0$.

Proof

One easily proves this by induction with the help of the Leibniz rules from Lemma 2.4. ∎

2.3. Properties of the evolving mass and stiffness matrices

We observe that the evolving mass matrix is symmetric and positive definite. The stiffness matrix is symmetric, and because we consider closed surfaces, only positive semidefinite and its null-space is spanned by the vector $(1, \dots, 1)^{\mathrm{T}}$.

We will use the notation: For a symmetric positive definite or semidefinite matrix $G(t) \in \mathbb{R}^{N\times N}$, we define the norm or semi-norm, respectively, for $w \in \mathbb{R}^N$:

$$|w|_{G(t)}^2 = \langle w\,|G(t)|\,w\rangle = w^{\mathrm{T}} G(t) w.$$

Note that for finite element functions $W_h(\cdot,t) = \sum_{i=1}^N w_i(t)\chi_i(\cdot,t) \in S_h(t)$ with the vector of nodal values $w(t) = (w_i(t)) \in \mathbb{R}^N$, we have

$$|w(t)|_{M(t)} = \|W_h(\cdot,t)\|_{L^2(\Gamma_h(t))} = \left(\int_{\Gamma_h(t)} |W_h|^2\right)^{1/2}, \tag{2.10a}$$

$$\begin{aligned} |w(t)|_{A(t)} &= \left\|\nabla_{\Gamma_h(t)} W_h(\cdot,t)\right\|_{L^2(\Gamma_h(t))} \\ &= \left(\int_{\Gamma_h(t)} |\nabla_{\Gamma_h} W_h|^2\right)^{1/2} := \sum_{E(t)\in\mathcal{T}_h(t)} \int_{E(t)} |\nabla_{\Gamma_h} W_h|^2. \end{aligned} \tag{2.10b}$$

We are ready now to state and prove the main result of this chapter.

Lemma 2.6

There are constants μ, κ, β (independent of the mesh-width h) such that

$$w^{\mathrm{T}}(M(s) - M(t))z \le (e^{\mu(s-t)} - 1)\; |w|_{M(t)}\, |z|_{M(t)} \tag{2.11}$$

$$w^{\mathrm{T}}(M^{-1}(s) - M(t)^{-1})z \le (e^{\mu(s-t)} - 1)\; |w|_{M(t)^{-1}}\, |z|_{M(t)^{-1}} \tag{2.12}$$

$$w^{\mathrm{T}}(A(s) - A(t))z \le (e^{\kappa(s-t)} - 1)\; |w|_{A(t)}\, |z|_{A(t)} \tag{2.13}$$

$$\begin{aligned} & w^{\mathrm{T}}\left((M^{-1}[A+M]M^{-1})(s) - (M^{-1}[A+M]M^{-1})(t)\right) z \\ & \qquad \le (e^{\beta(s-t)} - 1)\; |M^{-1}(t)w|_{A(t)+M(t)}\, |M^{-1}(t)z|_{A(t)+M(t)}, \end{aligned} \tag{2.14}$$

for all $w, z \in \mathbb{R}^N$ and $s, t \in [0, T]$.

We will apply this lemma with s close to t. Note that then $e^{\mu(s-t)} - 1 \le 2\mu(s-t)$, $e^{\kappa(s-t)} - 1 \le 2\kappa(s-t)$ and $e^{\beta(s-t)} - 1 \le 2\beta(s-t)$.

Proof

(a) For $w, z \in \mathbb{R}^N$, we define the discrete functions

$$W_h(x,t) = \sum_{j=1}^N w_j \chi_j(x,t) \quad \text{and} \quad Z_h(x,t) = \sum_{j=1}^N z_j \chi_j(x,t).$$

Note that by the transport property (2.2), we have $\partial_h^\bullet W_h = \partial_h^\bullet Z_h = 0$. Therefore, by the transport formula from Lemma 2.4 it follows that

$$\begin{aligned} w^{\mathrm{T}}\left(M(s)-M(t)\right)z &= \int_{\Gamma_h(s)} W_h(\cdot,s)Z_h(\cdot,s) - \int_{\Gamma_h(t)} W_h(\cdot,t)Z_h(\cdot,t) \\ &= \int_t^s \frac{d}{d\sigma}\int_{\Gamma_h(\sigma)} W_h(\cdot,\sigma)Z_h(\cdot,\sigma)\,d\sigma \\ &= \int_t^s \int_{\Gamma_h(\sigma)} W_h(\cdot,\sigma)Z_h(\cdot,\sigma)\nabla_{\Gamma_h(\sigma)}\cdot V_h\,d\sigma \\ &\le \mu \int_t^s \|W_h\|_{L^2(\Gamma_h(\sigma))}\|Z_h\|_{L^2(\Gamma_h(\sigma))}\,d\sigma \\ &= \mu \int_t^s |w|_{M(\sigma)}|z|_{M(\sigma)}\,d\sigma, \end{aligned}$$

where we have used that $\max_{\sigma\in[t,s]}\|\nabla_{\Gamma_h(\sigma)}\cdot V_h(\cdot,\sigma)\|_{L^\infty(\Gamma_h(\sigma))}$ is bounded by a constant μ independent of h and s,t, since V_h is the linear interpolant of the continuous velocity. With $z=w$, this inequality implies

$$|w|^2_{M(s)} \le |w|^2_{M(t)} + \mu\int_t^s |w|^2_{M(\sigma)}\,d\sigma, \qquad 0\le t\le s\le T,$$

and hence the Gronwall inequality yields

$$|w|^2_{M(s)} \le e^{\mu(s-t)}\,|w|^2_{M(t)}.$$

Inserting this bound for $|w|_{M(\sigma)}$ and $|z|_{M(\sigma)}$ in the above inequality yields the first inequality (2.11).

(b) With Lemma 2.4, we get for the matrix A

$$\begin{aligned} &w^{\mathrm{T}}\left(A(s)-A(t)\right)z \\ &\quad= \int_{\Gamma_h(s)} \nabla_{\Gamma_h(s)}W_h(\cdot,s)\cdot\nabla_{\Gamma_h(s)}Z_h(\cdot,s) - \int_{\Gamma_h(t)} \nabla_{\Gamma_h(t)}W_h(\cdot,t)\cdot\nabla_{\Gamma_h(t)}Z_h(\cdot,t) \\ &\quad= \int_t^s \frac{d}{d\sigma}\int_{\Gamma_h(\sigma)} \nabla_{\Gamma_h(\sigma)}W_h(\cdot,\sigma)\cdot\nabla_{\Gamma_h(\sigma)}Z_h(\cdot,\sigma)\,d\sigma. \end{aligned}$$

Lemma 2.4, keeping in mind that $\partial_h^\bullet W_h = \partial_h^\bullet Z_h = 0$ here, gives

$$\begin{aligned} &w^{\mathrm{T}}\left(A(s)-A(t)\right)z \\ &\quad= \int_t^s \int_{\Gamma_h(\sigma)} \mathcal{B}_h(V_h(\cdot,\sigma))\nabla_{\Gamma_h(\sigma)}W_h(\cdot,\sigma)\cdot\nabla_{\Gamma_h(\sigma)}Z_h(\cdot,\sigma)\,d\sigma \\ &\quad\le \kappa\int_t^s |w|_{A(\sigma)}|z|_{A(\sigma)}\,d\sigma \end{aligned}$$

since $\max_{\sigma\in[t,s]}\|\mathcal{B}_h(V_h(\cdot,\sigma)\|_{L^\infty(\Gamma_h(\sigma))}$ is uniformly bounded by a constant κ. Using this inequality together with the Gronwall inequality as above yields the third inequality (2.13).

(c) For the second inequality (2.12), we introduce the dual basis of $S_h(t)$ defined by

$$\big(\psi_i(\cdot,t)\big)_{i=1}^N = M(t)^{-1}\big(\chi_j(\cdot,t)\big)_{j=1}^N ,$$

and has the property that

$$\int_{\Gamma_h} \psi_i\chi_j = \delta_{ij} \quad \text{and} \quad \int_{\Gamma_h} \psi_i\psi_j = M^{-1}\big|_{i,j}.$$

The Leibniz formula (2.6) gives

$$0 = \frac{d}{dt}\int_{\Gamma_h} \psi_i\chi_j = \int_{\Gamma_h} \partial_h^\bullet\psi_i\chi_j + \psi_i\partial_h^\bullet\chi_j + \psi_i\chi_j\nabla_\Gamma\cdot V_h,$$

and since $\partial_h^\bullet\chi_j = 0$, it follows that

$$\int_{\Gamma_h} \partial_h^\bullet\psi_i\chi_j = -\int_{\Gamma_h} \psi_i\chi_j\nabla_\Gamma\cdot V_h \quad \text{for all } i,j = 1,\dots,N.$$

This yields that, for all $Z_h(\cdot,t) \in S_h(t)$ and functions of the form $\widetilde{W}_h(x,t) = \sum_{i=1}^N w_i\psi_i(\cdot,t)$ with time-independent coefficients w_i, we have

$$\int_{\Gamma_h} \partial_h^\bullet\widetilde{W}_h Z_h = -\int_{\Gamma_h} \widetilde{W}_h Z_h\nabla_\Gamma\cdot V_h. \tag{2.15}$$

For $w,z\in\mathbb{R}^N$, we now define

$$\widetilde{W}_h(\cdot,t) = \sum_{j=1}^N w_j\psi_j(\cdot,t) \in S_h(t) \quad \text{and} \quad \widetilde{Z}_h(\cdot,t) = \sum_{j=1}^N z_j\psi_j(\cdot,t) \in S_h(t).$$

Using the Leibniz formula in the third equality and (2.15) in the fourth equality we obtain

$$\begin{aligned}
w^{\mathrm{T}}\Big(M(s)^{-1} - M(t)^{-1}\Big)z &= \int_{\Gamma_h(s)} \widetilde{W}_h(\cdot,s)\widetilde{Z}_h(\cdot,s) - \int_{\Gamma_h(t)} \widetilde{W}_h(\cdot,t)\widetilde{Z}_h(\cdot,t) \\
&= \int_t^s \frac{d}{d\sigma}\int_{\Gamma_h(\sigma)} \widetilde{W}_h(\cdot,\sigma)\widetilde{Z}_h(\cdot,\sigma)\ \mathrm{d}\sigma \\
&= \int_t^s \int_{\Gamma_h(\sigma)} \big(\partial_h^\bullet\widetilde{W}_h\widetilde{Z}_h + \widetilde{W}_h\partial_h^\bullet\widetilde{Z}_h + \widetilde{W}_h\widetilde{Z}_h\nabla_{\Gamma_h(\sigma)}\cdot V_h\big)\ \mathrm{d}\sigma \\
&= \int_t^s \int_{\Gamma_h(\sigma)} -\widetilde{W}_h\widetilde{Z}_h\nabla_{\Gamma_h(\sigma)}\cdot V_h\ \mathrm{d}\sigma \\
&\leq \mu\int_t^s \big\|\widetilde{W}_h\big\|_{L_2(\Gamma_h(\sigma))}\big\|\widetilde{Z}_h\big\|_{L_2(\Gamma_h(\sigma))}\ \mathrm{d}\sigma \\
&= \mu\int_t^s |w|_{M(\sigma)^{-1}}\,|z|_{M(\sigma)^{-1}}\ \mathrm{d}\sigma.
\end{aligned}$$

Using this inequality together with the Gronwall inequality as above yields the third inequality (2.12).

(d) In order to proof the last inequality (2.14) we need to control the H^1-norm of the discrete material derivative of functions of the form:

$$\widetilde{W}_h(\cdot,t) = \sum_{i=1}^{N} w_i \psi_i(\cdot,t) = \sum_{i=1}^{N} (M(t)^{-1}w)_i \, \chi_i(\cdot,t) \in S_h(t),$$

where ψ_i are the functions introduced in part (c). Due to the fact that $\partial_h^\bullet \chi_i = 0$, the material derivatives of finite element functions $\phi_h \in S_h$ are again elements of S_h. Therefore with the help of the L^2-projection P_h into $S_h(t)$, we deduce from (2.15) that

$$\partial_h^\bullet \widetilde{W}_h(\cdot,t) = \sum_{i=1}^{N} w_i \partial_h^\bullet \psi_i(\cdot,t) = -P_h(\widetilde{W}_h \nabla_{\Gamma_h} \cdot V_h) \in S_h(t).$$

By standard arguments, we obtain

$$\|\partial_h^\bullet \widetilde{W}_h\|_{L^2(\Gamma_h)} = \|P_h(\widetilde{W}_h \nabla_{\Gamma_h} \cdot V_h)\|_{L^2(\Gamma_h)} \le \mu \|\widetilde{W}_h\|_{L^2(\Gamma_h)}. \tag{2.16}$$

We show next that

$$\|\nabla_{\Gamma_h}(\partial_h^\bullet \widetilde{W}_h)\|_{L^2(\Gamma_h)} \le c\left(\|\nabla_{\Gamma_h}\widetilde{W}_h\|_{L^2(\Gamma_h)} + \|\widetilde{W}_h\|_{L^2(\Gamma_h)}\right). \tag{2.17}$$

We use the inverse estimate ($\|\nabla_{\Gamma_h}\phi_h\|_{L^2(\Gamma_h)} \le ch^{-1}\|\phi_h\|_{L^2(\Gamma_h)}$ for $\phi_h \in S_h$) to find

$$\begin{aligned}
\|\nabla_{\Gamma_h}(\partial_h^\bullet \widetilde{W}_h)\|_{L^2(\Gamma_h)} &= \|\nabla_{\Gamma_h} P_h(\widetilde{W}_h \nabla_{\Gamma_h} \cdot V_h)\|_{L^2(\Gamma_h)} \\
&\le \|\nabla_{\Gamma_h} P_h(\widetilde{W}_h(\nabla_{\Gamma_h} \cdot V_h - (\nabla_\Gamma \cdot v)^{-l}))\|_{L^2(\Gamma_h)} \\
&\quad + \|\nabla_{\Gamma_h}(P_h(\widetilde{W}_h(\nabla_\Gamma \cdot v)^{-l}) - \widetilde{W}_h(\nabla_\Gamma \cdot v)^{-l})\|_{L^2(\Gamma_h)} \\
&\quad + \|\nabla_{\Gamma_h}(\widetilde{W}_h(\nabla_\Gamma \cdot v)^{-l})\|_{L^2(\Gamma_h)} \\
&\le \frac{c}{h}\|P_h(\widetilde{W}_h(\nabla_{\Gamma_h} \cdot V_h - (\nabla_\Gamma \cdot v)^{-l}))\|_{L^2(\Gamma_h)} \\
&\quad + \frac{c}{h}\|P_h(\widetilde{W}_h(\nabla_\Gamma \cdot v)^{-l}) - \widetilde{W}_h(\nabla_\Gamma \cdot v)^{-l}\|_{L^2(\Gamma_h)} \\
&\quad + c\|\widetilde{W}_h\|_{L^2(\Gamma_h)} + c\|\nabla_{\Gamma_h}\widetilde{W}_h\|_{L^2(\Gamma_h)}.
\end{aligned}$$

Here $f^{-l} : \Gamma_h \to \mathbb{R}$ denotes the extension of the function $f : \Gamma \to \mathbb{R}$ constantly in normal direction to Γ.

By interpolation estimates (cf. Lemma 6.2) and since $\widetilde{W}_h$ is piecewise linear on Γ_h and v is sufficiently smooth we have that

$$\|P_h(\widetilde{W}_h(\nabla_\Gamma \cdot v)^{-l}) - \widetilde{W}_h(\nabla_\Gamma \cdot v)^{-l}\|_{L^2(\Gamma_h)} \le ch^2(\|\widetilde{W}_h\|_{L^2(\Gamma_h)} + \|\nabla_{\Gamma_h}\widetilde{W}_h\|_{L^2(\Gamma_h)}).$$

Since V_h is the linear interpolant of v^{-l}, we observe for the remaining term:

$$\begin{aligned}
&\|P_h(\widetilde{W}_h(\nabla_{\Gamma_h} \cdot V_h - (\nabla_\Gamma \cdot v)^{-l}))\|_{L^2(\Gamma_h)} \\
&\qquad \le \|\widetilde{W}_h\|_{L^2(\Gamma_h)}\|\nabla_{\Gamma_h} \cdot V_h - (\nabla_\Gamma \cdot v)^{-l}\|_{L^\infty(\Gamma_h)} \le ch\|\widetilde{W}_h\|_{L^2(\Gamma_h)}.
\end{aligned}$$

All together yields to the stated inequality (2.17).

We are now ready to use similar techniques as in part (a)–(c) to prove the last inequality (2.14). With the notations introduced above, using the transport Lemma 2.4, the estimates (2.16) and (2.17) together with the Young's inequality we discover

$$
\begin{aligned}
& w^{\mathtt{T}} \Big((M^{-1}[A+M]M^{-1})(s) - (M^{-1}[A+M]M^{-1})(t) \Big)\, z \\
&\quad = \int_{\Gamma_h(s)} \nabla_{\Gamma_h(s)} \widetilde{W}_h(\cdot,s) \cdot \nabla_{\Gamma_h(s)} \widetilde{Z}_h(\cdot,s) - \int_{\Gamma_h(t)} \nabla_{\Gamma_h(t)} \widetilde{W}_h(\cdot,t) \cdot \nabla_{\Gamma_h(t)} \widetilde{Z}_h(\cdot,t) \\
&\quad = \int_t^s \frac{d}{d\sigma} \int_{\Gamma_h(\sigma)} \nabla_{\Gamma_h(\sigma)} \widetilde{W}_h(\cdot,\sigma) \cdot \nabla_{\Gamma_h(\sigma)} \widetilde{Z}_h(\cdot,\sigma) \,\mathrm{d}\sigma \\
&\quad = \int_t^s \int_{\Gamma_h(\sigma)} \Big(\nabla_{\Gamma_h(\sigma)} \partial_h^{\bullet} \widetilde{W}_h \cdot \nabla_{\Gamma_h(\sigma)} \widetilde{Z}_h + \nabla_{\Gamma_h(\sigma)} \widetilde{W}_h \cdot \nabla_{\Gamma_h(\sigma)} \partial_h^{\bullet} \widetilde{Z}_h \Big) \,\mathrm{d}\sigma \\
&\qquad + \int_t^s \int_{\Gamma_h(\sigma)} \mathcal{B}_h(V_h) \nabla_{\Gamma_h(\sigma)} \widetilde{W}_h \cdot \nabla_{\Gamma_h(\sigma)} \widetilde{Z}_h \,\mathrm{d}\sigma \\
&\quad \le \int_t^s \|\nabla_{\Gamma_h(\sigma)} \partial_h^{\bullet} \widetilde{W}_h\|_{L^2(\Gamma_h(\sigma))} \|\nabla_{\Gamma_h(\sigma)} \widetilde{Z}_h\|_{L^2(\Gamma_h(\sigma))} \,\mathrm{d}\sigma \\
&\qquad + \int_t^s \|\nabla_{\Gamma_h(\sigma)} \widetilde{W}_h\|_{L^2(\Gamma_h(\sigma))} \|\nabla_{\Gamma_h(\sigma)} \partial_h^{\bullet} \widetilde{Z}_h\|_{L^2(\Gamma_h(\sigma))} \,\mathrm{d}\sigma \\
&\qquad + \int_t^s \kappa \|\nabla_{\Gamma_h(\sigma)} \widetilde{W}_h\|_{L^2(\Gamma_h(\sigma))} \|\nabla_{\Gamma_h(\sigma)} \widetilde{Z}_h\|_{L^2(\Gamma_h(\sigma))} \,\mathrm{d}\sigma \\
&\quad \le \frac{1}{2} \beta \int_t^s \Big(|M(\sigma)^{-1} w|_{(A+M)(\sigma)}^2 + |M(\sigma)^{-1} z|_{(A+M)(\sigma)}^2 \Big) \,\mathrm{d}\sigma
\end{aligned}
$$

where we used the fact that

$$
\|\widetilde{W}_h\|_{L^2(\Gamma_h(\sigma))}^2 = |M(\sigma)^{-1} w|_{M(\sigma)}^2 \quad \text{and} \quad \|\nabla_{\Gamma_h(\sigma)} \widetilde{W}_h\|_{L^2(\Gamma_h(\sigma))}^2 = |M(\sigma)^{-1} w|_{A(\sigma)}^2.
$$

Letting $z = w$ gives

$$
|M(s)^{-1} w|_{(A+M)(s)}^2 \le |M(t)^{-1} w|_{(A+M)(t)}^2 + \beta \int_t^s |M(\sigma)^{-1} w|_{(A+M)(\sigma)}^2 \,\mathrm{d}\sigma.
$$

Using this inequality together with the Gronwall inequality as above completes the proof. ∎

From the ESFEM method, Lemma 2.6 is all what we will need in the stability analysis of the time discretization schemes considered in Chapter 3 and Chapter 4. We remark that our results are also valid for general ODE problems of the form 2.5 with matrices satisfying the above estimates.

In the following, we assume that $a = \nabla_{\Gamma_h} \cdot V_h$ and $B = \mathcal{B}_h(V_h)$ are sufficiently often continuously differentiable with respect to time. Then g_{kl} and G_{kl} from Lemma 2.5 are bounded independently of the grid size h and we can prove the following lemma which will be used to switch from the matrix-vector level to the function-space level. This will be done first in Chapter 5.

Lemma 2.7
For finite element functions $Z_h(\cdot,t) = \sum_{j=1}^N z_j(t)\chi_j(\cdot,t) \in S_h(t)$ *with the vector of nodal values* $z(t) = (z_j(t)) \in \mathbb{R}^N$*, there exists a constant* c *independent of the mesh-width* h *such that*

$$|(Mz)^{(k)}(t)|^2_{M(t)^{-1}} \le c \sum_{l=0}^k \|\partial_h^{(l)} Z_h\|^2_{L^2(\Gamma_h(t)} \tag{2.18}$$

and

$$|M(t)^{-1}(Mz)^{(k)}(t)|^2_{A(t)} \le c \sum_{l=0}^k \big(\|\partial_h^{(l)} Z_h\|^2_{L^2(\Gamma_h(t))} + \|\nabla_{\Gamma_h(t)}\partial_h^{(l)} Z_h\|^2_{L^2(\Gamma_h(t))}\big). \tag{2.19}$$

Proof
We omit the omnipresent argument t. We set $w = M^{-1}(Mz)^{(k)}$ and $W_h = \sum_{j=1}^N w_j\chi_j$. We then observe

$$\int_{\Gamma_h} W_h\chi_j = \sum_{k=1}^N w_k \int_{\Gamma_h} \chi_k\chi_j = (Mw)_j = (Mz)_j^{(k)} = \frac{d^k}{dt^k}\int_{\Gamma_h} Z_h\chi_j.$$

Then, by Lemma 2.5 we have that

$$\int_{\Gamma_h} W_h\phi_h = \int_{\Gamma_h} \partial_h^{(k)} Z_h\phi_h + \sum_{l=1}^k \int_{\Gamma_h} g_{kl}\partial_h^{(k-l)} Z_h\phi_h \quad \forall \phi_h \in S_h$$

This means that

$$W_h = \partial_h^{(k)} Z_h + \sum_{l=1}^k P_h(g_{kl}\partial_h^{(k-l)} Z_h)$$

with the L^2-projection P_h onto S_h. Here, we used the fact that the material derivatives of $Z_h \in S_h$ again are elements of S_h, since $\partial_h^\bullet \chi_i = 0$. Then,

$$|w|_M = \|W_h\|_{L^2(\Gamma_h)} \le \|\partial_h^{(k)} Z_h\|_{L^2(\Gamma_h)} + \sum_{l=1}^k \|g_{kl}\partial_h^{(k-l)} Z_h\|_{L^2(\Gamma_h)},$$

which yields (2.18). We write similarly

$$\begin{aligned} |w|_A &= \|\nabla_{\Gamma_h} W_h\|_{L^2(\Gamma_h)} \\ &\le \|\nabla_{\Gamma_h}\partial_h^{(k)} Z_h\|_{L^2(\Gamma_h)} + \sum_{l=1}^k \|\nabla_{\Gamma_h} P_h(g_{kl}\partial_h^{(k-l)} Z_h)\|_{L^2(\Gamma_h)}. \end{aligned} \tag{2.20}$$

Here, $g_{kl} = g_{kl}(a, \dot{a}, \dots, a^{(l)})$ are piecewise constant functions on the discrete surface Γ_h, since $a = \nabla_{\Gamma_h} \cdot V_h$.

We now show the proof of (2.19) for the case $k = 1$ and discuss the general case later. For $k = 1$, we have already proved in (2.17) that the last term on the right hand side of (2.20) is bounded by

$$\|\nabla_{\Gamma_h} P_h(aZ_h)\|_{L^2(\Gamma_h)} \le c\big(\|Z_h\|_{L^2(\Gamma_h)} + \|\nabla_{\Gamma_h} Z_h\|_{L^2(\Gamma_h)}\big)$$

we thus obtain the inequality

$$|w|_A \leq \|\nabla_{\Gamma_h} \partial_h^{\bullet} Z_h\|_{L^2(\Gamma_h)} + c\big(\|Z_h\|_{L^2(\Gamma_h)} + \|\nabla_{\Gamma_h} Z_h\|_{L^2(\Gamma_h)}\big).$$

This gives (2.19) in the case $k = 1$.

The case $k > 1$ is similar but more technical. We only give the basic ingredients for the proof. In this case one has to deal with polynomials of the time derivatives $\dot{a}, \dots, a^{(k)}$ of $a = \nabla_{\Gamma_h} \cdot V_h$. The most important formula is the material derivative of the tangential gradient. For a vector valued function b, one has the identity

$$\partial_h^{\bullet}(\nabla_{\Gamma_h} \cdot b) = \nabla_{\Gamma_h} \cdot \partial_h^{\bullet} b - \big(\mathcal{A} \nabla_{\Gamma_h} b\big) \tag{2.21}$$

with the matrix $\mathcal{A}_{lr} = \big(\nabla_{\Gamma_h}\big)_l V_{h,r} - \sum_{s=1}^{m+1} \nu_{h,s} \nu_{h,l} \big(\nabla_{\Gamma_h}\big)_r V_{h,s}$ $(l, r = 1, \dots, m+1)$. One then has to use this formula for $b = V_h$ and follow the ideas of the case $k = 1$. ∎

3. Time Discretization by Implicit Runge–Kutta Methods

In this chapter, we study the time discretization of the ODE system (2.5) resulting from the ESFEM method. We choose to apply implicit Runge–Kutta schemes which are known to be unconditionally stable when applied to PDEs on fixed domains. For algebraically stable and stiffly accurate Runge–Kutta methods such as Radau IIA collocation methods of arbitrary higher order, we prove the unconditional stability of the fully discrete scheme. Our stability analysis operates at the matrix-vector level and uses form the ESFEM method only the stated estimates for the evolving mass and stiffness matrices (Lemma 2.6). Thus, the analytical tools developed here could also be applied to similar ODE system obtained after the spatial discretization of PDEs on moving domains or obtained when applying the moving-mesh method.

3.1. Implicit Runge-Kutta methods

3.1.1. Method description

In order to compute approximations α_n to the solution $\alpha(t_n)$ of the ODE system (2.5), we consider an s-stage implicit Runge–Kutta (RK) method for the time discretization. We set for simplicity equidistant time points $t_n = t_{n-1} + \tau$ with step size $\tau > 0$ and $t_0 = 0$.

The approximations α_n to the solution $\alpha(t_n)$ are determined via the scheme (cf. [22, 27])

$$M_{ni}\alpha_{ni} = M_n\alpha_n + \tau \sum_{j=1}^{s} a_{ij}\dot{\alpha}_{nj}, \qquad i = 1, \cdots, s, \tag{3.1a}$$

$$M_{n+1}\alpha_{n+1} = M_n\alpha_n + \tau \sum_{i=1}^{s} b_i\dot{\alpha}_{ni}, \tag{3.1b}$$

where the internal stages satisfy

$$\dot{\alpha}_{ni} + A_{ni}\alpha_{ni} = 0 \qquad i = 1, \cdots, s,$$

with $A_{ni} = A(t_n + c_i\tau)$, $M_{ni} = M(t_n + c_i\tau)$ and $M_{n+1} = M(t_{n+1})$.

Here s is the number of stages and the method is uniquely defined via the so-called Butcher-tableau (cf. [27, Section IV.5]):

$$\begin{array}{c|c} c & \mathcal{A} \\ \hline & b^{\mathrm{T}} \end{array} := \begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array} .$$

3.1.2. Method assumptions

We assume:

- The method has stage order $q \geq 1$ and classical order $p \geq q+1$.
- The RK coefficient matrix (a_{ij}) is invertible, and we denote its inverse by (w_{ij}).
- The method is *algebraically stable*: the $s \times s$ matrix

$$(b_i a_{ij} + b_j a_{ji} - b_i b_j) \text{ is positive semi-definite, and all } b_i > 0\,, \tag{3.2}$$

- The method is *stiffly accurate*:

$$c_s = 1 \quad \text{and} \quad b_j = a_{sj} \quad \text{for} \quad j = 1, \ldots, s\,, \tag{3.3}$$

  which implies

$$\alpha_{n+1} = \alpha_{ns}.$$

Well-known examples are the collocation methods at Radau nodes, of stage order $q = s$ and classical order $p = 2s - 1$. The simplest method of this class is the backward Euler method with $s = 1$ and $a_{11} = c_1 = b_1 = 1$.

3.2. Defects and errors

Let us consider the perturbed ODE system

$$\begin{cases} \frac{d}{dt}\left(M(t)\widetilde{\alpha}(t)\right) + A(t)\widetilde{\alpha}(t) &= M(t)r(t) \\ \widetilde{\alpha}(0) &= \widetilde{\alpha}_0. \end{cases} \tag{3.4}$$

with a residual $r(t) \in R^N$. We will see in Chapter 5 that an arbitrary projection of the exact solution of the PDE (1.3) to the finite element space $S_h(t)$ satisfies a perturbed ODE system of the form (3.4). Thus, the analysis of this system will play a key role in estimating the difference between the fully discrete solution and the considered projection.

3.2.1. Defects and errors

The solution of (3.4) satisfies the RK relations up to a defect (quadrature error)

$$M_{ni}\widetilde{\alpha}(t_n + c_i\tau) = M_n\widetilde{\alpha}(t_n) + \tau \sum_{j=1}^{s} a_{ij}\dot{\widetilde{\alpha}}(t_n + c_j\tau) + \Delta_{ni} \qquad i = 1, \cdots, s, \tag{3.5a}$$

$$M_{n+1}\widetilde{\alpha}(t_{n+1}) = M_n\widetilde{\alpha}(t_n) + \tau \sum_{j=1}^{s} b_j\dot{\widetilde{\alpha}}(t_n + c_j\tau) + \delta_{n+1} \tag{3.5b}$$

By the assumption of stiff accuracy, we have

$$\delta_{n+1} = \Delta_{ns}.$$

For smooth solutions, we have by Taylor expansion (in suitable norms!)

$$\delta_{n+1} = \mathcal{O}(\tau^{p+1}), \ \Delta_{ni} = \mathcal{O}(\tau^{q+1}).$$

For the errors, we use the notations

$$\begin{aligned} e_n &= \alpha_n - \widetilde{\alpha}(t_n) \\ E_{ni} &= \alpha_{ni} - \widetilde{\alpha}(t_n + c_i\tau) \\ \dot{E}_{ni} &= \dot{\alpha}_{ni} - \dot{\widetilde{\alpha}}(t_n + c_i\tau), \end{aligned}$$

and subtract to obtain the *error equations*

$$M_{ni}E_{ni} = M_n e_n + \tau \sum_{j=1}^{s} a_{ij}\dot{E}_{nj} - \Delta_{ni}, \qquad i = 1, \cdots, s, \tag{3.6a}$$

$$M_{n+1}e_{n+1} = M_n e_n + \tau \sum_{i=1}^{s} b_i\dot{E}_{ni} - \delta_{n+1}, \tag{3.6b}$$

where the internal stages satisfy

$$\dot{E}_{ni} + A_{ni}E_{ni} = -M_{ni}r_{ni} \qquad i = 1, \cdots, s, \tag{3.7}$$

with $r_{ni} = r(t_n + c_i\tau)$.

3.3. Stability

The main result of this chapter is the following lemma. It states that the fully discrete scheme (combination of the ESFEM method from Chapter 2 and an algebraically stable and stiffly accurate Runge–method) is unconditionally stable.

Lemma 3.1
If the Runge–Kutta method is algebraically stable and stiffly accurate, then there exist $\tau_0 > 0$ *depending only on* μ, κ *of Lemma 2.6 such that for* $\tau \le \tau_0$ *and* $t_n \le T$*, the errors are bounded by*

$$|e_n|_{M_n}^2 + \tau \sum_{k=1}^{n} |e_k|_{A_k}^2 \le C \left(|e_0|_{M_0} + \tau \sum_{k=0}^{n-1} \sum_{i=1}^{s} \|M_{ki} r_{ki}\|_{*,t_{ki}}^2 + \tau \sum_{k=1}^{n} |\delta_k/\tau|_{M_k}^2 \right) + C\tau \sum_{k=0}^{n-1} \sum_{i=1}^{s} \left(|M_{ki}^{-1}\Delta_{ki}|_{M_{ki}}^2 + |M_{ki}^{-1}\Delta_{ki}|_{A_{ki}}^2 \right)$$

where $\|w\|_{*,t}^2 = w^{\mathsf{T}}(A(t)+M(t))^{-1}w$ *and* $t_{ki} = t_k + c_i\tau$*. The constant* C *is independent of* h, τ *and* n *(but depends on* μ, κ*, and* T*).*

Proof
The proof is based on the algebraic stability and stiff accuracy of the method and uses similar arguments as in the proof of Theorem 1.1 in [35] and Lemma 7.1 in [19].

(a) We start from (3.6b), take the squared norm at t_{n+1} and estimate the terms in

$$|M_{n+1}e_{n+1}|_{M_{n+1}^{-1}}^2 = \Big|M_n e_n + \tau \sum_{j=1}^{s} b_j \dot{E}_{nj}\Big|_{M_{n+1}^{-1}}^2 - 2\Big\langle M_n e_n + \tau \sum_{j=1}^{s} b_j \dot{E}_{nj} \,\Big|\, M_{n+1}^{-1} \,\Big|\, \delta_{n+1} \Big\rangle + |\delta_{n+1}|_{M_{n+1}^{-1}}^2 . \tag{3.8}$$

Expressing $M_n e_n$ by (3.6a), we obtain for the first term

$$|M_n e_n + \tau \sum_{j=1}^{s} b_j \dot{E}_{nj}|_{M_{n+1}^{-1}}^2 = |M_n e_n|_{M_{n+1}^{-1}}^2 + 2\tau \sum_{j=1}^{s} b_j \langle \dot{E}_{nj} \,|\, M_{n+1}^{-1} \,|\, M_{nj}E_{nj} + \Delta_{nj} \rangle + \tau^2 \sum_{i=1}^{s}\sum_{j=1}^{s} (b_i b_j - b_i a_{ij} - b_j a_{ji}) \langle \dot{E}_{ni} \,|\, M_{n+1}^{-1} \,|\, \dot{E}_{nj} \rangle , \tag{3.9}$$

where the last term is non-positive by the assumption of algebraic stability (3.2). In the second term we write $M_{n+1}^{-1} = M_n^{-1} + (M_{n+1}^{-1} - M_n^{-1})$. By condition (2.12), we have

$$\begin{aligned} |M_n e_n|_{M_{n+1}^{-1}}^2 &= \langle M_n e_n \,|\, M_{n+1}^{-1} \,|\, M_n e_n \rangle \\ &= \langle e_n \,|\, M_n \,|\, e_n \rangle + \langle M_n e_n \,|\, M_{n+1}^{-1} - M_n^{-1} \,|\, M_n e_n \rangle \\ &\le (1 + 2\mu\tau)\, |e_n|_{M_n}^2 . \end{aligned} \tag{3.10}$$

In the middle term we write

$$\langle \dot{E}_{nj} \,|\, M_{n+1}^{-1} \,|\, M_{nj}E_{nj} + \Delta_{nj} \rangle = \langle \dot{E}_{nj} \,|\, M_{nj}^{-1} \,|\, M_{nj}E_{nj} + \Delta_{nj} \rangle + \langle \dot{E}_{nj} \,|\, M_{n+1}^{-1} - M_{nj}^{-1} \,|\, M_{nj}E_{nj} + \Delta_{nj} \rangle \tag{3.11}$$

and estimate the two terms on the right separately.

(b) In view of (3.7), we have for the first term of (3.11)

$$
\begin{aligned}
\langle \dot{E}_{nj} \,|\, M_{nj}^{-1} \,|\, M_{nj}E_{nj} + \Delta_{nj} \rangle &= \langle \dot{E}_{nj} \,|\, E_{nj} \rangle + \langle \dot{E}_{nj} \,|\, M_{nj}^{-1} \,|\, \Delta_{nj} \rangle \\
&= - |E_{nj}|_{A_{nj}}^2 - \langle M_{nj} r_{nj} \,|\, E_{nj} + M_{nj}^{-1} \Delta_{nj} \rangle \\
&\quad - \langle E_{nj} \,|\, A_{nj} \,|\, M_{nj}^{-1} \Delta_{nj} \rangle
\end{aligned} \tag{3.12}
$$

For the second and third term of (3.12), we use the Cauchy-Schwarz inequality and Young's inequality to estimate

$$
\begin{aligned}
&\langle M_{nj} r_{nj} \,|\, E_{nj} + M_{nj}^{-1} \Delta_{nj} \rangle \\
&\quad = \langle (A_{nj} + M_{nj})^{-1/2} M_{nj} r_{nj} \,|\, (A_{nj} + M_{nj})^{1/2} \left(E_{nj} + M_{nj}^{-1} \Delta_{nj} \right) \rangle \\
&\quad \le \| M_{nj} r_{nj} \|_{*,nj} \left(|E_{nj} + M_{nj}^{-1} \Delta_{nj}|_{M_{nj}}^2 + |E_{nj} + M_{nj}^{-1} \Delta_{nj}|_{A_{nj}}^2 \right)^{1/2} \\
&\quad \le 2 \| M_{nj} r_{nj} \|_{*,nj}^2 + \frac{1}{4} \left(|E_{nj}|_{M_{nj}}^2 + |E_{nj}|_{A_{nj}}^2 \right) \\
&\qquad + \frac{1}{4} \left(|M_{nj}^{-1} \Delta_{nj}|_{M_{nj}}^2 + |M_{nj}^{-1} \Delta_{nj}|_{A_{nj}}^2 \right)
\end{aligned}
$$

$$
\begin{aligned}
\langle E_{nj} \,|\, A_{nj} \,|\, M_{nj}^{-1} \Delta_{nj} \rangle &\le |E_{nj}|_{A_{nj}} |M_{nj}^{-1} \Delta_{nj}|_{A_{nj}} \\
&\le \frac{1}{4} |E_{nj}|_{A_{nj}}^2 + 2 |M_{nj}^{-1} \Delta_{nj}|_{A_{nj}}^2 .
\end{aligned}
$$

Therefore, by (3.12), the first term on the right-hand side of (3.11) is bounded by

$$
\begin{aligned}
\langle \dot{E}_{nj} \,|\, M_{nj}^{-1} \,|\, M_{nj}E_{nj} + \Delta_{nj} \rangle \le &- \frac{1}{2} |E_{nj}|_{A_{nj}}^2 + \frac{1}{4} |E_{nj}|_{M_{nj}}^2 \\
&+ C \left(|M_{nj}^{-1} \Delta_{nj}|_{M_{nj}}^2 + |M_{nj}^{-1} \Delta_{nj}|_{A_{nj}}^2 \right)
\end{aligned} \tag{3.13}
$$

(c) For the last term on the right-hand side of (3.11, we rewrite (3.6a) as

$$
\dot{E}_{nj} = \tau^{-1} \sum_{i=1}^{s} w_{ji} (M_{ni} E_{ni} - M_n e_n + \Delta_{ni})
$$

and use (2.11)-(2.12) with sufficiently small τ as in (3.10) to get the bound

$$
\begin{aligned}
\langle \dot{E}_{nj} \,|\, M_{n+1}^{-1} - M_{nj}^{-1} \,|\, M_{nj}E_{nj} + \Delta_{nj} \rangle &\le C\tau |\dot{E}_{nj}|_{M_{nj}^{-1}} \cdot \left(|E_{nj}|_{M_{nj}} + |\Delta_{nj}|_{M_{nj}^{-1}} \right) \\
&\le C |e_n|_{M_n}^2 + C \sum_{i=1}^{s} |E_{ni}|_{M_{ni}}^2 \\
&\quad + C \sum_{i=1}^{s} |\Delta_{ni}|_{M_{ni}^{-1}}^2 .
\end{aligned} \tag{3.14}
$$

(d) In order to estimate the second term on the right hand side of (3.8), we use the error equations (3.6) together with the assumption that the the method is stiffly accurate (3.3) to find

$$M_n e_n + \tau \sum_{j=1}^{s} b_j \dot{E}_{nj} = M_n e_n + \tau \sum_{j=1}^{s} a_{sj} \dot{E}_{nj} = M_{ns} E_{ns} + \Delta_{ns} = M_{n+1} E_{ns} + \delta_{n+1}.$$

Then an application of the Cauchy-Schwarz inequality and Young's inequality gives

$$\begin{aligned} 2 \langle M_n e_n + \tau \sum_{j=1}^{s} b_j \dot{E}_{nj} \mid M_{n+1}^{-1} \mid \delta_{n+1} \rangle &\le 2 \, |M_{n+1} E_{ns} + \delta_{n+1}|_{M_{n+1}^{-1}} \, |\delta_{n+1}|_{M_{n+1}^{-1}} \\ &\le \tau \, |E_{ns}|^2_{M_{n+1}} + (1 + 2\tau)\tau \, |\delta_{n+1}/\tau|_{M_{n+1}^{-1}} . \end{aligned} \tag{3.15}$$

(e) Combining (3.8)–(3.15) and keeping in mind that $b_i > 0$, we have shown

$$\begin{aligned} &|e_{n+1}|^2_{M_{n+1}} - |e_n|^2_{M_n} + \frac{1}{2} \tau \sum_{i=1}^{s} b_i |E_{ni}|^2_{A_{ni}} \\ &\quad \le C\tau |e_n|^2_{M_n} + C\tau \sum_{i=1}^{s} |E_{ni}|^2_{M_{ni}} + C\tau \sum_{i=1}^{s} \|M_{ni} r_{ni}\|^2_{*,ni} \\ &\qquad + C\tau \sum_{i=1}^{s} \Big(|M_{ni}^{-1} \Delta_{ni}|^2_{M_{ni}} + |M_{ni}^{-1} \Delta_{ni}|^2_{A_{ni}} \Big) + C\tau |\delta_{n+1}/\tau|_{M_{n+1}^{-1}} . \end{aligned} \tag{3.16}$$

In order to be able to apply the discrete Gronwall inequality, we still need to estimate the terms $|E_{ni}|^2_{M_{ni}}$. This is what we do next.

We multiply the equation (3.6a) by E_{ni}^{T} and obtain

$$|E_{ni}|^2_{M_{ni}} = \langle e_n \mid M_n \mid E_{ni} \rangle + \tau \sum_{j=1}^{s} a_{ij} \langle \dot{E}_{nj} \mid E_{ni} \rangle - \langle \Delta_{ni} \mid E_{ni} \rangle .$$

The first term on the right-hand side is estimated for sufficiently small τ as

$$\begin{aligned} \langle e_n \mid M_n \mid E_{ni} \rangle &\le |e_n|_{M_n} \, |E_{ni}|_{M_n} \\ &\le \frac{1}{2} \epsilon |E_{ni}|^2_{M_n} + \frac{1}{2} \epsilon^{-1} |e_n|^2_{M_n} \\ &\le C\epsilon |E_{ni}|^2_{M_{ni}} + \frac{1}{2} \epsilon^{-1} |e_n|^2_{M_n} \end{aligned}$$

with a small constant $\epsilon > 0$. Similarly, the last term is bounded by

$$\begin{aligned} -\langle \Delta_{ni} \mid E_{ni} \rangle &= -\langle M_{ni}^{-1} \Delta_{ni} \mid M_{ni} \mid E_{ni} \rangle \\ &\le \tfrac{1}{2} \epsilon |E_{ni}|^2_{M_{ni}} + \tfrac{1}{2} \epsilon^{-1} |M_{ni}^{-1} \Delta_{ni}|^2_{M_{ni}} . \end{aligned}$$

For the middle term we proceed as in part (b). We rewrite with the help of (3.7) the expressions $\langle \dot{E}_{nj} \mid E_{ni} \rangle$ as

$$\langle \dot{E}_{nj} \mid E_{ni} \rangle = -\langle E_{nj} \mid A_{nj} \mid E_{ni} \rangle - \langle M_{nj} r_{nj} \mid E_{ni} \rangle,$$

then the Cauchy-Schwarz inequality, Young's inequality and conditions (2.11)–(2.13) yield

$$\langle \dot{E}_{nj} \mid E_{ni} \rangle \le C|E_{nj}|^2_{A_{nj}} + C|E_{ni}|^2_{A_{ni}} + C|E_{ni}|^2_{M_{ni}} + C\|M_{nj} r_{nj}\|^2_{*,nj}.$$

Combining the above bounds and choosing ϵ sufficiently small (but independent of τ), we achieve

$$|E_{ni}|^2_{M_{ni}} \le C|e_n|^2_{M_n} + C\tau \sum_{k=1}^{s} |E_{nk}|^2_{A_{ni}} + C\tau \sum_{k=1}^{s} \|M_{nk} r_{nk}\|^2_{*,nk} + C|M_{ni}^{-1}\Delta_{ni}|^2_{M_{ni}}. \tag{3.17}$$

(f) Inserting the bound (3.17) into (3.16) yields

$$\begin{aligned} |e_{n+1}|^2_{M_{n+1}} - |e_n|^2_{M_n} + \frac{1}{4}\tau \sum_{i=1}^{s} b_i |E_{ni}|^2_{A_{ni}} &\le C\tau |e_n|^2_{M_n} + C\tau \sum_{i=1}^{s} \|M_{ni} r_{ni}\|^2_{*,ni} \\ &+ C\tau \sum_{i=1}^{s} \Big(|M_{ni}^{-1}\Delta_{ni}|^2_{M_{ni}} + |M_{ni}^{-1}\Delta_{ni}|^2_{A_{ni}} \Big) + C\tau |\delta_{n+1}/\tau|_{M_{n+1}^{-1}}. \end{aligned} \tag{3.18}$$

We now sum over n and apply the discrete Gronwall inequality to achieve the stated result. ∎

4. Time Discretization by Backward Difference Formulas

We apply the backward difference formulas (BDF) to the ODE system (2.5) resulting from the space discretization of the parabolic equation on evolving surfaces. In the same frame work as in the previous Chapter 3, we study here the stability of the fully discrete method (ESFEM coupled with BDF). Using results from Dahlquist's G-stability theory [7] and Nevanlinna & Odeh's multiplier technique [42] together with the properties of the spatial semi-discretization (Lemma 2.6), we prove that the fully discrete scheme is unconditionally stable for the BDF methods up to order 5. To the best of our knowledge, this is the first time that these powerful techniques have been used in the study of time discretizations of parabolic differential equations [38].

4.1. BDF time discretization

Let us first recall the ODE system from Chapter 2:

$$\begin{cases} \frac{d}{dt}\left(M(t)\alpha(t)\right) + A(t)\alpha(t) &= 0 \\ \alpha(0) &= \alpha_0. \end{cases} \tag{4.1}$$

For the numerical integration of system (4.1), we consider the k-step BDF method with step size $\tau > 0$ given by

$$\frac{1}{\tau}\sum_{j=0}^{k} \delta_j M(t_{n-j})\alpha_{n-j} + A(t_n)\alpha_n = 0, \quad n \geq k, \tag{4.2}$$

with given starting values $\alpha_0, \ldots, \alpha_{k-1}$.

The method coefficients δ_j are determined from the relation

$$\delta(\zeta) = \sum_{j=0}^{k} \delta_j \zeta^j = \sum_{\ell=1}^{k} \frac{1}{\ell}(1-\zeta)^\ell. \tag{4.3}$$

The method is known to have order k and to be 0-stable for $k \leq 6$ (cf. [27, Chapter V]). Notice that the 1-step BDF method is the backward Euler method with $\delta_0 = 1$ and $\delta_1 = -1$.

4.2. Defects and errors

As in the previous Chapter 3, we consider the perturbed ODE system

$$\begin{cases} \frac{d}{dt}\left(M(t)\widetilde{\alpha}(t)\right) + A(t)\widetilde{\alpha}(t) &= M(t)r(t) \\ \widetilde{\alpha}(0) &= \widetilde{\alpha}_0. \end{cases} \tag{4.4}$$

The solution $\widetilde{\alpha}(t)$ of the perturbed system (4.4) when inserted into the above BDF scheme (4.2) yields defect d_n in

$$\frac{1}{\tau}\sum_{j=0}^{k} \delta_j M(t_{n-j})\widetilde{\alpha}(t_{n-j}) + A(t_n)\widetilde{\alpha}(t_n) = -d_n. \tag{4.5}$$

For the error, we use the notation

$$e_n = \alpha_n - \widetilde{\alpha}_n, \tag{4.6}$$

and subtract to obtain the *error equation*

$$\frac{1}{\tau}\sum_{j=0}^{k} \delta_j M(t_{n-j})e_{n-j} + A(t_n)e_n = d_n, \qquad n \geq k. \tag{4.7}$$

4.3. Basic results from Dahlquist (1978) and Nevanlinna & Odeh (1981)

We will use the following result from Dahlquist's G-stability theory.

Lemma 4.1 (Dahlquist [7]; see also [4], Section V.6 [27])
Let $\delta(\zeta)$ and $\mu(\zeta)$ be polynomials of degree at most k (at least one of them of exact degree k) that have no common divisor. Let $\langle\cdot,\cdot\rangle$ be an inner product on $\mathbb{R}^N$ with associated norm $|\cdot|$. If

$$\operatorname{Re}\frac{\delta(\zeta)}{\mu(\zeta)} > 0 \quad \textit{for} \quad |\zeta| < 1,$$

then there exists a symmetric positive definite matrix $G = (g_{ij}) \in \mathbb{R}^{k\times k}$ and real $\gamma_0, \dots, \gamma_k$ such that for all $v_0, \dots, v_k \in \mathbb{R}^N$

$$\Big\langle \sum_{i=0}^{k} \delta_i v_{k-i}, \sum_{j=0}^{k} \mu_j v_{k-j} \Big\rangle = \sum_{i,j=1}^{k} g_{ij}\langle v_i, v_j\rangle - \sum_{i,j=1}^{k} g_{ij}\langle v_{i-1}, v_{j-1}\rangle + \Big|\sum_{i=0}^{k}\gamma_i v_i\Big|^2.$$

In combination with the preceding result for $\mu(\zeta) = 1 - \eta\zeta$, the following property of BDF methods up to order 5 will play a key role in our stability analysis.

Lemma 4.2 (Nevanlinna & Odeh [42])
If $k \le 5$, then there exists $0 \le \eta < 1$ such that for $\delta(\zeta) = \sum_{\ell=1}^{k} \frac{1}{\ell}(1-\zeta)^\ell$,

$$\mathrm{Re}\,\frac{\delta(\zeta)}{1-\eta\zeta} > 0 \quad \textit{for} \quad |\zeta| < 1.$$

The smallest possible value of η is found to be $\eta = 0, 0, 0.0836, 0.2878, 0.8160$ for $k = 1, \dots, 5$, respectively.

4.4. Stability

We are now ready to state and prove the main result of this chapter analogous to the stability Lemma 3.1 for the implicit Runge–Kutta method. Here, we also prove that the fully discrete scheme (4.2) (combination of the ESFEM method and the k- step BDF method with $k \le 5$) is unconditionally stable.

Lemma 4.3
For the k-step BDF method with $k \le 5$, there exist $\tau_0 > 0$ depending only on μ and κ of Lemma 2.6 such that for $\tau \le \tau_0$ and $t_n \le T$, the errors e_n given by (4.7) are bounded by

$$|e_n|_{M_n}^2 + \tau \sum_{j=k}^{n} |e_j|_{A_j}^2 \le C\,\tau \sum_{j=k}^{n} \|d_j\|_{*,t_j}^2 + C \max_{0\le i\le k-1} |e_i|_{M_i}^2$$

where $\|w\|_{*,t}^2 = w^{\mathrm{T}}(A(t)+M(t))^{-1}w, A(t_n) = A_n$ and $M(t_n) = M_n$. The constant C is independent of h, τ and n (but depends on μ, κ, and T).

Proof
We start from (4.7) and rewrite it as

$$M_n \sum_{j=0}^{k} \delta_j e_{n-j} + \tau A_n e_n = \tau d_n + \sum_{j=1}^{k} \delta_j \left(M_n - M_{n-j}\right) e_{n-j}.$$

We use a modified energy estimate. Instead of multiplying scalarly with e_n as would be familiar with the implicit Euler method, we proceed similarly to the proof of Theorem 4.1 in [42] and take the Euclidean inner product with $e_n - \eta e_{n-1}$, for $n \ge k+1$. This gives

$$I_n + II_n = III_n + IV_n, \tag{4.8}$$

where

$$\begin{aligned}
I_n &= \Big\langle \sum_{j=0}^{k} \delta_j e_{n-j} \,|\, M_n \,|\, e_n - \eta e_{n-1} \Big\rangle \\
II_n &= \tau \left\langle e_n \,|\, A_n \,|\, e_n - \eta e_{n-1} \right\rangle \\
III_n &= \tau \left\langle d_n, e_n - \eta e_{n-1} \right\rangle \\
IV_n &= \sum_{j=1}^{k} \delta_j \left\langle e_{n-j} \,|\, M_n - M_{n-j} \,|\, e_n - \eta e_{n-1} \right\rangle .
\end{aligned}$$

To estimate the first term we introduce the following notation: For

$$E_n = (e_n, \dots, e_{n-k+1})^{\mathtt{T}},$$

we set

$$|E_n|^2_{G,n} = \sum_{i,j=1}^{k} g_{ij} \langle e_{n-k+i} \,|\, M_n \,|\, e_{n-k+j} \rangle,$$

where $G = (g_{ij})$ is the symmetric positive definite matrix of Lemma 4.1 for the BDF polynomial $\delta(\zeta)$ of (4.3) and for $\mu(\zeta) = 1 - \eta\zeta$ with η of Lemma 4.2. This defines a norm on $\mathbb{R}^{kN}$ such that

$$c_0 \sum_{j=1}^{k} |e_{n-k+j}|^2_{M_n} \le |E_n|^2_{G,n} \le c_1 \sum_{j=1}^{k} |e_{n-k+j}|^2_{M_n},$$

where c_0 and c_1 denote the smallest and largest eigenvalue of G, respectively. Then we obtain by Lemmas 4.1 and 4.2 that

$$|E_n|^2_{G,n} - |E_{n-1}|^2_{G,n} \le I_n, \qquad n \ge k+1.$$

With (2.11) we have for sufficiently small τ ($\mu\tau \le 1$)

$$|E_{n-1}|^2_{G,n} - |E_{n-1}|^2_{G,n-1} \le 2\mu\tau \sum_{i,j=1}^{k} |g_{ij}| \, |e_{n-1-k+i}|_{M_{n-1}} \, |e_{n-1-k+j}|_{M_{n-1}}.$$

We can choose $\gamma > 0$ depending only on G such that

$$\sum_{i,j=1}^{k} |g_{ij}| \, |e_{n-1-k+i}|_{M_{n-1}} \, |e_{n-1-k+j}|_{M_{n-1}} \le \gamma |E_{n-1}|^2_{G,n-1}.$$

With (4.8), this yields the bound

$$|E_n|^2_{G,n} - |E_{n-1}|^2_{G,n-1} \le 2\gamma\mu\tau |E_{n-1}|^2_{G,n-1} + III_n + IV_n - II_n, \qquad n \ge k+1.$$

The term II_n/τ is estimated using the Cauchy-Schwarz inequality, Young's inequality and (2.13):

$$\begin{aligned}
\langle e_n \,|A_n|\, e_n - \eta e_{n-1} \rangle &= |e_n|^2_{A_n} - \eta \, \langle e_n | A_n | e_{n-1} \rangle \\
&\ge |e_n|^2_{A_n} - \frac{1}{2}\eta |e_n|^2_{A_n} - \frac{1}{2}\eta |e_{n-1}|^2_{A_n} \\
&\ge \frac{2-\eta}{2} |e_n|^2_{A_n} - \frac{1}{2}\eta(1 + 2\kappa\tau) |e_{n-1}|^2_{A_{n-1}}.
\end{aligned}$$

For III_n/τ we have, using (2.11) and (2.13) in the last step for sufficiently small τ,

$$\begin{aligned}
&\langle d_n, e_n - \eta e_{n-1}\rangle \\
&\quad = \Big\langle (A_n + M_n)^{-1/2} d_n, (A_n + M_n)^{1/2}(e_n - \eta e_{n-1})\Big\rangle \\
&\quad \le \|d_n\|_{*,n}\big(|e_n - \eta e_{n-1}|_{A_n}^2 + |e_n - \eta e_{n-1}|_{M_n}^2\big)^{1/2} \\
&\quad \le \frac{1}{1-\eta}\|d_n\|_{*,n}^2 + \frac{1-\eta}{4}\big(|e_n - \eta e_{n-1}|_{A_n}^2 + |e_n - \eta e_{n-1}|_{M_n}^2\big) \\
&\quad \le \frac{1}{1-\eta}\|d_n\|_{*,n}^2 + \frac{1-\eta}{2}\Big((|e_n|_{A_n}^2 + |e_n|_{M_n}^2) + \eta^2(|e_{n-1}|_{A_n}^2 + |e_{n-1}|_{M_n}^2)\Big) \\
&\quad \le \frac{1}{1-\eta}\|d_n\|_{*,n}^2 + \frac{1-\eta}{2}(|e_n|_{A_n}^2 + |e_n|_{M_n}^2) \\
&\qquad + \frac{1-\eta}{2}\eta^2\Big((1+2\kappa\tau)|e_{n-1}|_{A_{n-1}}^2 + (1+2\mu\tau)|e_{n-1}|_{M_{n-1}}^2\Big).
\end{aligned}$$

We estimate the term IV_n using the Cauchy-Schwarz inequality, Young's inequality and (2.11):

$$\begin{aligned}
\langle e_{n-j}|M_n - M_{n-j}|e_n - \eta e_{n-1}\rangle &= \langle e_{n-j}|M_n - M_{n-j}|e_n\rangle - \eta\,\langle e_{n-j}|M_n - M_{n-j}|e_{n-1}\rangle \\
&\le 2\mu j\tau|e_{n-j}|_{M_n}|e_n|_{M_n} + 2\eta\mu j\tau|e_{n-j}|_{M_n}|e_{n-1}|_{M_n} \\
&\le (1+\eta)\mu j\tau|e_{n-j}|_{M_n}^2 + \mu j\tau|e_n|_{M_n}^2 + \eta\mu j\tau|e_{n-1}|_{M_n}^2.
\end{aligned}$$

Thus we get by the equivalence of norms

$$IV_n \le C(\mu,\eta)\tau\Big(|E_n|_{G,n}^2 + |E_{n-1}|_{G,n-1}^2\Big).$$

Combining the above inequalities and summing up gives, for sufficiently small $\tau \le \tau_0$ (which depends only on κ and μ) and for $n \ge k+1$,

$$\begin{aligned}
&|E_n|_{G,n}^2 + (1-\eta)\frac{\tau}{4}\sum_{j=k+1}^{n}|e_j|_{A_j}^2 \\
&\qquad\qquad \le C(\mu,\eta)\tau\sum_{j=k}^{n-1}|E_j|_{G,j}^2 + C(\eta)\tau\sum_{j=k+1}^{n}\|d_j\|_{*,j}^2 + C\eta^2\tau|e_k|_{A_k}^2.
\end{aligned}$$

The discrete Gronwall inequality and the equivalence of norms thus yield the stated result with $k+1$ instead of k and an extra term $C(\mu,\eta)\tau c_1|e_k|_{M_k}^2 + C\eta^2\tau|e_k|_{A_k}^2$. To estimate $|e_k|_{M_k}^2 + \tau|e_k|_{A_k}^2$, we take the inner product of the error equation for $n = k$ with e_k to obtain

$$\delta_0|e_k|_{M_k}^2 + \tau|e_k|_{A_k}^2 = \tau\langle d_k, e_k\rangle - \sum_{j=1}^{k}\delta_j\langle M_{k-j}e_{k-j}, e_k\rangle.$$

Noting that $\delta_0 > 0$ and estimating the terms on the right-hand side in the same way as above, in particular using $\langle M_{k-j}e_{k-j}, e_k\rangle \le |e_{k-j}|_{M_{k-j}} \cdot |e_k|_{M_{k-j}}$ and $|e_k|_{M_{k-j}} \le (1+2j\tau\mu)|e_k|_{M_k}$, we obtain

$$|e_k|_{M_k}^2 + \tau|e_k|_{A_k}^2 \le C\tau\|d_k\|_{*,k}^2 + C\max_{0\le i\le k-1}|e_i|_{M_i}^2.$$

Inserting this bound into the previous estimate completes the proof. ∎

5. Error Bounds for a Projection to the Finite Element Space I

In order to connect the stability lemmas from Chapter 3 and Chapter 4 with the continuous solution of the parabolic equation (1.3), we study in this chapter the difference between the fully discrete numerical solution U_h^n and a projection of the exact solution $u(\cdot, t)$ of the parabolic equation to the finite element space $S_h(t)$ at time $t = t_n$.

5.1. The fully discrete solution

Let $\{\alpha_k\}_{k=0}^n$ be generated by the s-stage implicit Runge–Kutta method (3.1) or by the k-step BDF method (4.2). Then, from the vector $\alpha_n = (\alpha_1^n, \cdots, \alpha_N^n)^{\mathrm{T}}$, we obtain the fully discrete numerical solution on the discrete surface $\Gamma_h(t_n)$

$$U_h^n = \sum_{j=1}^{N} \alpha_j^n \chi_j(\cdot, t_n), \tag{5.1}$$

as approximation to the exact solution of the parabolic equation $u(\cdot, t_n)$.

5.2. Projection to $S_h(t)$

Let $P_h : H^1(\Gamma(t)) \to S_h(t) \subset H^1(\Gamma_h(t))$ be an arbitrary projection of the exact solution of the parabolic equation to the finite element space $S_h(t)$. We write

$$P_h u(\cdot, t) = \sum_{j=1}^{N} \widetilde{\alpha}_j(t) \chi_j(\cdot, t).$$

Note that this projection P_h could be the piecewise linear interpolation operator at the nodes or an L^2- projection or a Ritz projection. The finite element residual of the parabolic problem $R_h(\cdot, t) = \sum_{j=1}^{N} r_j(t) \chi_j(\cdot, t) \in S_h(t)$ is defined by

$$\int_{\Gamma_h(t)} R_h \phi_h = \frac{d}{dt} \int_{\Gamma_h(t)} P_h u \, \phi_h + \int_{\Gamma_h(t)} \nabla_{\Gamma_h(t)}(P_h u) \cdot \nabla_{\Gamma_h(t)} \phi_h - \int_{\Gamma_h(t)} P_h u \, \partial_h^{\bullet} \phi_h, \tag{5.2}$$

where ϕ_h is a temporally smooth function with $\phi_h(\cdot,t) \in S_h(t)$. Then the equivalent matrix version for the vector $r(t) = (r_j(t)) \in \mathbb{R}^N$, is

$$\frac{d}{dt}\left(M(t)\widetilde{\alpha}(t)\right) + A(t)\widetilde{\alpha}(t) = M(t)r(t), \tag{5.3}$$

where $\widetilde{\alpha}(t) = (\widetilde{\alpha}_j(t)) \in \mathbb{R}^N$. This formulation (5.3) corresponds to the perturbed ODE system (3.4) and (4.4).

5.3. Error bounds for the implicit Runge–Kutta methods

A direct application of the stability lemma for the implicit RK methods (Lemma 3.1) gives the following error estimates for the difference between the projection $P_h u(\cdot,t_n)$ and the fully discrete numerical solution U_h^n determined by the combination of the piecewise linear finite elements and the s-stage implicit RK method (scheme (3.1)).

Theorem 5.1
Consider the space discretization of the parabolic equation (1.3) *by the evolving surface finite element method and time discretization by the s-stage RK method satisfying the assumptions* (3.1.2). *Assume that the geometry and the solution of the parabolic equation are so regular that $P_h u$ has continuous discrete material derivatives up to order $q+2$. Then, there exists $\tau_0 > 0$ independent of h such that for $\tau \leq \tau_0$, the error $E_h^n = U_h^n - P_h u(\cdot,t_n)$ is bounded for $t_n = n\tau \leq T$ by*

$$\begin{aligned}\|E_h^n\|_{L^2(\Gamma_h(t_n))} &+ \Big(\tau\sum_{j=k}^{n}\|\nabla_{\Gamma_h(t_j)}E_h^j\|^2_{L^2(\Gamma_h(t_j))}\Big)^{1/2} \\ &\leq C\beta_{h,q}\tau^{q+1} + C\tau\Big(\sum_{k=0}^{n-1}\sum_{i=1}^{s}\|R_h(\cdot,t_k+c_i\tau)\|^2_{H_h^{-1}(\Gamma_h(t_k+c_i\tau))}\Big)^{1/2} + C\|E_h^0\|_{L^2(\Gamma_h(t_0))}.\end{aligned}$$

Here C is independent of h (but depends on T), and

$$\beta_{h,q}^2 = \int_0^T \sum_{\ell=0}^{q+2}\Big(\|\partial_h^{(\ell)}(P_h u)(t)\|^2_{L^2(\Gamma_h(t))}\Big) + \sum_{\ell=0}^{q+1}\Big(\|\nabla_{\Gamma_h(t)}\partial_h^{(\ell)}(P_h u)(t)\|^2_{L^2(\Gamma_h(t))}\Big)\,\mathrm{d}t$$

The norm used for R_h is

$$\|R_h\|_{H_h^{-1}(\Gamma_h)} := \sup_{0\neq\phi_h\in S_h}\frac{(R_h,\phi_h)_{L^2(\Gamma_h)}}{\|\phi_h\|_{H^1(\Gamma_h)}}.$$

Proof
We consider the errors

$$\begin{aligned} e_n &= \alpha_n - \widetilde{\alpha}(t_n) \\ E_{ni} &= U_{ni} - \widetilde{\alpha}(t_n + c_i\tau). \end{aligned}$$

Due to the stability Lemma 3.1 we have

$$
\begin{aligned}
|e_n|_{M_n}^2 + \tau \sum_{k=1}^{n} |e_k|_{A_k}^2 \leq C \left(|e_0|_{M_0}^2 + \tau \sum_{k=0}^{n-1} \sum_{i=1}^{s} \|M_{ki} r_{ki}\|_{*,t_{ki}}^2 + \tau \sum_{k=1}^{n} |\delta_k/\tau|_{M_k}^2 \right) \\
+ C\tau \sum_{k=0}^{n-1} \sum_{i=1}^{s} \left(|M_{ki}^{-1} \Delta_{ki}|_{M_{ki}}^2 + |M_{ki}^{-1} \Delta_{ki}|_{A_{ki}}^2 \right). \qquad (5.4)
\end{aligned}
$$

(a) We first note that by using the norm identity (2.10), it follows (omitting the argument t)

$$
\begin{aligned}
\|Mr\|_* &= \left(r^{\mathrm{T}} M (A+M)^{-1} Mr\right)^{1/2} = \|(A+M)^{-1/2} Mr\|_2 \\
&= \sup_{0 \neq w \in \mathbb{R}^N} \frac{r^{\mathrm{T}} M (A+M)^{-1/2} w}{(w^{\mathrm{T}} w)^{1/2}} = \sup_{0 \neq z \in \mathbb{R}^N} \frac{r^{\mathrm{T}} M z}{(z^{\mathrm{T}} (A+M) z)^{1/2}} \\
&= \sup_{0 \neq \phi_h \in S_h} \frac{(R_h, \phi_h)_{L^2(\Gamma_h)}}{\|\phi_h\|_{H^1(\Gamma_h)}} = \|R_h\|_{H_h^{-1}(\Gamma_h)}. \qquad (5.5)
\end{aligned}
$$

Therefore we have

$$
\tau \sum_{k=0}^{n-1} \sum_{i=1}^{s} \|M_{ki} r_{ki}\|_{*,t_{ki}}^2 = \tau \sum_{k=0}^{n-1} \sum_{i=1}^{s} \|R_h(\cdot, t_k + c_i\tau)\|_{H_h^{-1}(\Gamma_h(t_k + c_i\tau))}^2. \qquad (5.6)
$$

(b) By using Taylor series expansion and the definition of the stage order q and the classical order $p \geq q+1$, we find that the defects δ_{n+1} and Δ_{ni} appearing in the error equation (3.5) satisfy

$$
\delta_{n+1} = \tau^{q+1} \int_{t_n}^{t_{n+1}} K\left(\frac{t - t_n}{\tau}\right) (M\widetilde{\alpha})^{(q+2)}(t)\, \mathrm{d}t \qquad (5.7a)
$$

$$
\Delta_{ni} = \tau^{q} \int_{t_n}^{t_{n+1}} K_i\left(\frac{t - t_n}{\tau}\right) (M\widetilde{\alpha})^{(q+1)}(t)\, \mathrm{d}t, \qquad (5.7b)
$$

with bounded Peano kernels K and K_i. We shall make use of Lemma 2.7 which shows that for $Z_h(\cdot,t) = \sum_{j=1}^N z_j(t)\chi_j(\cdot,t) \in S_h(t)$ with $z(t) = (z_j(t)) \in \mathbb{R}^N$:

$$
|(Mz)^{(k)}(t)|_{M(t)^{-1}}^2 \leq c \sum_{l=0}^{k} \|\partial_h^{(l)} Z_h\|_{L^2(\Gamma_h(t)}^2
$$

and

$$
|M(t)^{-1}(Mz)^{(k)}(t)|_{A(t)}^2 \leq c \sum_{l=0}^{k} (\|\partial_h^{(l)} Z_h\|_{L^2(\Gamma_h(t))}^2 + \|\nabla_{\Gamma_h(t)} \partial_h^{(l)} Z_h\|_{L^2(\Gamma_h(t))}^2).
$$

These estimates together with (2.12), (2.14) and the ODE system (5.3) yield

$$
\begin{aligned}
|\,(M\widetilde{\alpha})^{(q+2)}\,(t)|^2_{M(\sigma)^{-1}} &\le 2|\,(M\widetilde{\alpha})^{(q+2)}\,(t)|^2_{M(t)^{-1}} \\
&\le C\sum_{\ell=0}^{q+2}\Big(\|\partial_h^{(\ell)}(P_hu)(t)\|^2_{L^2(\Gamma_h(t))}\Big) \\
|M(\sigma)^{-1}\,(M\widetilde{\alpha})^{(q+1)}\,(t)|^2_{(A+M)(\sigma)} &\le 2|M(t)^{-1}\,(M\widetilde{\alpha})^{(q+1)}\,(t)|^2_{(A+M)(t)} \\
&\le C\sum_{\ell=0}^{q+1}\Big(\|\partial_h^{(\ell)}(P_hu)(t)\|^2_{L^2(\Gamma_h(t))} + \|\nabla_{\Gamma_h(t)}\partial_h^{(\ell)}(P_hu)(t)\|^2_{L^2(\Gamma_h(t))}\Big)
\end{aligned}
$$

provided that $\mu|t-\sigma|<1$ and $\beta|t-\sigma|<1$. Inserting these bounds into (5.7) yield

$$
\tau\sum_{k=1}^{n}|\delta_k/\tau|^2_{M_k^{-1}} + \tau\sum_{k=0}^{n-1}\sum_{i=1}^{s}\Big(|M_{ki}^{-1}\Delta_{ki}|^2_{M_{ki}} + |M_{ki}^{-1}\Delta_{ki}|^2_{A_{ki}}\Big) \le C\left(\tau^{q+1}\right)^2\beta^2_{h,s} \tag{5.8}
$$

(c) Inserting the bounds (5.6) and (5.8) into (5.4) and using the norm identity (2.10) completes the proof. ■

If the classical order p of the Runge–Kutta method is equal to $q+1$, then the above Theorem 5.1 shows that the order in time of the fully discrete scheme is optimal order $\mathcal{O}(\tau^{q+1})$. However, for p greater than $q+1$, we need stronger regularity conditions in order to obtain the classical order $\mathcal{O}(\tau^p)$. In the following, we assume that:

$$
\left|M(t)^{-1}\frac{d^{k_j-1}}{dt^{k_j-1}}\Big(A(t)M(t)^{-1}\Big)\dots\frac{d^{k_1-1}}{dt^{k_1-1}}\Big(A(t)M(t)^{-1}\Big)\frac{d^l}{dt^l}\left(M(t)\widetilde{\alpha}(t)\right)\right|_{M(t)} \le \gamma \tag{5.9a}
$$

$$
\left|M(t)^{-1}\frac{d^{k_j-1}}{dt^{k_j-1}}\Big(A(t)M(t)^{-1}\Big)\dots\frac{d^{k_1-1}}{dt^{k_1-1}}\Big(A(t)M(t)^{-1}\Big)\frac{d^l}{dt^l}\left(M(t)\widetilde{\alpha}(t)\right)\right|_{A(t)} \le \gamma \tag{5.9b}
$$

for all $k_i \ge 1$ and $l \ge q+1$ with $k_1+\dots+k_j+l \le p+1$. The zeroth derivative of the matrix $A(t)M(t)^{-1}$ is just the the matrix $A(t)M(t)^{-1}$ itself. Under these regularity conditions, we are able to prove the next convergence result of full order $\mathcal{O}(\tau^p)$.

Theorem 5.2

Consider the space discretization of the parabolic equation (1.3) *by the evolving surface finite element method and time discretization by the s-stage RK method satisfying the assumptions* (3.1.2) *with* $p>q+1$. *Under suitable regularity conditions such that conditions* (5.9) *are satisfied, the error* $E_h^n = U_h^n - P_hu(\cdot,t_n)$ *is bounded, for sufficiently small* $\tau \le \tau_0$ *and for* $t_n = n\tau \le T$, *by*

$$
\begin{aligned}
&\|E_h^n\|_{L^2(\Gamma_h(t_n))} + \Big(\tau\sum_{j=k}^{n}\|\nabla_{\Gamma_h(t_j)}E_h^j\|^2_{L^2(\Gamma_h(t_j))}\Big)^{1/2} \\
&\qquad \le C_0\tau^p + C\tau\Big(\sum_{k=0}^{n-1}\sum_{i=1}^{s}\|R_h(\cdot,t_k+c_i\tau)\|^2_{H_h^{-1}(\Gamma_h(t_k+c_i\tau))}\Big)^{1/2} + C\|E_h^0\|_{L^2(\Gamma_h(t_0))}.
\end{aligned}
$$

Here C_0 *is independent of* h *(but depends on* T *and* γ*).*

PROOF
The main idea of the proof is to modify the defects Δ_{ni} appearing in (5.4) so they are of order p. To do so, we follow Lubich & Ostermann in their proof of Theorem 1 in [36] and first split the matrices $A_{ni}M_{ni}^{-1}$ and the defects Δ_{ni} by Taylor series expansion as follows

$$\begin{aligned}
A_{ni}M_{ni}^{-1} &= T_{ni} + B_{ni} \\
&= \sum_{k=0}^{m-1} \frac{(c_i\tau)^k}{k!}(AM^{-1})^{(k)}(t_n) + \int_{t_n}^{t_n+c_i\tau} \frac{(t_n + c_i\tau - t)^{m-1}}{(m-1)!}(AM^{-1})^{(m)}(t)\,\mathrm{d}t \\
\Delta_{ni} &= D_{ni} + Q_{ni} \\
&= \sum_{l=q+1}^{p} \tau^l \xi_i^{(l)} \widetilde{y}^{(l)}(t_n) + \tau^p \int_{t_n}^{t_{n+1}} K_i\left(\frac{t-t_n}{\tau}\right)\widetilde{y}^{(p+1)}(t)\,\mathrm{d}t
\end{aligned}$$

with bounded Peano kernels K_i and $\xi_i^{(l)} = \frac{1}{l!}\left(l\sum_{j=1}^{s} a_{ij}c_j^{l-1} - c_i^l\right)$ and $m = p - q - 1$. We denote by $f^{(k)}(t)$ the k-th time derivative of $f(t)$ if $k \geq 1$ and $f^{(0)}(t) = f(t)$. The $N \times N-$identity matrix is denoted by I_N and we put:

$$\boldsymbol{\mathcal{O}} = \mathcal{O} \otimes I_{2N}, \qquad \boldsymbol{b}^{\mathrm{T}} = b^{\mathrm{T}} \otimes I_{2N},$$

where $\otimes$ denotes *the Kronecker product* of two matrices. We also use the notation:

$$\boldsymbol{\Delta}_n = (\Delta_{n1}, \dots, \Delta_{ns})^{\mathrm{T}}, \quad \boldsymbol{M}_n = \mathrm{diag}(M_{n1}, \dots, M_{ns})^{\mathrm{T}}, \quad \text{etc.}$$

Then, we introduce the new internal stages:

$$\begin{aligned}
\widehat{\boldsymbol{E}}_n &= \boldsymbol{E}_n + \boldsymbol{M}_n^{-1}\widehat{\boldsymbol{D}}_n, \qquad \text{with} \quad \widehat{\boldsymbol{D}}_n = \sum_{k=0}^{m-1} (\tau\boldsymbol{\mathcal{O}}\boldsymbol{T_n})^k\,\boldsymbol{D}_n, \\
\dot{\widehat{\boldsymbol{E}}}_n &= -\boldsymbol{A}_n\widehat{\boldsymbol{E}}_n - \boldsymbol{M}_n\boldsymbol{r}_n = \dot{\boldsymbol{E}}_n - \boldsymbol{A}_n\boldsymbol{M}_n^{-1}\widehat{\boldsymbol{D}}_n.
\end{aligned}$$

Thereby, we rewrite the error equations (3.6) as

$$\begin{aligned}
M_{ni}\widehat{E}_{ni} &= M_n e_n - \tau\sum_{j=1}^{s} a_{ij}\dot{\widehat{E}}_{nj} - \Delta'_{ni}, \qquad i = 1, \cdots, s, \\
M_{n+1}e_{n+1} &= M_n e_n + \tau\sum_{i=1}^{s} b_i\dot{\widehat{E}}_{ni} - \delta'_{n+1},
\end{aligned}$$

where the modified defects satisfy

$$\begin{aligned}
\boldsymbol{\Delta}'_n &= \boldsymbol{Q}_n + \tau\boldsymbol{\mathcal{O}}\boldsymbol{B}_n\widehat{\boldsymbol{D}}_n + (\tau\boldsymbol{\mathcal{O}}\boldsymbol{T_n})^m\,\boldsymbol{D_n} \\
\delta'_{n+1} &= \delta_{n+1} + \tau\boldsymbol{b}^{\mathrm{T}}\boldsymbol{B}_n\widehat{\boldsymbol{D}}_n + \tau\boldsymbol{b}^{\mathrm{T}}\boldsymbol{T_n}\widehat{\boldsymbol{D}}_n.
\end{aligned} \tag{5.10}$$

Similar to the estimate (5.4), we then obtain

$$\begin{aligned}
|e_n|_{M_n}^2 + \tau\sum_{k=1}^{n} |e_k|_{A_k}^2 &\leq C\left(|e_0|_{M_0}^2 + \tau\sum_{k=0}^{n-1}\sum_{i=1}^{s} \|M_{ki}r_{ki}\|_{*,t_{ki}}^2 + \tau\sum_{k=1}^{n} |\delta'_k/\tau|_{M_k}^2\right) \\
&\quad + C\tau\sum_{k=0}^{n-1}\sum_{i=1}^{s}\left(|M_{ki}^{-1}\Delta'_{ki}|_{M_{ki}}^2 + |M_{ki}^{-1}\Delta'_{ki}|_{A_{ki}}^2\right).
\end{aligned} \tag{5.11}$$

As a result of the regularity conditions (5.9), we discover that

$$|M_{ki}^{-1}\Delta'_{ki}|^2_{M_{ki}} + |M_{ki}^{-1}\Delta'_{ki}|^2_{A_{ki}} \le C_0\tau^p. \tag{5.12}$$

We now come to the last part of the proof, where we show that $|\delta'_k/\tau|_{M_k}$ is also of order $\mathcal{O}(\tau^p)$. By the regularity condition (5.9), the first and second term of (5.10) clearly are of order $\mathcal{O}(\tau^{p+1})$. Therefore, our problem reduces to show that $\tau\boldsymbol{b}^{\mathrm{T}}\boldsymbol{T_n}\widehat{\boldsymbol{D}}_n$ is of order $\mathcal{O}(\tau^{p+1})$. We first observe that $\tau\boldsymbol{b}^{\mathrm{T}}\boldsymbol{T_n}\widehat{\boldsymbol{D}}_n$ is just a linear combination of terms of the form

$$b^{\mathrm{T}}\mathcal{O}\mathcal{C}^{k_j-1}\dots\mathcal{O}\mathcal{C}^{k_1-1}\boldsymbol{\xi}^{(l)}\cdot(AM^{-1})^{(k_j-1)}(t_n)\dots(AM^{-1})^{(k_1-1)}(t_n)\widetilde{\alpha}^{(l)}(t_n)\cdot\tau^{|k|+l+1} \tag{5.13}$$

where $\mathcal{C} = \operatorname{diag}(c_1, c_2, \dots, c_s)$ and $|k| = \sum_{i=1}^{j} k_i, \quad k_i \in \{1, \dots, m\}$ with $j \le m$. Thanks to the order conditions of the Runge–Kutta method (see [24, p. 56]), we have

$$b^{\mathrm{T}}\mathcal{O}\mathcal{C}^{k_j-1}\dots\mathcal{O}\mathcal{C}^{k_1-1}\boldsymbol{\xi}^{(l)} = 0 \quad \text{for} \quad |k| + l + 1 \le p.$$

Therefore, all the terms of (5.13) vanish for $|k| + l + 1 \le p$. Thus, by the regularity conditions (5.9), we find

$$|\delta'_k/\tau|_{M_k} \le C_0\tau^p \tag{5.14}$$

Inserting the bounds (5.12), (5.14) and (5.6) into (5.11) and using the norm identity (2.10) completes the proof. ∎

5.4. Error bounds for the BDF methods

We use the stability lemma for the BDF methods (Lemma 4.3) together with the norm identity (2.10) to prove the following error estimates for the difference between the projection $P_h u(\cdot, t_n)$ and the fully discrete numerical solution U_h^n (ESFEM/BDF).

Theorem 5.3
Consider the space discretization of the parabolic equation (1.3) *by the evolving surface finite element method and time discretization by the BDF method of order $k \le 5$. Assume that the geometry and the solution of the parabolic equation are so regular that $P_h u$ has continuous discrete material derivatives up to order $k+1$. Then, there exists $\tau_0 > 0$ independent of h such that for $\tau \le \tau_0$, the error $E_h^n = U_h^n - P_h u(\cdot, t_n)$ is bounded for $t_n = n\tau \le T$ by*

$$\|E_h^n\|_{L^2(\Gamma_h(t_n))} + \Big(\tau\sum_{j=k}^{n}\|\nabla_{\Gamma_h(t_j)}E_h^j\|^2_{L^2(\Gamma_h(t_j))}\Big)^{1/2}$$
$$\le C\widetilde{\beta}_{h,k}\tau^k + \Big(\tau\sum_{j=k}^{n}\|R_h(\cdot,t_j)\|^2_{H_h^{-1}(\Gamma_h(t_j))}\Big)^{1/2} + C\max_{0\le i\le k-1}\|E_h^i\|_{L^2(\Gamma_h(t_i))}.$$

Here C is independent of h (but depends on T), and

$$\widetilde{\beta}_{h,k}^2 = \int_0^T\sum_{\ell=0}^{k+1}\|\partial_h^{(\ell)}(P_h u)(t)\|^2_{L^2(\Gamma_h(t))}\,dt.$$

Proof
We consider the error

$$e_n = \alpha_n - \widetilde{\alpha}(t_n),$$

and get the error equation (4.7) with

$$d_n = M(t_n)r(t_n) + \frac{d}{dt}(M\widetilde{\alpha})(t_n) - \frac{1}{\tau}\sum_{j=0}^{k}\delta_j(M\widetilde{\alpha})(t_{n-j}). \tag{5.15}$$

Lemma 4.3 with d_n of (5.15) shows that

$$|e_n|_{M_n}^2 + \tau\sum_{j=k}^{n}|e_j|_{A_j}^2 \le C\,\tau\sum_{j=k}^{n}\|d_j\|_{*,t_j}^2 + C\max_{0\le i\le k-1}|e_i|_{M_i}^2. \tag{5.16}$$

We first note by (5.5) that

$$\|M(t_n)r(t_n)\|_{*,t_n} = \|R_h(\cdot,t_n)\|_{H_h^{-1}(\Gamma_h(t_n))}. \tag{5.17}$$

By using Taylor expansion and the definition of order k of the k-step BDF method, one finds that the backward differentiation error of a smooth function can be represented with a scalar Peano kernel $K(\theta)$,

$$g'(t) - \frac{1}{\tau}\sum_{j=0}^{k}\delta_j g(t-j\tau) = \tau^k\int_0^k K(\theta)g^{(k+1)}(t-\theta\tau)\,d\theta.$$

We use this formula for $g = M\widetilde{\alpha}$ and set $w = M^{-1}(M\widetilde{\alpha})^{(k+1)}$, so that

$$\frac{d}{dt}(M\widetilde{\alpha})(t_n) - \frac{1}{\tau}\sum_{j=0}^{k}\delta_j(M\widetilde{\alpha})(t_{n-j}) = \tau^k\int_0^k K(\theta)(Mw)(t_n-\theta\tau)\,d\theta.$$

We note

$$\begin{aligned}\|M(t)w\|_{*,s}^2 &= w^{\mathrm{T}}M(t)\big(A(s)+M(s)\big)^{-1}M(t)w\\ &= w^{\mathrm{T}}M(t)M(s)^{-1/2}\big(M(s)^{-1/2}A(s)M(s)^{-1/2}+I\big)^{-1}M(s)^{-1/2}M(t)w\\ &\le \|M(s)^{-1/2}M(t)w\|_2^2 = w^{\mathrm{T}}M(t)M(s)^{-1}M(t)w.\end{aligned}$$

This is further estimated using Lemma 2.6:

$$w^{\mathrm{T}}M(t)M(s)^{-1}M(t)w = w^{\mathrm{T}}M(t)w + w^{\mathrm{T}}M(t)(M(s)^{-1}-M(t)^{-1})M(t)w \le 2\,w^{\mathrm{T}}M(t)w,$$

provided that $2\mu|t-s|\le 1$. For such t and s we have thus shown that

$$\|M(t)w\|_{*,s}^2 \le 2\,|w|_t^2.$$

Lemma 2.7 shows that for $w = M^{-1}(M\widetilde{\alpha})^{(k+1)}$ with $\widetilde{\alpha}$ the vector of nodal values of $P_h u$, we have

$$|w(t)|_t^2 \leq C \sum_{l=0}^{k+1} \|(P_h u)^{(l)}(t)\|^2_{L^2(\Gamma_h(t))}.$$

Combining these estimates yields

$$\begin{aligned}
&\Big\| \frac{d}{dt}(M\widetilde{\alpha})(t_n) - \frac{1}{\tau}\sum_{j=0}^{k}\delta_j (M\widetilde{\alpha})(t_{n-j})\Big\|^2_{*,t_n} \\
&\leq \tau^{2k} c \int_0^k \|(Mw)(t_n - \theta\tau)\|^2_{*,t_n}\, d\theta \\
&\leq \tau^{2k}\, 2c \int_0^k |w(t_n - \theta\tau)|^2_{t_n-\theta\tau}\, d\theta \\
&\leq \tau^{2k}\, 2cC \int_0^k \sum_{l=0}^{k+1} \|(P_h u)^{(l)}(t_n - \theta\tau)\|^2_{L^2(\Gamma_h(t_n-\theta\tau))}\, d\theta. \qquad (5.18)
\end{aligned}$$

Plugging (5.17) and (5.18) into (5.15), then into (5.16) and finally using the norm identity (2.10) closes the proof. ■

Remark 5.4

1. *If P_h is the piecewise linear interpolation operator at the nodes, then $\beta_{h,q}$ as well as $\widetilde{\beta}_{h,k}$ are clearly bounded uniformly in h. However, one can expect only suboptimal bound for the corresponding residual,i.e., $\|R_h(t)\|_{H_h^{-1}(\Gamma_h(t))} = \mathcal{O}(h)$. Thus, in order to prove optimal-order error bounds, we have to deal with the question:*

   Is there a projection P_h such that $\beta_{h,q}$ as well as $\widetilde{\beta}_{h,k}$ are bounded uniformly in h and at the same time $\|R_h(t)\|_{H_h^{-1}(\Gamma_h(t))}$ is of optimal order $\mathcal{O}(h^2)$?

   A positive answer to this question can be found in Chapter 8.

2. *We can also compare the fully discrete solution with the semi-discrete solution U_h of* (2.4) *(then $R_h = 0$). For the corresponding error $U_h^n - U_h(\cdot, t_n)$, we obtain a similar bound where R_h does not appear and the factor in front of the τ^{q+1} term (for the implicit Runge–Kutta) and the τ^k term (for the BDF method) are bounded in terms of higher-order discrete material derivatives of U_h instead of $P_h u$. We then need regularity results for the semi-discrete solution U_h, such as that of Theorem 9.1 in [19], which shows that*

$$\sup_{(0,T)} \|U_h^{(m)}\|^2_{L^2(\Gamma_h)} + \int_0^T \|\nabla_{\Gamma_h} U_h^{(m)}\|^2_{L^2(\Gamma_h)}\, dt \leq c \sum_{\ell=0}^{m} \|\partial_h^{(l)} U_h(\cdot, 0)\|^2_{L^2(\Gamma_{h0})}.$$

6. Lifts

We summarize a number of results from [13, 14, 15] and prove geometric approximation estimates about lifts of functions from the discretized to the original surface. These estimates together with the Ritz map which we will introduce in Chapter 7 are crucial in order to prove that the semidiscrete residual appearing in (5.2) is of optimal order.

6.1. Estimates between surface finite elements and their lifts

We denote by $d(x,t), x \in \mathbb{R}^{m+1}, t \in [0,T]$ the *signed distance function* to the smooth closed surface $\Gamma(t)$ and let $\mathcal{N}(t)$ be a neighbourhood of $\Gamma(t)$ such that for every $x \in \mathcal{N}(t)$ and $t \in [0,T]$ there exists a unique $p(x,t) \in \Gamma(t)$ which is the normal projection of x onto $\Gamma(t)$, i.e.

$$x - p(x,t) = d(x,t)\nu(p(x,t),t). \tag{6.1}$$

We assume $\Gamma_h(t) \subset \mathcal{N}(t)$. Thus for each triangle $E(t)$ in $\Gamma_h(t)$ there is a unique curved triangle $e(t) = p(E(t),t) \subset \Gamma(t)$, and this induces an exact triangulation of $\Gamma(t)$ with curved edges. Furthermore we assume that $\Gamma_h(t)$ consists of triangles $E(t)$ in $\mathcal{T}_h(t)$ with inner radius bounded below by $\sigma_h \geq ch$ for some $c > 0$.

For any continuous function $\eta_h : \Gamma_h \to \mathbb{R}$ we define its lift $\eta_h^l : \Gamma \to \mathbb{R}$ by

$$\eta_h^l(p,t) = \eta_h(x,t), \qquad p \in \Gamma(t),$$

where $x \in \Gamma_h(t)$ is such that $p = p(x,t)$. Then we have the lifted finite element space

$$S_h^l(t) = \{\varphi_h = \phi_h^l \;:\; \phi_h \in S_h(t)\}.$$

Note that $\chi_j^l(\cdot,t)(j = 1,\ldots,J)$ form a basis of $S_h^l(t)$.

We denote by δ_h the quotient between the smooth and discrete surface measures dA and dA_h, defined by $\delta_h dA_h = dA$.

We further introduce Pr and Pr_h as the projections onto the tangent planes of Γ and Γ_h respectively and the Weingarten map $\mathcal{H}\,(\mathcal{H}_{ij} = \partial_{x_j}\nu_i)$. Defining $\mathcal{Q}_h = \frac{1}{\delta_h}(I - d\mathcal{H})PrPr_hPr(I - d\mathcal{H})$ we get the relation [15, Lemma 5.5]

$$\nabla_{\Gamma_h}\eta(x) \cdot \nabla_{\Gamma_h}\phi(x) = \delta_h \mathcal{Q}_h \nabla_\Gamma \eta^l(p) \cdot \nabla_\Gamma \phi^l(p). \tag{6.2}$$

Lemma 6.1
Assume $\Gamma(t)$ and $\Gamma_h(t)$ satisfy the requirements stated above. Then we have

$$\|d\|_{L^\infty(\Gamma_h)} \le ch^2, \quad \|1-\delta_h\|_{L^\infty(\Gamma_h)} \le ch^2, \quad \|\nu - \nu_h\|_{L^\infty(\Gamma_h)} \le ch,$$
$$\|Pr - \mathcal{Q}_h\|_{L^\infty(\Gamma_h)} \le ch^2, \quad \left\|\partial_h^{(\ell)} d\right\|_{L^\infty(\Gamma_h)} \le ch^2, \quad \left\|\partial_h^{(\ell)} \delta_h\right\|_{L^\infty(\Gamma_h)} \le ch^2,$$
$$\left\|Pr(\partial_h^{(\ell)}\mathcal{Q}_h)Pr\right\|_{L^\infty(\Gamma_h)} \le ch^2,$$

where the superscript (ℓ) denotes the ℓth discrete material derivative.

Proof
A proof for the first four estimates can be found in [14, Lemma 5.1]. To prove the other estimates, we consider a single element $E(t) \subset \Gamma_h(t)$, and w.l.o.g. we assume $E \in \mathbb{R}^2 \times \{0\}$. Since $\partial_h^{(\ell)} d = 0$ in the vertices of the triangle E, the linear interpolant $I_h \partial_h^{(\ell)} d$ vanishes on E. By the standard interpolation estimates it follows that

$$\left\|\partial_h^{(\ell)} d\right\|_{L^\infty(E)} = \left\|\partial_h^{(\ell)} d - I_h\partial_h^{(\ell)} d\right\|_{L^\infty(E)} \le ch^2 \left\|\partial_h^{(\ell)} d\right\|_{W^{2,\infty}(E)} \le ch^2.$$

Similarly,

$$\left\|\partial_{x_j}(\partial_h^{(\ell)} d)\right\|_{L^\infty(E)} \le ch \qquad \text{for} \quad j=1,2.$$

Since $\nu_j = \partial_{x_j} d$ and $\partial_h^\bullet(\partial_{x_j} f) = \partial_{x_j}(\partial_h^\bullet f) - \partial_{x_j} V_h \cdot \nabla f$, we obtain recursively

$$\left\|\partial_h^{(\ell)} \nu_j\right\|_{L^\infty(E)} \le ch \qquad \text{for} \quad j=1,2.$$

For $x = (x_1, x_2, 0) \in E$ we have by (6.1)

$$p_{x_j} = e_j - \nu_j \nu - d\nu_{x_j} \qquad (j = 1,2),$$

where $e_j \in \mathbb{R}^3$ denotes the jth standard basis vector. Then direct computation yields

$$\delta_h = \|p_{x_1} \times p_{x_2}\| = |\nu_3| + dR(\nu, \nu_{x_1}, \nu_{x_2}) = \sqrt{1 - \nu_1^2 - \nu_2^2} + dR(\nu, \nu_{x_1}, \nu_{x_2})$$

with some smooth remainder function R. Since $|d|, |\partial_h^{(\ell)} d| = \mathcal{O}(h^2)$ and $|\nu_j|, |\partial_h^{(\ell)} \nu_j| = \mathcal{O}(h)$ for $j = 1,2$, it follows that $|\partial_h^{(\ell)} \nu_3| \le ch^2$ and

$$\left\|\partial_h^{(\ell)} \delta_h\right\|_{L^\infty(E)} \le ch^2.$$

Let us now prove the last estimate for $\ell = 1$. The general case follows recursively with similar arguments. We note that for $\mathcal{Q}_h$ in (6.2), we have with some smooth remainder function R:

$$\mathcal{Q}_h = \frac{1}{\delta_h} Pr Pr_h Pr + dR(\delta_h, Pr, Pr_h, \mathcal{H}).$$

Since $|d|, |\partial_h^\bullet d| = \mathcal{O}(h^2)$, $\delta_h = 1 + \mathcal{O}(h^2)$ and $|\partial_h^\bullet \delta_h| = \mathcal{O}(h^2)$, we find

$$Pr\,(\partial_h^\bullet \mathcal{Q}_h)\,Pr = Pr\partial_h^\bullet\,(PrPr_hPr)\,Pr + \mathcal{O}(h^2). \tag{6.3}$$

Using the fact that $\partial_h^\bullet \nu \cdot \nu = 0$, we get

$$\begin{aligned} Pr\partial_h^\bullet\,(PrPr_hPr)\,Pr &= Pr\partial_h^\bullet\,(PrPr_hPr - Pr)\,Pr \\ &= -Pr\partial_h^\bullet\left(Pr\nu_h\nu_h^\intercal Pr\right)Pr. \end{aligned} \tag{6.4}$$

We keep in mind that in our situation $\nu_h = e_3$. Thus

$$|Pr\nu_h| = |\nu_h - (\nu_h \cdot \nu)\nu| = |e_3 - \nu_3\nu| = \sqrt{1-\nu_3^2} = \sqrt{\nu_1^2+\nu_2^2} = \mathcal{O}(h), \tag{6.5a}$$

$$|\partial_h^\bullet(Pr\nu_h)| = |-(\partial_h^\bullet\nu_3)\nu - \nu_3\partial_h^\bullet\nu| = \mathcal{O}(h). \tag{6.5b}$$

Inserting the bounds (6.5) into (6.4) and finally into (6.3) completes the proof. ∎

6.2. Error bound of the lifted interpolation

We shall make use of the following interpolation estimate given in [13, Lemma 5]:

Lemma 6.2

For a given $\eta \in H^2(\Gamma)$,

$$\|\eta - I_h\eta\|_{L^2(\Gamma)} + h\,\|\nabla_\Gamma(\eta - I_h\eta)\|_{L^2(\Gamma)} \le ch^2\left(\left\|\nabla_\Gamma^2\eta\right\|_{L^2(\Gamma)} + h\,\|\nabla_\Gamma\eta\|_{L^2(\Gamma)}\right),$$

where $I_h\eta \in S_h^l$ is the lift of the pointwise linear interpolation $\widetilde{I}_h\eta \in S_h$.

6.3. Velocity of lifted material points and material derivatives

By the definition (2.1) of the discrete material velocity V_h for a material point $X(t)$ on $\Gamma_h(t)$, we get the associated material velocity on $\Gamma(t)$: For $y(t) = p(X(t), t)$, we have

$$\dot{y}(t) = v_h(y(t), t)$$

with

$$\begin{aligned} v_h\,(y,t) &= \frac{\partial p}{\partial t}\,(x,t) + V_h\,(x,t)\cdot\nabla p\,(x,t) \\ &= (Pr - d\mathcal{H})(x,t)V_h(x,t) - \partial_t d(x,t)\nu(x,t) - d(x,t)\partial_t\nu(x,t), \end{aligned} \tag{6.6}$$

for $y = p(x,t)$. We note that $-\partial_t d(x,t)\nu(x,t)$ is just the normal component of $v(p,t)$, and the other two terms on the right-hand side of (6.6) are tangent to $\Gamma(t)$ in p. It follows that

$$v_h - v \text{ is a tangent vector.} \tag{6.7}$$

The discrete material derivatives on $\Gamma_h(t)$ and $\Gamma(t)$ then read

$$\partial_h^\bullet \phi_h = \frac{\partial \phi_h}{\partial t} + V_h \cdot \nabla \phi_h,$$
$$\partial_h^\bullet \varphi_h = \frac{\partial \varphi_h}{\partial t} + v_h \cdot \nabla \varphi_h.$$

It was shown in [15, Lemma 4.1] that the basis functions of $S_h^l(t)$ also satisfy the *transport property*

$$\partial_h^\bullet \varphi_j = \partial_h^\bullet \phi_j^l = 0. \tag{6.8}$$

Therefore the discrete material derivative and the lifting process commute in the following sense: For $\varphi_h = \phi_h^l \in S_h^l$,

$$\partial_h^\bullet \varphi_h = (\partial_h^\bullet \phi_h)^l = \sum_{j=1}^{J} \dot{\phi}_{h,j} \chi_j^l,$$

where $\phi_{h,j}(t) = \phi_h(a_j(t), t) = \varphi_h(a_j(t), t)$.

We have the following bounds for the difference between the different velocities:

Lemma 6.3
The error between the continuous velocity v and the lifted discrete velocity v_h on the smooth surface Γ satisfies the bounds, for $\ell \geq 0$,

$$\|\partial_h^{(\ell)}(v - v_h)\|_{L^\infty(\Gamma)} + h\|\nabla_\Gamma \partial_h^{(\ell)}(v - v_h)\|_{L^\infty(\Gamma)} \leq C_\ell\, h^2. \tag{6.9}$$

PROOF
The definition (6.6) of v_h together with the fact that $V_h = I_h v$ give (cf. [15, Lemma 5.6])

$$|v(p,t) - v_h(p,t)| = |Pr(v - I_h v)(p,t) + d(\mathcal{H} I_h v(p,t) + \partial_t \nu)| \leq Ch^2.$$

For $\ell = 1$, we have by the transport property (6.8) and Lemma 6.1

$$\begin{aligned} |\partial_h^\bullet(v - v_h)| &\leq |(\partial_h^\bullet Pr)(v - I_h v)| + |Pr(\partial_h^\bullet v - I_h \partial_h^\bullet v)| \\ &\quad + |(\partial_h^\bullet d)(\mathcal{H} I_h v + \partial_t \nu)| + |d \partial_h^\bullet(\mathcal{H} I_h v + \partial_t \nu)| \\ &\leq Ch^2. \end{aligned}$$

Using the fact that $\nabla_\Gamma d = \nabla_\Gamma \partial_h^\bullet d = 0$ and Lemma 6.1, we obtain

$$\begin{aligned} |\nabla_\Gamma(v - v_h)| &\leq c\,|v - I_h v| + c\,|\nabla_\Gamma(v - I_h v)| + ch^2 \leq ch, \\ |\nabla_\Gamma \partial_h^\bullet(v - v_h)| &\leq c\,|v - I_h v| + c\,|\nabla_\Gamma(v - I_h v)| + c\,|\partial_h^\bullet v - I_h \partial_h^\bullet v| \\ &\quad + c\,|\nabla_\Gamma(\partial_h^\bullet v - I_h \partial_h^\bullet v)| + ch^2 \\ &\leq ch. \end{aligned}$$

For $\ell > 1$ the proof uses the same arguments. ∎

6.4. Lifts and bilinear forms

We define the bilinear forms for $w, \varphi \in H^1(\Gamma)$ as

$$a(w,\varphi) = \int_\Gamma \nabla_\Gamma w \cdot \nabla_\Gamma \varphi, \tag{6.10a}$$

$$m(w,\varphi) = \int_\Gamma w\varphi, \tag{6.10b}$$

where the forms also depend on time t. We write $a(w,\varphi;t)$ etc. when we want to make the dependence on t explicit.

The discrete analogs of the above bilinear forms for $W_h, \phi_h \in S_h$ are defined by

$$a_h(W_h,\phi_h) = \sum_{E\in\mathcal{T}_h} \int_E \nabla_{\Gamma_h} W_h \cdot \nabla_{\Gamma_h} \phi_h, \tag{6.11a}$$

$$m_h(W_h,\phi_h) = \int_{\Gamma_h} W_h\phi_h. \tag{6.11b}$$

We are interested in the time derivatives of these bilinear forms. For this we need some more bilinear forms:

$$g(v;w,\varphi) = \int_\Gamma (\nabla_\Gamma \cdot v)\, w\varphi, \tag{6.12a}$$

$$b(v;w,\varphi) = \int_\Gamma \mathcal{B}(v) \nabla_\Gamma w \cdot \nabla_\Gamma \varphi \tag{6.12b}$$

with the matrix

$$\mathcal{B}(v)_{ij} = \delta_{ij} \nabla_\Gamma \cdot v - \left((\nabla_\Gamma)_i v_j + (\nabla_\Gamma)_j v_i \right), \quad i,j = 1,\dots,m+1.$$

Their discrete analogs read

$$g_h(V_h;W_h,\phi_h) = \int_{\Gamma_h} (\nabla_{\Gamma_h} \cdot V_h)\, W_h\phi_h, \tag{6.13a}$$

$$b_h(V_h;W_h,\phi_h) = \sum_{E\in\mathcal{T}_h} \int_E \mathcal{B}_h(V_h) \nabla_{\Gamma_h} W_h \cdot \nabla_{\Gamma_h} \phi_h \tag{6.13b}$$

with

$$\mathcal{B}_h(V_h)_{ij} = \delta_{ij} \nabla_{\Gamma_h} \cdot V_h - \left((\nabla_{\Gamma_h})_i V_{hj} + (\nabla_{\Gamma_h})_j V_{hi} \right), \quad i,j = 1,\dots,m+1.$$

We shall make use of the following transport lemma [15, Lemma 4.2].

Lemma 6.4
For $\varphi, w, \partial^\bullet \varphi, \partial^\bullet w, \partial_h^\bullet \varphi, \partial_h^\bullet w \in H^1(\Gamma)$ we have:

$$\frac{d}{dt} m(w,\varphi) = m(\partial^\bullet w,\varphi) + m(w,\partial^\bullet \varphi) + g(v;w,\varphi),$$
$$\frac{d}{dt} a(w,\varphi) = a(\partial^\bullet w,\varphi) + a(w,\partial^\bullet \varphi) + b(v;w,\varphi).$$

The same formulas hold when $\partial^\bullet$ and v are replaced with $\partial_h^\bullet$ and v_h, respectively. Furthermore for $W_h, \phi_h \in S_h$ we have the following analogs:

$$\begin{aligned}\frac{d}{dt}m_h(W_h,\phi_h) &= m_h(\partial_h^\bullet W_h,\phi_h) + m_h(W_h,\partial_h^\bullet\phi_h) + g_h(V_h;W_h,\phi_h),\\ \frac{d}{dt}a_h(W_h,\phi_h) &= a_h(\partial_h^\bullet W_h,\phi_h) + a_h(W_h,\partial_h^\bullet\phi_h) + b_h(V_h;W_h,\phi_h).\end{aligned}$$

We show the following bounds for the lifting process.

Lemma 6.5
For any $(W_h, \phi_h) \in S_h \times S_h$ with the corresponding lifts $(w_h, \varphi_h) \in S_h^l \times S_h^l$ we have

$$\begin{aligned}&|m(w_h,\varphi_h) - m_h(W_h,\phi_h)| \le ch^2\|w_h\|_{L^2(\Gamma)}\|\varphi_h\|_{L^2(\Gamma)},\\ &|a(w_h,\varphi_h) - a_h(W_h,\phi_h)| \le ch^2\|\nabla_\Gamma w_h\|_{L^2(\Gamma)}\|\nabla_\Gamma\varphi_h\|_{L^2(\Gamma)},\\ &|g(v_h;w_h,\varphi_h) - g_h(V_h;W_h,\phi_h)| \le ch^2\|w_h\|_{L^2(\Gamma)}\|\varphi_h\|_{L^2(\Gamma)},\\ &|b(v_h;w_h,\varphi_h) - b_h(V_h;W_h,\phi_h)| \le ch^2\|\nabla_\Gamma w_h\|_{L^2(\Gamma)}\|\nabla_\Gamma\varphi_h\|_{L^2(\Gamma)}.\end{aligned}$$

Proof
The first two estimates have been shown in [15, Lemma 5.5]. To prove the third estimate, we apply the Transport Lemma 6.4 once on Γ_h and a second time on Γ, to get the following identities:

$$\begin{aligned}\frac{d}{dt}m(w_h,\varphi_h) &= \frac{d}{dt}m_h(W_h,\phi_h\cdot\delta_h)\\ &= m_h(\partial_h^\bullet W_h,\phi_h\cdot\delta_h) + m_h(W_h,\partial_h^\bullet\phi_h\cdot\delta_h) + m_h(W_h,\phi_h\cdot\partial_h^\bullet\delta_h)\\ &\quad + g_h(V_h;W_h,\phi_h\cdot\delta_h)\\ &= m(\partial_h^\bullet w_h,\varphi_h) + m(w_h,\partial_h^\bullet\varphi_h) + g(v_h;w_h,\varphi_h).\end{aligned}$$

Due to the fact that $\partial_h^\bullet w_h = (\partial_h^\bullet W_h)^l$, using Lemma 6.1 and the equivalence of norms between the continuous and discrete surface, it follows

$$\begin{aligned}|g(v_h;w_h,\varphi_h) - g_h(V_h;W_h,\phi_h)| &= |m_h(W_h,\phi_h\cdot\partial_h^\bullet\delta_h) + g_h(V_h;W_h,\phi_h\cdot(\delta_h-1))|\\ &\le c\left(\|\partial_h^\bullet\delta_h\|_{L^\infty(\Gamma_h)} + \|\delta_h - 1\|_{L^\infty(\Gamma_h)}\right)\|w_h\|_{L^2(\Gamma)}\|\varphi_h\|_{L^2(\Gamma)}\\ &\le ch^2\|w_h\|_{L^2(\Gamma)}\|\varphi_h\|_{L^2(\Gamma)}.\end{aligned}$$

Similarly we prove the last estimate. We use Lemma 6.4 and the relation (6.2) to find

$$\begin{aligned}&\frac{d}{dt}\int_{\Gamma_h}\nabla_{\Gamma_h}W_h\nabla_{\Gamma_h}\phi_h = \int_\Gamma \mathcal{Q}_h^l\nabla_\Gamma w_h\nabla_\Gamma\varphi_h\\ &= \int_\Gamma \mathcal{Q}_h^l\nabla_\Gamma\partial_h^\bullet w_h\nabla_\Gamma\varphi_h + \int_\Gamma \mathcal{Q}_h^l\nabla_\Gamma w_h\nabla_\Gamma\partial_h^\bullet\varphi_h + \int_\Gamma \partial_h^\bullet\mathcal{Q}_h^l\nabla_\Gamma w_h\nabla_\Gamma\varphi_h\\ &\quad + \int_\Gamma \mathcal{B}(v_h)\mathcal{Q}_h^l\nabla_\Gamma w_h\nabla_\Gamma\varphi_h\\ &= \int_{\Gamma_h}\nabla_{\Gamma_h}\partial_h^\bullet W_h\nabla_{\Gamma_h}\phi_h + \int_{\Gamma_h}\nabla_{\Gamma_h}W_h\nabla_{\Gamma_h}\partial_h^\bullet\phi_h + \int_{\Gamma_h}\mathcal{B}_h(V_h)\nabla_{\Gamma_h}W_h\nabla_{\Gamma_h}\phi_h.\end{aligned}$$

Therefore, the relation $\partial_h^\bullet w_h = (\partial_h^\bullet W_h)^l$, (6.2) and Lemma 6.1 yield

$$\begin{aligned}
&|b_h(V_h; W_h, \phi_h) - b(v_h; w_h, \varphi_h)| \\
&\qquad = \left| \int_\Gamma \partial_h^\bullet \mathcal{Q}_h^l \nabla_\Gamma w_h \nabla_\Gamma \varphi_h + \int_\Gamma \mathcal{B}(v_h) \left(\mathcal{Q}_h^l - I \right) \nabla_\Gamma w_h \nabla_\Gamma \varphi_h \right| \\
&\qquad \leq ch^2 \|\nabla_\Gamma w_h\|_{L^2(\Gamma)} \|\nabla_\Gamma \varphi_h\|_{L^2(\Gamma)},
\end{aligned}$$

which completes the proof. ■

7. The Ritz Map for Evolving Surfaces

In the following, we introduce a modified Ritz projection for partial differential equations on evolving surfaces. We start by motivating the definition for the parabolic equation. Then, we state a general definition of a Ritz map, one of its version will be used for the parabolic equation and another version for the wave equation. Since we are dealing with moving surfaces and moving meshes, it turned out that in general the material derivative and the Ritz map do not commute. Nevertheless, we are able to prove optimal estimates for the error in the Ritz map and the error in its material derivative.

7.1. A modified Ritz projection

It turns out to be convenient in the error analysis to use a modified Ritz projection $\widetilde{\mathcal{P}}_h : H^1(\Gamma(t)) \to S_h(t)$ defined as follows; we use the bilinear forms of Section 6.4 and the lifted discrete velocity of Section 6.3. To motivate the definition, we rewrite the weak form (1.4) of the parabolic equation in terms of the bilinear forms,

$$\frac{d}{dt} m(u, \varphi) + a(u, \varphi) = m(u, \partial^\bullet \varphi),$$

and use the Leibniz formula with the discrete material derivative $\partial_h^\bullet$ on Γ and note $\partial_h^\bullet \varphi = \partial^\bullet \varphi + (v_h - v) \cdot \nabla_\Gamma \varphi$, because $v_h - v$ is a tangent vector (see (6.7)). Then, this equation becomes

$$m(\partial_h^\bullet u, \varphi) + g(v_h; u, \varphi) + m(u, (v_h - v) \cdot \nabla_\Gamma \varphi) + a(u, \varphi) = 0. \tag{7.1}$$

We now define a Ritz map that collects the last two terms on the left-hand side of this equation, which are the only terms that contain the surface gradient of the test function φ. Since $a(\cdot, \cdot)$ is only positive semi-definite, we consider the positive definite bilinear forms

$$\begin{aligned} a^*(w, \varphi) &= a(w, \varphi) + m(w, \varphi), && w, \varphi \in H^1(\Gamma) \\ a_h^*(W_h, \phi_h) &= a_h(W_h, \phi_h) + m_h(W_h, \phi_h), && W_h, \phi_h \in S_h. \end{aligned}$$

We note that $a^*(w, w) = \|w\|^2_{H^1(\Gamma)}$. We write $a^*(w, \varphi; t)$ etc. to make the dependence on t explicit. In the error analysis for the wave equation, it turned out that we need a different Ritz map then the one needed for the parabolic equation. For this reason, we give the following general definition.

Definition 7.1
For given $z \in H^1(\Gamma(t))$ and $\zeta \in L^2(\Gamma(t))$, there is a unique $\widetilde{\mathcal{P}}_h z \in S_h(t)$ such that for all $\phi_h \in S_h(t)$ we have, with the corresponding lift $\varphi_h = \phi_h^l$,

$$a_h^*(\widetilde{\mathcal{P}}_h z, \phi_h; t) = a^*(z, \varphi_h; t) + m(\zeta, (v_h(\cdot, t) - v(\cdot, t)) \cdot \nabla_{\Gamma(t)} \varphi_h; t). \tag{7.2}$$

We define $\mathcal{P}_h z \in S_h^l(t)$ as the lift of $\widetilde{\mathcal{P}}_h z$, i.e., $\mathcal{P}_h z = (\widetilde{\mathcal{P}}_h z)^l$.

7.2. Error in the Ritz map

Theorem 7.2
The error in the Ritz map satisfies the bounds, for $0 \le t \le T$ and $h \le h_0$ with sufficiently small h_0,

$$\|z - \mathcal{P}_h z\|_{L^2(\Gamma(t))} + h \left\| \nabla_{\Gamma(t)} (z - \mathcal{P}_h z) \right\|_{L^2(\Gamma(t))} \le C h^2 \left(\|z\|_{H^2(\Gamma(t))} + \|\zeta\|_{L^2(\Gamma(t))} \right). \tag{7.3}$$

Proof
We omit the omnipresent argument t in the following. We first note that in view of (6.9) and Lemma 6.5, we have for all $\varphi_h \in S_h^l$:

$$\begin{aligned} a^*(z - \mathcal{P}_h z, \varphi_h) &= a_h^*(\widetilde{\mathcal{P}}_h z, \phi_h) - a^*(\mathcal{P}_h z, \varphi_h) - m(\zeta, (v_h - v) \cdot \nabla_\Gamma \varphi_h) \\ &\le C h^2 \|\mathcal{P}_h z\|_{H^1(\Gamma)} \|\varphi_h\|_{H^1(\Gamma)} + C h^2 \|\zeta\|_{L^2(\Gamma)} \|\varphi_h\|_{H^1(\Gamma)} . \end{aligned} \tag{7.4}$$

This relation will serve as a substitute for the Galerkin orthogonality in standard finite element theory on fixed domains. Together with the interpolation error bound of Lemma 6.2 this yields

$$\begin{aligned} \|z - \mathcal{P}_h z\|_{H^1(\Gamma)}^2 &= a^*(z - \mathcal{P}_h z, z - I_h z) + a^*(z - \mathcal{P}_h z, I_h z - \mathcal{P}_h z) \\ &\le \|z - \mathcal{P}_h z\|_{H^1(\Gamma)} \|z - I_h z\|_{H^1(\Gamma)} + C h^2 (\|\mathcal{P}_h z\|_{H^1(\Gamma)} + \|\zeta\|_{L^2(\Gamma)}) \|I_h z - \mathcal{P}_h z\|_{H^1(\Gamma)} \\ &\le C h \|z - \mathcal{P}_h z\|_{H^1(\Gamma)} \|z\|_{H^2(\Gamma)} + C h^2 \left(\|\mathcal{P}_h z\|_{H^1(\Gamma)} + \|\zeta\|_{L^2(\Gamma)} \right) \|I_h z - \mathcal{P}_h z\|_{H^1(\Gamma)} . \end{aligned}$$

Using once more Lemma 6.2 we estimate

$$\begin{aligned} &\left(\|\mathcal{P}_h z\|_{H^1(\Gamma)} + \|\zeta\|_{L^2(\Gamma)} \right) \|I_h z - \mathcal{P}_h z\|_{H^1(\Gamma)} \\ &\quad \le \left(\|\mathcal{P}_h z - z\|_{H^1(\Gamma)} + \|z\|_{H^1(\Gamma)} + \|\zeta\|_{L^2(\Gamma)} \right) \cdot \left(C h \|z\|_{H^2(\Gamma)} + \|z - \mathcal{P}_h z\|_{H^1(\Gamma)} \right) \\ &\quad \le 2 \|z - \mathcal{P}_h z\|_{H^1(\Gamma)}^2 + \|z\|_{H^1(\Gamma)}^2 + \|\zeta\|_{L^2(\Gamma)}^2 + C h^2 \|z\|_{H^2(\Gamma)}^2 . \end{aligned}$$

Combining both of the above inequalities yields, for sufficiently small h,

$$\|z - \mathcal{P}_h z\|_{H^1(\Gamma)}^2 \le C h^2 \left(\|z\|_{H^2(\Gamma)}^2 + \|\zeta\|_{L^2(\Gamma)}^2 \right), \tag{7.5}$$

which implies the gradient estimate in (7.3).

Now we use the Aubin-Nitsche trick to prove the $\mathcal{O}(h^2)$ bound of the $L^2(\Gamma)$ error, and solve the problem

$$-\Delta_\Gamma w + w = z - \mathcal{P}_h z \quad \text{on } \Gamma.$$

Then by the elliptic theory on smooth surfaces (see [3] and [47] for more details), $w \in H^2(\Gamma)$ satisfies the bound

$$\|w\|_{H^2(\Gamma)} \leq c \|z - \mathcal{P}_h z\|_{L^2(\Gamma)} . \tag{7.6}$$

The Cauchy–Schwarz inequality, the interpolation estimate of Lemma 6.2 and the bounds (7.5) and (7.4) yield

$$\begin{aligned}
\|z - \mathcal{P}_h z\|_{L^2(\Gamma)}^2 &= a^*(z - \mathcal{P}_h z, w) \\
&= a^*(z - \mathcal{P}_h z, w - I_h w) + a^*(z - \mathcal{P}_h z, I_h w) \\
&\leq Ch^2 \left(\|z\|_{H^2(\Gamma)} + \|\zeta\|_{L^2(\Gamma)} \right) \|w\|_{H^2(\Gamma)} \\
&\quad + Ch^2 \Big(\|\mathcal{P}_h z\|_{H^1(\Gamma)} + \|\zeta\|_{L^2(\Gamma)} \Big) \|I_h w\|_{H^1(\Gamma)} .
\end{aligned}$$

Noting, from (7.5) and Lemma 6.2,

$$\begin{aligned}
&\|\mathcal{P}_h z\|_{H^1(\Gamma)} \leq \|z\|_{H^1(\Gamma)} + Ch \left(\|z\|_{H^2(\Gamma)} + \|\zeta\|_{L^2(\Gamma)} \right) \\
&\|I_h w\|_{H^1(\Gamma)} \leq \|w\|_{H^1(\Gamma)} + Ch \|w\|_{H^2(\Gamma)} ,
\end{aligned}$$

we obtain

$$\|z - \mathcal{P}_h z\|_{L^2(\Gamma)}^2 \leq Ch^2 \left(\|z\|_{H^2(\Gamma)} + \|\zeta\|_{L^2(\Gamma)} \right) \|w\|_{H^2(\Gamma)} .$$

Applying the bound (7.6) completes the proof. ■

7.3. Error in the material derivatives of the Ritz map

In general, $\partial_h^\bullet \mathcal{P}_h z \neq \mathcal{P}_h \partial_h^\bullet z$, but what we actually need, is the following result.

Theorem 7.3

The error in the material derivatives of the Ritz map satisfies the bounds, for $\ell \geq 1$, $0 \leq t \leq T$ and $h \leq h_0$ with sufficiently small h_0,

$$\begin{aligned}
&\left\| \partial_h^{(\ell)} \left(z - \mathcal{P}_h z \right)(t) \right\|_{L^2(\Gamma(t))} + h \left\| \nabla_\Gamma \Big(\partial_h^{(\ell)} \left(z - \mathcal{P}_h z \right)(t) \Big) \right\|_{L^2(\Gamma(t))} \\
&\quad \leq C_\ell \, h^2 \sum_{i=0}^{\ell} \left(\left\| \partial^{(i)} z(t) \right\|_{H^2(\Gamma(t))} + \left\| \partial^{(i)} \zeta(t) \right\|_{L^2(\Gamma(t))} + \left\| \partial^{(i-1)} \zeta(t) \right\|_{H^1(\Gamma(t))} \right),
\end{aligned} \tag{7.7}$$

with $\partial^{(-1)}\zeta(t) := 0$.

Proof
We prove this bound only for $\ell = 1$. The general case follows with similar arguments.

We take the time derivative of Equation (7.2) and use the Transport Lemma 6.4, the relation

$$\partial_h^\bullet \nabla_\Gamma f = \nabla_\Gamma \partial_h^\bullet f - \mathcal{D}(v_h)\nabla_\Gamma f \quad \text{with} \quad \mathcal{D}(v_h)_{ij} = (\nabla_\Gamma)_i v_{hj} - \sum_{l=1}^{m+1} \nu_l \nu_i (\nabla_\Gamma)_j v_{h,l},$$

which is proved in [18, Lemma 2.6], and the definition of the Ritz projection (7.2) to arrive at

$$\begin{aligned} a^*(\partial_h^\bullet z - \partial_h^\bullet \mathcal{P}_h z, \varphi_h) = & -b(v_h; z - \mathcal{P}_h z, \varphi_h) - g(v_h; z - \mathcal{P}_h z, \varphi_h) \\ & + F_1(\varphi_h) + F_2(\varphi_h) \end{aligned} \tag{7.8}$$

for $\varphi_h \in S_h^l$,where

$$\begin{aligned} F_1(\varphi_h) &= a_h^*(\partial_h^\bullet \widetilde{\mathcal{P}}_h z, \phi_h) - a^*(\partial_h^\bullet \mathcal{P}_h z, \varphi_h) + b_h(V_h; \widetilde{\mathcal{P}}_h z, \phi_h) - b(v_h; \mathcal{P}_h z, \varphi_h) \\ &\quad + g_h(V_h; \widetilde{\mathcal{P}}_h z, \phi_h) - g(v_h; \mathcal{P}_h z, \varphi_h), \\ F_2(\varphi_h) &= -m(\partial_h^\bullet \zeta, (v_h - v)\cdot \nabla_\Gamma \varphi_h) - g(v_h; \zeta, (v_h - v)\cdot \nabla_\Gamma \varphi_h) \\ &\quad - m(\zeta, (\partial_h^\bullet [v - v_h])\cdot \nabla_\Gamma \varphi_h) + m(\zeta, (v_h - v)\cdot \mathcal{D}(v_h)\nabla_\Gamma \varphi_h). \end{aligned}$$

We start by bounding $F_1(\varphi_h)$ and $F_2(\varphi_h)$. Lemma 6.5 yields

$$|F_1(\varphi_h)| \le Ch^2 \left(\|\partial_h^\bullet \mathcal{P}_h z\|_{H^1(\Gamma)} + \|\mathcal{P}_h z\|_{H^1(\Gamma)} \right) \|\varphi_h\|_{H^1(\Gamma)}. \tag{7.9}$$

In view of (6.9) and the fact that $(v - v_h)$ is a tangent vector, it follows that

$$\begin{aligned} \|\partial_h^\bullet \zeta\|_{L^2(\Gamma)} &\le \|\partial_h^\bullet \zeta - \partial^\bullet \zeta\|_{L^2(\Gamma)} + \|\partial^\bullet \zeta\|_{L^2(\Gamma)} \\ &= \|(v_h - v)\cdot \nabla_\Gamma \zeta\|_{L^2(\Gamma)} + \|\partial^\bullet \zeta\|_{L^2(\Gamma)} \\ &\le ch^2 \|\nabla_\Gamma \zeta\|_{L^2(\Gamma)} + \|\partial^\bullet \zeta\|_{L^2(\Gamma)}. \end{aligned}$$

Thus we get the bound

$$|F_2(\varphi_h)| \le Ch^2 \left(\|\partial^\bullet \zeta\|_{L^2(\Gamma)} + \|\zeta\|_{H^1(\Gamma)} \right) \|\varphi_h\|_{H^1(\Gamma)}. \tag{7.10}$$

We use the relation (6.9) to find

$$\|\partial_h^\bullet z\|_{H^1(\Gamma)} \le \|\partial^\bullet z\|_{H^1(\Gamma)} + ch \|z\|_{H^2(\Gamma)}.$$

Then inserting $\varphi_h = \partial_h^\bullet \mathcal{P}_h z$ in (7.8), and using Theorem 7.2, (7.9) and (7.10), for $h \le h_0$, we obtain

$$\|\partial_h^\bullet \mathcal{P}_h z\|_{H^1(\Gamma)} \le C \|\partial^\bullet z\|_{H^1(\Gamma)} + Ch \|z\|_{H^2(\Gamma)} + Ch \|\zeta\|_{H^1(\Gamma)} + Ch^2 \|\partial^\bullet \zeta\|_{L^2(\Gamma)}.$$

Combining the above bounds, we estimate the right hand side of (7.8), for sufficiently small $h \leq h_0$, as follows:

$$a^*(\partial_h^\bullet z - \partial_h^\bullet \mathcal{P}_h z, \varphi_h) \\ \leq Ch \left(\|z\|_{H^2(\Gamma)} + \|\zeta\|_{H^1(\Gamma)} + h \|\partial^\bullet \zeta\|_{L^2(\Gamma)} + h \|\partial^\bullet z\|_{H^1(\Gamma)} \right) \|\varphi_h\|_{H^1(\Gamma)} . \quad (7.11)$$

So we obtain

$$\|\partial_h^\bullet z - \partial_h^\bullet \mathcal{P}_h z\|_{H^1(\Gamma)}^2 \\ = a^*(\partial_h^\bullet z - \partial_h^\bullet \mathcal{P}_h z, \partial_h^\bullet z - I_h \partial^\bullet z) + a^*(\partial_h^\bullet z - \partial_h^\bullet \mathcal{P}_h z, I_h \partial^\bullet z - \partial_h^\bullet \mathcal{P}_h z) \\ \leq \|\partial_h^\bullet z - \partial_h^\bullet \mathcal{P}_h z\|_{H^1(\Gamma)} \|\partial_h^\bullet z - I_h \partial^\bullet z\|_{H^1(\Gamma)} \\ + Ch \left(\|z\|_{H^2(\Gamma)} + \|\zeta\|_{H^1(\Gamma)} + h \|\partial^\bullet \zeta\|_{L^2(\Gamma)} + h \|\partial^\bullet z\|_{H^1(\Gamma)} \right) \|I_h \partial^\bullet z - \partial_h^\bullet \mathcal{P}_h z\|_{H^1(\Gamma)} \quad (7.12)$$

The interpolation error bound of Lemma 6.2 and (6.9) yield

$$\|\partial_h^\bullet z - I_h \partial^\bullet z\|_{H^1(\Gamma)} = \|\partial_h^\bullet z - \partial^\bullet z\|_{H^1(\Gamma)} + \|\partial^\bullet z - I_h \partial^\bullet z\|_{H^1(\Gamma)} \\ \leq Ch \|z\|_{H^2(\Gamma)} + Ch \|\partial^\bullet z\|_{H^2(\Gamma)} ,$$

and similarly

$$\|I_h \partial^\bullet z - \partial_h^\bullet \mathcal{P}_h z\|_{H^1(\Gamma)} \leq Ch \|\partial^\bullet z\|_{H^2(\Gamma)} + Ch \|z\|_{H^2(\Gamma)} + \|\partial_h^\bullet z - \partial_h^\bullet \mathcal{P}_h z\|_{H^1(\Gamma)} .$$

Applying the last two estimates to (7.12) and using Young's inequality, for $h \leq h_0$, yield

$$\|\partial_h^\bullet z - \partial_h^\bullet \mathcal{P}_h z\|_{H^1(\Gamma)}^2 \leq Ch^2 \left(\|z\|_{H^2(\Gamma)}^2 + \|\partial^\bullet z\|_{H^2(\Gamma)}^2 + \|\zeta\|_{H^1(\Gamma)}^2 + \|\partial^\bullet \zeta\|_{L^2(\Gamma)}^2 \right) , \quad (7.13)$$

which implies the gradient estimate in (7.7).

To prove the $L^2(\Gamma)$ estimate, we use as before the Aubin-Nitsche trick and solve the problem

$$-\Delta_\Gamma w + w = \partial_h^\bullet z - \partial_h^\bullet \mathcal{P}_h z \quad \text{on } \Gamma.$$

Then by the elliptic theory it follows

$$\|w\|_{H^2(\Gamma)} \leq c \|\partial_h^\bullet z - \partial_h^\bullet \mathcal{P}_h z\|_{L^2(\Gamma)} . \quad (7.14)$$

A calculation that is nearly identical to [15, proof of Theorem 6.2] gives

$$-b(v_h; z - \mathcal{P}_h z, I_h w) \leq Ch^2 \left(\|z\|_{H^2(\Gamma)} + \|\zeta\|_{L^2(\Gamma)} \right) \|w\|_{H^2(\Gamma)} .$$

Therefore combining (7.8), (7.9), (7.10) and Theorem 7.2 yields

$$a^*(\partial_h^\bullet z - \partial_h^\bullet \mathcal{P}_h z, I_h w) \leq Ch^2 \left(\|z\|_{H^2(\Gamma)} + \|\partial^\bullet z\|_{H^1(\Gamma)} + \|\zeta\|_{H^1(\Gamma)} + \|\partial^\bullet \zeta\|_{L^2(\Gamma)} \right) \|w\|_{H^2(\Gamma)} .$$

Together with (7.13) and Lemma 6.2 this yields

$$\begin{aligned}
\|\partial_h^\bullet z - \partial_h^\bullet \mathcal{P}_h z\|_{L^2(\Gamma)}^2 &= a^*(\partial_h^\bullet z - \partial_h^\bullet \mathcal{P}_h z, w) \\
&= a^*(\partial_h^\bullet z - \partial_h^\bullet \mathcal{P}_h z, w - I_h w) + a^*(\partial_h^\bullet z - \partial_h^\bullet \mathcal{P}_h z, I_h w) \\
&\leq C h^2 \left(\|z\|_{H^2(\Gamma)} + \|\partial^\bullet z\|_{H^2(\Gamma)} + \|\zeta\|_{H^1(\Gamma)} + \|\partial^\bullet \zeta\|_{L^2(\Gamma)} \right) \|w\|_{H^2(\Gamma)} \,.
\end{aligned}$$

Finally applying the bound (7.14) completes the proof. ∎

8. Error Estimates I

This chapter shows the main results of the first part of this thesis. To begin with, we prove that the finite element residual R_h defined in (5.2) is of optimal order when we take the projection $P_h u$ to be the Ritz map $\widetilde{\mathcal{P}}_h u$ defined in (7.2). Then, combining the results from the previous chapters and this optimal bound of the residual, we finally achieve optimal order of convergence in space and time of the full discretization schemes (ESFEM coupled with implicit RK method as well as with BDF method) in the natural time-dependent norms.

8.1. Bound of the semidiscrete residual

We define the Ritz map for the the parabolic equation on evolving surfaces by setting $\zeta = u$ in (7.2), i.e.,

$$a_h^*(\widetilde{\mathcal{P}}_h u, \phi_h) = a^*(u, \varphi_h) + m(u, (v(\cdot,t) - v_h(\cdot,t)) \cdot \nabla_{\Gamma(t)} \varphi_h) \quad \forall \phi_h^l = \varphi_h \in S_h^l. \qquad (8.1)$$

We now replace the projection $P_h u$ appearing in the definition (5.2) of the the finite element residual R_h with the the Ritz map $\widetilde{\mathcal{P}}_h u$ given by (8.1). This will permit us to show the optimal rate of convergence $\mathcal{O}(h^2)$ for this residual.

Lemma 8.1
Assume that the solution u of the parabolic equation is sufficiently smooth. Then, there exist $C > 0$ and $h_0 > 0$ such that for $h \leq h_0$ and $0 \leq t \leq T$, the finite element residual of the Ritz map for the parabolic problem is bounded by

$$\|R_h(\cdot,t)\|_{H^{-1}(\Gamma_h(t))} \leq C h^2. \qquad (8.2)$$

Proof
We start by rewriting the residual equation (5.2) for $R_h \in S_h$ with $P_h = \widetilde{\mathcal{P}}_h$ as

$$\begin{aligned} m_h(R_h, \phi_h) &= \frac{d}{dt} m_h(\widetilde{\mathcal{P}}_h u, \phi_h) + a_h(\widetilde{\mathcal{P}}_h u, \phi_h) - m_h(\widetilde{\mathcal{P}}_h u, \partial_h^\bullet \phi_h) \\ &= m_h(\partial_h^\bullet \widetilde{\mathcal{P}}_h u, \phi_h) + g_h(V_h; \widetilde{\mathcal{P}}_h u, \phi_h) + a_h(\widetilde{\mathcal{P}}_h u, \phi_h), \end{aligned} \qquad (8.3)$$

where we have used the Transport Lemma 6.4. Next we rewrite the weak from (1.4) of the parabolic equation in terms of the bilinear forms with $\varphi = \varphi_h$ as

$$\frac{d}{dt}\, m(\partial^\bullet u, \varphi_h) + a(u, \varphi_h) = m(u, \partial^\bullet \varphi_h),$$

and use the the Leibniz formula with the discrete material derivative $\partial_h^\bullet$ on Γ to obtain

$$m(\partial_h^\bullet u, \varphi_h) + g(v_h; u, \varphi_h) + a(u, \varphi_h) = m(u, \partial^\bullet \varphi_h - \partial_h^\bullet \varphi_h).$$

Combining this equation with (8.3) and using the definition of the Ritz map (8.1) yields

$$m_h(R_h, \phi_h) = F_1(\varphi_h) + F_2(\varphi_h) + F_3(\varphi_h) \qquad \varphi_h = \phi_h^l \in S_h^l, \tag{8.4}$$

where

$$\begin{aligned} F_1(\varphi_h) &= m_h(\partial_h^\bullet \widetilde{\mathcal{P}}_h u, \phi_h) - m(\partial_h^\bullet u, \varphi_h), \\ F_2(\varphi_h) &= g_h(V_h; \widetilde{\mathcal{P}}_h u, \phi_h) - g(v_h; u, \varphi_h), \\ F_3(\varphi_h) &= m(u, \varphi_h) - m_h(\widetilde{\mathcal{P}}_h u, \phi_h), \end{aligned}$$

Applying Lemma 6.5, using $(\partial_h^\bullet \widetilde{\mathcal{P}}_h u)^l = \partial_h^\bullet \mathcal{P}_h u$ and applying Theorem 7.3 with $\ell = 1$ yields

$$\begin{aligned} |F_1(\varphi_h)| &= m_h(\partial_h^\bullet \widetilde{\mathcal{P}}_h u, \phi_h) - m(\partial_h^\bullet \mathcal{P}_h u, \varphi_h) + m(\partial_h^\bullet \mathcal{P}_h u - \partial_h^\bullet u, \varphi_h) \\ &\le Ch^2 \left\|\varphi_h\right\|_{L^2(\Gamma)}, \end{aligned}$$

and with the same arguments

$$\begin{aligned} |F_2(\varphi_h)| &\le Ch^2 \left\|\varphi_h\right\|_{L^2(\Gamma)}, \\ |F_3(\varphi_h)| &\le Ch^2 \left\|\varphi_h\right\|_{L^2(\Gamma)}. \end{aligned}$$

Inserting the above bounds into (8.4) and noting the equivalence of the L^2-norms between the original and discretized surfaces completes the proof. ■

Looking at the proof of the above lemma, we have even shown that the L^2- norm of R_h is of order 2. In the definition and the proof, one could simply take the Ritz map (8.1) with $\zeta = 0$ and end up with a definition which is more similar to the classical Ritz projection and then have to estimate the extra term $F_4(\varphi_h) = m(u, (v - v_h) \cdot \nabla_\Gamma \varphi_h) \le Ch^2 \|\nabla_\Gamma \varphi_h\|_{L^2(\Gamma)}$. This will also lead to the optimal bound in the H_h^{-1}-norm, but not in the L^2-norm which we actually do not need anyway. However, we will later see that for the wave equation it is crucial to choose $\zeta = \partial_h^\bullet u$ in the definition of the Ritz map.

8.2. Error bound for the full discretization

In this section, we compare the lifts of the fully discrete numerical solution $u_h^n := (U_h^n)^l$ with the exact solution $u(\cdot, t_n)$ of the parabolic equation (1.3).

Let $\{\alpha_k\}_{k=0}^n$ be generated by the s-stage implicit Runge–Kutta method (3.1) or by the k-step BDF method (4.2). Then as in (5.1), we obtain the lift of the fully discrete numerical solution

$$u_h^n := (U_h^n)^l = \sum_{j=1}^{N} \alpha_j^n \chi_j^l(\cdot, t_n),$$

which is a lifted finite element function defined on the surface $\Gamma(t_n)$. Next, we state and prove the main results of the first part of this thesis.

Theorem 8.2 (ESFEM/RK)
Consider the space discretization of the parabolic equation (1.3) *by the evolving surface finite element method and time discretization by the s-stage implicit Runge–Kutta method* (3.1) *satisfying the assumptions 3.1.2. Let u be a sufficiently smooth solution of the parabolic equation* (1.3) *and assume that the discrete initial data satisfy*

$$\left\| u_h^0 - (\mathcal{P}_h u)(\cdot, t_0) \right\|_{L^2(\Gamma(0))} \leq C_0 h^2.$$

Then, there exist $h_0 > 0$ and $\tau_0 > 0$ such that for $h \leq h_0$ and $\tau \leq \tau_0$, the following error bound holds for $t_n = n\tau \leq T$:

$$\|u_h^n - u(\cdot, t_n)\|_{L_2(\Gamma(t_n))} + h\Big(\tau \sum_{j=k}^{n} \|\nabla_{\Gamma(t_j)} u_h^j - \nabla_{\Gamma(t_j)} u(\cdot, t_j)\|_{L_2(\Gamma(t_j))}^2\Big)^{1/2} \leq C\left(\tau^{q+1} + h^2\right),$$

Assuming that the regularity conditions (5.9) *are satisfied, we obtain τ^p instead of τ^{q+1}. The constant C is independent of h, τ, and n subject to the stated conditions.*

Theorem 8.3 (ESFEM/BDF)
Consider the space discretization of the parabolic equation (1.3) *by the evolving surface finite element method and time discretization by the BDF method of order $k \leq 5$. Let u be a sufficiently smooth solution of the parabolic equation* (1.3) *and assume that the discrete initial data satisfy*

$$\max_{0 \leq i \leq k-1} \left\| u_h^i - (\mathcal{P}_h u)(\cdot, t_i) \right\|_{L^2(\Gamma(0))} \leq C_0 h^2.$$

Then, there exist $h_0 > 0$ and $\tau_0 > 0$ such that for $h \leq h_0$ and $\tau \leq \tau_0$, the following error bound holds for $t_n = n\tau \leq T$:

$$\|u_h^n - u(\cdot, t_n)\|_{L_2(\Gamma(t_n))} + h\Big(\tau \sum_{j=k}^{n} \|\nabla_{\Gamma(t_j)} u_h^j - \nabla_{\Gamma(t_j)} u(\cdot, t_j)\|_{L_2(\Gamma(t_j))}^2\Big)^{1/2} \leq C\left(\tau^{k} + h^2\right),$$

The constant C is independent of h, τ, and n subject to the stated conditions.

PROOF
We decompose the global error into two components as

$$u_h^n - u(\cdot, t_n) = \Big(u_h^n - \mathcal{P}_h u(\cdot, t_n)\Big) + \Big(\mathcal{P}_h u(\cdot, t_n) - u(t_n)\Big). \tag{8.5}$$

Taking into account that the L^2 and H^1 norms on the discretized and original surface are equivalent (Lemma 6.1), in order to estimate the first part of (8.5), we just need to combine the theorems and lemmas from the previous chapters. For example, for the k-step BDF method, using Theorem 5.3 together with Lemma 8.1 (residual bound) and Theorems 7.2 and 7.3 (for estimating $\widetilde{\beta}_{h,k}$) one finds that the first part is of order $\mathcal{O}(\tau^k + h^2)$. The second part of (8.5) is already taken care of in Theorems 7.2 and 7.3. ∎

Remark 8.4

It is well known, that Runge–Kutta time discretization schemes suffer from order reduction phenomena when they are applied to partial differential equations with non-periodic boundary conditions on plane domains (cf. [34, 36, 43]). In particular, condition (13.22) *fails to hold uniformly in the mesh size on surfaces with boundary. However, for smooth solutions of equations on smooth closed surfaces, it can be expected that the regularity condition* (5.9) *holds true.*

9. Numerical Experiments I

We present numerical experiments for the homogeneous as well as the inhomogeneous parabolic equation on evolving surfaces confirming some of our theoretical results. The fully discrete methods (cf. Section 5.1) are implemented by using the finite element toolbox ALBERTA [44], Matlab, and the DUNE-FEM module [5]. For the implementation of the 3- stage implicit Runge–Kutta method (Radau IIA), we make use of the code RADAU5 of Hairer & Wanner [26, 27]. The visualization is done by using the application ParaView [29].

Example 9.1
We consider the numerical example [14, Example 7.3] and solve the parabolic equation

$$\partial^{\bullet} u + u \, \nabla_\Gamma \cdot v - \Delta_\Gamma u = f \quad \text{on } \Gamma(t), \tag{9.1}$$

where the surface $\Gamma(t)$ is an ellipsoid with time dependent axis and given as the level set

$$\Gamma(t) = \left\{ x \in \mathbb{R}^3 \, : \, \frac{x_1^2}{1 + 0.25 \sin(\pi \cdot t)} + x_2^2 + x_3^2 - 1 = 0 \right\}.$$

The right hand side f is calculated so that the exact solution is given by

$$u(x,t) = e^{-6t} x_1 x_2.$$

Fully discrete scheme for the inhomogeneous parabolic equation on evolving surfaces: We treated so far only the homogeneous parabolic equation on evolving surfaces, we mention again that it is straightforward to extend our results to the inhomogeneous case. The fully discrete scheme for the inhomogeneous equation has to be updated with a right hand side similar to the inhomogeneous parabolic equation on a fixed domain. For example, the implicit RK method (3.1) becomes:

The s- stage implicit RK method for the inhomogeneous parabolic equation on evolving surfaces reads

$$M_{ni}\alpha_{ni} = M_n \alpha_n - \tau \sum_{j=1}^{s} a_{ij} A_{nj} \alpha_{nj} + \tau \sum_{j=1}^{s} a_{ij} F_{nj}, \qquad i = 1, \cdots, s, \tag{9.2a}$$

$$M_{n+1}\alpha_{n+1} = M_n \alpha_n - \tau \sum_{i=1}^{s} b_i A_{ni} \alpha_{ni} + \tau \sum_{i=1}^{s} b_i F_{ni}, \tag{9.2b}$$

where $(F_{ni})_{j=1}^{N} = \left(\int_{\Gamma_h(t_{ni})} f^{-l} \chi_j \right)_{j=1}^{N}$, with $t_{ni} = t_n + c_i \tau$.

1. **Experiment (backward Euler):** Let $\{\mathcal{T}_h^i\}_{i=0}^k$ and $\{\tau_i\}_{i=0}^k$ be a sequence of meshes of a surface by uniform refinement and a sequence of time steps respectively. The uniform refinement is such that $h_i \approx \frac{1}{2}h_{i-1}$. We set $\tau_i = \frac{1}{4}\tau_{i-1}$ to obtain the time step sequence, starting with $\tau_0 = 0.1$. For each mesh $\mathcal{T}_h^i$ together with the corresponding time step size τ_i, we solve the parabolic equation using the piecewise linear finite elements in combination with the backward Euler method. Then, we compute the error between the lifted numerical solution and the exact solution for $0 \leq t \leq 1$ in the following norms:

$$L^\infty\left(L^2\right): \quad \max_{0\leq n\leq N} \|u_h^n - u(\cdot, t_n)\|_{L^2(\Gamma(t_n))},$$

$$L^2\left(H^1\right): \quad \left(\tau \sum_{n=0}^{N} \left\|\nabla_{\Gamma(t_n)} u_h^n - \nabla_{\Gamma(t_n)} u(\cdot, t_n)\right\|^2_{L^2(\Gamma(t_n))}\right)^{\frac{1}{2}}.$$

Assuming that the error Err_i satisfies $Err_i = C\left(h_i + \tau_i^{1/2}\right)^{EOC}$. Then, it follows that $\frac{Err_{i-1}}{Err_i} = 2^{EOC}$. Thus, the experimental order of convergence (EOC) is determined by

$$EOC = \frac{\log \frac{Err_{i-1}}{Err_i}}{\log 2}, \qquad i = 1, \cdots k.$$

In Table 9.1, we list the errors and the corresponding EOCs. As theoretically expected from Theorem 8.2, we observe $EOC \approx 2$ for the $L^\infty\left(L^2\right)$, whereas $EOC \approx 1$ for the $L^2\left(H^1\right)$ norm.

Table 9.1.: Errors and observed orders of convergence for the backward Euler.

Level	DOF	$L^\infty(L^2)$	EOC	$L^2(H^1)$	EOC
0	318	$6.33 \cdot 10^{-2}$	–	$1.50 \cdot 10^{-1}$	–
1	1266	$1.85 \cdot 10^{-2}$	1.77	$5.34 \cdot 10^{-2}$	1.49
2	5058	$4.83 \cdot 10^{-3}$	1.93	$2.24 \cdot 10^{-2}$	1.25
3	20226	$1.22 \cdot 10^{-3}$	1.98	$1.05 \cdot 10^{-2}$	1.08
4	80898	$3.06 \cdot 10^{-4}$	1.99	$5.21 \cdot 10^{-3}$	1.02
5	323586	$7.67 \cdot 10^{-5}$	1.99	$2.60 \cdot 10^{-3}$	1.00

2. **Experiment (BDF2):** We repeat the first experiment with the BDF2 method instead of the backward Euler method. Now, we choose $\tau_i = \frac{1}{2}\tau_{i-1}$ with $\tau_0 = 0.2$. Here, the error is assumed to satisfy $Err_i = C(h_i + \tau_i)^{EOC}$. Then as above we get

$$EOC = \frac{\log \frac{Err_{i-1}}{Err_i}}{\log 2}.$$

The Table 9.2 shows that the experimental orders of convergence, $EOC \approx 2$ for the $L^\infty(L^2)$ norm as well as $EOC \approx 1$ for the $L^2(H^1)$ norm, coincide with the theoretical ones (cf. Theorem 8.3).

Table 9.2.: Errors and observed orders of convergence for the BDF2.

Level	DOF	$L^\infty(L^2)$	EOC	$L^2(H^1)$	EOC
0	318	$4.33 \cdot 10^{-2}$	–	$1.51 \cdot 10^{-1}$	–
1	1266	$1.88 \cdot 10^{-2}$	1.20	$6.13 \cdot 10^{-2}$	1.30
2	5058	$6.21 \cdot 10^{-3}$	1.59	$2.54 \cdot 10^{-2}$	1.26
3	20226	$1.76 \cdot 10^{-3}$	1.81	$1.14 \cdot 10^{-2}$	1.15
4	80898	$4.67 \cdot 10^{-4}$	1.91	$5.41 \cdot 10^{-3}$	1.07
5	323586	$1.20 \cdot 10^{-4}$	1.96	$2.64 \cdot 10^{-3}$	1.03
6	1294338	$3.04 \cdot 10^{-5}$	1.98	$1.31 \cdot 10^{-3}$	1.01

3. **Experiment (Radau IIA):** In this experiment, we examine the convergence of the 3- stage Radau IIA method (3.1). The method is given via the Butcher tableau:

The 3-stage Radau IIA method

$$
\begin{array}{c|ccc}
\frac{4-\sqrt{6}}{10} & \frac{88-7\sqrt{6}}{360} & \frac{296-169\sqrt{6}}{1800} & \frac{-2+3\sqrt{6}}{225} \\
\frac{4+\sqrt{6}}{10} & \frac{296+169\sqrt{6}}{1800} & \frac{88+7\sqrt{6}}{360} & \frac{-2-3\sqrt{6}}{225} \\
1 & \frac{16-\sqrt{6}}{36} & \frac{16+\sqrt{6}}{36} & \frac{1}{9} \\
\hline
 & \frac{16-\sqrt{6}}{36} & \frac{16+\sqrt{6}}{36} & \frac{1}{9}
\end{array}
$$

We compare the fully discrete solution with the piecewise linear interpolant of the exact solution on the discrete surface $\Gamma_h(t)$. We consider the sequence of meshes $\{\mathcal{T}_h^\ell(t)\}_{\ell=1}^4$ with $2^{2\ell+6}+2$ meshpoints and a time step size sequence $\{\tau_i\}_{i=0}^{17}$. For each mesh $\mathcal{T}_h^\ell$, we solve the parabolic equation on the time interval $0 \le t \le 1$ using the time step size τ_i for $i = 0, \cdots, 17$. Then, we collect the errors $e(x,t) = u_n(x) - u(x,t)$ (with $n\tau = t$) at the mesh points of the surface into a vector $e \in \mathbb{R}^N$ and consider the norm and semi-norm defined by the mass and stiffness matrix, respectively, at time t,

$$
\begin{aligned}
\text{Error (M):} \quad & \left(\langle e \,|M(t)|\, e\rangle\right)^{1/2}, \\
\text{Error (A):} \quad & \left(\langle e \,|A(t)|\, e\rangle\right)^{1/2}.
\end{aligned}
$$

In Figure 9.1, we plot the error for the Radau IIA in these norms versus the time step size. We recognize two regions: In the region where the time discretization error dominates the spatial one, we observe that the experimental convergence rate coincide with the classical order $2 \times 3 + 1 = 5$ of the method. In the complementary region, for smaller time steps, we observe a faster convergence with respect to the spatial refinement in the L^2-norm than in the energy seminorm. The observed results match the theoretical ones perfectly (cf. Theorem 8.2).

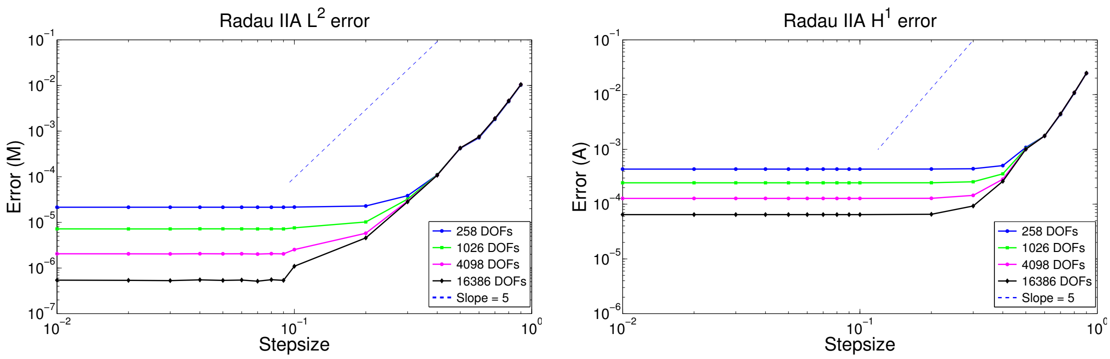


Figure 9.1.: Errors of Radau IIA scheme in the L^2-norm (left: Error (M)) and the energy seminorm (right: Error (A)) vs. time step size for four spatial refinements at time t=1.

4. **Experiment (Adaptive Radau IIA):** We repeat the 3. Experiment (Radau IIA) with variable time steps as provided by the RADAU5 code of [27]. In Figure 9.2, we plot the errors in the M-norm as well as in the A-seminorm versus the computing time in seconds on a standard PC for ten local error tolerances ranging from $Atol = Rtol = 10^{-1}$ to $Atol = Rtol = 10^{-10}$.

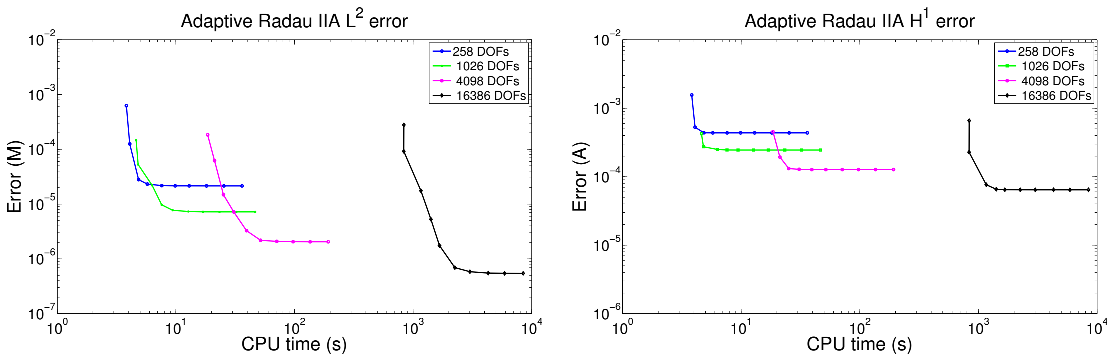


Figure 9.2.: Errors of the Radau IIA in the L^2-norm (left: Error(M)) and the energy seminorm (right: Error(A)) vs. CPU time for four spatial refinements and ten tolerances at time t=1.

5. **Experiment (BDF):** In this experiment, we examine the convergence of the BDF schemes (4.2) of order $k = 4$ and $k = 5$. This is done exactly as in the Experiment 2 for the implicit Runge–Kutta method by using the BDF scheme for the time discretization instead. The starting values $u_0, \cdots, u_{k-1}$ are taken to be the exact solution values at the nodes, i.e., for $j = 0, \cdots, k-1$, we set $(u_j)_i = u(a_i(t_j), t_j)$ for $i = 1, \ldots, N$, with $t_j = j\tau$. In Figures 9.3 and 9.4, we plot the errors in the M-norm as well as in the A-seminorm at time $t = 1$ versus the time step size. In analogy to the 3. Experiment for the Radau IIA method, the optimal convergence order in time is observed in the region where the temporal error is dominant. In the other region where the spatial error is dominant, we see that, the convergence with respect to the spatial refinement in the L^2- norm is faster than the one in the H^1-seminorm. Both conclusions are in agreement with the convergence results as stated in Theorem 8.3.

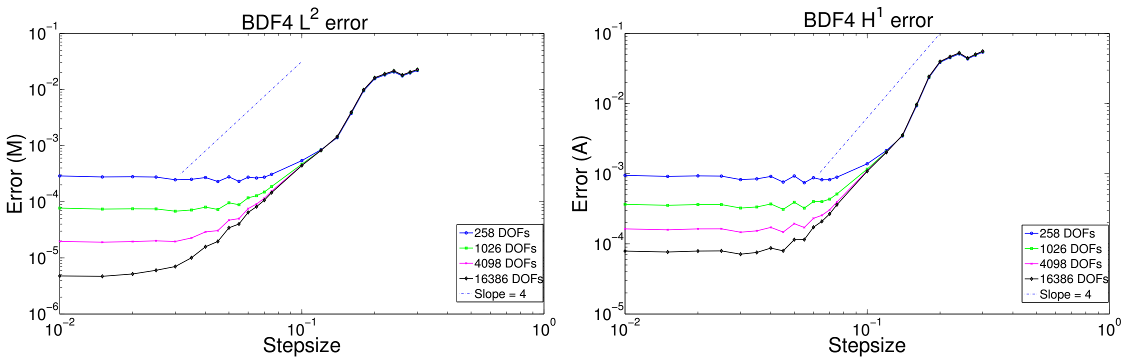


Figure 9.3.: Errors of the BDF4 scheme in the L^2- norm (left: Error (M)) and the energy seminorm (right: Error(A)) vs. timestep size for four spatial refinements at time $t = 1$.

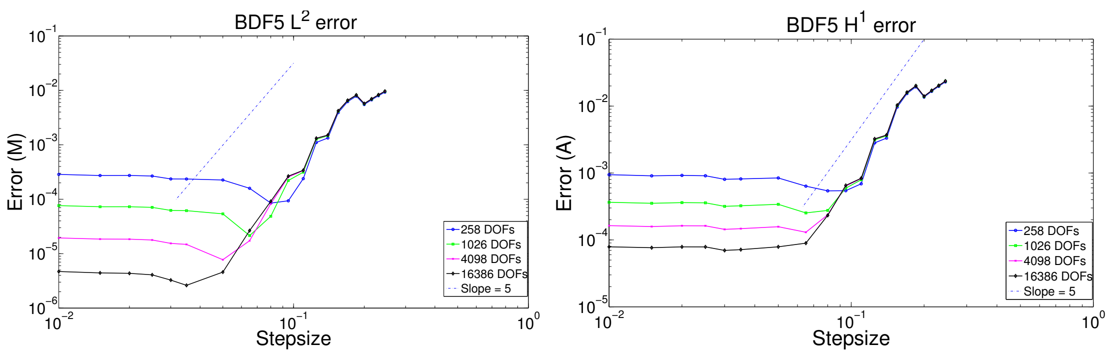
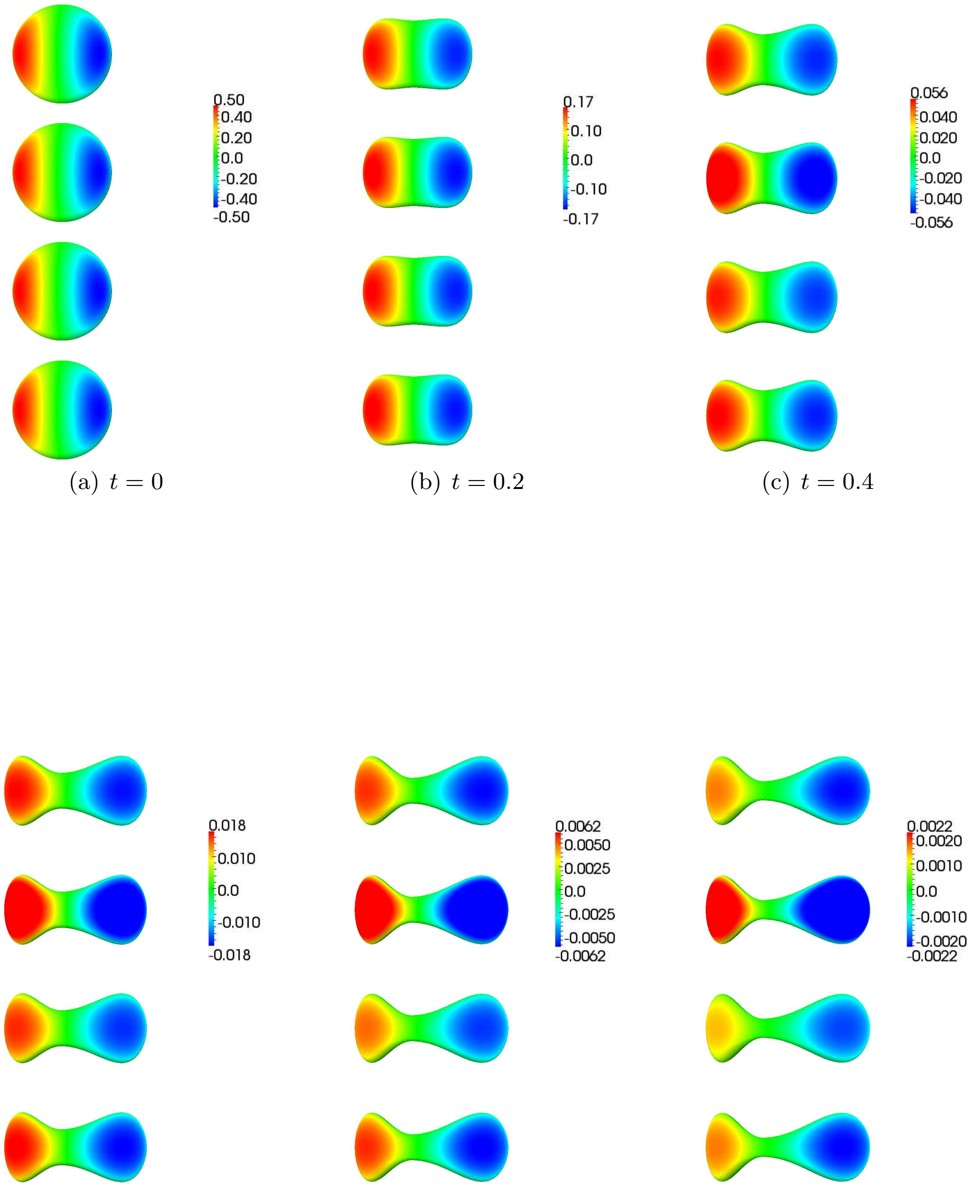


Figure 9.4.: Errors of the BDF5 schemes in the L^2- norm (left: Error (M)) and the energy seminorm (right: Error (A)) vs. timestep size for four spatial refinements at time $t = 1$.

Example 9.2
We choose a time-dependent surface of the form

$$\Gamma(t) := \left\{ x_1 + \max(0, x_1)t, \frac{g(x,t)x_2}{\sqrt{x_2^2 + x_3^2}}, \frac{g(x,t)x_3}{\sqrt{x_2^2 + x_3^2}} : x \in \Gamma(0) = S^2 \right\},$$
$$g(x,t) = e^{-2t}\sqrt{x_2^2 + x_3^2} + (1 - e^{-2t}) \left(\left(1 - x_1^2\right) \left(x_1^2 + 0.05\right) + x_1^2\sqrt{(1 - x_1^2)} \right). \tag{9.3}$$

We consider the parabolic equation (9.1) posed on the above surface on the time interval $[0, 1]$, with right hand side $f = 0$ and initial data $u(x, 0) = x_1 x_2$. The surface evolves from an initially spherical shape at $t = 0$ to a “baseball bat” like shape. In this experiment, we compare three BDF methods, namely, the backward Euler method (BDF1), BDF2 and BDF4. First, we construct a reference solution by taking the discrete surface $\Gamma_h(t)$ with 4098 meshpoints and the small time step size $\tau = 10^{-4}$ and then apply the ESFEM coupled with BDF1 method. Next, we take the same mesh but a different time step size $\tau = 5 \times 10^{-2}$ and conduct three experiments with BDF1, BDF2 and BDF4. The starting values for BDF2 as well as for BDF4 are determined by the constructed reference solution. In Figure 9.5, we show snapshots of the discrete solution for the four different experiments. Reading from top to bottom, each subfigure presents the reference solution, the solution by BDF1, by BDF2, and by BDF4. As theoretically expected, we observe a convergence to the reference solution when the order of the scheme is increased. The computational time of the reference solution with the small time step size is 264 seconds, whereas the computational time of the schemes with the larger time step is approximately 3 seconds.



(a) $t = 0$ (b) $t = 0.2$ (c) $t = 0.4$

(d) $t = 0.6$ (e) $t = 0.8$ (f) $t = 1$

Figure 9.5.: Snapshots of the discrete solution of equation (9.1) on a time-dependent surface of the form (9.3). Reading from top to bottom, each subfigure shows results of the BDF1 scheme with the uniformly small time step size $\tau = 10^{-4}$ and the BDF1, BDF2 and BDF4 schemes with the larger time step size $\tau = 5 \times 10^{-2}$.

Part II.

Full Discretization of Wave Equations on Evolving Surfaces

10. Wave Equations on Evolving Surfaces

In this chapter, we derive a linear wave equation on a given time-dependent surface which is the natural analog of the classical acoustic wave equation on a fixed spatial domain. We begin with some basic definitions and results from elementary differential geometry that are necessary to describe the mathematical model. Next, we use the Hamilton variational principle to derive the wave equation on an evolving surface, where we consider a Lagrangian that is the analog of the Lagrangian for the acoustic wave equation on a fixed domain. We introduce the weak formulation and prove the well-posedness of the initial value problem.

10.1. Basic notation

For a time interval $t \in [0,T]$, we consider a smoothly evolving family of smooth m-dimensional compact closed hypersurfaces $\Gamma(t)$ in $\mathbb{R}^{m+1}$ without boundary. The unit outward pointing normal is denoted by ν and depends smoothly on time t.

We assume that the surface $\Gamma(t)$ is generated by the smooth map

$$\Phi : \Gamma_0 \times [0,T] \longrightarrow \mathbb{R}^{n+1}, \;\; \Phi(\Gamma_0, t) = \Gamma(t),$$

where $\Gamma_0 = \Gamma(0)$, and assume that $\Phi_t(\cdot) = \Phi(\cdot, t) : \Gamma_0 \longrightarrow \Gamma(t)$ is a diffeomorphism for every $t \in [0,T]$. We can then represent the surface $\Gamma(t)$ as

$$\Gamma(t) = \{x = \Phi(x_0, t) \,|\, x_0 \in \Gamma_0\}\,.$$

The *velocity* of the material points $x(t)$ on the surface $\Gamma(t)$ is given by

$$\dot{x}(t) = v(x(t), t) = \partial_t \Phi\left(\Phi_t^{-1}(x(t)), t\right) \qquad \text{for} \quad x(t) \in \Gamma(t).$$

We define the space-time surface as

$$G_T = \bigcup_{t\in[0,T]} \Gamma(t) \times \{t\}.$$

In the following, we omit the omnipresent argument t in the surface $\Gamma(t)$, wherever it is clear which surface is considered or whenever the stated relations are valid independently of the time t.

The *tangential gradient* of a smooth function $g : \Gamma \to \mathbb{R}$ is given by

$$\nabla_\Gamma g = \nabla \bar{g} - \nabla \bar{g} \cdot \nu \, \nu,$$

where $\bar{g}$ is an extension of g to an open neighborhood of Γ, $\nabla \bar{g}$ denotes the usual $(m+1)$-dimensional gradient and $a \cdot b = \sum_{j=1}^{m+1} a_j b_j$ for vectors a and b in $\mathbb{R}^{m+1}$. The tangential gradient only depends on the values of g on the surface Γ and is independent of the choice of the extension with $\nabla_\Gamma g \cdot \nu = 0$.

The *Laplace-Beltrami* operator on Γ is the tangential divergence of the tangential gradient

$$\Delta_\Gamma g = \nabla_\Gamma \cdot \nabla_\Gamma g = \sum_{j=1}^{m+1} (\nabla_\Gamma)_j (\nabla_\Gamma)_j g,$$

and the Green's formula on $\Gamma (\partial \Gamma = \emptyset)$ reads

$$\int_\Gamma \nabla_\Gamma g \cdot \nabla_\Gamma \varphi = - \int_\Gamma \varphi \Delta_\Gamma g. \tag{10.1}$$

The *material derivative* of a smooth function $g : G_T \to \mathbb{R}$ is given by

$$\partial^\bullet g = \frac{\partial g}{\partial t} + v \cdot \nabla g, \tag{10.2}$$

which only depends on the values of the function g on the space-time surface G_T. For a more detailed discussion concerning surface gradients and material derivatives, we refer the reader to [21, 14].

We use the notation $L^k(\Gamma)$ and $H^k(\Gamma)$ for the standard Sobolev spaces on a surface Γ for $1 \le k \le \infty$. We will also work with the Sobolev spaces:

$$\begin{aligned}
L^2(G_T; L^k) &= \left\{ g : G_T \longrightarrow \mathbb{R} \, : \, \int_0^T \|g(\cdot, t)\|^2_{L^k(\Gamma(t)} \, \mathrm{d}t < \infty \right\}, \\
L^2(G_T; H^k) &= \left\{ g : G_T \longrightarrow \mathbb{R} \, : \, \int_0^T \|g(\cdot, t)\|^2_{H^k(\Gamma(t)} \, \mathrm{d}t < \infty \right\}, \\
L^\infty(G_T; L^k) &= \left\{ g : G_T \longrightarrow \mathbb{R} \, : \, \operatorname{ess} \sup_{0 \le t \le T} \|g(\cdot, t)\|_{L^k(\Gamma(t)} < \infty \right\}, \\
L^\infty(G_T; H^k) &= \left\{ g : G_T \longrightarrow \mathbb{R} \, : \, \operatorname{ess} \sup_{0 \le t \le T} \|g(\cdot, t)\|_{H^k(\Gamma(t)} < \infty \right\},
\end{aligned}$$

with $1 \le k \le \infty$. Due to the fact that Φ_t is a diffeomorphism between Γ_0 and $\Gamma(t)$, we note the relation

$$g \in H^k(\Gamma(t)) \Longleftrightarrow \widehat{g} \in H^k(\Gamma_0),$$

for the functions $g(\cdot, t) : \Gamma(t) \longrightarrow \mathbb{R}$ and $\widehat{g} = g \circ \Phi_t : \Gamma_0 \longrightarrow \mathbb{R}$. For more information about Sobolev spaces, we refer to the monographs [2] and [47].

10.2. Hamilton's principle of stationary action

With the *Lagrangian* (kinetic energy minus potential energy)

$$\mathcal{L}(u, \partial^\bullet u, t) = \frac{1}{2}\int_{\Gamma(t)} |\partial^\bullet u|^2 - \frac{1}{2}\int_{\Gamma(t)} \left|\nabla_{\Gamma(t)} u\right|^2 \tag{10.3}$$

we consider the *action integral*

$$\mathcal{S}[u] = \int_0^T \mathcal{L}(u(t), \partial^\bullet u(t), t)\,\mathrm{d}t \tag{10.4}$$

for $u(t) = u(\cdot, t) \in H^1(\Gamma(t))$. The analogous action integral on a fixed domain Ω instead of moving surfaces $\Gamma(t)$ is minimized by solutions of the classical acoustic wave equation $\partial_t^2 u - \Delta u = 0$. In our situation, we arrive at the following partial differential equation which is called the Jenner equation in [16].

Lemma 10.1
If $u : G_T \to \mathbb{R}$ is a smooth function that extremizes the action integral $\mathcal{S}[u]$ among all smooth functions on G_T with given end-points $u(\cdot, 0)$ and $u(\cdot, T)$, then u is a solution of the Euler–Lagrange partial differential equation

$$\partial^\bullet\partial^\bullet u(x,t) + \partial^\bullet u(x,t)\ \nabla_{\Gamma(t)} \cdot v(x,t) - \Delta_{\Gamma(t)} u(x,t) = 0 \tag{10.5}$$

for $x \in \Gamma(t)$ and $0 \le t \le T$.

We refer to (10.5) as the *wave equation on the evolving surface*. An inhomogeneity $f(x,t)$ on the right-hand side of (10.7) is obtained by adding the term $\int_{\Gamma(t)} fu$ to the Lagrangian. Note that it is easy and straightforward to extend all of the upcoming results to the inhomogeneous problem.

Proof
The result is a consequence of the Leibniz formula on surfaces [14, Lemma 2.2]:

$$\frac{d}{dt}\int_{\Gamma(t)} g = \int_{\Gamma(t)} \partial^\bullet g + g\nabla_{\Gamma(t)} \cdot v. \tag{10.6}$$

Computing variations of the action while keeping the endpoints of $u(., t)$ fixed ($\delta u(0) = \delta u(T) = 0$), using (10.6) and partial integration, we get

$$\begin{aligned}\delta\mathcal{S}[u] &= \frac{d}{d\epsilon}\Big|_{\epsilon=0} S\left(u + \epsilon\delta u\right) = \int_0^T \int_{\Gamma(t)} \left(\partial^\bullet u\, \partial^\bullet \delta u - \nabla_{\Gamma(t)} u \nabla_{\Gamma(t)} \delta u\right) \mathrm{d}t \\ &= \int_0^T \frac{d}{dt}\int_{\Gamma(t)} \partial^\bullet u\, \delta u\, \mathrm{d}t - \int_0^T\int_{\Gamma(t)} \left(\partial^\bullet\partial^\bullet u\, \delta u + \partial^\bullet u\, \delta u\, \nabla_{\Gamma(t)} \cdot v + \nabla_{\Gamma(t)} u \nabla_{\Gamma(t)} \delta u\right) \mathrm{d}t \\ &= -\int_0^T \int_{\Gamma(t)} \left(\partial^\bullet\partial^\bullet u + \partial^\bullet u \nabla_{\Gamma(t)} \cdot v - \Delta_{\Gamma(t)} u\right) \delta u\, \mathrm{d}t = 0.\end{aligned}$$

With the fundamental lemma of the calculus of variations we obtain the result. ∎

10.3. The mathematical model

We consider the initial value problem for the linear wave equation on evolving surfaces

$$\begin{cases} \partial^\bullet \partial^\bullet u(x,t) + \partial^\bullet u(x,t)\ \nabla_{\Gamma(t)} \cdot v(x,t) - \Delta_{\Gamma(t)} u(x,t) &= 0 \quad \text{on } G_T \\ u(\cdot,0) &= u_0 \quad \text{on } \Gamma(0) \\ \partial^\bullet u(\cdot,0) &= \dot{u}_0 \quad \text{on } \Gamma(0) \end{cases} \tag{10.7}$$

with given initial data $u_0 \in H^2(\Gamma(0))$ and $\dot{u}_0 \in H^1(\Gamma(0))$.

Definition 10.2 (Bilinear forms)
As in Chapter 6, we define the bilinear forms for $w, \varphi \in H^1(\Gamma)$ as

$$a(w,\varphi) = \int_\Gamma \nabla_\Gamma w \cdot \nabla_\Gamma \varphi, \tag{10.8a}$$

$$m(w,\varphi) = \int_\Gamma w\varphi, \tag{10.8b}$$

$$g(v;w,\varphi) = \int_\Gamma (\nabla_\Gamma \cdot v)\, w\varphi, \tag{10.8c}$$

where the forms also depend on time t.

Definition 10.3 (Weak solution)
We say a function

$$u \in L^2(G_T;H^1) \text{ with } \partial^\bullet u \in L^2(G_T;H^1),\ \partial^\bullet\partial^\bullet u \in L^2(G_T;L^2),$$

is a weak solution of the wave equation (10.7), if:

- *For almost $t \in [0,T]$*

$$m(\partial^\bullet\partial^\bullet u, \varphi) + g(v;\partial^\bullet u,\varphi) + a(u,\varphi) = 0 \quad \text{for all } \varphi(\cdot,t) \in H^1(\Gamma(t)). \tag{10.9}$$

- $u(\cdot,0) = u_0$ *and* $\partial^\bullet u(\cdot,0) = \dot{u}_0$.

Lemma 10.4 (Weak form)
A weak solution u satisfies for almost every $t \in [0,T]$,

$$\frac{d}{dt} m(\partial^\bullet u,\varphi) + a(u,\varphi) = m(\partial^\bullet u, \partial^\bullet \varphi), \tag{10.10}$$

for all $\varphi \in L^2(G_T;H^1)$ with $\partial^\bullet \varphi \in L^2(G_T;L^2)$.

Proof
By multiplying the above equation (10.7) by a test function φ, integrating over Γ and performing integration by parts, we obtain

$$\begin{aligned} 0 &= m(\partial^\bullet\partial^\bullet u,\varphi) + g(v;\partial^\bullet u,\varphi) + a(u,\varphi) \\ &= m(\partial^\bullet\partial^\bullet u,\varphi) + m(\partial^\bullet u,\partial^\bullet\varphi) + g(v;\partial^\bullet u,\varphi) + a(u,\varphi) - m(\partial^\bullet u,\partial^\bullet\varphi) \\ &= \frac{d}{dt} m(\partial^\bullet u,\varphi) + a(u,\varphi) - m(\partial^\bullet u,\partial^\bullet\varphi) \end{aligned}$$

where we made use of the transport Lemma 6.4. ■

Theorem 10.5 (Existence and uniqueness of weak solution)
There exists a unique weak solution of the wave equation (10.7) *with*

$$u \in L^\infty(G_T; H^2), \partial^\bullet u \in L^\infty(G_T; H^1)$$
$$\partial^\bullet \partial^\bullet u \in L^\infty(G_T; L^2)$$

Proof
Let $\{\varphi_j^0\}_{j\in\mathbb{N}}$ be the eigenfunctions of the the Laplace-Beltrami operator on Γ_0 which form an orthonormal basis of $L^2(\Gamma_0)$ and orthogonal basis of $H^1(\Gamma_0)$. With the help of the diffeomorphism

$$\Phi_t : \Gamma_0 \longrightarrow \Gamma(t),$$

we define

$$\varphi_j(\Phi_t(\cdot), t) = \varphi_j^0(\cdot).$$

For any function $g \in H^1(\Gamma(t))$ and $\Gamma(t) \ni x = \Phi_t(y)$, we then have

$$g(x,t) = g(\Phi_t(y), t) = \sum_{j=1}^{\infty} \alpha_j(t)\varphi_j^0(y) = \sum_{j=1}^{\infty} \alpha_j(t)\varphi_j(x,t). \tag{10.11}$$

We also note the transport property

$$\partial^\bullet \varphi_j(x,t) = \frac{d}{dt}\varphi_j(\Phi(y,t),t) = \frac{d}{dt}\varphi_j^0(y) = 0. \tag{10.12}$$

We now proceed similarly to the proof of Theorem 3 in [20, Section 7.2].

Galerkin ansatz: We consider the approximation of the problem (10.10) on $X_N(t) = \text{span}\{\varphi_1, \cdots, \varphi_N\}$: Find $u_N(\cdot,t) = \sum_{j=1}^N q_j(t)\varphi_j(\cdot,t) \in X_N(t)$ such that

- For almost every $t \in [0,T]$,

$$\frac{d}{dt}m(\partial^\bullet u_N, \varphi) + a(u_N, \varphi) = m(\partial^\bullet u_N, \partial^\bullet \varphi) \quad \text{for all } \varphi \in X_N(t). \tag{10.13}$$

- $u_N(\cdot,0) = \sum_{j=0}^N m(u_0,\varphi_j)\varphi_j$ and $\partial^\bullet u_N(\cdot,0) = \sum_{j=0}^N m(\dot{u}_0,\varphi_j)\varphi_j$.

Using the transport property (10.12), we find that $\partial^\bullet u_N(\cdot,t)$ as well as $\partial^\bullet\partial^\bullet u_N(\cdot,t)$ belong to the finite dimensional space $X_N(t)$. With the standard theory of ordinary differential equations, one easily show that there exists a unique solution u_N of the system (10.13).

Energy estimates: We prove some energy estimates which we will need when sending $N \to \infty$:

(1) We choose $\varphi = \partial^\bullet u_N$ in (10.13) and use the transport Lemma 6.4 to obtain

$$\frac{d}{dt}m(\partial^\bullet u_N, \partial^\bullet u_N) + a(u_N, \partial^\bullet u_N) = m(\partial^\bullet u_N, \partial^\bullet\partial^\bullet u_N)$$
$$= \frac{1}{2}\frac{d}{dt}m(\partial^\bullet u_N, \partial^\bullet u_n) - \frac{1}{2}g(v; \partial^\bullet u_N, \partial^\bullet u_N).$$

Again with the transport lemma and Cauchy-Schwarz inequality , it follows that

$$\frac{d}{dt}m(\partial^\bullet u_N, \partial^\bullet u_N) + \frac{d}{dt}a(u_N, u_N) = b(v; u_N, u_N) - g(v, \partial^\bullet u_N, \partial^\bullet u_N)$$
$$\frac{d}{dt}\left\|\partial^\bullet u_N\right\|^2_{L^2(\Gamma(t))} + \frac{d}{dt}\left\|\nabla_{\Gamma(t)}u_N\right\|^2_{L^2(\Gamma(t))} \leq C\left(\left\|\partial^\bullet u_N\right\|^2_{L^2(\Gamma(t))} + \left\|\nabla_{\Gamma(t)}u_N\right\|^2_{L^2(\Gamma(t))}\right).$$

Applying Gronwall's lemma, we arrive at the first estimate

$$\sup_{t\in[0,T]}\left\|\partial^\bullet u_N\right\|^2_{L^2(\Gamma(t))} + \sup_{t\in[0,T]}\left\|\nabla_{\Gamma(t)}u_N\right\|^2_{L^2(\Gamma(t))}$$
$$\leq C\left(\left\|\partial^\bullet u_N(0)\right\|^2_{L^2(\Gamma(0))} + \left\|\nabla_{\Gamma(0)}u_N(0)\right\|^2_{L^2(\Gamma(0))}\right). \quad (10.14)$$

(2) By the transport Lemma 6.4, we also have

$$\frac{d}{dt}m(u_N, u_N) = 2m(\partial^\bullet u_N, u_N) + g(v; u_N, u_N).$$

Thus using the Cauchy-Schwarz inequality and the above estimate (10.14), we get

$$\frac{d}{dt}\left\|u_N\right\|^2_{L^2(\Gamma(t))} \leq C\left\|u_N\right\|^2_{L^2(\Gamma(t))} + C\left(\left\|\partial^\bullet u_N(0)\right\|^2_{L^2(\Gamma(0))} + \left\|\nabla_{\Gamma(0)}u_N(0)\right\|^2_{L^2(\Gamma(0))}\right).$$

Once again applying Gronwall's lemma, we obtain the second estimate

$$\sup_{t\in[0,T]}\left\|u_N\right\|^2_{L^2(\Gamma(t))} \leq C\left(\left\|\partial^\bullet u_N(0)\right\|^2_{L^2(\Gamma(0))} + \left\|u_N(0)\right\|^2_{H^1(\Gamma(0))}\right). \quad (10.15)$$

(3) It remains to bound $\partial^\bullet\partial^\bullet u_N$ in L^2. To do so, we first take the time derivative of the Equation (10.13) with $\varphi = \varphi_j$ and use the Transport Lemma 6.4 twice to find

$$m(\partial^{(3)}u_N, \varphi_j) + g(v; \partial^{(2)}u_N, \varphi_j) + a(\partial^\bullet u_N, \varphi_j)$$
$$+ b(v; u_N, \varphi_j) + \frac{d}{dt}g(v; \partial^\bullet u_N, \varphi_j) = 0, \quad (10.16)$$

where the superscript (ℓ) denotes the ℓ-th material derivative. By the transport lemma, we note that $(^\cdot = d/dt)$

$$\frac{d}{dt}g(v; \partial^\bullet u_N, \varphi_j) = \frac{d}{dt}\int_\Gamma(\nabla_\Gamma \cdot v)\partial^\bullet u_N\varphi_j$$
$$= \int_\Gamma(\nabla_\Gamma \cdot v)^\cdot\partial^\bullet u_N\varphi_j + \int_\Gamma(\nabla_\Gamma \cdot v)\partial^{(2)}u_N\varphi_j + \int_\Gamma(\nabla_\Gamma \cdot v)^2\partial^\bullet u_N\varphi_j$$
$$=: F_1(\varphi_j).$$

Next, we multiply the equation (10.16) by $q_j''(t)$, sum over j and use the Cauchy-Schwarz inequality, Young's inequality and the Transport Lemma 6.4 to estimate

$$
\begin{aligned}
m(\partial^{(3)}u_N, \partial^{(2)}u_N) + g(v; \partial^{(2)}u_N, \partial^{(2)}u_N) + \\
+ a(\partial^\bullet u_N, \partial^{(2)}u_N) + b(v; u_N, \partial^{(2)}u_N) = -F_1(\partial^{(2)}u_N),
\end{aligned}
$$

as

$$
\begin{aligned}
&\frac{d}{dt}\|\partial^{(2)}u_N\|^2_{L^2(\Gamma(t))} + \frac{d}{dt}\|\nabla_\Gamma \partial^\bullet u_N\|^2_{L^2(\Gamma(t))} \\
&\quad \leq C\left(\|\partial^{(2)}u_N\|^2_{L^2(\Gamma(t))} + \|\partial^\bullet u_N\|^2_{H^1(\Gamma(t))}\right) - 2b(v; u_N, \partial^{(2)}u_N), \quad (10.17)
\end{aligned}
$$

where we have used that $\sup_{t\in[0,T]}(\|\nabla_\Gamma \cdot v\|_{L^\infty(\Gamma(t))} + \|(\nabla_\Gamma \cdot v)^\cdot\|_{L^\infty(\Gamma(t))})$ is bounded, since the velocity v of the surface is smooth, to bound

$$
|F_1(\partial^{(2)}u_N)| \leq C\left(\|\partial^{(2)}u_N\|^2_{L^2(\Gamma)} + \|\partial^\bullet u_N\|^2_{L^2(\Gamma)}\right).
$$

The next step is to estimate $b(v; u_N, \partial^{(2)}u_N)$. The Transport Lemma 6.4 and the relation

$$
\partial^\bullet \nabla_\Gamma f = \nabla_\Gamma \partial^\bullet f - \mathcal{D}(v)\nabla_\Gamma f \quad \text{with} \quad \mathcal{D}(v)_{ij} = (\nabla_\Gamma)_i v_j - \sum_{l=1}^{m+1} \nu_l \nu_i (\nabla_\Gamma)_j v_l,
$$

which is proved in [18, Lemma 2.6] yield

$$
\begin{aligned}
&\int_0^t b(v; u_N(s), \partial^{(2)}u_N(s))\,\mathrm{d}s = \int_0^t \left(\int_{\Gamma(s)} \mathcal{B}(v)\nabla_\Gamma \partial^{(2)}u_N \nabla_\Gamma u_N\right)\mathrm{d}s \\
&= \int_0^t \left(\int_{\Gamma(s)} \partial^\bullet(\mathcal{B}(v)\nabla_\Gamma \partial^\bullet u_N \nabla_\Gamma u_N) - (\partial^\bullet \mathcal{B}(v))\nabla_\Gamma \partial^\bullet u_N \nabla_\Gamma u_N\right)\mathrm{d}s \\
&\quad - \int_0^t \left(\int_{\Gamma(s)} \mathcal{B}(v)\nabla_\Gamma \partial^\bullet u_N \partial^\bullet \nabla_\Gamma u_N) - \mathcal{B}(v)\mathcal{D}(v)\nabla_\Gamma \partial^\bullet u_N \nabla_\Gamma u_N\right)\mathrm{d}s \\
&= \int_0^t \frac{d}{ds}\left(\int_{\Gamma(s)} \mathcal{B}(v)\nabla_\Gamma \partial^\bullet u_N \nabla_\Gamma u_N\right)\mathrm{d}s - \int_0^t \left(\int_{\Gamma(s)} \mathcal{B}(v)\nabla_\Gamma \partial^\bullet u_N \nabla_\Gamma u_N \nabla_\Gamma \cdot v\right)\mathrm{d}s \\
&\quad - \int_0^t \left(\int_{\Gamma(s)} (\partial^\bullet \mathcal{B}(v))\nabla_\Gamma \partial^\bullet u_N \nabla_\Gamma u_N\right)\mathrm{d}s \\
&\quad - \int_0^t \left(\int_{\Gamma(s)} \mathcal{B}(v)\nabla_\Gamma \partial^\bullet u_N \partial^\bullet \nabla_\Gamma u_N) - \mathcal{B}(v)\mathcal{D}(v)\nabla_\Gamma \partial^\bullet u_N \nabla_\Gamma u_N\right)\mathrm{d}s \\
&\leq \frac{1}{4}\|\nabla_\Gamma \partial^\bullet u_N(t)\|^2_{L^2(\Gamma(t))} + C\|\nabla_\Gamma u_N(t)\|^2_{L^2(\Gamma(t))} + C\|\nabla_\Gamma \partial^\bullet u_N(0)\|^2_{L^2(\Gamma(0))} \\
&\quad + C\|\nabla_\Gamma u_N(0)\|^2_{L^2(\Gamma(0))} + C\int_0^t \|\nabla_\Gamma u_N\|^2_{L^2(\Gamma(s))}\mathrm{d}s + C\int_0^t \|\nabla_\Gamma \partial^\bullet u_N\|^2_{L^2(\Gamma(s))}\mathrm{d}s.
\end{aligned}
$$

Integrating the equation (10.17) and using Cauchy-Schwarz inequality, Young's inequality and the above estimate, we arrive at

$$\begin{aligned}
&\|\partial^{(2)}u_N(t)\|^2_{L^2(\Gamma(t))} + \frac{1}{2}\|\nabla_\Gamma \partial^\bullet u_N(t)\|^2_{L^2(\Gamma(t))} \\
&\leq C\int_0^t (\|\partial^{(2)}u_N(s)\|^2_{L^2(\Gamma(s))} + \|\nabla_\Gamma \partial^\bullet u_N(s)\|^2_{L^2(\Gamma(s))})\mathrm{d}s \\
&+ C\int_0^t (\|\partial^\bullet u_N(s)\|^2_{L^2(\Gamma(s))} + \|\nabla_\Gamma u_N(s)\|^2_{L^2(\Gamma(s))})\mathrm{d}s + C\|\nabla_\Gamma u_N(t)\|^2_{L^2(\Gamma(t))} \\
&\quad + C\|\nabla_\Gamma \partial^\bullet u_N(0)\|^2_{L^2(\Gamma(0))} + C\|\nabla_\Gamma u_N(0)\|^2_{L^2(\Gamma(0))} + \|\partial^{(2)}u_N(0)\|^2_{L^2(\Gamma(0))}.
\end{aligned} \tag{10.18}$$

Inserting the bounds (10.14) and (10.15) into (10.18) and applying Gronwall's inequality, it follows that

$$\begin{aligned}
&\sup_{t\in[0,T]} \|\partial^{(2)}u_N(t)\|^2_{L^2(\Gamma(t))} + \sup_{t\in[0,T]} \|\nabla_\Gamma \partial^\bullet u_N(t)\|^2_{L^2(\Gamma(t))} \\
&\leq C\left(\|\partial^{(2)}u_N(0)\|^2_{L^2(\Gamma(0))} + \|\nabla_{\Gamma(0)}\partial^\bullet u_N(0)\|^2_{L^2(\Gamma(0))}\right) \\
&\qquad\qquad + C\left(\|\partial^\bullet u_N(0)\|^2_{L^2(\Gamma(0))} + \|u_N(0)\|^2_{H^1(\Gamma(0))}\right)
\end{aligned} \tag{10.19}$$

(4) Keeping in mind that the basis functions $\{\varphi_j\}_{j=1}^\infty$ are the eigenfunction of $-\Delta_{\Gamma(0)}$, we deduce for the initial data

$$\begin{aligned}
\|u_N(0)\|^2_{H^1(\Gamma(0))} &\leq C\|u_0\|^2_{H^1(\Gamma(0))} \\
\|\partial^\bullet u_N(0)\|^2_{H^1(\Gamma(0))} &\leq C\|\dot{u}_0\|^2_{H^1(\Gamma(0))}.
\end{aligned}$$

Since $\partial^{(2)}u_N(0) \in X_N(0)$, we have from (10.13) and the Transport Lemma 6.4 that

$$\begin{aligned}
m(\partial^{(2)}u_N(0), \partial^{(2)}u_N(0)) = &-a(u_N(0), \partial^{(2)}u_N(0)) - g(v; \partial^\bullet u_N(0), \partial^{(2)}u_N(0)) \\
&\leq \|\Delta_{\Gamma_0}u_N(0)\|_{L^2(\Gamma(0))}\|\partial^{(2)}u_N(0)\|_{L^2(\Gamma(0))} \\
&\quad + C\|\partial^\bullet u_N(0)\|_{L^2(\Gamma(0))}\|\partial^{(2)}u_N(0)\|_{L^2(\Gamma(0))}.
\end{aligned}$$

Thus

$$\|\partial^{(2)}u_N(0)\|_{L^2(\Gamma(0))} \leq \|\Delta_{\Gamma_0}u_N(0)\|_{L^2(\Gamma(0))} + C\|\partial^\bullet u_N(0)\|_{L^2(\Gamma(0))}.$$

We also have that $\Delta^2_{\Gamma_0}u_N(0) \in X_N(0)$ and $m(u_N(0), \varphi_j^0) = m(u_0, \varphi_j^0)$ for $j = 0, \dots, N$, therefore

$$\begin{aligned}
\|\Delta_{\Gamma_0}u_N(0)\|^2_{L^2(\Gamma(0))} &= m(\Delta_{\Gamma_0}u_N(0), \Delta_{\Gamma_0}u_N(0)) = m(u_N(0), \Delta^2_{\Gamma_0}u_N(0)) \\
&= m(u_0, \Delta^2_{\Gamma_0}u_N(0)) = m(\Delta_{\Gamma_0}u_0, \Delta_{\Gamma_0}u_N(0)) \\
&\leq \|\Delta_{\Gamma_0}u_0\|_{L^2(\Gamma(0))}\|\Delta_{\Gamma_0}u_N(0)\|_{L^2(\Gamma(0))}.
\end{aligned}$$

Thus, we find

$$\|\partial^{(2)}u_N(0)\|_{L^2(\Gamma(0))} \leq C(\|\Delta_{\Gamma_0}u_0\|_{L^2(\Gamma(0))} + \|\dot{u}_0\|_{L^2(\Gamma(0))}).$$

(5) Inserting the estimates for the initial data into (10.14), (10.15) and (10.19), we discover

$$\sup_{t\in[0,T]} \|u_N(t)\|^2_{H^1(\Gamma(t))} + \sup_{t\in[0,T]} \|\partial^\bullet u_N(t)\|^2_{H^1(\Gamma(t))} + \sup_{t\in[0,T]} \|\partial^{(2)} u_N(t)\|^2_{L^2(\Gamma(t))} \\ \leq C(\|u_0\|_{H^2(\Gamma(0))} + \|\dot{u}_0\|_{H^1(\Gamma(0))}). \quad (10.20)$$

Passing to limits: From the energy estimates (10.20), we infer that there exists a subsequence $\{u_{N_l}\}_{l=1}^\infty \subset \{u_N\}_{N=1}^\infty$ and a $u \in L^2(G_T; H^1)$, with $\partial^\bullet u \in L^2(G_T; H^1), \partial^\bullet\partial^\bullet u \in L^2(G_T; L^2)$ such that

$$\begin{cases} u_{N_l} \rightharpoonup u & \text{weakly in} \quad L^2(G_T; H^1) \\ \partial^\bullet u_{N_l} \rightharpoonup \partial^\bullet u & \text{weakly in} \quad L^2(G_T; H^1) \\ \partial^\bullet\partial^\bullet u_{N_l} \rightharpoonup \partial^\bullet\partial^\bullet u & \text{weakly in} \quad L^2(G_T; L^2) \end{cases}$$

Since the functions $\varphi_j(\cdot, t)$ are dense in $H^1(\Gamma(t))$ cf. (10.11), we deduce

$$m(\partial^\bullet\partial^\bullet u, \varphi) + g(v; \partial^\bullet u, \varphi) + a(u, \varphi) = 0 \quad \text{for all } \varphi(\cdot, t) \in H^1(\Gamma(t)).$$

In a standard way (cf. [20, Section 7.2.2], one can verify that

$$u(\cdot, 0) = u_0 \ \text{ and } \partial^\bullet u(\cdot, 0) = \dot{u}_0.$$

Thus, u is a weak solution of the wave equation (10.7).

Uniqueness: For a weak solution u of (10.7), using the same arguments as above (10.15), we discover

$$\sup_{t\in[0,T]} \|u\|^2_{L^2(\Gamma(t))} \leq C\left(\|\dot{u}_0\|^2_{L^2(\Gamma(0))} + \|u_0\|^2_{H^1(\Gamma(0))}\right)$$

From the linearity of the problem and the application of this estimate to the difference of two weak solutions, we see that there can be only one weak solution.

Regularity: From the energy estimates (10.20), we deduce that the limit function u satisfies

$$\sup_{t\in[0,T]} \|u\|^2_{H^1(\Gamma(t))} + \sup_{t\in[0,T]} \|\partial^\bullet u\|^2_{H^1(\Gamma(t))} + \sup_{t\in[0,T]} \|\partial^{(2)} u\|^2_{L^2(\Gamma(t))} \\ \leq C(\|u_0\|_{H^2(\Gamma(0))} + \|\dot{u}_0\|_{H^1(\Gamma(0))}) \quad (10.21)$$

By the elliptic theory on smooth surfaces (see [3] and [47] for more details) and the relation

$$a(u, \varphi) = -m(\partial^\bullet\partial^\bullet u, \varphi) - g(v; \partial^\bullet u, \varphi) \quad \text{for all } \varphi(\cdot, t) \in H^1(\Gamma(t)),$$

it follows that $u(\cdot, t) \in H^2(\Gamma(t))$ and

$$\|u\|^2_{H^2(\Gamma(t))} \leq C(\|\partial^{(2)} u\|^2_{L^2(\Gamma(t))} + \|\partial^\bullet u\|^2_{L^2(\Gamma(t))}).$$

Combining this estimate and (10.21) completes the proof. ∎

11. Variational Space Discretization

This chapter describes the variational space discretization of the wave equation using the evolving surface finite element (ESFEM) method of Dziuk & Elliott [14]. The variational principle is discretized with piecewise linear evolving surface finite elements, which will lead to a time dependent Hamiltonian system.

11.1. Recap: The evolving surface finite element method

Following [14], the smooth surface $\Gamma(t)$ is interpolated at nodes $a_i(t) \in \Gamma(t)$ $(i = 1, \ldots, N)$ by a discrete polygonal surface $\Gamma_h(t)$, where h denotes the grid size. These nodes move with velocity $da_i(t)/dt = v(a_i(t), t)$. The discrete surface

$$\Gamma_h(t) = \bigcup_{E(t) \in \mathcal{T}_h(t)} E(t)$$

is the union of m-dimensional simplices $E(t)$ that is assumed to form an admissible triangulation $\mathcal{T}_h(t)$; see [14] for details. The finite element space on the discrete surface $\Gamma_h(t)$ is chosen as

$$S_h(t) = \{\phi_h \in C^0(\Gamma_h(t)) \;:\; \phi_h|_E \in \mathbb{P}_1 \text{ for all } E \in \mathcal{T}_h(t)\},$$

where $\mathbb{P}_1$ denotes the space of polynomials of degree at most 1. Let $\chi_j(\cdot, t)$ $(j = 1, \ldots, N)$ be the nodal basis of $S_h(t)$, given by $\chi_j(a_i(t), t) = \delta_{ji}$ for all i, so that

$$S_h(t) = \operatorname{span}\{\chi_1(\cdot, t), \ldots, \chi_N(\cdot, t)\}.$$

We define a velocity for material points $X(t)$ on the surface $\Gamma_h(t)$ by

$$\dot{X}(t) = V_h(X(t), t), \quad V_h(x, t) := \sum_{j=1}^{N} v(a_j(t), t)\chi_j(x, t), \quad x \in \Gamma_h(t). \tag{11.1}$$

Then the discrete material derivative on $\Gamma_h(t)$ is given by

$$\partial_h^\bullet \phi_h = \frac{\partial \phi_h}{\partial t} + V_h \cdot \nabla \phi_h. \tag{11.2}$$

The construction is such that the discrete material derivatives of the basis functions satisfy the *transport property* [14, Proposition 5.4]:

$$\partial_h^\bullet \chi_j = 0. \tag{11.3}$$

The discrete surface gradient is defined piecewise as

$$\nabla_{\Gamma_h} g = \nabla g - \nabla g \cdot \nu_h \nu_h,$$

where ν_h denotes the normal to the discrete surface.

After the discretization of the surface and setting the appropriate definitions on the discrete surface $\Gamma_h(t)$, we now formulate the semi-discrete Hamilton principle as follows.

Problem 11.1 (The semi-discrete Hamilton principle)
We replace the Lagrangian (10.3) *with the Lagrangian on the discretized surface*

$$\mathcal{L}_h\left(U_h, \partial_h^\bullet U_h, t\right) = \frac{1}{2}\int_{\Gamma_h(t)} |\partial_h^\bullet U_h|^2 - \frac{1}{2}\int_{\Gamma_h(t)} |\nabla_{\Gamma_h} U_h|^2 \tag{11.4}$$

and minimize the action integral

$$\mathcal{S}_h[U_h] = \int_0^T \mathcal{L}_h\left(U_h(t), \partial_h^\bullet U_h(t), t\right)\, dt \tag{11.5}$$

for $U_h(t) = U_h(\cdot, t) \in S_h(t)$.

With $U_h(\cdot, 0) = U_h^0$ *and* $\partial_h^\bullet U_h(\cdot, 0) = \dot{U}_h^0$, *where* U_h^0 *and* $\dot{U}_h^0 \in S_h(0)$ *are appropriate approximations of* u_0 *and* $\dot{u}_0$, *respectively.*

Remark 11.2
The problem (11.1) *turns out to be equivalent to the Galerkin discretization of* (10.10)*: For all temporally smooth* ϕ_h *with* $\phi_h(\cdot, t) \in S_h(t)$ *and for all* t,

$$\frac{d}{dt}\int_{\Gamma_h(t)} \partial_h^\bullet U_h\, \phi_h + \int_{\Gamma_h(t)} \nabla_{\Gamma_h(t)} U_h \cdot \nabla_{\Gamma_h(t)} \phi_h = \int_{\Gamma_h(t)} \partial_h^\bullet U_h \partial_h^\bullet \phi_h. \tag{11.6}$$

11.2. Matrix-vector formulation and Hamiltonian system

We denote the discrete solution

$$U_h(\cdot, t) = \sum_{j=1}^N q_j(t)\chi_j(\cdot, t) \ \in S_h(t)$$

and define $q(t) \in \mathbb{R}^N$ as the nodal vector with entries $q_j(t) = U_h(a_j(t), t)$. Then by the transport property (11.3), we have

$$\partial_h^\bullet U_h(\cdot, t) = \sum_{j=1}^N \dot{q}_j(t)\chi_j(\cdot, t) \ \in S_h(t),$$

where $\dot{q}_j = dq_j/dt$. We often abbreviate $U_h(t) = U_h(\cdot, t)$, $\partial_h^\bullet U_h(t) = \partial_h^\bullet U_h(\cdot, t)$, $\chi_j(t) = \chi_j(\cdot, t)$, etc.

The evolving mass matrix $M(t)$ and the stiffness matrix $A(t)$ are defined by

$$M(t)_{ij} = \int_{\Gamma_h(t)} \chi_i(t)\chi_j(t), \qquad A(t)_{ij} = \int_{\Gamma_h(t)} \nabla_{\Gamma_h(t)}\chi_i(t) \cdot \nabla_{\Gamma_h(t)}\chi_j(t)$$

for $i, j = 1, \ldots, N$. The mass matrix is symmetric and positive definite. The stiffness matrix is symmetric and only positive semidefinite. Its null-space is spanned by the vector $(1, \ldots, 1)^{\mathrm{T}}$ because we consider closed surfaces.

With these matrices, the discrete Lagrangian becomes

$$\mathcal{L}_h(U_h, \partial_h^\bullet U_h, t) = \frac{1}{2}\dot{q}^{\mathrm{T}} M(t)\dot{q} - \frac{1}{2}q^{\mathrm{T}} A(t) q =: \mathcal{L}_h(q, \dot{q}, t) \tag{11.7}$$

with an obvious doubling of notation. A simple calculation gives the following result.

Lemma 11.3
The minimizer of the action integral

$$\mathcal{S}_h[q] = \int_0^T \mathcal{L}_h(q(t), \dot{q}(t), t)\, dt \tag{11.8}$$

is a solution of the Euler-Lagrange equation

$$\frac{d}{dt}\left(M(t)\dot{q}(t)\right) + A(t)q(t) = 0. \tag{11.9}$$

With $q(0) = q_0 = (U_h^0(a_j))$ *and* $\dot{q}(0) = \dot{q}_0 = (\dot{U}_h^0(a_j))$.

By introducing the conjugate *momenta*

$$p(t) := \frac{\partial \mathcal{L}_h}{\partial \dot{q}}(q(t), \dot{q}(t), t) = M(t)\dot{q}(t),$$

we reformulate (11.9) as the Hamiltonian system

$$\dot{p}(t) = -A(t)q(t) \tag{11.10a}$$
$$\dot{q}(t) = M(t)^{-1}p(t) \tag{11.10b}$$

corresponding to the time-dependent Hamiltonian

$$H(q, p, t) = \frac{1}{2}p^{\mathrm{T}} M(t)^{-1} p + \frac{1}{2}q^{\mathrm{T}} A(t) q.$$

Putting the pieces together, we obtain the initial value problem:

Problem 11.4 (The Hamiltonian system)
The system (11.10) *can be written in the variable* $y(t) = (p(t), q(t))^{\mathrm{T}}$ *as* Hamilton's equations

$$\begin{cases} \dot{y}(t) &= J^{-1}H(t)y(t) \\ y(0) &= y_0 = (q_0, p_0)^{\mathrm{T}} = (q_0, M(0)\dot{q}_0)^{\mathrm{T}}, \end{cases} \tag{11.11}$$

with

$$J = \begin{pmatrix} 0 & I_N \\ -I_N & 0 \end{pmatrix}, \qquad H(t) = \begin{pmatrix} M(t)^{-1} & 0 \\ 0 & A(t) \end{pmatrix} \in \mathbb{R}^{2N\times 2N}, \tag{11.12}$$

and I_N *is the identity matrix of dimension* N*.*

For a symmetric positive definite or semidefinite matrix $G(t) \in \mathbb{R}^{N\times N}$, we define the norm or semi-norm, respectively, for $w \in \mathbb{R}^N$:

$$|w|^2_{G(t)} = \langle w\, |G(t)|\, w\rangle = w^{\mathrm{T}}G(t)w.$$

The following lemma from Chapter 2 (Lemma 2.6) will be the only result needed from the evolving surface finite element method in order to prove stability estimates for various time discretization schemes.

Lemma 11.5
There are constants μ, κ *(independent of the mesh-width* h*) such that*

$$w^{\mathrm{T}}(M(s) - M(t))z \le \mu|s-t|\; |w|_{M(t)}\, |z|_{M(t)} \tag{11.13}$$

$$w^{\mathrm{T}}(M(s)^{-1} - M(t)^{-1})z \le \mu|s-t|\; |w|_{M(t)^{-1}}\, |z|_{M(t)^{-1}} \tag{11.14}$$

$$w^{\mathrm{T}}(A(s) - A(t))z \le \kappa|s-t|\; |w|_{A(t)}\, |z|_{A(t)} \tag{11.15}$$

for all $w, z \in \mathbb{R}^N$ *and* $s, t \in [0, T]$.

11.3. Time dependent energy norm

With the symmetric positive definite matrix

$$\widehat{H}(t) = \begin{pmatrix} M(t)^{-1} & 0 \\ 0 & A(t) + M(t) \end{pmatrix} \in \mathbb{R}^{2N\times 2N},$$

we define the associate time-dependent energy norm for $y = (p, q)^{\mathrm{T}}$ on $\mathbb{R}^{2N}$:

$$\|y\|_t^2 = \langle q\,|A(t) + M(t)|\,q\rangle + \left\langle p \,\middle|\, M(t)^{-1} \,\middle|\, p\right\rangle = \left\langle y \,\middle|\, \widehat{H}(t) \,\middle|\, y\right\rangle = y^{\mathrm{T}}\widehat{H}(t)y. \tag{11.16}$$

Note that for finite element functions $U_h(\cdot, t) = \sum_{j=1}^N q_j(t)\chi_j(\cdot, t) \in S_h(t)$ with the vector of nodal values $q(t) = (q_j(t)) \in \mathbb{R}^N$ and $p(t) = M(t)\dot{q}(t)$, for $y(t) = (p(t), q(t))^{\mathrm{T}}$, we have

$$\begin{aligned} \|y(t)\|_t^2 &= \langle q(t)\,|M(t)|\,q(t)\rangle + \langle q(t)\,|A(t)|\,q(t)\rangle + \left\langle p(t) \,\middle|\, M(t)^{-1} \,\middle|\, p(t)\right\rangle \\ &= \|U_h(\cdot,t)\|^2_{L_2(\Gamma_h(t))} + \|\nabla_{\Gamma_h(t)}U_h(\cdot,t)\|^2_{L_2(\Gamma_h(t))} + \|\partial_h^{\bullet}U_h(\cdot,t)\|^2_{L_2(\Gamma_h(t))}. \end{aligned} \tag{11.17}$$

In the stability analysis we will make use of the following estimates:

Lemma 11.6
With μ and κ from Lemma 11.5 and the definitions above, we have

$$y^{\mathtt{T}} \widehat{H}(t) J^{-1} H(t) y \leq \frac{1}{2} \|y\|_t^2 \tag{11.18}$$

$$y^{\mathtt{T}} \left(\widehat{H}(s) - \widehat{H}(t) \right) z \leq (\mu + \kappa) |s - t| \, \|y\|_t \, \|z\|_t \tag{11.19}$$

for all $y, z \in \mathbb{R}^{2N}$ and $s, t \in [0, T]$.

Proof
Using the above definitions, the fact that $\langle p \,|(A+M)^{-1}|\, p \rangle \leq \langle p \,|M^{-1}|\, p \rangle$, the Cauchy-Schwarz inequality, and Young's inequality yield (omitting the argument t)

$$\begin{aligned} y^{\mathtt{T}} \widehat{H}(t) J^{-1} H(t) y &= p^T q \\ &\leq |p|_{(A+M)^{-1}} |q|_{A+M} \\ &\leq \frac{1}{2} \left(|p|^2_{(A+M)^{-1}} + |q|^2_{A+M} \right) \\ &\leq \frac{1}{2} \left(|p|^2_{M^{-1}} + |q|^2_{A+M} \right) \end{aligned}$$

which prove the first inequality (11.18).

The second inequality is a straightforward application of Lemma 11.5. ■

12. Variational Time Discretization

In the following, we study the variational time discretization of the Hamiltonian system (Problem 11.4). For a given set of a discrete time point $0 = t_0 < t_1 < \cdots < t_L \leq T$ with uniform step size τ, we want to compute an approximation q_n of the exact solution $q(t_n)$ of the *Euler-Lagrange equation* (11.9) at time $t = t_n$. This will not be done in the usual way by approximating the *Euler-Lagrange equations* directly, but by minimizing an approximate action to obtain a *discrete Euler-Lagrange equation*, which will give us a scheme to compute q_n for all $0 \leq n \leq L$. In particular, we study the stability of a version of the leapfrog or Störmer–Verlet method under the natural analog of the CFL condition that is required for a fixed surface. Further, we consider the Gauß–Runge–Kutta (GRK) methods, aiming for higher-order accuracy in time and unconditional stability of the fully discrete scheme.

12.1. Recap: Variational integrators

We give a brief review of variational integrators which have been studied by Suris [45], Veselov [46] and in a series of papers by Marsden and coauthors. For a comprehensive discussion of variational integrators we refer the reader to Marsden and West [40] and [24, Section VI.6].
We use an approximation

$$\mathcal{L}_{h,\tau}\left(q_n, q_{n+1}, t_n\right) \approx \int_{t_n}^{t_{n+1}} \mathcal{L}_h\left(q(t), \dot{q}(t), t\right) \, \mathrm{d}t. \tag{12.1}$$

Then the action integral over the whole time interval is approximated by the *discrete action sum*

$$\mathcal{S}_{h,\tau}(\{q_n\}_0^L) = \sum_{n=0}^{L-1} \mathcal{L}_{h,\tau}(q_n, q_{n+1}, t_n).$$

Computing variations of this discrete action sum with the boundary points q_0 and q_L held fixed, gives the *discrete Euler-Lagrange equations*

$$D_2\mathcal{L}_{h,\tau}(q_{n-1}, q_n, t_{n-1}) + D_1\mathcal{L}_{h,\tau}(q_n, q_{n+1}, t_n) = 0, \qquad 1 \leq n \leq L-1, \tag{12.2}$$

where D_1 and D_2 denote the partial derivative with respect to the first and second argument of $\mathcal{L}_{h,\tau}$, respectively.

If we take initial conditions (q_0, q_1) then the discrete Euler-Lagrange equations (12.2) implicitly define a two-step integrator

$$(q_{n-1}, q_n) \to (q_n, q_{n+1})$$

that calculates recursively the sequence $\{q_n\}_0^L$ by solving in every step the discrete Euler-Lagrange equations.
Since we rewrote our problem (11.10) in a Hamiltonian position-momenta form, we want to have an integrator also in this form. We define the *discrete momenta* at every time step n as

$$p_n := D_2\mathcal{L}_{h,\tau}(q_{n-1}, q_n, t_{n-1}) = -D_1\mathcal{L}_{h,\tau}(q_n, q_{n+1}, t_n),$$

where the second equality holds in view of (12.2). With this definition the variational integrator in the position-momenta form is written as the one-step method

$$p_n = -D_1\mathcal{L}_{h,\tau}(q_n, q_{n+1}, t_n) \tag{12.3a}$$
$$p_{n+1} = D_2\mathcal{L}_{h,\tau}(q_n, q_{n+1}, t_n). \tag{12.3b}$$

If we take initial conditions (q_0, p_0), then we solve the first equation for q_1, then evaluate the second equation to get p_1, and repeat this procedure to get the full sequence $\{q_n\}_0^L$.

In the following, we will use the time dependent energy norm introduced in Chapter 11,i.e, for $y = (p, q)^{\mathsf{T}}$ on $\mathbb{R}^{2N}$:

$$\|y\|_t^2 = \langle q \,| A(t) + M(t) |\, q\rangle + \left\langle p \,\middle|\, M(t)^{-1} \,\middle|\, p\right\rangle. \tag{12.4}$$

12.2. The leapfrog or Störmer–Verlet method

12.2.1. Method formulation

For a given step size τ, we choose $\mathcal{L}_{h,\tau}(q_n, q_{n+1}, t_n)$ by approximating $q(t)$ as the linear interpolant of q_n and q_{n+1} and approximating the first part of the integral (12.1) with the two terms of (11.7) by the midpoint rule and the second part by the trapezoidal rule. This gives

$$\begin{aligned}\mathcal{L}_{h,\tau}(q_n, q_{n+1}, t_n) = {} & \frac{\tau}{2}\left\langle \dot{q}_{n+\frac{1}{2}} \,\middle|\, M_{n+\frac{1}{2}} \,\middle|\, \dot{q}_{n+\frac{1}{2}}\right\rangle \\ & - \frac{\tau}{4}\Big(\langle q_n \,| A_n |\, q_n\rangle + \langle q_{n+1} \,| A_{n+1} |\, q_{n+1}\rangle\Big)\end{aligned}$$

with $\dot{q}_{n+\frac{1}{2}} = (q_{n+1} - q_n)/\tau,\ A_n = A(t_n)$ and $M_{n+1/2} = M(t_n + \frac{1}{2}\tau)$.

Then we compute the scheme (12.3),

$$\begin{aligned} p_n &= -D_1\mathcal{L}_{h,\tau}(q_n, q_{n+1}, t_n) = M_{n+\frac{1}{2}}\dot{q}_{n+\frac{1}{2}} + \frac{\tau}{2}A_n q_n \\ p_{n+1} &= D_2\mathcal{L}_{h,\tau}(q_n, q_{n+1}, t_n) = M_{n+\frac{1}{2}}\dot{q}_{n+\frac{1}{2}} - \frac{\tau}{2}A_{n+1} q_{n+1}. \end{aligned}$$

Inserting the term of $\dot{q}_{n+\frac{1}{2}}$ and solving the first equation for q_{n+1}, we obtain:

A version of the *leapfrog* or *Störmer–Verlet* method (see, e.g., [23]) to the system (11.10):

$$q_{n+1} = q_n + \tau M_{n+\frac{1}{2}}^{-1} p_n - \frac{1}{2}\tau^2 M_{n+\frac{1}{2}}^{-1} A_n q_n \tag{12.5a}$$

$$p_{n+1} = p_n - \frac{\tau}{2} A_n q_n - \frac{\tau}{2} A_{n+1} q_{n+1}, \tag{12.5b}$$

or equivalently

$$p_{n+1/2} = p_n - \frac{\tau}{2} A_n q_n \tag{12.6a}$$

$$q_{n+1} = q_n + \tau M_{n+\frac{1}{2}}^{-1} p_{n+1/2} \tag{12.6b}$$

$$p_{n+1} = p_{n+1/2} - \frac{\tau}{2} A_{n+1} q_{n+1}. \tag{12.6c}$$

The scheme is explicit except for solving a linear system with the mass matrix in each time step.

From the vectors $q_n = (q_j^n)$ and $\dot{q}_n = (\dot{q}_j^n) := M(t_n)^{-1} p_n$ we obtain the finite element functions on the discrete surface $\Gamma_h(t_n)$

$$U_h^n = \sum_{j=1}^{N} q_j^n \chi_j(t_n), \quad \partial_h^\bullet U_h^n = \sum_{j=1}^{N} \dot{q}_j^n \chi_j(t_n) \tag{12.7}$$

as approximations to $u(t_n)$ and $\partial^\bullet u(t_n)$, respectively.

12.2.2. Defects and errors

Let $\widetilde{q}_n$ and $\widetilde{p}_n$ be reference values that we want to compare with q_n and p_n, respectively (e.g., $\widetilde{q}_n = q(t_n)$ and $\widetilde{p}_n = p(t_n)$). Inserted into (12.5) they yield defects d_{n+1}^q and d_{n+1}^p in

$$\widetilde{q}_{n+1} = \widetilde{q}_n + \tau M_{n+\frac{1}{2}}^{-1} \widetilde{p}_n - \frac{1}{2}\tau^2 M_{n+\frac{1}{2}}^{-1} A_n \widetilde{q}_n + d_{n+1}^q \tag{12.8a}$$

$$\widetilde{p}_{n+1} = \widetilde{p}_n - \frac{\tau}{2} A_n \widetilde{q}_n - \frac{\tau}{2} A_{n+1} \widetilde{q}_{n+1} + d_{n+1}^p. \tag{12.8b}$$

For the errors we use the notation

$$e_n^q = q_n - \widetilde{q}_n \tag{12.9a}$$

$$e_n^p = p_n - \widetilde{p}_n \tag{12.9b}$$

and subtract to get the *error equation*

$$e^q_{n+1} = e^q_n + \tau M^{-1}_{n+\frac{1}{2}} e^p_n - \frac{1}{2}\tau^2 M^{-1}_{n+\frac{1}{2}} A_n e^q_n - d^q_{n+1} \tag{12.10a}$$

$$e^p_{n+1} = e^p_n - \frac{\tau}{2} A_n e^q_n - \frac{\tau}{2} A_{n+1} e^q_{n+1} - d^p_{n+1}. \tag{12.10b}$$

12.2.3. The CFL condition

From now on we assume that the step size τ fulfills the following restriction:

$$\frac{1}{4}\tau^2 \rho\left(M(t)^{-1/2} A(t) M(t)^{-1/2}\right) \le 1 - \theta \tag{12.11}$$

for all $0 \le t \le T$ and for a fixed $0 < \theta < 1$, where $\rho(\cdot)$ denotes the spectral radius. For a quasi-uniform triangulation we have $\rho\left(M(t)^{-1/2} A(t) M(t)^{-1/2}\right) \sim h^{-2}$, so that we have a time step restriction $\tau \le ch$.

Under the CFL condition (12.11), the symmetric matrix

$$\widehat{A}(t) = A(t) - \frac{1}{4}\tau^2 A(t) M(t)^{-1} A(t) \quad \text{is positive semidefinite,} \tag{12.12}$$

and there exists C_θ such that for every $e^q \in \mathbb{R}^N$ we have

$$\langle e^q | \widehat{A}(t) | e^q \rangle \le \langle e^q | A(t) | e^q \rangle \le C_\theta \langle e^q | \widehat{A}(t) | e^q \rangle. \tag{12.13}$$

12.2.4. Stability

We denote by $e_n = (e^q_n, e^p_n)$ the error vector at time t_n and by $d_n = (d^q_n, d^p_n)$ the defect vector in (12.10). With this notation we prove the following stability result.

Lemma 12.1 (leapfrog)
There exists $\tau_0 > 0$ depending only on μ and κ of Lemma 11.5 and on θ of (12.11) *such that for step sizes $\tau \le \tau_0$ satisfying the CFL condition* (12.11)*, the error for the leapfrog method (scheme 12.5) is bounded, for $t_n = n\tau \le T$, by*

$$\|e_n\|_{t_n} \le C\Big(\|e_0\|_{t_0} + \sum_{k=1}^{n} \|d_k\|_{t_k}\Big).$$

The constant C is independent of h, τ, and n subject to the stated conditions (but depends on μ, κ, θ, and T).

Proof
We use a time-dependent modified energy norm on $\mathbb{R}^{2N}$: for $e = (e^p, e^q) \in \mathbb{R}^{2N}$,

$$\|e\|^2_{t,CFL} = \langle e^q | M(t) + \widehat{A}(t) | e^q \rangle + \langle e^p | M(t)^{-1} | e^p \rangle. \tag{12.14}$$

Thanks to the CFL condition (12.11), there is a constant C_θ such that

$$\|e\|_{t,CFL} \le \|e\|_t \le C_\theta \|e\|_{t,CFL}\,. \tag{12.15}$$

We prove the lemma in three steps.

(a) *Local error:* Here we analyze the error after *one* step, starting with $e_n = 0$. Thus the error equation (12.10) simply reads

$$e^q_{n+1} = -d^q_{n+1} \tag{12.16a}$$
$$e^p_{n+1} = -\frac{\tau}{2} A_{n+1} e^q_{n+1} - d^p_{n+1}. \tag{12.16b}$$

Using the semi-norm equivalence (12.13) for the first equation of (12.16) yields

$$\begin{aligned}\langle e^q_{n+1} | A_{n+1} + M_{n+1} | e^q_{n+1} \rangle &= \langle d^q_{n+1} | M_{n+1} + A_{n+1} | d^q_{n+1} \rangle \\ &\le C_\theta \left\langle d^q_{n+1} \middle| M_{n+1} + \widehat{A}_{n+1} \middle| d^q_{n+1} \right\rangle . \end{aligned} \tag{12.17}$$

Furthermore we get by the second equation of (12.16)

$$\left\langle e^p_{n+1} + d^p_{n+1} \middle| M^{-1}_{n+1} \middle| e^p_{n+1} + d^p_{n+1} \right\rangle = \frac{1}{4}\tau^2 \left\langle e^q_{n+1} \middle| A_{n+1} M^{-1}_{n+1} A_{n+1} \middle| e^q_{n+1} \right\rangle .$$

Thus we obtain

$$\begin{aligned}\left\langle e^p_{n+1} \middle| M^{-1}_{n+1} \middle| e^p_{n+1} \right\rangle = \frac{1}{4}\tau^2 \left\langle e^q_{n+1} \middle| A_{n+1} M^{-1}_{n+1} A_{n+1} \middle| e^q_{n+1} \right\rangle \\ - 2 \left\langle e^p_{n+1} \middle| M^{-1}_{n+1} \middle| d^p_{n+1} \right\rangle - \left\langle d^p_{n+1} \middle| M^{-1}_{n+1} \middle| d^p_{n+1} \right\rangle .\end{aligned}$$

We estimate the second term on the right-hand side by the Cauchy–Schwarz inequality and Young's inequality to obtain

$$\begin{aligned}\frac{1}{2} \left\langle e^p_{n+1} \middle| M^{-1}_{n+1} \middle| e^p_{n+1} \right\rangle - \frac{1}{4}\tau^2 \left\langle e^q_{n+1} \middle| A_{n+1} M^{-1}_{n+1} A_{n+1} \middle| e^q_{n+1} \right\rangle \\ \le 2 \left\langle d^p_{n+1} \middle| M^{-1}_{n+1} \middle| d^p_{n+1} \right\rangle . \end{aligned} \tag{12.18}$$

Therefore, adding (12.17) to (12.18) yields

$$\|e_{n+1}\|_{t_{n+1},CFL} \le C_\theta \ \|d_{n+1}\|_{t_{n+1},CFL} . \tag{12.19}$$

(b) *Error propagation:* We now consider one step of the error equations without defects and estimate $\|e_{n+1}\|_{t_{n+1}}$ in terms of $\|e_n\|_{t_n}$:

$$e^q_{n+1} = e^q_n + \tau M^{-1}_{n+\frac{1}{2}} e^p_n - \frac{1}{2}\tau^2 M^{-1}_{n+\frac{1}{2}} A_n e^q_n \tag{12.20a}$$
$$e^p_{n+1} = e^p_n - \frac{\tau}{2} A_n e^q_n - \frac{\tau}{2} A_{n+1} e^q_{n+1}. \tag{12.20b}$$

We start by direct computation taking the squared A-seminorm of e^q_{n+1} at time t_{n+1}

and the squared M^{-1}-norm of e^p_{n+1} at time $t_{n+\frac{1}{2}}$ to find

$$\begin{aligned}
&\langle e^q_{n+1} \left| A_{n+1} \right| e^q_{n+1} \rangle \\
&\quad= \langle e^q_n \left| A_{n+1} \right| e^q_n \rangle + 2\tau \left\langle e^q_n \left| A_{n+1} \right| M^{-1}_{n+\frac{1}{2}} e^p_n \right\rangle - \tau^2 \left\langle e^q_n \left| A_{n+1} \right| M^{-1}_{n+\frac{1}{2}} A_n e^q_n \right\rangle \\
&\quad+ \tau^2 \left\langle e^p_n \left| M^{-1}_{n+\frac{1}{2}} A_{n+1} M^{-1}_{n+\frac{1}{2}} \right| e^p_n \right\rangle - \tau^3 \left\langle e^p_n \left| M^{-1}_{n+\frac{1}{2}} A_{n+1} M^{-1}_{n+\frac{1}{2}} \right| A_n e^q_n \right\rangle \\
&\quad+ \frac{1}{4}\tau^4 \left\langle e^q_n \left| A_n M^{-1}_{n+\frac{1}{2}} A_{n+1} M^{-1}_{n+\frac{1}{2}} A_n \right| e^q_n \right\rangle . \\
&\left\langle e^p_{n+1} \left| M^{-1}_{n+\frac{1}{2}} \right| e^p_{n+1} \right\rangle \\
&\quad= \left\langle e^p_n \left| M^{-1}_{n+\frac{1}{2}} \right| e^p_n \right\rangle - \tau \left\langle e^p_n \left| M^{-1}_{n+\frac{1}{2}} \right| A_n e^q_n \right\rangle - \tau \left\langle e^p_n \left| M^{-1}_{n+\frac{1}{2}} \right| A_{n+1} e^q_{n+1} \right\rangle \\
&\quad+ \frac{1}{4}\tau^2 \left\langle e^q_n \left| A_n M^{-1}_{n+\frac{1}{2}} A_n \right| e^q_n \right\rangle + \frac{1}{2}\tau^2 \left\langle A_n e^q_n \left| M^{-1}_{n+\frac{1}{2}} \right| A_{n+1} e^q_{n+1} \right\rangle \\
&\quad+ \frac{1}{4}\tau^2 \left\langle e^q_{n+1} \left| A_{n+1} M^{-1}_{n+\frac{1}{2}} A_{n+1} \right| e^q_{n+1} \right\rangle .
\end{aligned}$$

Expressing e^q_{n+1} by (12.20a), it follows that

$$\begin{aligned}
&\left\langle e^p_{n+1} \left| M^{-1}_{n+\frac{1}{2}} \right| e^p_{n+1} \right\rangle \\
&= \left\langle e^p_n \left| M^{-1}_{n+\frac{1}{2}} \right| e^p_n \right\rangle - \tau \left\langle e^p_n \left| M^{-1}_{n+\frac{1}{2}} \right| A_n e^q_n \right\rangle - \tau \left\langle e^p_n \left| M^{-1}_{n+\frac{1}{2}} \right| A_{n+1} e^q_n \right\rangle \\
&- \tau^2 \left\langle e^p_n \left| M^{-1}_{n+\frac{1}{2}} A_{n+1} M^{-1}_{n+\frac{1}{2}} \right| e^p_n \right\rangle + \frac{1}{2}\tau^3 \left\langle e^p_n \left| M^{-1}_{n+\frac{1}{2}} A_{n+1} M^{-1}_{n+\frac{1}{2}} \right| A_n e^q_n \right\rangle \\
&+ \frac{1}{4}\tau^2 \left\langle e^q_n \left| A_n M^{-1}_{n+\frac{1}{2}} A_n \right| e^q_n \right\rangle + \frac{1}{2}\tau^2 \left\langle A_n e^q_n \left| M^{-1}_{n+\frac{1}{2}} \right| A_{n+1} e^q_n \right\rangle \\
&+ \frac{1}{2}\tau^3 \left\langle A_n e^q_n \left| M^{-1}_{n+\frac{1}{2}} A_{n+1} M^{-1}_{n+\frac{1}{2}} \right| e^p_n \right\rangle - \frac{1}{4}\tau^4 \left\langle e^q_n \left| A_n M^{-1}_{n+\frac{1}{2}} A_{n+1} M^{-1}_{n+\frac{1}{2}} A_n \right| e^q_n \right\rangle \\
&+ \frac{1}{4}\tau^2 \left\langle e^q_{n+1} \left| A_{n+1} M^{-1}_{n+\frac{1}{2}} A_{n+1} \right| e^q_{n+1} \right\rangle .
\end{aligned}$$

Adding both expressions leads to

$$\begin{aligned}
&\left\langle e^q_{n+1} \left| A_{n+1} - \frac{1}{4}\tau^2 A_{n+1} M^{-1}_{n+\frac{1}{2}} A_{n+1} \right| e^q_{n+1} \right\rangle + \left\langle e^p_{n+1} \left| M^{-1}_{n+\frac{1}{2}} \right| e^p_{n+1} \right\rangle \\
&= \langle e^q_n \left| A_{n+1} \right| e^q_n \rangle + \left\langle e^p_n \left| M^{-1}_{n+\frac{1}{2}} \right| e^p_n \right\rangle - \frac{1}{2}\tau^2 \left\langle A_{n+1} e^q_n \left| M^{-1}_{n+\frac{1}{2}} \right| A_n e^q_n \right\rangle \\
&\qquad + \frac{1}{4}\tau^2 \left\langle A_n e^q_n \left| M^{-1}_{n+\frac{1}{2}} \right| A_n e^q_n \right\rangle + \left\langle e^q_n \left| A_{n+1} - A_n \right| \tau M^{-1}_{n+\frac{1}{2}} e^p_n \right\rangle . \qquad (12.21)
\end{aligned}$$

We estimate the terms on the right-hand side of (12.21) separately, starting by the first and second term, then the third and the fourth together, and in the end the last term.

In the first and second term on the right hand side of (12.21) we write $A_{n+1} = (A_{n+1} - A_n) + A_n$ and $M^{-1}_{n+\frac{1}{2}} = \left(M^{-1}_{n+\frac{1}{2}} - M^{-1}_n\right) + M^{-1}_n$ respectively. Then conditions (11.15) and (11.14) yield

$$\begin{aligned} \langle e^q_n \,| A_{n+1} |\, e^q_n \rangle &= \langle e^q_n \,| A_{n+1} - A_n |\, e^q_n \rangle + \langle e^q_n \,| A_n |\, e^q_n \rangle \\ &\le (1 + \kappa\tau) \, \langle e^q_n \,| A_n |\, e^q_n \rangle \end{aligned} \tag{12.22}$$

$$\left\langle e^p_n \,\middle| M^{-1}_{n+\frac{1}{2}} \middle|\, e^p_n \right\rangle \le (1 + \mu\tau) \left\langle e^p_n \,\middle| M^{-1}_n \middle|\, e^p_n \right\rangle . \tag{12.23}$$

In the third term of (12.21) we also write $A_{n+1} = (A_{n+1} - A_n) + A_n$ and add it to the fourth term on the right side of (12.21) to get

$$\begin{aligned} &-\frac{1}{2}\tau^2 \left\langle A_{n+1} e^q_n \,\middle| M^{-1}_{n+\frac{1}{2}} \middle|\, A_n e^q_n \right\rangle + \frac{1}{4}\tau^2 \left\langle A_n e^q_n \,\middle| M^{-1}_{n+\frac{1}{2}} \middle|\, A_n e^q_n \right\rangle \\ &= \left\langle e^q_n \middle| A_{n+1} - A_n \middle| -\frac{1}{2}\tau^2 M^{-1}_{n+\frac{1}{2}} A_n e^q_n \right\rangle - \frac{1}{4}\tau^2 \left\langle e^q_n \,\middle| A_n M^{-1}_{n+\frac{1}{2}} A_n \middle|\, e^q_n \right\rangle . \end{aligned} \tag{12.24}$$

We start by the first term on the right hand side and use condition (11.15) and Young's inequality to get

$$\begin{aligned} \left\langle e^q_n \middle| A_{n+1} - A_n \middle| -\frac{1}{2}\tau^2 M^{-1}_{n+\frac{1}{2}} A_n e^q_n \right\rangle &\le C\tau \, |e^q_n|_{A_n} \left| \frac{1}{2}\tau^2 M^{-1}_{n+\frac{1}{2}} A_n e^q_n \right|_{A_n} \\ &\le C\tau \left(|e^q_n|^2_{A_n} + \frac{1}{4} \left| \frac{1}{2}\tau^2 M^{-1}_{n+\frac{1}{2}} A_n e^q_n \right|^2_{A_n} \right) . \end{aligned}$$

Using the CFL condition (12.11), similar arguments to those used for (12.22) and (12.23), and (12.13) yield that this is further bounded by

$$\begin{aligned} \left\langle e^q_n \middle| A_{n+1} - A_n \middle| -\frac{1}{2}\tau^2 M^{-1}_{n+\frac{1}{2}} A_n e^q_n \right\rangle &\le C\tau \left(|e^q_n|^2_{A_n} + \frac{1}{4} \left| \frac{1}{2}\tau^2 M^{-1}_{n+\frac{1}{2}} A_n e^q_n \right|^2_{A_{n+\frac{1}{2}}} \right) \\ &\le C\tau \left(|e^q_n|^2_{A_n} + \frac{1}{4}\tau^2 \, |A_n e^q_n|^2_{M^{-1}_{n+\frac{1}{2}}} \right) \\ &\le C\tau \left(|e^q_n|^2_{A_n} + \frac{1}{4}\tau^2 \, |A_n e^q_n|^2_{M^{-1}_n} \right) \\ &\le C_\theta \, \tau \left\langle e^q_n \,\middle| \widehat{A}_n \middle|\, e^q_n \right\rangle . \end{aligned}$$

For the last term of (12.24) we write $M^{-1}_{n+\frac{1}{2}} = \left(M^{-1}_{n+\frac{1}{2}} - M^{-1}_n\right) + M^{-1}_n$ and use condition (11.14), the CFL condition (12.11) and (12.13) to get

$$\begin{aligned}
&-\frac{1}{4}\tau^2 \left\langle e_n^q \left| A_n M_{n+\frac{1}{2}}^{-1} A_n \right| e_n^q \right\rangle \\
&\qquad = -\frac{1}{4}\tau^2 \left\langle A_n e_n^q \left| M_{n+\frac{1}{2}}^{-1} - M_n^{-1} \right| A_n e_n^q \right\rangle - \frac{1}{4}\tau^2 \left\langle e_n^q \left| A_n M_n^{-1} A_n \right| e_n^q \right\rangle \\
&\qquad \le C\tau \left\langle \frac{1}{4}\tau^2 M_n^{-1} A_n e_n^q \left| A_n \right| e_n^q \right\rangle - \frac{1}{4}\tau^2 \left\langle e_n^q \left| A_n M_n^{-1} A_n \right| e_n^q \right\rangle \\
&\qquad \le C_\theta\ \tau \left\langle e_n^q \left| \widehat{A}_n \right| e_n^q \right\rangle - \frac{1}{4}\tau^2 \left\langle e_n^q \left| A_n M_n^{-1} A_n \right| e_n^q \right\rangle .
\end{aligned}$$

Combining the above bounds yields

$$\begin{aligned}
&-\frac{1}{2}\tau^2 \left\langle A_{n+1} e_n^q \left| M_{n+\frac{1}{2}}^{-1} \right| A_n e_n^q \right\rangle + \frac{1}{4}\tau^2 \left\langle A_n e_n^q \left| M_{n+\frac{1}{2}}^{-1} \right| A_n e_n^q \right\rangle \\
&\qquad\qquad \le -\frac{1}{4}\tau^2 \left\langle e_n^q \left| A_n M_n^{-1} A_n \right| e_n^q \right\rangle + C_\theta\ \tau \left\langle e_n^q \left| \widehat{A}_n \right| e_n^q \right\rangle . \qquad (12.25)
\end{aligned}$$

For the last term on the right-hand side of (12.21), we use condition (11.15), Young's inequality, the CFL condition (12.11) to estimate

$$\begin{aligned}
\left\langle e_n^q \middle| A_{n+1} - A_n \middle| \tau M_{n+\frac{1}{2}}^{-1} e_n^p \right\rangle &\le C\tau \left(\langle e_n^q \left| A_n \right| e_n^q \rangle + \frac{1}{4} \left\langle \tau M_{n+\frac{1}{2}}^{-1} e_n^p \middle| A_n \middle| \tau M_{n+\frac{1}{2}}^{-1} e_n^p \right\rangle \right) \\
&\le C\tau \left(\langle e_n^q \left| A_n \right| e_n^q \rangle + \left\langle e_n^p \left| M_{n+\frac{1}{2}}^{-1} \right| e_n^p \right\rangle \right) \\
&\le C_\theta\ \tau \left(\left\langle e_n^q \left| \widehat{A}_n \right| e_n^q \right\rangle + \left\langle e_n^p \left| M_n^{-1} \right| e_n^p \right\rangle \right) . \qquad (12.26)
\end{aligned}$$

Now we take the squared M-norm of e_{n+1}^q at time $t_{n+\frac{1}{2}}$ to find

$$\begin{aligned}
&\left\langle e_{n+1}^q \left| M_{n+\frac{1}{2}} \right| e_{n+1}^q \right\rangle \\
&= \left\langle e_n^q \left| M_{n+\frac{1}{2}} \right| e_n^q \right\rangle + 2\tau \langle e_n^q | e_n^p \rangle - \tau^2 \langle e_n^q \left| A_n \right| e_n^q \rangle + \tau^2 \left\langle e_n^p \left| M_{n+\frac{1}{2}}^{-1} \right| e_n^p \right\rangle \\
&\qquad\qquad - \tau^3 \left\langle e_n^p \left| M_{n+\frac{1}{2}}^{-1} \right| A_n e_n^q \right\rangle + \frac{1}{4}\tau^4 \left\langle e_n^q \left| A_n M_{n+\frac{1}{2}}^{-1} A_n \right| e_n^q \right\rangle .
\end{aligned}$$

The Cauchy–Schwarz inequality, the CFL condition (12.11) and the bound (11.13) yield

$$\begin{aligned}
\left\langle e_n^q \left| M_{n+\frac{1}{2}} \right| e_n^q \right\rangle &\le (1 + \mu\tau) \langle e_n^q \left| M_n \right| e_n^q \rangle \\
2\tau \langle e_n^q | e_n^p \rangle &\le \tau \left(|e_n^q|_{M_n}^2 + |e_n^p|_{M_n^{-1}}^2 \right) \\
-\tau^2 \left\langle e_n^q \left| A_n - \frac{1}{4}\tau^2 A_n M_{n+\frac{1}{2}}^{-1} A_n \right| e_n^q \right\rangle &\le \left(-\tau^2 + C_\theta \tau^3 \right) \left\langle e_n^q \left| \widehat{A}_n \right| e_n^q \right\rangle \\
\tau^3 \left\langle e_n^p \left| M_{n+\frac{1}{2}}^{-1} \right| A_n e_n^q \right\rangle &\le \tau^3 |e_n^p|_{M_{n+\frac{1}{2}}^{-1}} \, |A_n e_n^q|_{M_{n+\frac{1}{2}}^{-1}} \\
&\le C\tau \left(|e_n^p|_{M_n^{-1}}^2 + C_\theta \left\langle e_n^q \left| \widehat{A}_n \right| e_n^q \right\rangle \right) .
\end{aligned}$$

Thus we have

$$\left\langle e^q_{n+1} \left| M_{n+\frac{1}{2}} \right| e^q_{n+1} \right\rangle \leq (1+C\tau)\, |e^q_n|^2_{M_n} + C\tau |e^p_n|^2_{M_n^{-1}} + C_\theta \tau \left\langle e^q_n \left| \widehat{A}_n \right| e^q_n \right\rangle . \tag{12.27}$$

Combining (12.21)-(12.26) and the above bound (12.27) yields

$$\left\langle e^q_{n+1} \left| M_{n+\frac{1}{2}} + A_{n+1} - \frac{\tau^2}{4} A_{n+1} M^{-1}_{n+\frac{1}{2}} A_{n+1} \right| e^q_{n+1} \right\rangle + \left\langle e^p_{n+1} \left| M^{-1}_{n+\frac{1}{2}} \right| e^p_{n+1} \right\rangle \leq (1+C_\theta \tau)\, \|e_n\|^2_{t_n,CFL} . \tag{12.28}$$

This is almost the desired estimate, except that we have here $M_{n+1/2}$ instead of M_{n+1}. It remains to show that we have a bound of the same type also with M_{n+1}. Since by (11.13) and (11.14),

$$\left\langle e^q_{n+1} \left| M_{n+1} - M_{n+\frac{1}{2}} \right| e^q_{n+1} \right\rangle \leq \mu\tau \left\langle e^q_{n+1} \left| M_{n+1/2} \right| e^q_{n+1} \right\rangle$$
$$\left\langle e^p_{n+1} \left| M^{-1}_{n+1} - M^{-1}_{n+\frac{1}{2}} \right| e^p_{n+1} \right\rangle \leq \mu\tau \left\langle e^p_{n+1} \left| M^{-1}_{n+1/2} \right| e^p_{n+1} \right\rangle$$

and by (11.14) and (12.12),

$$\left\langle e^q_{n+1} \left| \frac{\tau^2}{4} A_{n+1} (M^{-1}_{n+1} - M^{-1}_{n+\frac{1}{2}}) A_{n+1} \right| e^q_{n+1} \right\rangle \leq \mu\tau \left\langle e^q_{n+1} \left| \frac{\tau^2}{4} A_{n+1} M^{-1}_{n+1} A_{n+1} \right| e^q_{n+1} \right\rangle \leq \mu\tau \left\langle e^q_{n+1} \left| A_{n+1} \right| e^q_{n+1} \right\rangle ,$$

we obtain

$$\|e_{n+1}\|^2_{t_{n+1},CFL} \leq (1+\mu\tau) \Big(\left\langle e^q_{n+1} \left| M_{n+\frac{1}{2}} + A_{n+1} - \frac{\tau^2}{4} A_{n+1} M^{-1}_{n+\frac{1}{2}} A_{n+1} \right| e^q_{n+1} \right\rangle + \left\langle e^p_{n+1} \left| M^{-1}_{n+\frac{1}{2}} \right| e^p_{n+1} \right\rangle \Big),$$

which together with (12.28) finally yields

$$\|e_{n+1}\|_{t_{n+1},CFL} \leq (1+C\tau)\, \|e_n\|_{t_n,CFL} .$$

(c) *Error accumulation:* A standard application of Lady Windermere's fan (see [25, 27]) and the equivalence of norms (12.15) completes the proof. ∎

Lemma 12.1 shows that the fully discrete scheme (combination of ESFEM and Leapfrog method 12.5) is stable under the CFL condition (12.11). To overcome this time step restriction due to the CFL condition, we consider in the next two sections fully implicit variational time integrators; namely, the Gauß–Runge–Kutta methods, and we show that they are unconditionally stable.

12.3. The implicit midpoint rule

12.3.1. Method formulation

For a given step size τ, we choose $\mathcal{L}_{h,\tau}(q_n, q_{n+1}, t_n)$ by approximating $q(t)$ as the linear interpolant of q_n and q_{n+1} and approximating the whole integral (12.1) by the midpoint rule. This gives

$$\mathcal{L}_{h,\tau}(q_n, q_{n+1}, t_n) = \frac{\tau}{2}\left\langle \dot{q}_{n+\frac{1}{2}} \middle| M_{n+\frac{1}{2}} \middle| \dot{q}_{n+\frac{1}{2}} \right\rangle - \frac{\tau}{2}\left\langle q_{n+\frac{1}{2}} \middle| A_{n+\frac{1}{2}} \middle| q_{n+\frac{1}{2}} \right\rangle,$$

with $\dot{q}_{n+\frac{1}{2}} = (q_{n+1} - q_n)/\tau,\ q_{n+\frac{1}{2}} = (q_{n+1} + q_n)/2, A_{n+\frac{1}{2}} = A\left(t_n + \frac{1}{2}\tau\right)$ and $M_{n+\frac{1}{2}} = M\left(t_n + \frac{1}{2}\tau\right)$. Then we compute the scheme (12.3)

$$\begin{aligned}
p_n &= -D_1\mathcal{L}_d(q_n, q_{n+1}, \tau) \\
&= M_{n+\frac{1}{2}} v_{n+\frac{1}{2}} + \frac{\tau}{2} A_{n+\frac{1}{2}} q_{n+\frac{1}{2}} \\
p_{n+1} &= D_2\mathcal{L}_d(q_n, q_{n+1}, \tau) \\
&= M_{n+\frac{1}{2}} v_{n+\frac{1}{2}} - \frac{\tau}{2} A_{n+\frac{1}{2}} q_{n+\frac{1}{2}}.
\end{aligned}$$

We set $p_{n+\frac{1}{2}} = M_{n+\frac{1}{2}}\dot{q}_{n+\frac{1}{2}}$ and solve the first equation for $p_{n+\frac{1}{2}}$ to obtain the implicit *midpoint* rule

$$\begin{aligned}
p_{n+\frac{1}{2}} &= p_n - \frac{\tau}{2} A_{n+\frac{1}{2}} q_{n+\frac{1}{2}} \\
q_{n+\frac{1}{2}} &= q_n + \frac{\tau}{2} M^{-1}_{n+\frac{1}{2}} p_{n+\frac{1}{2}} \\
q_{n+1} &= q_n + \tau M^{-1}_{n+\frac{1}{2}} p_{n+\frac{1}{2}} \\
p_{n+1} &= p_n - \tau A_{n+\frac{1}{2}} q_{n+\frac{1}{2}}.
\end{aligned}$$

We use the notation $y_n = (p_n, q_n)$ and $Y_{n+\frac{1}{2}} = \left(p_{n+\frac{1}{2}}, q_{n+\frac{1}{2}}\right)^T$ to obtain:

The implicit midpoint rule applied to the Hamiltonian system (Problem 11.4) reads

$$Y_{n+\frac{1}{2}} = y_n + \frac{\tau}{2} J^{-1} H_{n+\frac{1}{2}} Y_{n+\frac{1}{2}} \tag{12.29a}$$

$$y_{n+1} = y_n + \tau J^{-1} H_{n+\frac{1}{2}} Y_{n+\frac{1}{2}}, \tag{12.29b}$$

with $H_{n+\frac{1}{2}} = H\left(t_n + \frac{1}{2}\tau\right)$.

12.3.2. Defects and errors

Let us consider the perturbed scheme

$$\widetilde{Y}_{n+\frac{1}{2}} = \widetilde{y}_n + \frac{\tau}{2} J^{-1} H_{n+\frac{1}{2}} \widetilde{Y}_{n+\frac{1}{2}} + \Delta_{n+\frac{1}{2}} \tag{12.30a}$$

$$\widetilde{y}_{n+1} = \widetilde{y}_n + \tau J^{-1} H_{n+\frac{1}{2}} \widetilde{Y}_{n+\frac{1}{2}} + \delta_{n+1}, \tag{12.30b}$$

where $\Delta_{n+\frac{1}{2}}$ and δ_{n+1} are the defects obtained when inserting the values $\widetilde{Y}_{n+\frac{1}{2}}$ and $\widetilde{y}_n$ (e.g., $\widetilde{Y}_{n+\frac{1}{2}} = y(t_n + \frac{1}{2}\tau)$ and $\widetilde{y}_n = y(t_n)$) into (12.29).
By subtracting (12.30) from (12.29) and stetting $E_{n+\frac{1}{2}} = Y_{n+\frac{1}{2}} - \widetilde{Y}_{n+\frac{1}{2}}$ and $e_n = y_n - \widetilde{y}_n$, we get the *error equations*

$$E_{n+\frac{1}{2}} = e_n + \frac{1}{2}\tau \dot{E}_{n+\frac{1}{2}} - \Delta_{n+\frac{1}{2}} \tag{12.31a}$$

$$e_{n+1} = e_n + \tau \dot{E}_{n+\frac{1}{2}} - \delta_{n+1}, \tag{12.31b}$$

where

$$\dot{E}_{n+\frac{1}{2}} = J^{-1} H_{n+\frac{1}{2}} E_{n+\frac{1}{2}}. \tag{12.31c}$$

12.3.3. Stability

In analogy to the leapfrog method, we state and prove the main result of this section which shows that the fully discrete method with the implicit midpoint rule (scheme (12.29)) is unconditionally stable.

Lemma 12.2 (implicit midpoint rule)
There exists $\tau_0 > 0$ depending only on μ and κ of Lemma 2.6 such that for $\tau \le \tau_0$, the error for the implicit midpoint rule is bounded , for $t_n = n\tau \le T$, by

$$\|e_n\|_{t_n} \le C \left(\|e_0\|_{t_0} + \left\|\Delta_{\frac{1}{2}}\right\|_{t_0} + \sum_{j=1}^{n-1} \left\|\delta_j + \Delta_{j+\frac{1}{2}} - \Delta_{j-\frac{1}{2}}\right\|_{t_j} + \left\|\delta_n - \Delta_{n-\frac{1}{2}}\right\|_{t_n} \right).$$

The constant C is independent of h, τ and n (but depends on $\mu, \kappa,$ and T).

Proof
The first step is to modify the errors e_n and the defects δ_{n+1} in such a way that we obtain new error equations of the form (12.31), where the first equation contains no defects. For this purpose, we follow the idea of Kraaijevanger in his study of the B-convergence of the implicit midpoint rule [31] and define, for given n, the new errors $\{\widetilde{e}_k\}_{k=0}^{n}$ and the new

defects $\left\{\widetilde{\delta}_k\right\}_{k=0}^{n}$ in the following way:

$$\begin{aligned}
\widetilde{e}_k &= e_k - \Delta_{k+\frac{1}{2}} && k = 0, \cdots, n-1 \\
\widetilde{e}_n &= e_n \\
\widetilde{\delta}_0 &= \Delta_{\frac{1}{2}} \\
\widetilde{\delta}_k &= \delta_k + \Delta_{k+\frac{1}{2}} - \Delta_{k-\frac{1}{2}} && k = 1, \cdots, n-1 \\
\widetilde{\delta}_n &= \delta_n - \Delta_{n-\frac{1}{2}}.
\end{aligned}$$

This gives the desired error equations for $k = 1, \cdots, n-1$:

$$E_{k+\frac{1}{2}} = \widetilde{e}_k + \frac{1}{2}\tau \dot{E}_{n+\frac{1}{2}} \tag{12.32a}$$

$$\widetilde{e}_{k+1} = \widetilde{e}_k + \tau \dot{E}_{n+\frac{1}{2}} - \widetilde{\delta}_{k+1}. \tag{12.32b}$$

Now, we start from (12.32b) by taking the squared norm of $(\widetilde{e}_{k+1} + \widetilde{\delta}_{k+1})$ at $(t_{k+\frac{1}{2}} = t_k + \frac{1}{2}\tau)$ and estimate the terms in

$$\left\|\widetilde{e}_{k+1} + \widetilde{\delta}_{k+1}\right\|_{t_{k+\frac{1}{2}}}^2 = \left\|\widetilde{e}_k\right\|_{t_{k+\frac{1}{2}}}^2 + 2\tau \left\langle \widetilde{e}_k \left| \widehat{H}_{k+\frac{1}{2}} \right| \dot{E}_{k+\frac{1}{2}} \right\rangle + \tau^2 \left\| \dot{E}_k \right\|_{t_{k+\frac{1}{2}}}^2 .$$

Expressing $\widetilde{e}_k$ by (12.32a), using (12.31c) and relation (11.18), it follows that

$$\left\|\widetilde{e}_{k+1} + \widetilde{\delta}_{k+1}\right\|_{t_{k+\frac{1}{2}}}^2 \le \left\|\widetilde{e}_k\right\|_{t_{k+\frac{1}{2}}}^2 + \tau \left\|E_{k+\frac{1}{2}}\right\|_{t_{k+\frac{1}{2}}}^2 . \tag{12.33}$$

In order to bound the norm of $E_{k+\frac{1}{2}}$, we first multiply the equation (12.32a) by $E_{k+\frac{1}{2}}^{\mathtt{T}} \widehat{H}_{k+\frac{1}{2}}$ and obtain

$$\left\|E_{k+\frac{1}{2}}\right\|_{t_{k+\frac{1}{2}}}^2 = \left\langle \widetilde{e}_k \left| \widehat{H}_{k+\frac{1}{2}} \right| E_{k+\frac{1}{2}} \right\rangle + \frac{1}{2}\tau \left\langle E_{k+\frac{1}{2}} \left| \widehat{H}_{k+\frac{1}{2}} \right| \dot{E}_{k+\frac{1}{2}} \right\rangle .$$

Then, using the relation (11.18), the Cauchy-Schwarz inequality and Young's inequality, for sufficiently small τ, yield

$$\left\|E_{k+\frac{1}{2}}\right\|_{t_{k+\frac{1}{2}}}^2 \le C \left\|\widetilde{e}_k\right\|_{t_{k+\frac{1}{2}}}^2 . \tag{12.34}$$

Next, we write $\widetilde{H}_{k+1} = \widetilde{H}_{k+\frac{1}{2}} + \left(\widetilde{H}_{k+1} - \widetilde{H}_{k+\frac{1}{2}}\right)$ and use the condition (11.19) to estimate

$$\begin{aligned}
\left\|\widetilde{e}_{k+1} + \widetilde{\delta}_{k+1}\right\|_{t_{k+1}}^2 &= \left\langle \widetilde{e}_{k+1} + \widetilde{\delta}_{k+1} \left| \widetilde{H}_{k+1} \right| \widetilde{e}_{k+1} + \widetilde{\delta}_{k+1} \right\rangle \\
&= \left\langle \widetilde{e}_{k+1} + \widetilde{\delta}_{k+1} \left| \widetilde{H}_{k+\frac{1}{2}} \right| \widetilde{e}_{k+1} + \widetilde{\delta}_{k+1} \right\rangle \\
&\quad + \left\langle \widetilde{e}_{k+1} + \widetilde{\delta}_{k+1} \left| \widetilde{H}_{k+1} - \widetilde{H}_{k+\frac{1}{2}} \right| \widetilde{e}_{k+1} + \widetilde{\delta}_{k+1} \right\rangle \\
&\le (1 + C\tau) \left\|\widetilde{e}_{k+1} + \widetilde{\delta}_{k+1}\right\|_{t_{k+\frac{1}{2}}}^2 .
\end{aligned} \tag{12.35}$$

In the same way, we find

$$\|\widetilde{e}_k\|^2_{t_{k+\frac{1}{2}}} \leq (1 + C\tau) \|\widetilde{e}_k\|^2_{t_k} . \tag{12.36}$$

Combining (12.33)–(12.36) yields

$$\|\widetilde{e}_{k+1}\|_{t_{k+1}} \leq (1 + C\tau) \|\widetilde{e}_k\|_{t_k} + \left\|\widetilde{\delta}_{k+1}\right\|_{t_{k+1}} .$$

Summing over k and knowing that $\widetilde{e}_0 = e_0 - \delta_0$ gives

$$\|\widetilde{e}_{t_n}\|_n \leq C\tau \sum_{j=0}^{n-1} \|\widetilde{e}_j\|_{t_j} + \sum_{j=0}^{n} \left\|\widetilde{\delta}_j\right\|_{t_j} + \|e_0\|_{t_0} .$$

Thus, using a discrete Gronwall inequality and the fact that $\widetilde{e}_n = e_n$ yield the stated result. ■

12.4. Gauß–Runge–Kutta methods

For a given step size τ, we choose $\mathcal{L}_{h,\tau}(q_n, q_{n+1}, t_n)$ by approximating $q(t)$ by a polynomial of degree s and approximating the whole integral (12.1) by the Gauß quadrature. Then, we obtain the s- stage Gauß–Runge–Kutta (GRK) method (cf. [24, Section VI.6] and [40] for more details). In the following, we will then see that we have a class of fully discrete variational schemes with an arbitrarily high order in time. Let us now start by giving a brief review of the GRK methods.

12.4.1. Method formulation and properties

For a given step size $\tau > 0$, the s-stage GRK method applied to the Hamiltonian system (11.11) reads

$$Y_{ni} = y_n + \tau \sum_{j=1}^{s} a_{ij} \dot{Y}_{nj}, \qquad i = 1, \cdots, s, \tag{12.37a}$$

$$y_{n+1} = y_n + \tau \sum_{i=1}^{s} b_i \dot{Y}_{ni}, \tag{12.37b}$$

where the internal stages satisfy

$$\dot{Y}_{ni} = J^{-1} H_{ni} Y_{ni} \qquad i = 1, \cdots, s,$$

with $H_{ni} = H(t_n + c_i\tau)$.

The method is uniquely defined via the so-called Butcher-tableau (cf. [27, Section IV.5]):

$$\begin{array}{c|c} c & \mathcal{A} \\ \hline & b^{\mathrm{T}} \end{array} := \begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array} .$$

Here, the $\{b_i\}_{i=1}^s$ are the weights of the s-stage Gauß-quadrature and the $\{c_i\}_{i=1}^s$ are the nodes of this quadrature transformed to the interval $[0,1]$. The coefficients of the matrix $\mathcal{A}$ are determined from the conditions

$$\sum_{j=1}^{s} a_{ij} c_j^{k-1} = \frac{c_i^k}{k} \qquad i, k = 1, \cdots, s.$$

Note that the implicit midpoint rule is the 1-stage GRK method with

$$\begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & 1 \end{array} .$$

Now, we summarize the various properties of the method (cf. [27, Section IV.14]), which are crucial in order to show the upcoming stability estimates.

- The GRK method is *algebraically stable*, i.e.,

$$b_i \geq 0, \qquad i = 1, \cdots, s, \tag{12.38a}$$
$$b_i a_{ij} + b_j a_{ji} - b_i b_j = 0 \qquad i, j = 1, \cdots, s. \tag{12.38b}$$

- The matrix $\mathcal{A}$ is invertible and we denote its inverse by $\mathcal{A}^{-1} = [w_{ij}]$. Further, $0 < c_i < 1\,(i = 1, \ldots, s)$, and by defining

$$\alpha := \min_{i=1,\ldots,s} \frac{1}{2c_i\,(1-c_i)}, \quad \mathcal{B} = \operatorname{diag}(b_1, b_2, \ldots, b_s), \quad \mathcal{C} = \operatorname{diag}(c_1, c_2, \ldots, c_s),$$
$$\mathcal{D} = \operatorname{diag}(d_1, d_2, \ldots, d_s) := \mathcal{B}\left(\mathcal{C}^{-1} - I\right),$$

  we have the *coercivity* condition

$$w^{\mathrm{T}} \mathcal{D} \mathcal{A}^{-1} w \geq \alpha w^{\mathrm{T}} \mathcal{D} w \qquad \text{for all } w \in \mathbb{R}^s, \tag{12.39}$$

  with $\alpha > 0$ and $d_i > 0$.

- The s-stage GRK method is of stage order s and classical order $2s$.

12.4.2. Defects and errors

Let $\widetilde{y}_n, \widetilde{Y}_{ni}$ and $\dot{\widetilde{Y}}_{ni}$ be reference values that we want to compare with y_n, Y_{ni} and $\dot{Y}_{ni}$, respectively (e.g., $\widetilde{Y}_{ni} = y(t_n + c_i\tau), \dot{\widetilde{Y}}_{ni} = \dot{y}(t_n + c_i\tau)$ and $\widetilde{y}_n = y(t_n)$). When inserted into (12.37), they yield defects δ_{n+1} and Δ_{ni} in

$$\widetilde{Y}_{ni} = \widetilde{y}_n + \tau \sum_{j=1}^{s} a_{ij} \dot{\widetilde{Y}}_{nj} + \Delta_{ni}, \qquad i = 1, \cdots, s, \tag{12.40a}$$

$$\widetilde{y}_{n+1} = \widetilde{y}_n + \tau \sum_{i=1}^{s} b_i \dot{\widetilde{Y}}_{ni} + \delta_{n+1}, \tag{12.40b}$$

where the new internal stages $\widetilde{Y}_{ni}$ satisfy

$$\dot{\widetilde{Y}}_{ni} = J^{-1} H_{ni} \widetilde{Y}_{ni}, \qquad i = 1, \cdots, s.$$

For the errors, we introduce the notations

$$e_n = y_n - \widetilde{y}_n \tag{12.41a}$$

$$E_{ni} = Y_{ni} - \widetilde{Y}_{ni} \tag{12.41b}$$

$$\dot{E}_{ni} = \dot{Y}_{ni} - \dot{\widetilde{Y}}_{ni}, \tag{12.41c}$$

and subtract (12.40) from (12.37) to get the *error equations*

$$E_{ni} = e_n + \tau \sum_{j=1}^{s} a_{ij} \dot{E}_{nj} - \Delta_{ni}, \qquad i = 1, \cdots, s, \tag{12.42a}$$

$$e_{n+1} = e_n + \tau \sum_{i=1}^{s} b_i \dot{E}_{ni} - \delta_{n+1}, \tag{12.42b}$$

where

$$\dot{E}_{ni} = J^{-1} H_{ni} E_{ni}, \qquad i = 1, \cdots, s. \tag{12.43}$$

12.4.3. Error equations in compact form

We rewrite the Runge–Kutta scheme (12.42) in a more compact form. The $s \times s$ and the $2N \times 2N-$identity matrices will be denoted by I_s and I_{2N}, respectively. The vector with all components equal to one in $\mathbb{R}^s$ is denoted by $\mathbb{1}$. Then, we put:

$$\boldsymbol{\mathcal{O}} = \mathcal{O} \otimes I_{2N}, \qquad \boldsymbol{b}^{\mathsf{T}} = b^{\mathsf{T}} \otimes I_{2N}, \qquad \mathbb{1} = \mathbb{1} \otimes I_{2N},$$

where $\otimes$ denotes *the Kronecker product* of two matrices. Further, with the vectors

$$\boldsymbol{\Delta}_n = (\Delta_{n1}, \dots, \Delta_{ns})^{\mathsf{T}}, \quad \boldsymbol{E}_n = (E_{n1}, \dots, E_{ns})^{\mathsf{T}}, \quad \dot{\boldsymbol{E}}_n = (\dot{E}_{n1}, \dots, \dot{E}_{ns})^{\mathsf{T}},$$

and the block diagonal matrices

$$\boldsymbol{J}^{-1} = I_s \otimes J^{-1}, \qquad \boldsymbol{H}_n = \operatorname{diag}\left(H_{n1}, H_{n2}, \ldots, H_{ns}\right),$$

the Runge-Kutta relations (12.42) and (12.43) can be written as

$$\boldsymbol{E}_n = \mathbb{1} e_n + \tau \boldsymbol{\mathcal{Q}} \dot{\boldsymbol{E}}_n - \boldsymbol{\Delta}_n, \tag{12.44a}$$

$$e_{n+1} = e_n + \tau \boldsymbol{b}^{\mathrm{T}} \dot{\boldsymbol{E}}_n - \delta_{n+1}, \tag{12.44b}$$

with $\boldsymbol{E}_n$ satisfying the relation

$$\dot{\boldsymbol{E}}_n = \boldsymbol{J}^{-1} \boldsymbol{H}_n \, \boldsymbol{E}_n. \tag{12.45}$$

For a vector $\boldsymbol{E} = (E_1, E_2, \ldots, E_s)^{\mathrm{T}} \in \mathbb{R}^{2N \cdot s}$ $\left(E_i \in \mathbb{R}^{2N}\right)$, we define the norm

$$|||\boldsymbol{E}|||_t^2 = \left\langle \boldsymbol{E} \,\middle|\, I_s \otimes \widehat{H}(t) \,\middle|\, \boldsymbol{E} \right\rangle = \boldsymbol{E}^{\mathrm{T}} \left(I_s \otimes \widehat{H}(t)\right) \boldsymbol{E} = \sum_{i=1}^{s} \|E_i\|_t^2 \,.$$

12.4.4. Stability

The following stability lemma will play a key role in estimating the total error.

Lemma 12.3 (GRK)
There exists $\tau_0 > 0$ depending only on μ and κ of Lemma 2.6 such that for $\tau \leq \tau_0$, the error for the s-stage GRK method (with $s \geq 2$) is bounded, for $t_n = n\tau \leq T$, by

$$\|e_n\|_{t_n} \leq C \left(\|e_0\|_{t_0} + \sum_{j=0}^{n-1} |||\boldsymbol{\Delta}_j|||_{t_j} + \sum_{j=1}^{n} \|\delta_j\|_{t_j} \right).$$

The constant C is independent of h, τ and n (but depends on μ, κ, and T).

Proof
We prove this lemma in three steps:

(a) *Local error:* Here, we analyze the error after *one* step, starting with $e_n = 0$. Thus, the error equation (12.44) simply reads

$$\boldsymbol{E}_n = \tau \boldsymbol{\mathcal{Q}} \dot{\boldsymbol{E}}_n - \boldsymbol{\Delta}_n \tag{12.46a}$$

$$e_{n+1} = \tau \boldsymbol{b}^{\mathrm{T}} \dot{\boldsymbol{E}}_n - \delta_{n+1}. \tag{12.46b}$$

We multiply the equation (12.46a) by $\boldsymbol{E}_n^{\mathrm{T}} \widehat{\boldsymbol{H}}_n \left(\mathcal{D}\mathcal{Q}^{-1} \otimes I_{2N}\right)$ and obtain

$$\begin{aligned} \boldsymbol{E}_n^{\mathrm{T}} \widehat{\boldsymbol{H}}_n \left(\mathcal{D}\mathcal{Q}^{-1} \otimes I_{2N}\right) \boldsymbol{E}_n = \tau \boldsymbol{E}_n^{\mathrm{T}} \widehat{\boldsymbol{H}}_n \left(\mathcal{D} \otimes I_{2N}\right) \dot{\boldsymbol{E}}_n& \\ + \boldsymbol{E}_n^{\mathrm{T}} \widehat{\boldsymbol{H}}_n \left(\mathcal{D}\mathcal{Q}^{-1} \otimes I_{2N}\right) \boldsymbol{\Delta}_n&. \end{aligned} \tag{12.47}$$

We handle each term separately, starting by bounding the term on the left-hand side from below, and then bounding the terms on the right-hand side from above.

We write $\widehat{\boldsymbol{H}}_n = \left(I_s \otimes \widehat{H}_{n0}\right) + \left(\widehat{\boldsymbol{H}}_n - \left(I_s \otimes \widehat{H}_{n0}\right)\right)$, where $\widehat{H}_{n0} = \widehat{H}(t_n)$, and get

$$\begin{aligned}\boldsymbol{E}_n^{\mathrm{T}}\widehat{\boldsymbol{H}}_n\left(\mathcal{D}\mathcal{Q}^{-1}\otimes I_{2N}\right)\boldsymbol{E}_n &= \boldsymbol{E}_n^{\mathrm{T}}\left(I_s \otimes \widehat{H}_{n0}\right)\left(\mathcal{D}\mathcal{Q}^{-1}\otimes I_{2N}\right)\boldsymbol{E}_n \\ &\quad + \boldsymbol{E}_n^{\mathrm{T}}\left(\widehat{\boldsymbol{H}}_n - \left(I_s \otimes \widehat{H}_{n0}\right)\right)\left(\mathcal{D}\mathcal{Q}^{-1}\otimes I_{2N}\right)\boldsymbol{E}_n.\end{aligned} \tag{12.48}$$

Since $\widehat{H}_{n0}$ is symmetric and positive definite, we define $\widetilde{\boldsymbol{E}}_n = \left(I_s \otimes \widehat{H}_{n0}\right)^{1/2}\boldsymbol{E}_n$. Then, using the coercivity condition (12.39) and the fact that $d_i > 0$, for the first term on the right-hand side of (12.48), we get

$$\begin{aligned}\boldsymbol{E}_n^{\mathrm{T}}\left(I_s \otimes \widehat{H}_{n0}\right)\left(\mathcal{D}\mathcal{Q}^{-1}\otimes I_{2N}\right)\boldsymbol{E}_n &= \widetilde{\boldsymbol{E}}_n^{\mathrm{T}}\left(\mathcal{D}\mathcal{Q}^{-1}\otimes I_{2N}\right)\widetilde{\boldsymbol{E}}_n \\ &\geq \alpha\boldsymbol{E}_n^{\mathrm{T}}\left(\mathcal{D}\otimes \widehat{H}_{n0}\right)\boldsymbol{E}_n \\ &\geq c|||\boldsymbol{E}_n|||_{t_n}^2\end{aligned} \tag{12.49}$$

with a constant $c > 0$.
The last term on the right-hand side of (12.48) is estimated using condition (11.19) and Young's inequality as follows

$$\begin{aligned}\boldsymbol{E}_n^{\mathrm{T}}\left(\widehat{\boldsymbol{H}}_n - \left(I_s \otimes \widehat{H}_{n0}\right)\right)\left(\mathcal{D}\mathcal{Q}^{-1}\otimes I_{2N}\right)\boldsymbol{E}_n &= \sum_{i,j=1}^{s}\left(\mathcal{D}\mathcal{Q}^{-1}\right)_{ij}\left\langle E_{ni}\,\middle|\,\widehat{H}_{ni} - \widehat{H}_{n0}\,\middle|\,E_{nj}\right\rangle \\ &\leq C\tau\sum_{i,j}^{s}\|E_{ni}\|_{t_n}\|E_{nj}\|_{t_n} \\ &\leq C\tau\sum_{i,j}^{s}\left(\|E_{ni}\|_{t_n}^2 + \|E_{nj}\|_{t_n}^2\right) \\ &\leq C\tau|||\boldsymbol{E}_n|||_{t_n}^2.\end{aligned} \tag{12.50}$$

Therefore, we deduce by (12.48), (12.49) and (12.50), for sufficiently small τ, that

$$|||\boldsymbol{E}_n|||_{t_n}^2 \leq C\ \boldsymbol{E}_n^{\mathrm{T}}\widehat{\boldsymbol{H}}_n\left(\mathcal{D}\mathcal{Q}^{-1}\otimes I_{2N}\right)\boldsymbol{E}_n. \tag{12.51}$$

For the first term on the right-hand side of (12.47), we use the relations (12.45), (11.18), and (11.19) to get

$$\begin{aligned}\tau\boldsymbol{E}_n^{\mathrm{T}}\widehat{\boldsymbol{H}}_n\left(\mathcal{D}\otimes I_{2N}\right)\dot{\boldsymbol{E}}_n &= \tau\boldsymbol{E}_n^{\mathrm{T}}\widehat{\boldsymbol{H}}_n\left(\mathcal{D}\otimes I_{2N}\right)\boldsymbol{J}^{-1}\boldsymbol{H}_n\boldsymbol{E}_n \\ &= \tau\sum_{i=1}^{s}d_iE_{ni}\widehat{H}_{ni}J^{-1}H_{ni}E_{ni} \\ &\leq C\tau\sum_{i=1}^{s}\|E_{ni}\|_{t_{ni}}^2 \\ &\leq C\tau|||\boldsymbol{E}_n|||_{t_n}^2.\end{aligned} \tag{12.52}$$

As above, the right-hand side of (12.47) is estimated using the Cauchy-Schwarz inequality and condition (11.19)

$$\boldsymbol{E}_n^{\mathrm{T}} \widehat{\boldsymbol{H}}_n \left(\mathcal{D}\mathcal{Q}^{-1} \otimes I_{2N}\right) \boldsymbol{\Delta}_n \leq (1 + C\tau) \;\; |||\boldsymbol{E}_n|||_{t_n} \cdot |||\boldsymbol{\Delta}_n|||_{t_n}. \tag{12.53}$$

Combining (12.47), (12.51), (12.52) and (12.53), for sufficiently small τ, yields

$$|||\boldsymbol{E}_n|||_{t_n} \leq C \;\; |||\boldsymbol{\Delta}_n|||_{t_n}. \tag{12.54}$$

Now, we go back to (12.46b) and rewrite with the help of (12.46a)

$$e_{n+1} = \left(b^{\mathrm{T}} \mathcal{Q}^{-1} \otimes I_{2N}\right) (\boldsymbol{E}_n + \boldsymbol{\Delta}_n) - \delta_{n+1},$$

then, using the Cauchy-Schwarz inequality, Young's inequality, (12.54) and condition (11.19), it follows that

$$\begin{aligned} \|e_{n+1} + \delta_{n+1}\|_{t_{n+1}} &\leq C \;\; \left(|||\boldsymbol{E}_n|||_{t_{n+1}} + |||\boldsymbol{\Delta}_n|||_{t_{n+1}}\right) \\ &\leq C \;\; |||\boldsymbol{\Delta}_n|||_{t_n}. \end{aligned}$$

For the local error, we thus find

$$\|e_{n+1}\|_{t_{n+1}} \leq C \;\; |||\boldsymbol{\Delta}_n|||_{t_n} + \|\delta_{n+1}\|_{t_{n+1}}. \tag{12.55}$$

(b) *Error propagation:* Here, we analyze the error after one step of the GRK method between two numerical solutions starting from different start values. Instead of (12.42), we thus have the following error equations

$$E_{ni} = e_n + \tau \sum_{j=1}^{s} a_{ij} \dot{E}_{nj}, \qquad i = 1, \cdots, s, \tag{12.56a}$$

$$e_{n+1} = e_n + \tau \sum_{i=1}^{s} b_i \dot{E}_{ni}, \tag{12.56b}$$

with

$$\dot{E}_{ni} = J^{-1} H_{ni} E_{ni}, \qquad i = 1, \cdots, s. \tag{12.57}$$

We start from (12.56b) by taking the squared energy norm at t_{n+1} and then express e_n by (12.56a) to find

$$\begin{aligned} \|e_{n+1}\|_{t_{n+1}}^2 = \; & \|e_n\|_{t_{n+1}}^2 + 2\tau \sum_{j=1}^{s} b_j \left\langle E_{nj} \middle| \widehat{H}_{n+1} \middle| \dot{E}_{nj} \right\rangle \\ & - \tau^2 \sum_{i=1}^{s} \sum_{j=1}^{s} b_i a_{ij} + b_j a_{ji} - b_i b_j \left\langle \dot{E}_{ni} \middle| \widehat{H}_{n+1} \middle| \dot{E}_{nj} \right\rangle. \end{aligned} \tag{12.58}$$

The first term on the right-hand side of (12.58) is estimated using condition (11.19)

$$\begin{aligned} \|e_n\|^2_{t_{n+1}} &= \left\langle e_n \left| \widehat{H}_n \right| e_n \right\rangle + \left\langle e_n \left| \widehat{H}_{n+1} - \widehat{H}_n \right| e_n \right\rangle \\ &\leq (1 + C\tau) \|e_n\|^2_{t_n} . \end{aligned} \tag{12.59}$$

For the second term, we use the relations (11.19), (12.57) and (11.18) to estimate

$$\begin{aligned} \left\langle E_{nj} \left| \widehat{H}_{n+1} \right| \dot{E}_{nj} \right\rangle &= \left\langle E_{nj} \left| \widehat{H}_{n+1} - \widehat{H}_{nj} \right| \dot{E}_{nj} \right\rangle + \left\langle E_{nj} \left| \widehat{H}_{nj} \right| \dot{E}_{nj} \right\rangle \\ &\leq C\,\tau \|E_{nj}\|_{t_n + c_j\tau} \left\| \dot{E}_{nj} \right\|_{t_n + c_j\tau} + \frac{1}{2} \|E_{nj}\|^2_{t_n + c_j\tau} \\ &\leq C\,\tau \|E_{nj}\|_{t_n} \left\| \dot{E}_{nj} \right\|_{t_n} + C \|E_{nj}\|^2_{t_n} . \end{aligned} \tag{12.60}$$

As in the first step by the local error (12.54), with $\Delta_{nj} = e_n$, we estimate

$$\|E_{nj}\|_{t_n} \leq C \ \|e_n\|_{t_n} . \tag{12.61}$$

On the other hand, rewriting (12.56a) as

$$\dot{E}_{nj} = \tau^{-1} \sum_{i=1}^{s} w_{ij} \left(E_{ni} - e_n\right),$$

and using (12.61), it follows that

$$\left\| \dot{E}_{nj} \right\|_{t_n} \leq C\,\tau^{-1} \|e_n\|_{t_n} .$$

Therefore, by (12.60) and (12.61), we find

$$\left\langle E_{nj} \left| \widehat{H}_{n+1} \right| \dot{E}_{nj} \right\rangle \leq C \ \|e_n\|^2_{t_n} . \tag{12.62}$$

Thanks to the algebraic stability of the method (12.38), the last term on the right-hand side of (12.58) vanishes. Thus, by (12.58), (12.59) and (12.62), we obtain

$$\|e_{n+1}\|_{t_{n+1}} \leq (1 + C\tau) \|e_n\|_{t_n} . \tag{12.63}$$

(c) *Error accumulation:* A standard application of Lady Windermere's fan (see [25, 27]) completes the proof. ∎

13. Error Bounds for a Projection to the Finite Element Space II

In the previous Chapter 12, we studied the stability of the fully discrete scheme on the Matrix-vector level, now it is the time to connect the stated results to the PDE world. We will thus analyze the error between the fully discrete numerical solution U_h^n and a projection of the exact solution $u(\cdot, t)$ of the wave equation to the finite element space $S_h(t)$ at time $t = t_n$. We will show, how the problem of estimating the total error reduces to estimating the semidiscrete residual of the projection considered here.

13.1. The fully discrete solution

Let $y_n = (p_n, q_n)^T$ be generated by the leapfrog method (12.5) or by the s-stage GRK method (12.37) (Keeping in mind that the 1-stage GRK is the implicit midpoint rule). Then, from the vectors $q_n = (q_j^n)$ and $\dot{q}_n = (\dot{q}_j^n) := M(t_n)^{-1} p_n$ we obtain the fully discrete numerical solution and its numerical material derivative

$$U_h^n = \sum_{j=1}^{N} q_j^n \chi_j(\cdot, t_n), \qquad \partial_h^\bullet U_h^n = \sum_{j=1}^{N} \dot{q}_j^n \chi_j(\cdot, t_n), \tag{13.1}$$

which are finite element functions defined on the surface $\Gamma_h(t_n)$.

13.2. Projection to $S_h(t)$

Let $P_h : H^1(\Gamma(t)) \to S_h(t) \subset H^1(\Gamma_h(t))$ be an arbitrary projection of the exact solution of the wave equation to the finite element space $S_h(t)$. We set

$$P_h u(\cdot, t) = \sum_{j=1}^{N} \widetilde{q}_j(t) \chi_j(\cdot, t), \qquad \partial_h^\bullet (P_h u)(\cdot, t) = \sum_{j=1}^{N} \dot{\widetilde{q}}_j(t) \chi_j(\cdot, t).$$

Note that this projection P_h could be the piecewise linear interpolation operator at the nodes or an L^2- projection or a Ritz projection.

We define the finite element residual $R_h(\cdot,t) = \sum_{j=1}^N r_j(t)\chi_j(\cdot,t) \in S_h(t)$ by

$$\begin{aligned}&\int_{\Gamma_h(t)} R_h(\cdot,t)\phi_h(\cdot,t)\\ &= \frac{d}{dt}\int_{\Gamma_h(t)} \partial_h^\bullet(P_h u)(\cdot,t)\,\phi_h(\cdot,t) + \int_{\Gamma_h(t)} \nabla_{\Gamma_h(t)}(P_h u)(\cdot,t)\cdot\nabla_{\Gamma_h(t)}\phi_h(\cdot,t)\\ &\qquad - \int_{\Gamma_h(t)} \partial_h^\bullet(P_h u)(\cdot,t)\,\partial_h^\bullet\phi_h(\cdot,t),\end{aligned} \tag{13.2}$$

where ϕ_h is a temporally smooth function with $\phi_h(\cdot,t) \in S_h(t)$. The equivalent matrix version with the vectors $\widetilde{q}(t) = (\widetilde{q}_j(t)) \in \mathbb{R}^N$ and $r(t) = (r_j(t)) \in \mathbb{R}^N$ is

$$\frac{d}{dt}\Big(M(t)\dot{\widetilde{q}}(t)\Big) + A(t)\widetilde{q}(t) = M(t)r(t). \tag{13.3}$$

We reformulate (13.3) as

$$\dot{\widetilde{p}}(t) = -A(t)\widetilde{q}(t) + M(t)r(t) \tag{13.4a}$$
$$\dot{\widetilde{q}}(t) = M(t)^{-1}\widetilde{p}(t). \tag{13.4b}$$

Further, we set $\widetilde{y}(t) = (\widetilde{p}(t),\widetilde{q}(t))^{\mathrm{T}}$ and $\Lambda(t) = (M(t)r(t),0)^{\mathrm{T}}$, to get

$$\dot{\widetilde{y}}(t) = J^{-1}H(t)\widetilde{y}(t) + \Lambda(t). \tag{13.5}$$

In the next three sections, we will make use of the stability results for the leapfrog method (Lemma 12.1), the implicit midpoint rule (Lemma 12.2), and for the general GRK method (Lemma 12.3) and translate them back into a function-space framework using the norm identity (11.17) in order to schow error estimates for the difference between the fully discrete solution U_h^n and the projection $P_h u(\cdot,t_n)$.

13.3. Error bounds for the leapfrog method

Theorem 13.1
Let U_h^n and $\partial_h^\bullet U_h^n$ be determined by the leapfrog method (13.1)*. Under the CFL condition* (12.11) *and suitable regularity conditions on the exact solution u of the wave equation* (10.7)*, such that $P_h u$ has continuous discrete material derivatives up to order* 4*. Then, there exists $\tau_0 > 0$ independent of h such that for $\tau \le \tau_0$, the errors $E_h^n = U_h^n - P_h u(\cdot,t_n)$ and $\partial_h^\bullet E_h^n = \partial_h^\bullet U_h^n - \partial_h^\bullet(P_h u)(\cdot,t_n)$ are bounded for $t_n = n\tau \le T$ by*

$$\begin{aligned}&\|E_h^n\|_{L^2(\Gamma_h(t_n))} + \|\nabla_{\Gamma_h} E_h^n\|_{L^2(\Gamma_h(t_n))} + \|\partial_h^\bullet E_h^n\|_{L^2(\Gamma_h(t_n))}\\ &\le C\left(\left\|E_h^0\right\|_{L^2(\Gamma_h(t_0))} + \left\|\nabla_{\Gamma_h} E_h^0\right\|_{L^2(\Gamma_h(t_0))} + \left\|\partial_h^\bullet E_h^0\right\|_{L^2(\Gamma_h(t_0))}\right)\\ &\qquad + C\widetilde{\beta}_h\tau^2 + C\tau\sum_{k=0}^n \|R_h(\cdot,t_k)\|_{L^2(\Gamma_h(t_k))}.\end{aligned}$$

Here C is independent of h (but depends on T and θ), and

$$\widetilde{\beta}_h = \int_0^T \left(\|\nabla_{\Gamma_h} \partial_h^{(3)} P_h u(\cdot,t)\|_{L^2(\Gamma_h(t))} + \sum_{\ell=1}^{4} \|\partial_h^{(\ell)} P_h u(\cdot,t)\|_{L^2(\Gamma_h(t))} \right) \mathrm{d}t,$$

where the superscript (ℓ) denotes the ℓ-th discrete material derivative.

Proof

Considering the errors

$$\begin{aligned} e_n^q &= q_n - \widetilde{q}(t_n) \\ e_n^p &= p_n - \widetilde{p}(t_n), \end{aligned}$$

the defects appearing in the error equation (12.10) satisfy

$$\begin{aligned} d_{n+1}^q &= \widetilde{q}\,(t_{n+1}) - \widetilde{q}\,(t_n) - \tau M_{n+\frac{1}{2}}^{-1} \widetilde{p}\,(t_n) + \frac{1}{2}\tau^2 M_{n+\frac{1}{2}}^{-1} A_n \widetilde{q}\,(t_n) \\ d_{n+1}^p &= \widetilde{p}\,(t_{n+1}) - \widetilde{p}\,(t_n) + \frac{\tau}{2} A_n \widetilde{q}\,(t_n) + \frac{\tau}{2} A_{n+1} \widetilde{q}\,(t_{n+1}). \end{aligned}$$

By (13.4) and Taylor expansion, we obtain

$$\begin{aligned} d_{n+1}^q &= \tau^3 \int_0^1 K_1(\theta) \dddot{\widetilde{q}}\,(t_n + \theta\tau)\,\mathrm{d}\theta + \tau^3 M_{n+\frac{1}{2}}^{-1} \int_0^{\frac{1}{2}} K_2(\theta) \ddot{\widetilde{p}}(t_n + \theta\tau)\,\mathrm{d}\theta \\ &\quad + \frac{1}{2}\tau^2 M_{n+\frac{1}{2}}^{-1} M_n r_n && (13.6) \\ d_{n+1}^p &= \tau^2 \int_0^1 K_3(\theta) \ddot{\widetilde{p}}\,(t_n + \theta\tau)\,\mathrm{d}\theta + \frac{\tau}{2} M_n r_n + \frac{\tau}{2} M_{n+1} r_{n+1}, && (13.7) \end{aligned}$$

with bounded Peano kernels K_1, K_2 and K_3.

Using Lemma 11.5 and the norm identity (11.17) we first have

$$\begin{aligned} &|\dddot{\widetilde{q}}\,(t)|_{M(s)} + |\dddot{\widetilde{q}}\,(t)|_{A(s)} \\ &\qquad \le \sqrt{2} \left(\|\partial_h^{(3)} P_h u(\cdot,t)\|_{L^2(\Gamma_h(t))} + \|\nabla_{\Gamma_h} \partial_h^{(3)} P_h u(\cdot,t)\|_{L^2(\Gamma_h(t))} \right) \end{aligned} \qquad (13.8)$$

provided that $\mu|t-s| \le 1$ and $\kappa|t-s| \le 1$. Now by Lemma 11.5 and the CFL condition (12.11) we estimate for $t \in [t_n, t_{n+1}]$

$$\begin{aligned} \tau^3 |M_{n+\frac{1}{2}}^{-1} \ddot{\widetilde{p}}(t)|_{M_{n+1}} &\le \sqrt{2}\tau^3 |M_{n+\frac{1}{2}}^{-1} \ddot{\widetilde{p}}(t)|_{M_{n+\frac{1}{2}}} \le 2\tau^3 |\ddot{\widetilde{p}}(t)|_{M(t)^{-1}} \\ \tau^3 |M_{n+\frac{1}{2}}^{-1} \ddot{\widetilde{p}}(t)|_{A_{n+1}} &\le C_\theta \tau^2 |\ddot{\widetilde{p}}(t)|_{M_{n+\frac{1}{2}}^{-1}} \le 2C_\theta \tau^2 |\ddot{\widetilde{p}}(t)|_{M(t)^{-1}}. \end{aligned}$$

Therefore in view of (13.5) we find for sufficiently small τ:

$$\tau^3 \left(|M_{n+\frac{1}{2}}^{-1} \ddot{\widetilde{p}}(t)|_{M_{n+1}} + |M_{n+\frac{1}{2}}^{-1} \ddot{\widetilde{p}}(t)|_{A_{n+1}} \right) \le C\tau^2 |(M\widetilde{q})^{(3)}(t)|_{M(t)^{-1}}. \qquad (13.9)$$

Lemma 2.7 shows that for $w_h(t) = \sum_{j=1}^N w_j(t)\chi_j(t)$ with $w(t) = (w_j(t))$:

$$|(Mw)^{(k)}|^2_{M^{-1}} \le c \sum_{j=0}^{k} \|\partial_h^{(\ell)} w_h\|^2_{L^2(\Gamma_h)}. \tag{13.10}$$

Thus, (13.10) and (13.9) yield

$$\tau^3 \left(|M^{-1}_{n+\frac{1}{2}} \ddot{\widetilde{p}}(t)|_{M_{n+1}} + |M^{-1}_{n+\frac{1}{2}} \ddot{\widetilde{p}}(t)|_{A_{n+1}} \right) \le C\tau^2 \sum_{\ell=1}^{3} \|\partial_h^{(\ell)} P_h u(\cdot,t)\|_{L^2(\Gamma_h(t))}.$$

Again by Lemma 11.5 and the CFL condition (12.11) used similarly to (13.9), and by the norm identity (11.17), we get the bound

$$\tau^2 \left(|M^{-1}_{n+\frac{1}{2}} M_n r_n|_{M_{n+1}} + |M^{-1}_{n+\frac{1}{2}} M_n r_n|_{A_{n+1}} \right) \le C\tau \|R_h(\cdot,t_n)\|_{L^2(\Gamma_h(t_n))}. \tag{13.11}$$

Combining (13.8) and (13.11), we thus have by (13.6)

$$\sum_{k=1}^{n} |d_k^q|_{M_k} + |d_k^q|_{A_k} \le C\tau^2 \beta_h + C\tau \sum_{k=0}^{n} \|R_h(\cdot,t_k)\|_{L^2(\Gamma_h(t_k))}. \tag{13.12}$$

For d_{k+1}^p of (13.7) we use the same arguments (Lemma 11.5 and (13.10)) as above, to find

$$\begin{aligned} |\dddot{\widetilde{p}}(t)|_{M(s)^{-1}} &\le C|\dddot{\widetilde{p}}(t)|_{M(t)^{-1}} = C|\left(M\widetilde{q}\right)^{(4)}(t)|_{M(t)^{-1}} \\ &\le C \sum_{\ell=1}^{4} \|\partial_h^{(\ell)} P_h u(\cdot,t)\|_{L^2(\Gamma_h(t))}. \end{aligned}$$

Thus, it follows that

$$\sum_{k=1}^{n} |d_k^p|_{M_k^{-1}} \le C\tau^2 \beta_h + C\tau \sum_{k=0}^{n} \|R_h(\cdot,t_k)\|_{L^2(\Gamma_h(t_k))}. \tag{13.13}$$

Inserting the bounds (13.12) and (13.13) into Lemma 12.1 and using the norm identity (11.17) completes the proof. ■

13.4. Error bounds for the implicit midpoint rule

Theorem 13.2
Let U_h^n and $\partial_h^\bullet U_h^n$ be determined by the 1*-stage GRK method* (13.1) *(implicit midpoint rule). Under sufficient regularity conditions on the exact solution u of the wave equation* (10.7)*, such that $P_h u$ has continuous discrete material derivatives up to order* 4*. Then,*

there exists $\tau_0 > 0$ independent of h such that for $\tau \le \tau_0$, the errors $E_h^n = U_h^n - P_h u(\cdot, t_n)$ and $\partial_h^\bullet E_h^n = \partial_h^\bullet U_h^n - \partial_h^\bullet (P_h u)(\cdot, t_n)$ are bounded for $t_n = n\tau \le T$ by

$$\begin{aligned}
&\|E_h^n\|_{L^2(\Gamma_h(t_n))} + \|\nabla_{\Gamma_h} E_h^n\|_{L^2(\Gamma_h(t_n))} + \|\partial_h^\bullet E_h^n\|_{L^2(\Gamma_h(t_n))} \\
&\le C\left(\left\|E_h^0\right\|_{L^2(\Gamma_h(t_0))} + \left\|\nabla_{\Gamma_h} E_h^0\right\|_{L^2(\Gamma_h(t_0))} + \left\|\partial_h^\bullet E_h^0\right\|_{L^2(\Gamma_h(t_0))}\right) \\
&\qquad\qquad + C\beta_h \tau^2 + C\tau \sum_{k=0}^{n-1} \|R_h(\cdot, t_k + \frac{1}{2}\tau)\|_{L^2(\Gamma_h(t_k + \frac{1}{2}\tau))}.
\end{aligned}$$

Here, C is independent of h (but depends on T), and

$$\begin{aligned}
\beta_h = \int_0^T \Big(&\|\nabla_{\Gamma_h} \partial_h^{(2)} (P_h u)(\cdot, t)\|_{L^2(\Gamma_h(t))} + \|\nabla_{\Gamma_h} \partial_h^{(3)} (P_h u)(\cdot, t)\|_{L^2(\Gamma_h(t))} \\
&+ \sum_{\ell=1}^{4} \|\partial_h^{(\ell)} (P_h u)(\cdot, t)\|_{L^2(\Gamma_h(\cdot, t))}\Big)\, \mathrm{d}t.
\end{aligned}$$

PROOF

The proof is similar to that of the previous Theorem 13.1. In order to keep the fully discrete methods independent, we give all of the details explicitly again.

Considering the errors

$$\begin{aligned}
e_n &= y_n - \widetilde{y}(t_n) \\
E_{n+\frac{1}{2}} &= Y_{n+\frac{1}{2}} - \widetilde{y}(t_{n+\frac{1}{2}}),
\end{aligned}$$

the defects appearing in the error equations for the implicit midpoint rule (12.31) satisfy

$$\begin{aligned}
\Delta_{k-\frac{1}{2}} &= \widetilde{y}(t_{k-\frac{1}{2}}) - \widetilde{y}(t_{k-1}) - \frac{1}{2}\tau J^{-1} H_{k-\frac{1}{2}} \widetilde{y}(t_{k-\frac{1}{2}}) \\
\delta_k &= \widetilde{y}(t_k) - \widetilde{y}(t_{k-1}) - \tau J^{-1} H_{k-\frac{1}{2}} \widetilde{y}(t_{k-\frac{1}{2}}).
\end{aligned}$$

By (13.5) and Taylor expansion, we obtain

$$\Delta_{\frac{1}{2}} = \frac{1}{2}\tau\Lambda(t_{\frac{1}{2}}) + \int_0^{t_{\frac{1}{2}}} \left(\frac{t_{\frac{1}{2}} - t}{2}\right) \ddot{\widetilde{y}}(t)\, \mathrm{d}t \tag{13.14a}$$

$$\begin{aligned}
\delta_k + \Delta_{k+\frac{1}{2}} - \Delta_{k-\frac{1}{2}} &= \frac{1}{2}\tau\Lambda(t_{k-\frac{1}{2}}) + \frac{1}{2}\tau\Lambda(t_{k+\frac{1}{2}}) \\
&\quad + \tau^2 \int_{t_{k-\frac{1}{2}}}^{t_{k+\frac{1}{2}}} K\left(\frac{t - t_{k-\frac{1}{2}}}{\tau}\right) \dddot{\widetilde{y}}(t)\, \mathrm{d}t
\end{aligned} \tag{13.14b}$$

$$\delta_n - \Delta_{n-\frac{1}{2}} = \frac{1}{2}\tau\Lambda(t_{n-\frac{1}{2}}) + \int_{t_{n-\frac{1}{2}}}^{t_n} \left(\frac{t_{n-\frac{1}{2}} - t}{2}\right) \ddot{\widetilde{y}}(t)\, \mathrm{d}t, \tag{13.14c}$$

with bounded Peano kernel K.

By Lemma 11.5 with $\mu|t - \sigma| \le 1$ and the norm identity (11.17), we first note that

$$\|\Lambda(t)\|_\sigma^2 = \left\langle M(t)r(t) \,\middle|\, M(\sigma)^{-1} \,\middle|\, M(t)r(t)\right\rangle \le 2|r(t)|_{M(t)}^2 = 2\|R_h(\cdot, t)\|_{L^2(\Gamma_h(t))}^2. \tag{13.15}$$

Lemma 2.7 shows that for $Z_h(\cdot,t) = \sum_{j=1}^m z_j(t)\chi_j(\cdot,t)$ with $z(t) = (z_j(t))$:

$$|(Mz)^{(k)}(t)|^2_{M(t)^{-1}} \le C \sum_{\ell=0}^{k} \|\partial_h^{(\ell)} Z_h(\cdot,t)\|^2_{L^2(\Gamma_h(t))}, \tag{13.16}$$

where $f^{(k)}(t)$ denotes the k-th time derivative of $f(t)$ if $k \ge 1$ and $f^{(0)}(t) = f(t)$. The system (13.5), Lemma 11.5, (13.16) and the norm identity (11.17) yield

$$\begin{aligned}\left\|\widetilde{y}^{(k)}(t)\right\|^2_\sigma &= |\widetilde{p}^{(k)}(t)|^2_{M(\sigma)^{-1}} + |\widetilde{q}^{(k)}(t)|^2_{(A+M)(\sigma)} \\ &\le 2|(M\dot{\widetilde{q}})^{(k)}(t)|^2_{M(t)^{-1}} + 2|\widetilde{q}^{(k)}(t)|^2_{(A+M)(t)} \\ &\le C\sum_{\ell=1}^{k+1}\left(\|\partial_h^{(\ell)}(P_hu)(\cdot,t)\|^2_{L^2(\Gamma_h(t))}\right) + 2\|\nabla_{\Gamma_h}\partial_h^{(k)}(P_hu)(\cdot,t)\|^2_{L^2(\Gamma_h(t))} \end{aligned}\tag{13.17}$$

The identities (13.14) together with the bounds (13.15) and (13.17) yield

$$\begin{aligned}\left\|\Delta_{\frac12}\right\|_{t_0} + \left\|\delta_n - \Delta_{n-\frac12}\right\|_{t_n} + C\sum_{j=1}^{n-1}\left\|\delta_j + \Delta_{j+\frac12} - \Delta_{j-\frac12}\right\|_{t_j} \\ \le C\tau^2\beta_h + C\tau\sum_{k=0}^{n-1}\|R_h(\cdot,t_{k+\frac12})\|_{L^2(\Gamma_h(t_{k+\frac12}))}.\end{aligned}$$

Inserting this bound into Lemma 12.2 and using the identity (11.17) closes proof. ■

13.5. Error bounds for the Gauß–Runge–Kutta methods

We prove for general GRK method the following result similar to Theorem 13.2. We will then use the stability Lemma 12.3 and the norm identity (11.17).

Theorem 13.3
For $s \ge 2$, let U_h^n and $\partial_h^\bullet U_h^n$ be determined by the s-stage GRK method (13.1)*. Under sufficient regularity conditions on the exact solution u of the wave equation* (10.7)*, such that P_hu has continuous discrete material derivatives up to order $s+2$. Then, there exists $\tau_0 > 0$ independent of h such that for $\tau \le \tau_0$, the errors $E_h^n = U_h^n - P_hu(\cdot,t_n)$ and $\partial_h^\bullet E_h^n = \partial_h^\bullet U_h^n - \partial_h^\bullet(P_hu)(\cdot,t_n)$ are bounded for $t_n = n\tau \le T$ by*

$$\begin{aligned}&\|E_h^n\|_{L^2(\Gamma_h(t_n))} + \|\nabla_{\Gamma_h}E_h^n\|_{L^2(\Gamma_h(t_n))} + \|\partial_h^\bullet E_h^n\|_{L^2(\Gamma_h(t_n))} \\ &\le C\left(\left\|E_h^0\right\|_{L^2(\Gamma_h(t_0))} + \left\|\nabla_{\Gamma_h}E_h^0\right\|_{L^2(\Gamma_h(t_0))} + \left\|\partial_h^\bullet E_h^0\right\|_{L^2(\Gamma_h(t_0))}\right) \\ &\qquad + C\beta_{h,s}\tau^s + C\tau\sum_{k=0}^{n-1}\sum_{i=1}^{s}\|R_h(\cdot,t_k+c_i\tau)\|_{L^2(\Gamma_h(t_k+c_i\tau))}.\end{aligned}$$

Here, C is independent of h (but depends on T), and

$$\beta_{h,s} = \int_0^T\left(\|\nabla_{\Gamma_h}\partial_h^{(s+1)}(P_hu)(\cdot,t)\|_{L^2(\Gamma_h(t))} + \sum_{\ell=1}^{s+2}\|\partial_h^{(\ell)}(P_hu)(\cdot,t)\|_{L^2(\Gamma_h(t))}\right)\mathrm{d}t.$$

Proof
Considering the errors

$$\begin{aligned} e_n &= y_n - \widetilde{y}(t_n) \\ E_{ni} &= Y_{ni} - \widetilde{y}(t_n + c_i\tau), \end{aligned}$$

we rewrite the Runge-kutta relation (12.44), with $\boldsymbol{\Lambda}_n = (\Lambda_{n1}, \ldots, \Lambda_{ns})^{\mathsf{T}}$, as

$$\boldsymbol{E}_n = \mathbb{1} e_n + \tau \boldsymbol{\mathcal{Q}} \boldsymbol{J}^{-1} \boldsymbol{H}_n \, \boldsymbol{E}_n - (\tau \boldsymbol{\mathcal{Q}} \boldsymbol{\Lambda}_n + \boldsymbol{\Delta}_n) \tag{13.18a}$$

$$e_{n+1} = e_n + \tau \boldsymbol{b}^{\mathsf{T}} \boldsymbol{J}^{-1} \boldsymbol{H}_n \, \boldsymbol{E}_n - \left(\tau \boldsymbol{b}^{\mathsf{T}} \boldsymbol{\Lambda}_n + \delta_{n+1} \right). \tag{13.18b}$$

Due to the stability Lemma 12.3, we get

$$\|e_n\|_{t_n} \leq C \left(\|e_0\|_{t_0} + \tau \sum_{j=0}^{n-1} |||\boldsymbol{\Lambda}_j|||_{t_j} + \sum_{j=0}^{n-1} |||\boldsymbol{\Delta}_j|||_{t_j} + \sum_{j=1}^{n} \|\delta_j\|_{t_j} \right). \tag{13.19}$$

In view of (13.15), we have

$$\tau \sum_{k=0}^{n-1} |||\boldsymbol{\Lambda}_k|||_{t_k} \leq C\tau \sum_{k=0}^{n-1} \sum_{i=1}^{s} \|R_h(\cdot, t_k + c_i\tau)\|_{L^2(\Gamma_h(t_k + c_i\tau))}. \tag{13.20}$$

By using Taylor series expansion, we find that the defects δ_{n+1} and Δ_{ni} appearing in the error equation (13.18) satisfy

$$\begin{aligned} \delta_{n+1} &= \tau^s \int_{t_n}^{t_{n+1}} K\left(\frac{t - t_n}{\tau} \right) \widetilde{y}^{(s+1)}(t) \, \mathrm{d}t \\ \Delta_{ni} &= \tau^s \int_{t_n}^{t_{n+1}} K_i\left(\frac{t - t_n}{\tau} \right) \widetilde{y}^{(s+1)}(t) \, \mathrm{d}t, \end{aligned}$$

with bounded Peano kernels K and K_i. By (13.17), we thus have

$$\begin{aligned} \|\delta_{n+1}\|_{t_{n+1}} \leq \tau^s \sqrt{2} C \int_{t_n}^{t_{n+1}} \sum_{\ell=1}^{s+2} \left(\|\partial_h^{(\ell)} (P_h u)(\cdot, t)\|_{L^2(\Gamma_h(t))} \right) \, \mathrm{d}t \\ + \tau^s \sqrt{2} C \int_{t_n}^{t_{n+1}} \|\nabla_{\Gamma_h} \partial_h^{(s+1)} (P_h u)(\cdot, t)\|_{L^2(\Gamma_h(t))} \, \mathrm{d}t, \end{aligned} \tag{13.21a}$$

$$\begin{aligned} \|\Delta_{ni}\|_{t_n} \leq \tau^s \sqrt{2} C \int_{t_n}^{t_{n+1}} \sum_{\ell=1}^{s+2} \left(\|\partial_h^{(\ell)} (P_h u)(\cdot, t)\|_{L^2(\Gamma_h(t))} \right) \, \mathrm{d}t \\ + \tau^s \sqrt{2} C \int_{t_n}^{t_{n+1}} \|\nabla_{\Gamma_h} \partial_h^{(s+1)} (P_h u)(\cdot, t)\|_{L^2(\Gamma_h(t))} \, \mathrm{d}t. \end{aligned} \tag{13.21b}$$

Inserting the bounds (13.20) and (13.21) into (13.19) and using the norm identity (11.17) completes the proof. ∎

For the 1-stage GRK method, Theorem 13.2 shows that the order in time of the fully discrete scheme is equal to the classical order $\mathcal{O}(\tau^2)$. However, Theorem 13.3 for general

s-stage GRK method shows only order $\mathcal{O}(\tau^s)$. In order to obtain the classical order $\mathcal{O}(\tau^{2s})$, stronger regularity conditions are needed.

For $s \geq 2$, we assume that:

$$\left\| J^{-1}H^{(k_j-1)}(t)\dots J^{-1}H^{(k_1-1)}(t)\widetilde{y}^{(l)}(t)\right\|_t \leq \gamma \tag{13.22a}$$

$$\left\| J^{-1}H^{(s)}(\sigma)J^{-1}H^{(k_j-1)}(t)\dots J^{-1}H^{(k_1-1)}(t)\widetilde{y}^{(l)}(t)\right\|_t \leq \gamma, \tag{13.22b}$$

for all $0 \leq k_i \leq s-1$ and $l \geq s+1$ with $k_1+\dots+k_j+l \leq 2s+1$ and $|\sigma - t| \leq \tau$. For $k_i = 0$, the matrix $H^{(-1)}(t)$ is meant to be the identity matrix. Thereby, we get the following convergence result of full order $\mathcal{O}(\tau^{2s})$.

Theorem 13.4

Under suitable regularity conditions on the exact solution u of the wave equation (10.7) *such that conditions* (13.22) *are satisfied. Then, there exists $\tau_0 > 0$ independent of h such that for $\tau \leq \tau_0$, the errors $E_h^n = U_h^n - P_h u(\cdot, t_n)$ and $\partial_h^\bullet E_h^n = \partial_h^\bullet U_h^n - \partial_h^\bullet (P_h u)(\cdot, t_n)$ are bounded for $t_n = n\tau \leq T$, by*

$$\begin{aligned}
&\|E_h^n\|_{L^2(\Gamma_h(t_n))} + \|\nabla_{\Gamma_h} E_h^n\|_{L^2(\Gamma_h(t_n))} + \|\partial_h^\bullet E_h^n\|_{L^2(\Gamma_h(t_n))} \\
&\leq C\left(\left\|E_h^0\right\|_{L^2(\Gamma_h(t_0))} + \left\|\nabla_{\Gamma_h} E_h^0\right\|_{L^2(\Gamma_h(t_0))} + \left\|\partial_h^\bullet E_h^0\right\|_{L^2(\Gamma_h(t_0))}\right) \\
&\qquad + C_0\tau^{2s} + C\tau \sum_{k=0}^{n-1}\sum_{i=1}^{s} \|R_h(t_k + c_i\tau)\|_{L^2(\Gamma_h(t_k+c_i\tau))}.
\end{aligned}$$

Here, C_0 is independent of h (but depends on T and γ)

PROOF

The main idea of the proof is to modify the defects appearing in (13.18) so they are of order $2s+1$. To do so, we follow Lubich & Ostermann in their proof of Theorem 1 in [36] and first split the matrix H_{ni} and the defects Δ_{ni} as follows

$$H_{ni} = T_{ni} + B_{ni} = \sum_{k=0}^{s-1} \frac{(c_i\tau)^k}{k!} H^{(k)}(t_n) + \int_{t_n}^{t_n+c_i\tau} \frac{(t_n + c_i\tau - t)^{s-1}}{(s-1)!} H^{(s)}(t)\,\mathrm{d}t$$

$$\Delta_{ni} = D_{ni} + R_{ni} = \sum_{l=s+1}^{2s} \tau^l \xi_i^{(l)} \widetilde{y}^{(l)}(t_n) + \tau^{2s}\int_{t_n}^{t_{n+1}} K_i\left(\frac{t-t_n}{\tau}\right)\widetilde{y}^{(2s+1)}(t)\,\mathrm{d}t$$

with bounded Peano kernels K_i and $\xi_i^{(l)} = \frac{1}{l!}\left(l\sum_{j=1}^{s} a_{ij}c_j^{l-1} - c_i^l\right)$.

We introduce the vectors $\boldsymbol{D_n} = (D_{ni})_{i=1}^s$ and $\boldsymbol{R_n} = (R_{ni})_{i=1}^s$, the block diagonal matrices

$$\boldsymbol{T_n} = \operatorname{diag}(T_{n1}, T_{n2}, \dots, T_{ns}) \quad \text{and} \quad \boldsymbol{B}_n = \operatorname{diag}(B_{n1}, B_{n2}, \dots, B_{ns}),$$

and the new internal stages

$$\widehat{\boldsymbol{E}}_n = \boldsymbol{E}_n + \widehat{\boldsymbol{D}}_n, \qquad \text{with} \quad \widehat{\boldsymbol{D}}_n = \sum_{k=0}^{s-1}\left(\tau \boldsymbol{\mathcal{Q}}\boldsymbol{J}^{-1}\boldsymbol{T_n}\right)^k \boldsymbol{D}_n.$$

Next, we rewrite the error equations (13.18) as

$$\begin{aligned} e_{n+1} &= e_n + \tau \boldsymbol{b}^{\mathrm{T}} \boldsymbol{J}^{-1} \boldsymbol{H}_n \widehat{\boldsymbol{E}}_n - \left(\tau \boldsymbol{b}^{\mathrm{T}} \boldsymbol{\Lambda}_n + \boldsymbol{\delta}'_{n+1}\right) \\ \widehat{\boldsymbol{E}}_n &= \mathbb{1} e_n + \tau \mathcal{Q} \boldsymbol{J}^{-1} \boldsymbol{H}_n \widehat{\boldsymbol{E}}_n - \left(\tau \mathcal{Q} \boldsymbol{\Lambda}_n + \boldsymbol{\Delta}'_n\right), \end{aligned}$$

where the modified defects satisfy

$$\begin{aligned} \delta'_{n+1} &= \delta_{n+1} + \tau \boldsymbol{b}^{\mathrm{T}} \boldsymbol{J}^{-1} \boldsymbol{B}_n \widehat{\boldsymbol{D}}_n + \tau \boldsymbol{b}^{\mathrm{T}} \boldsymbol{J}^{-1} \boldsymbol{T_n} \widehat{\boldsymbol{D}}_n \\ \boldsymbol{\Delta}'_n &= \boldsymbol{R}_n + \tau \mathcal{Q} \boldsymbol{J}^{-1} \boldsymbol{B}_n \widehat{\boldsymbol{D}}_n + \left(\tau \mathcal{Q} \boldsymbol{J}^{-1} \boldsymbol{T_n}\right)^s \boldsymbol{D_n}. \end{aligned} \tag{13.23}$$

By the stability Lemma 12.3, we have

$$\|e_n\|_{t_n} \leq C \left(\|e_0\|_{t_0} + \tau \sum_{j=0}^{n-1} |||\boldsymbol{\Lambda}_j|||_{t_j} + \sum_{j=0}^{n-1} |||\boldsymbol{\Delta}'_j|||_{t_j} + \sum_{j=1}^{n} \left\|\delta'_j\right\|_{t_j} \right). \tag{13.24}$$

By the regularity conditions (13.22), for $j = (0, \ldots, n-1)$, we observe that

$$|||\boldsymbol{\Delta}'_j|||_{t_j} \leq C_0 \tau^{2s+1}. \tag{13.25}$$

Now, we come to the last part of the proof, where we show that δ'_j is also of order $\mathcal{O}\left(\tau^{2s+1}\right)$. By the regularity condition (13.22), the first and second term of (13.23) clearly are of order $\mathcal{O}\left(\tau^{2s+1}\right)$. Therefore, our problem reduces to show that $\tau \boldsymbol{b}^{\mathrm{T}} \boldsymbol{J}^{-1} \boldsymbol{T_n} \widehat{\boldsymbol{D}}_n$ is of order $\mathcal{O}\left(\tau^{2s+1}\right)$. We start by introducing the following notation:

$$\mathcal{C} = \operatorname{diag}(c_1, c_2, \ldots, c_s) \quad \text{and} \quad \xi^{(l)} = \left(\xi_i^{(l)}\right)_{i=1}^s.$$

Then, we see that $\tau \boldsymbol{b}^{\mathrm{T}} \boldsymbol{J}^{-1} \boldsymbol{T_n} \widehat{\boldsymbol{D}}_n$ consists of a linear combination of expressions of the form

$$b^{\mathrm{T}} \mathcal{Q} \mathcal{C}^{k_j - 1} \ldots \mathcal{Q} \mathcal{C}^{k_1 - 1} \xi^{(l)} \cdot J^{-1} H^{(k_j - 1)}(t_n) \ldots J^{-1} H^{(k_1 - 1)}(t_n) \widetilde{y}^{(l)}(t_n) \cdot \tau^{|k| + l + 1} \tag{13.26}$$

where $|k| = \sum_{i=1}^{j} k_i, \quad k_i \in \{1, \ldots, s\}$ and $j \leq s$.

By the order conditions of the Runge–Kutta method (see [24, p. 56]), we have

$$b^{\mathrm{T}} \mathcal{Q} \mathcal{C}^{k_j - 1} \ldots \mathcal{Q} \mathcal{C}^{k_1 - 1} \xi^{(l)} = 0 \quad \text{for} \quad |k| + l + 1 \leq 2s,$$

therefore, all the expressions of (13.26) vanish for $|k| + l + 1 \leq 2s$. Thus, by the regularity conditions (13.22), for $j = (1, 2, \ldots, n)$, we get

$$\left\|\delta'_j\right\|_{t_j} \leq C_0 \tau^{2s+1}. \tag{13.27}$$

Inserting the bounds (13.25), (13.27) and (13.20) into (13.24) and using the norm identity (11.17) completes the proof. ∎

Remark 13.5

1. *If P_h is the piecewise linear interpolation operator at the nodes, then $\widetilde{\beta}_h$, β_h as well as $\beta_{h,s}$ are clearly bounded uniformly in h. However, we were only able to prove that $\|R_h(\cdot,t)\|_{L^2(\Gamma_h(t))} = \mathcal{O}(1)$. Thus as in the parabolic case the remaining question here is:*
   Can we find a projection P_h such that $\widetilde{\beta}_h$, β_h as well as $\beta_{h,s}$ are bounded uniformly in h and $\|R_h(\cdot,t)\|_{L^2(\Gamma_h(t))}$ is of optimal order $\mathcal{O}(h^2)$?

   A positive answer for this question was not obvious and it was the main reason to define such a Ritz map introduced in Chapter 7.

2. *We can also compare the fully discrete solution with the semi-discrete solution U_h of (11.6). For the corresponding error $U_h^n - U_h(\cdot,t_n)$, we obtain a similar bound where R_h does not appear and the factor in front of the τ^s term is bounded in terms of higher-order discrete material derivatives of U_h instead of $P_h u$. Then we would of had to show regularity results for the semi-discrete solution U_h.*

14. Error Estimates II

In the following, we prove optimal error bounds for the fully discrete methods considered in the previous chapters for the wave equation. Keeping in mind the previous results, the problem of bounding the total error reduces to finding an appropriate projection $P_h u$ such that the Residual appearing in (13.2) is of optimal order $\mathcal{O}(h^2)$. Thus, we first show how our Ritz map introduced in Chapter 7 is a sufficient choice, thereby we make use of the geometric approximation estimates stated in Chapter 6. Finally, we prove optimal error estimates for the difference between the lifts of the fully discrete numerical solution and the exact solution of the wave equation, as well as the difference between the numerical material derivative of the lifts of the fully discrete numerical solution and the material derivative of the exact solution.

14.1. Ritz map and residual bound

We first recall some definitions that we already used in the previous chapters.

We denote by $d(x,t), x \in \mathbb{R}^{m+1}, t \in [0,T]$ the *signed distance function* to the smooth closed surface $\Gamma(t)$ and let $\mathcal{N}(t)$ be a neighborhood of $\Gamma(t)$ such that for every $x \in \mathcal{N}(t)$ and $t \in [0,T]$ there exists a unique $p(x,t) \in \Gamma(t)$ which is the normal projection of x onto $\Gamma(t)$, i.e.,

$$x - p(x,t) = d(x,t)\nu(p(x,t),t). \tag{14.1}$$

We assume $\Gamma_h(t) \subset \mathcal{N}(t)$. Thus, for each triangle $E(t)$ in $\Gamma_h(t)$, there is a unique curved triangle $e(t) = p(E(t),t) \subset \Gamma(t)$, and this induces an exact triangulation of $\Gamma(t)$ with curved edges. Furthermore, we assume that $\Gamma_h(t)$ consists of triangles $E(t)$ in $\mathcal{T}_h(t)$ with inner radius bounded below by $\sigma_h \geq ch$ for some $c > 0$.

For any continuous function $\eta_h : \Gamma_h \to \mathbb{R}$, we define its lift $\eta_h^l : \Gamma \to \mathbb{R}$ by

$$\eta_h^l(p,t) = \eta_h(x,t), \qquad p \in \Gamma(t),$$

where $x \in \Gamma_h(t)$ is such that $p = p(x,t)$. Then, we have the lifted finite element space

$$S_h^l(t) = \{\varphi_h = \phi_h^l \ : \ \phi_h \in S_h(t)\}.$$

Now, we show how we choose the appropriate projection, so that the residual appearing in (13.2) is of optimal order $\mathcal{O}(h^2)$. As in the case for the parabolic equation, it turns out also to be convenient in the error analysis for the wave equation on evolving surfaces to use a modified Ritz projection $\widetilde{\mathcal{P}}_h(t) : H^1(\Gamma(t)) \to S_h(t)$ defined in the following way, where we use the bilinear forms of Section 6.4 and the lifted discrete velocity of Section 6.3. To motivate the definition, we rewrite the weak form (10.10) of the wave equation in terms of the bilinear forms,

$$\frac{d}{dt} m(\partial^\bullet u, \varphi) + a(u, \varphi) = m(\partial^\bullet u, \partial^\bullet \varphi),$$

and use the Leibniz formula with the discrete material derivative $\partial_h^\bullet$ on Γ and note $\partial_h^\bullet \varphi = \partial^\bullet \varphi + (v_h - v) \cdot \nabla_\Gamma \varphi$, because $v_h - v$ is a tangent vector (see (6.7)). Then, this equation becomes

$$\begin{aligned} m(\partial_h^\bullet \partial_h^\bullet u, \varphi) + g(v_h; \partial^\bullet u, \varphi) + m(\partial_h^\bullet \partial^\bullet u - \partial_h^\bullet \partial_h^\bullet u, \varphi) \\ + m(\partial^\bullet u, (v_h - v) \cdot \nabla_\Gamma \varphi) + a(u, \varphi) = 0. \end{aligned} \tag{14.2}$$

We now define a Ritz map that collects the last two terms on the left-hand side of this equation, which are the only terms that contain the surface gradient of the test function φ. Note the difference to the parabolic case, that one have $m(\partial^\bullet u, (v - v_h) \cdot \nabla_\Gamma \varphi)$ instead of $m(u, (v - v_h) \cdot \nabla_\Gamma \varphi)$. Since $a(\cdot, \cdot)$ is only positive semi-definite, we consider the positive definite bilinear forms

$$\begin{aligned} a^*(w, \varphi) &= a(w, \varphi) + m(w, \varphi), && w, \varphi \in H^1(\Gamma) \\ a_h^*(W_h, \phi_h) &= a_h(W_h, \phi_h) + m_h(W_h, \phi_h), && W_h, \phi_h \in S_h. \end{aligned}$$

We note that $a^*(w, w) = \|w\|^2_{H^1(\Gamma)}$.

Definition 14.1
For given $z \in H^1(\Gamma(t))$ and $\partial^\bullet z \in L^2(\Gamma(t))$, there is a unique $\widetilde{\mathcal{P}}_h(t) z \in S_h(t)$ such that for all $\phi_h \in S_h(t)$ we have, with the corresponding lift $\varphi_h = \phi_h^l$,

$$a_h^*(\widetilde{\mathcal{P}}_h z, \phi_h) = a^*(z, \varphi_h) + m(\partial^\bullet z, (v_h(\cdot, t) - v(\cdot, t)) \cdot \nabla_{\Gamma(t)} \varphi_h). \tag{14.3}$$

We define $\mathcal{P}_h z \in S_h^l(t)$ as the lift of $\widetilde{\mathcal{P}}_h z$, i.e., $\mathcal{P}_h z = (\widetilde{\mathcal{P}}_h z)^l$.

We immediately see that this definition is the same as the one considered in Chapter 7 when we set $\zeta = \partial^\bullet z$. Thus, we have the following results from Theorem 7.2 and Theorem 7.3.

Lemma 14.2
The error in the Ritz map satisfies the bounds, for $0 \le t \le T$ and $h \le h_0$ with sufficiently small h_0,

$$\|z - \mathcal{P}_h z\|_{L^2(\Gamma(t))} + h \left\| \nabla_{\Gamma(t)} (z - \mathcal{P}_h z) \right\|_{L^2(\Gamma(t))} \le C h^2 \left(\|z\|_{H^2(\Gamma(t))} + \|\partial^\bullet z\|_{L^2(\Gamma(t))} \right). \tag{14.4}$$

Lemma 14.3
The error in the material derivatives of the Ritz map satisfies the bounds, for $\ell \geq 1$, $0 \leq t \leq T$ and $h \leq h_0$ with sufficiently small h_0,

$$\left\| \partial_h^{(\ell)} (z - \mathcal{P}_h z) \right\|_{L^2(\Gamma(t))} + h \left\| \nabla_\Gamma \Big(\partial_h^{(\ell)} (z - \mathcal{P}_h z) \Big) \right\|_{L^2(\Gamma(t))} \leq C_\ell \, h^2 \sum_{i=0}^{\ell} \left(\left\| \partial^{(i)} z \right\|_{H^2(\Gamma(t))} + \left\| \partial^{(i+1)} z \right\|_{L^2(\Gamma(t))} \right). \quad (14.5)$$

An optimal-order bound of the residual $R_h(\cdot, t) \in S_h(t)$ of (13.2) is then achieved if we take the mapping P_h to be the Ritz map $\widetilde{P}_h$ defined in (14.3).

Lemma 14.4
Assume that the solution u of the wave equation is sufficiently smooth. Then, there exist $C > 0$ and $h_0 > 0$ such that for $h \leq h_0$ and $0 \leq t \leq T$,

$$\|R_h(\cdot, t)\|_{L^2(\Gamma_h(t))} \leq Ch^2. \quad (14.6)$$

Proof
We start by rewriting the residual equation (13.2) for $R_h \in S_h$ with $P_h = \widetilde{\mathcal{P}}_h$ as

$$\begin{aligned} m_h(R_h, \phi_h) &= \frac{d}{dt} m_h(\partial_h^\bullet \widetilde{\mathcal{P}}_h u, \phi_h) + a_h(\widetilde{\mathcal{P}}_h u, \phi_h) - m_h(\partial_h^\bullet \widetilde{\mathcal{P}}_h u, \partial_h^\bullet \phi_h) \\ &= m_h(\partial_h^\bullet \partial_h^\bullet \widetilde{\mathcal{P}}_h u, \phi_h) + g_h(V_h; \partial_h^\bullet \widetilde{\mathcal{P}}_h u, \phi_h) + a_h(\widetilde{\mathcal{P}}_h u, \phi_h), \end{aligned}$$

where we have used the Transport Lemma 6.4. Combining this equation with (7.1) and using the definition of the Ritz map (14.3) yield

$$m_h(R_h, \phi_h) = F_1(\varphi_h) + F_2(\varphi_h) + F_3(\varphi_h), \qquad \varphi_h = \phi_h^l \in S_h^l, \quad (14.7)$$

where

$$\begin{aligned} F_1(\varphi_h) &= m_h(\partial_h^\bullet \partial_h^\bullet \widetilde{\mathcal{P}}_h u, \phi_h) - m(\partial_h^\bullet \partial_h^\bullet u, \varphi_h), \\ F_2(\varphi_h) &= g_h(V_h; \partial_h^\bullet \widetilde{\mathcal{P}}_h u, \phi_h) - g(v_h; \partial^\bullet u, \varphi_h), \\ F_3(\varphi_h) &= m(\partial_h^\bullet \partial_h^\bullet u - \partial_h^\bullet \partial^\bullet u, \varphi_h), \\ F_4(\varphi_h) &= m(u, \varphi_h) - m_h(\widetilde{\mathcal{P}}_h u, \phi_h). \end{aligned}$$

Applying Lemma 6.5, using $(\partial_h^\bullet \partial_h^\bullet \widetilde{\mathcal{P}}_h u)^l = \partial_h^\bullet \partial_h^\bullet \mathcal{P}_h u$ and applying Lemma 14.3 with $\ell = 2$ yields

$$\begin{aligned} |F_1(\varphi_h)| &= \left| m_h(\partial_h^\bullet \partial_h^\bullet \widetilde{\mathcal{P}}_h u, \phi_h) - m(\partial_h^\bullet \partial_h^\bullet \mathcal{P}_h u, \varphi_h) + m(\partial_h^\bullet \partial_h^\bullet \mathcal{P}_h u - \partial_h^\bullet \partial_h^\bullet u, \varphi_h) \right| \\ &\leq ch^2 \|\varphi_h\|_{L^2(\Gamma)} \, . \end{aligned}$$

Using the same arguments, it follows that

$$\begin{aligned} |F_2(\varphi_h)| &\leq ch^2 \|\varphi_h\|_{L^2(\Gamma)} \, , \\ |F_4(\varphi_h)| &\leq ch^2 \|\varphi_h\|_{L^2(\Gamma)} \, . \end{aligned}$$

Furthermore Lemma 6.3 yields

$$|F_3(\varphi_h)| = |m(\partial_h^\bullet[(v - v_h) \cdot \nabla_\Gamma u], \varphi_h)| \leq ch^2 \|\varphi_h\|_{L^2(\Gamma)}\,.$$

Inserting the above bounds into (8.4) with $\phi_h = R_h$ and noting the equivalence of L^2-norms between the original and discretized surfaces completes the proof. ∎

We remark that it is crucial to choose $\zeta = \partial^\bullet u$ in the definition of the Ritz map for the wave equation, otherwise one will have only suboptimal order $\mathcal{O}(h)$ for the residual R_h measured in the L^2-norm.

14.2. Error bound for the full discretization

In this section, we compare the lifts of the fully discrete numerical solution $u_h^n := (U_h^n)^l$ and its numerical material derivative $\partial_h^\bullet u_h^n := (\partial_h^\bullet U_h^n)^l$ with the exact solution $u(\cdot, t_n)$ of the wave equation (10.7) and its material derivative $\partial^\bullet u(\cdot, t_n)$, respectively.

Let $y_n = (p_n, q_n)^\mathrm{T}$ be generated by the leapfrog method (12.5) or by the s-stage GRK method (12.37) (keeping in mind that the 1-stage GRK method is the implicit midpoint rule (12.29)). As in (13.1), we obtain the lifts of the fully discrete numerical solution and its numerical material derivative from

$$u_h^n := (U_h^n)^l = \sum_{j=1}^N q_j^n \chi_j^l(\cdot, t_n), \qquad \partial_h^\bullet u_h^n := (\partial_h^\bullet U_h^n)^l = \sum_{j=1}^N \dot{q}_j^n \chi_j^l(\cdot, t_n), \tag{14.8}$$

which are lifted finite element functions defined on the surface $\Gamma(t_n)$. Then, the main results of this part read as follows:

Theorem 14.5 (ESFEM/leapfrog)
Consider the variational space discretization of the wave equation (10.7) *by the evolving surface finite element method and the variational time discretization by the leapfrog method. Let u be a sufficiently smooth solution of the wave equation* (10.7) *and assume that the discrete initial data satisfy*

$$\begin{aligned} \left\| u_h^0 - (\mathcal{P}_h u)(\cdot, 0) \right\|_{L^2(\Gamma(0))} + \left\| \nabla_{\Gamma(0)} u_h^0 - \nabla_{\Gamma(0)} (\mathcal{P}_h u)(\cdot, 0) \right\|_{L^2(\Gamma(0))} & \\ + \left\| \partial_h^\bullet u_h^0 - \partial_h^\bullet (\mathcal{P}_h u)(\cdot, 0) \right\|_{L^2(\Gamma(0))} &\leq C_0 h^2. \end{aligned}$$

Then, there exist $h_0 > 0$ and $\tau_0 > 0$ such that for $h \leq h_0$ and $\tau \leq \tau_0$ satisfying the CFL condition (12.11)*, the following error bound holds for $0 \leq t_n = n\tau \leq T$:*

$$\begin{aligned} \|u_h^n - u(.,t_n)\|_{L^2(\Gamma(t_n))} + h \left\| \nabla_{\Gamma(t_n)} u_h^n - \nabla_{\Gamma(t_n)} u(.,t_n) \right\|_{L^2(\Gamma(t_n))} & \\ + \|\partial_h^\bullet u_h^n - \partial^\bullet u(.,t_n)\|_{L^2(\Gamma(t_n))} &\leq C(h^2 + \tau^2). \end{aligned}$$

The constant C is independent of h, τ, and n subject to the stated conditions.

Theorem 14.6 (ESFEM/GRK)
Consider the variational space discretization of the wave equation (10.7) *by the evolving surface finite element method and the variational time discretization by the s-stage GRK method. Let u be a sufficiently smooth solution of the wave equation* (10.7) *and assume that the discrete initial data satisfy*

$$\left\|u_h^0 - (\mathcal{P}_h u)(\cdot,0)\right\|_{L^2(\Gamma(0))} + \left\|\nabla_{\Gamma(0)} u_h^0 - \nabla_{\Gamma(0)}(\mathcal{P}_h u)(\cdot,0)\right\|_{L^2(\Gamma(0))} + \left\|\partial_h^\bullet u_h^0 - \partial_h^\bullet(\mathcal{P}_h u)(\cdot,0)\right\|_{L^2(\Gamma(0))} \le C_0 h^2.$$

Then, there exist $h_0 > 0$ and $\tau_0 > 0$ such that for $h \le h_0$ and $\tau \le \tau_0$, the following error bound holds for $0 \le t_n = n\tau \le T$:

$$\|u_h^n - u(.,t_n)\|_{L^2(\Gamma(t_n))} + h\left\|\nabla_{\Gamma(t_n)} u_h^n - \nabla_{\Gamma(t_n)} u(.,t_n)\right\|_{L^2(\Gamma(t_n))} + \|\partial_h^\bullet u_h^n - \partial^\bullet u(.,t_n)\|_{L^2(\Gamma(t_n))} \le C\big(h^2 + \tau^s\big).$$

For the implicit midpoint rule ($s = 1$), the bound holds with τ^2 instead of τ^s. For general s, assuming that the regularity conditions (13.22) *are satisfied, we obtain τ^{2s} instead of τ^s. The constant C is independent of h, τ, and n subject to the stated conditions.*

Proof
The total error is divided into two parts such as

$$u_h^n - u(\cdot,t_n) = \Big(u_h^n - \mathcal{P}_h u(\cdot,t_n)\Big) + \Big(\mathcal{P}_h u(\cdot,t_n) - u(\cdot,t_n)\Big). \tag{14.9}$$

Taking into account that the L^2 and H^1 norms on the discretized and original surface are equivalent (Lemma 6.1) and the fact that $\|\partial^\bullet u - \partial_h^\bullet u\|_{L^2(\Gamma)} \le Ch^2$ (Lemma 6.3), in order to estimate the first part of (14.9), we need only to combine the theorems and lemmas from the previous chapters. For example, the implicit midpoint rule ($s = 1$): we use Theorem 13.2 together with Lemma 14.4 (residual bound) and Lemmas 14.2 and 14.3 (for estimating β_h), to find that the first part is of order $\mathcal{O}(\tau^2 + h^2)$. The second part of (14.9) is already taken care of in Lemmas 14.2 and 14.3. ■

The condition on the starting values is satisfied with the choice

$$u_h^0 = (\mathcal{P}_h u)(0), \qquad \partial_h^\bullet u_h^0 = I_h \partial^\bullet u(0).$$

For the nodal vectors q^0 and $p^0 = M(0)\dot{q}^0$ this corresponds to the entries

$$q_j^0 = (\mathcal{P}_h u)(a_j(0),0), \qquad \dot{q}_j^0 = \dot{u}_0(a_j(0)).$$

Instead of using the Ritz map $\mathcal{P}_h$ defined by (7.2) we can use the simpler approximation u_h^0 given by the more standard Ritz projection

$$a_h^*(u_h^0, \phi_h; 0) = a^*(u_0, \varphi_h; 0) \quad \text{for all } \phi_h \in S_h(0), \quad \varphi_h = \phi_h^l$$

with a sufficiently accurate approximation to the integrals on the right-hand side. By the estimates of Theorem 7.2 (with 0 in place of ζ at $t = 0$ and the fact that $|v - v_h| \le Ch^2$), this approximation still satisfies the condition on the initial data in both Theorems 14.5 and 14.6. While this simplified projection is sufficient for determining the numerical initial values, it cannot replace the Ritz map of (14.3) in the second-order error analysis (see the proof of Lemma 14.4).

This construction of the starting values requires solving a linear system with the extended stiffness matrix $A(0) + M(0)$ for q^0. As for the classical wave equation on a fixed domain, the simpler choice of the linear interpolant $u_h^0 = I_h u(0)$ does not guarantee second-order convergence (cf. [12]).

Remark 14.7
As already mentioned in Remark 8.4, Runge–Kutta time discretization of partial differential equations on plane domains suffers from order reduction phenomena which depends on the boundary conditions (cf. [34, 36, 43]). Thus, we only expect that the convergence order of the s- stage GRK method, when applied to a wave equation posed on surfaces with boundary, is only equal to $s + \ell$ with $\ell \ge 0$ depending on the boundary conditions. This means that condition (13.22) *will mostly fail to hold uniformly in the mesh size on surfaces with boundary. However, we expect that the regularity condition* (13.22) *holds true for smooth solutions of wave equations on smooth closed surfaces.*

15. Numerical Experiments II

In this chapter, we present numerical experiments to illustrate some of our convergence results for the wave equation. The fully discrete methods (schemes (12.5), (12.37)) are implemented by using the DUNE-FEM module, which is based on the Distributed and Unified Numerics Environment (DUNE), see [5, 10, 11]. The visualization is done by using the application ParaView [29]. For more details about the implementation of the evolving surface finite element method, we refer to Dziuk & Elliott [14].

Example 15.1
In this example, we consider the inhomogeneous wave equation

$$\partial^\bullet \partial^\bullet u + \partial^\bullet u \; \nabla_\Gamma \cdot v - \Delta_\Gamma u = f \quad \text{on } \Gamma(t), \tag{15.1}$$

where

$$\Gamma(t) = \left\{ x \in \mathbb{R}^3 \, : \, \frac{x_1^2}{1 + 0.25 \sin(\pi \cdot t)} + x_2^2 + x_3^2 - 1 = 0 \right\}.$$

The right hand side f is calculated so that the exact solution is given by

$$u(x,t) = \sin(\sqrt{6}t) x_1 x_2.$$

Fully discrete scheme for the inhomogeneous wave equation: We treated so far only the homogeneous wave equation on evolving surfaces, we mention again that it is straightforward to extend our results to the inhomogeneous case. The fully discrete scheme for the inhomogeneous equation has to be updated only with a right hand side similar to the inhomogeneous wave equation on a fixed domain. For example, the leapfrog scheme (12.6) becomes:

The *leapfrog* or *Störmer–Verlet* method for the inhomogeneous wave equation on evolving surfaces reads

$$p_{n+1/2} = p_n - \frac{\tau}{2} A_n q_n + \frac{\tau}{2} F_n \tag{15.2a}$$

$$q_{n+1} = q_n + \tau M^{-1}_{n+\frac{1}{2}} p_{n+1/2} \tag{15.2b}$$

$$p_{n+1} = p_{n+1/2} - \frac{\tau}{2} A_{n+1} q_{n+1} + \frac{\tau}{2} F_{n+1}, \tag{15.2c}$$

where $(F_n)_{j=1}^N = \left(\int_{\Gamma_h(t_n)} f^{-l} \chi_j \right)_{j=1}^N$.

1. **Experiment (Leapfrog)**: Let $\{\mathcal{T}_h^i(t)\}_{i=0}^k$ and $\{\tau_i\}_{i=0}^k$ be a sequence of meshes on the surface $\Gamma(t)$ by uniform refinement and a sequence of time steps respectively. The uniform refinement is such that $h_i \approx \frac{1}{2}h_{i-1}$. We proved in Theorem 14.5 that the rate of convergence in τ and h are the same. Thus, we choose $\tau_i = \frac{1}{2}\tau_{i-1}$ to construct the time step size sequence $\{\tau_i\}_{i=0}^k$. Further, in order to satisfy the CFL condition, we start with $\tau_0 = 5 \times 10^{-2}$. For each mesh $\mathcal{T}_h^i$ together with the corresponding time step size τ_i, we solve the wave equation (15.1) using the piecewise linear finite elements in combination with the leapfrog method (scheme 15.2). Then, we compute the error between the lifted numerical solution (14.8) and the exact solution for $0 \le t \le 1$ in the following norms:

$$L^\infty\left(L^2\right): \qquad \max_{0\le n\le N} \|u_h^n - u(t_n)\|_{L^2(\Gamma(t_n))},$$

$$L^\infty\left(H^1\right): \qquad \max_{0\le n\le N} \left\|\nabla_{\Gamma(t_n)} u_h^n - \nabla_{\Gamma(t_n)} u(t_n)\right\|_{L^2(\Gamma(t_n))},$$

$$L^\infty\left(L^2\right)^\bullet: \qquad \max_{0\le n\le N} \|\partial_h^\bullet u_h^n - \partial^\bullet u(t_n)\|_{L^2(\Gamma(t_n))}.$$

Assuming that the error Er_i satisfies $Er_i = C\left(h_i + \tau_i\right)^{EOC}$, it follows that $\frac{Er_{i-1}}{Er_i} = 2^{EOC}$. Thus, the experimental order of convergence (EOC) is determined by

$$EOC = \frac{\log \frac{Er_{i-1}}{Er_i}}{\log 2}, \qquad i = 1, \cdots k.$$

In Table 15.1, we list the errors and the corresponding EOCs. As theoretically expected from Theorem 14.5, we observe $EOC \approx 2$ for the $L^\infty\left(L^2\right)$ as well as for the $L^\infty\left(L^2\right)^\bullet$ norm, whereas $EOC \approx 1$ for the $L^\infty\left(H^1\right)$ norm.

Table 15.1.: Errors and observed orders of convergence for the 1. Experiment (Leapfrog).

Level	DOF	$L^\infty(L^2)$	EOC	$L^\infty(H^1)$	EOC	$L^\infty(L^2)^\bullet$	EOC
0	318	$2.05 \cdot 10^{-2}$	–	$1.77 \cdot 10^{-1}$	–	$2.26 \cdot 10^{-2}$	–
1	1266	$5.27 \cdot 10^{-3}$	1.95	$8.91 \cdot 10^{-2}$	0.99	$5.88 \cdot 10^{-3}$	1.94
2	5058	$1.34 \cdot 10^{-3}$	1.97	$4.27 \cdot 10^{-2}$	1.05	$1.47 \cdot 10^{-3}$	2.00
3	20226	$3.35 \cdot 10^{-4}$	2.00	$2.18 \cdot 10^{-2}$	0.96	$3.74 \cdot 10^{-4}$	1.97
4	80898	$8.35 \cdot 10^{-5}$	2.00	$1.11 \cdot 10^{-2}$	0.96	$9.50 \cdot 10^{-5}$	1.98
5	323586	$2.08 \cdot 10^{-5}$	1.99	$5.58 \cdot 10^{-3}$	0.99	$2.37 \cdot 10^{-5}$	1.99

2. **Experiment (Implicit midpoint)**: We repeat the first experiment with the implicit midpoint rule instead of the leapfrog method for the time discretization. We choose a time step size $\tau_0 = 0.125$ in order to obtain at least the same accuracy as by

the Leapfrog method. In Table 15.2, as in the case by the leapfrog method, we observe again $EOC \approx 2$ for the $L^\infty\left(L^2\right)$ as well as for the $L^\infty\left(L^2\right)^\bullet$ norm, whereas $EOC \approx 1$ for the $L^\infty\left(H^1\right)$ norm. This shows that the theoretical convergence results (Theorem 14.6) are optimal.

Table 15.2.: Errors and observed orders of convergence for the 2. Experiment (Implicit midpoint).

Level	DOF	$L^\infty(L^2)$	EOC	$L^\infty(H^1)$	EOC	$L^\infty(L^2)^\bullet$	EOC
0	318	$5.23 \cdot 10^{-3}$	–	$1.74 \cdot 10^{-1}$	–	$2.18 \cdot 10^{-2}$	–
1	1266	$1.43 \cdot 10^{-3}$	1.87	$8.87 \cdot 10^{-2}$	0.97	$5.47 \cdot 10^{-3}$	1.99
2	5058	$3.68 \cdot 10^{-4}$	1.95	$4.45 \cdot 10^{-2}$	0.99	$1.37 \cdot 10^{-3}$	1.99
3	20226	$9.30 \cdot 10^{-5}$	1.98	$2.23 \cdot 10^{-2}$	0.99	$3.44 \cdot 10^{-4}$	1.99
4	80898	$2.33 \cdot 10^{-5}$	1.99	$1.11 \cdot 10^{-2}$	0.99	$8.61 \cdot 10^{-5}$	1.99
5	323586	$5.83 \cdot 10^{-6}$	1.99	$5.58 \cdot 10^{-3}$	0.99	$2.15 \cdot 10^{-5}$	1.99
6	1294338	$1.45 \cdot 10^{-6}$	1.99	$2.79 \cdot 10^{-3}$	0.99	$5.38 \cdot 10^{-6}$	1.99

3. **Experiment (GRK)**: In this experiment, we examine the convergence of the GRK time discretization with s-stages. We observed, when applying the 2-stage GRK method to the resulting ODE system after the space discretization by the evolving surface finite element method, the total error is dominated by the spatial error. For this reason, we shall compare the fully discrete solution with the exact solution of the ODE system. Since this solution is not available, we compute reference solutions q_{ref} and p_{ref} via the 3-stage GRK method with a small time step size $\tau_{ref} = 10^{-4}$. Next, we construct the time step size sequence $\{\tau_i\}_{i=0}^{7}$ by setting $\tau_i = \frac{1}{2}\tau_{i-1}$ with $\tau_0 = 0.5$. For each time step size τ_i, we solve the ODE system on the time interval $0 \leq t \leq 1$ to obtain the numerical solutions q_{τ_i} and p_{τ_i} using 4 different schemes, namely, the Leapfrog method, the implicit midpoint rule, the 2-stage and the 3- stage GRK methods. In Figure 15.1, we plot the errors at time $t = 1$ versus the time step size in the following norms

$$\begin{aligned}
\text{Error (M)}: &\quad \left(\langle q_{ref} - q_{\tau_i} \left| M(t) \right| q_{ref} - q_{\tau_i} \rangle\right)^{1/2}, \\
\text{Error (A)}: &\quad \left(\langle q_{ref} - q_{\tau_i} \left| A(t) \right| q_{ref} - q_{\tau_i} \rangle\right)^{1/2}, \\
\text{Error (M}^{-1}\text{)}: &\quad \left(\left\langle p_{ref} - p_{\tau_i} \left| M(t)^{-1} \right| p_{ref} - p_{\tau_i} \right\rangle\right)^{1/2}.
\end{aligned}$$

Additionally, we plot the spatial error which dominates the total error. For all schemes, we clearly observe that the experimental convergence rates in time match perfect with the theoretical ones.

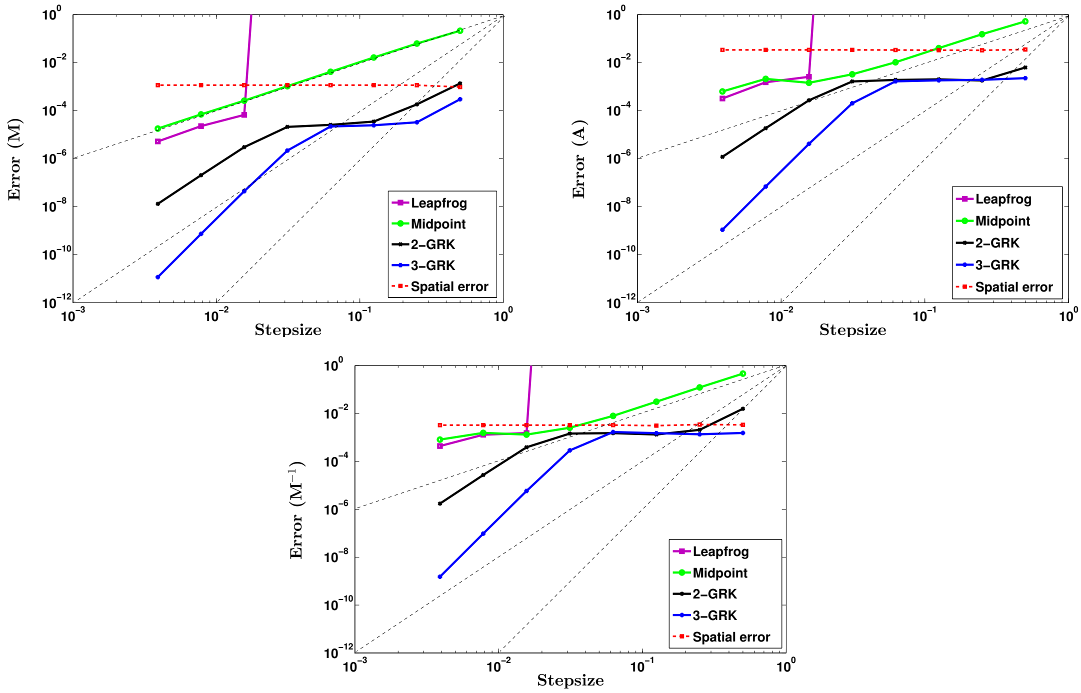


Figure 15.1.: Errors vs. time step size for four different time discretization schemes as well as the spatial error at time $t = 1$.

Example 15.2
In this example, we show how the time step size restriction can be inconvenient. Let us consider the start values $u_0 = 10$ and $\dot{u}_0 = 0$. Then, independently of the choice of the moving surface $\Gamma(t)$, the exact solution of the wave equation (10.7) remains constant for all time (i.e., $u(x,t) = 10$). In Figure 15.2, we show snapshots of the discrete solution at times $t = 0, 1, 1.5, 2, 2.5$ (from top to bottom). Since the exact solution is constant, the torus is not supposed to change its color. On the left-hand side of Figure 15.2, the discrete solution is obtained by using the Leapfrog method. We start with a small step size $\tau = \frac{1}{128}$ in order to fulfill the CFL-condition at time $t = 0$. However, due to the movement of the mesh (i.e., h might decrease), there is no guarantee for the CFL-condition to remain fulfilled. E.g., see the last two snapshots on the left-hand side of Figure 15.2. One could, of course, use the smallest occurring h. However, in the present example, this does not give an accurate solution in a reasonable computing time. On the contrary, the implicit midpoint rule integrates this problem without difficulty. By choosing the time step size $\tau = \frac{1}{32}$, it takes only a few seconds to integrate until $t = 2.5$ and to obtain a good approximation of the exact solution as we clearly recognize from the right-hand side of Figure 15.2.

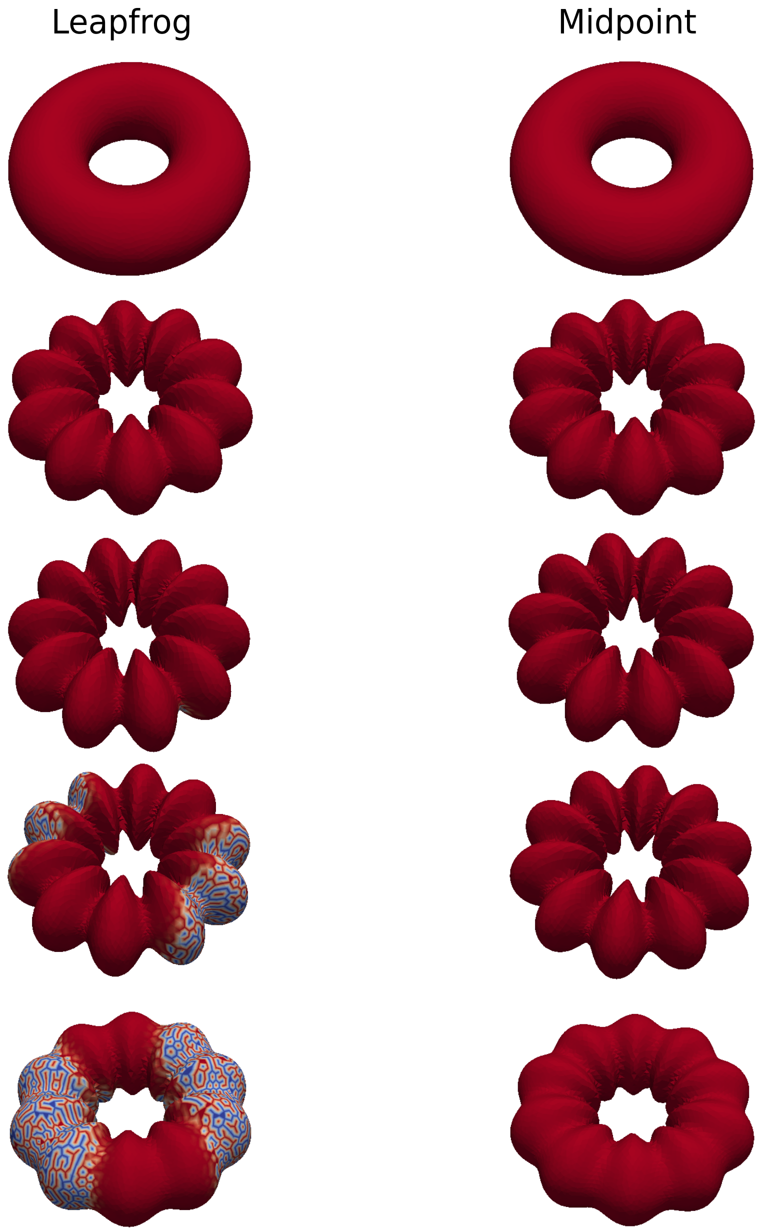


Figure 15.2.: Snapshots of the discrete solution of the wave equation using the Leapfrog method (left) and the implicit midpoint rule (right). The exact solution is constant: $u = 10$.

Example 15.3
We choose a time-dependent surface of the form

$$\Gamma(t) := \left\{ x_1 + \max(0, x_1)t, \frac{g(x,t)x_2}{\sqrt{x_2^2+x_3^2}}, \frac{g(x,t)x_3}{\sqrt{x_2^2+x_3^2}} : x \in \Gamma(0) = S^2 \right\}, \quad (15.3)$$

$$g(x,t) = e^{-2t}\sqrt{x_2^2+x_3^2} + (1-e^{-2t})\left(\left(1-x_1^2\right)\left(x_1^2+0.05\right) + x_1^2\sqrt{(1-x_1^2)}\right).$$

We consider the wave equation (15.1) posed on the above surface on the time interval $[0,3]$, with right hand side $f = 0$ and initial data $u(x,0) = e^{-5|x-x_0|^2} + e^{-5|x-x_1|^2}$, where $x_0 = (1,0,0), x_1 = (-1,0,0)$, and $\partial^\bullet u(x,0) = 0$. The surface evolves from an initially spherical shape at $t = 0$ to a "baseball bat" like shape. Simultaneously we observe a wave traveling from the right to the left and another from the left to the right. They superimpose for a short time and cross paths without any dissipation. We choose the time step $\tau = 5 \times 10^{-4}$, in order to satisfy the CFL condition (12.11). Figure 1 shows snapshots of the discrete solution at time $t = 0, 0.8, 1.2, 1.8, 2.2, 3$ from the left to the right.

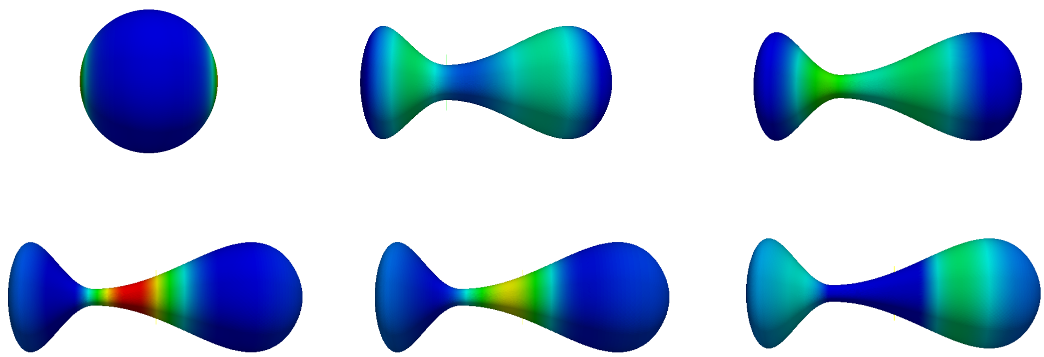


Figure 15.3.: Snapshots of the discrete solution of the wave equation on a time-dependent surface of the form (15.3) reading from the left to the right at time $t = 0, 0.8, 1.2, 1.8, 2.2, 3$.

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