

Runge–Kutta time discretization of parabolic differential equations on evolving surfaces

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A linear parabolic differential equation on a moving surface is first discretized in space by evolving surface finite elements and then in time by an implicit Runge–Kutta method. For algebraically stable and stiffly accurate Runge–Kutta methods, unconditional stability of the full discretization is proven and the convergence properties are analysed. Moreover, the implementation is described for the case of the Radau IIA time discretization. Numerical experiments illustrate the behaviour of the fully discrete method.

Keywords: parabolic PDE, evolving surface finite element method, implicit Runge–Kutta method

1. Introduction

Partial differential equations on surfaces appear in many applications. They arise in material sciences, fluid mechanics and bio-physics [1], [9], [4], and it is important to discretize these PDEs by efficient methods. The basic linear parabolic PDE on a moving surface is

$$\dot{u} + u\nabla_{\Gamma(t)} \cdot v - \Delta_{\Gamma(t)} u = f \quad \text{on } \Gamma(t). \quad (1.1)$$

The moving surface $\Gamma(t)$ with velocity $v = v(x, t)$ is given and the solution $u = u(x, t)$ ($x \in \Gamma(t), 0 \leq t \leq T$) has to be computed. In [2] the evolving surface finite element method (ESFEM) was introduced in order to solve this model problem of diffusion and advection on a given moving surface. The work [2] develops a spatial discretization of (1.1) with piecewise linear finite elements. The moving surface $\Gamma(t)$ is approximated by a moving discrete surface $\Gamma_h(t)$. An error analysis of this spatial discretization is given in [2] and [3].

The semi-discretization in space of (1.1) with piecewise linear surface finite elements leads to an ODE system of the form

$$\frac{d}{dt} (M(t)U(t)) + A(t)U(t) = F(t), \quad (1.2)$$

where $M(t)$ is the evolving mass matrix and $A(t)$ is the evolving stiffness matrix. $U(t)$ denotes the coefficient vector of the spatially discrete solution and $F(t)$ is the discrete right-hand side.

Here we treat implicit Runge–Kutta time discretizations for the spatially discretized problem (1.2), aiming for temporal stability uniformly in the space discretization and for higher-order bounds for the temporal error. Our key technical novelties are Lemma 4.1, which provides for an abstract framework in which we can treat the spatially discretized equation, and Lemma 7.1, which yields a stability estimate in the natural time-dependent norms for Runge–Kutta methods that are algebraically stable and stiffly accurate, such as the Radau IIA methods.

The paper is organized as follows: In Section 2 we recall the basic notation for PDEs on evolving surfaces. In Section 3 we describe the spatial discretization of (1.1) with piecewise linear finite elements and derive the ODE system. Section 5 contains the numerical procedure for the solution of the ODE system. Sections 7 and 8 are devoted to stability estimates and error bounds. In Section 10 we describe the implementation of the time-stepping method and in Section 11 we give computational examples.

2. Parabolic equations on evolving surfaces

Assume that $\Gamma(t)$, $t \in [0, T]$, is a smoothly evolving family of smooth d -dimensional hypersurfaces in \mathbb{R}^{d+1} . By $v = v(x, t)$ we denote the vector valued given smooth velocity of the surface. Each surface is assumed to be compact. The conservation of a scalar quantity $u = u(x, t)$, $x \in \Gamma(t)$, $t \in [0, T]$ with a linear diffusive flux on $\Gamma(t)$ can be modelled by the linear parabolic partial differential equation

$$\dot{u} + u \nabla_{\Gamma} \cdot v - \Delta_{\Gamma} u = f \text{ on } \Gamma \quad (2.1)$$

together with the initial condition $u = u_0$ on $\Gamma_0 = \Gamma(0)$. See [2] for a derivation of the PDE. By a dot we denote the material derivative

$$\dot{u} = \frac{\partial u}{\partial t} + v \cdot \nabla u, \quad (2.2)$$

where here and in the following $a \cdot b = \sum_{j=1}^{d+1} a_j b_j$ for vectors a and b in \mathbb{R}^{d+1} . ∇ denotes the usual $d + 1$ -dimensional gradient. The material derivative \dot{u} only depends on the values of the function u on the space-time surface

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

Note that in general the quantities $\frac{\partial u}{\partial t}$ or ∇u do not make sense on G_T and only their combination in the material derivative (2.2) is well defined.

By ∇_{Γ} we denote the surface or tangential gradient on the surface Γ . This gradient is the projection to the tangent space of the $d + 1$ -dimensional gradient. For a smooth function g defined in a neighbourhood of Γ we define

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

where n is a normal vector field to Γ . The components of the surface gradient are written as $\nabla_{\Gamma} g = ((\nabla_{\Gamma})_1 g, \dots, (\nabla_{\Gamma})_{d+1} g)$. The tangential gradient only depends on the values of g on

the surface Γ and not on the extension. For a more detailed discussion we refer to [5] and [2]. The Laplace-Beltrami operator on Γ then is defined as the tangential divergence of the tangential gradient:

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

Since Green's formula holds on surfaces (here without boundary), a weak form of (2.1) is derived easily:

$$\frac{d}{dt} \int_{\Gamma} u \varphi + \int_{\Gamma} \nabla_{\Gamma} u \cdot \nabla_{\Gamma} \varphi = \int_{\Gamma} u \dot{\varphi} + \int_{\Gamma} f \varphi. \quad (2.3)$$

for all smooth $\varphi : G_T \rightarrow \mathbb{R}$. Here one has used the Leibniz formula respectively the transport theorem on surfaces,

$$\frac{d}{dt} \int_{\Gamma} g = \int_{\Gamma} \dot{g} + g \nabla_{\Gamma} \cdot v.$$

We will use a similar rule for discrete surfaces, see Lemma 3.1.

3. The evolving surface finite element method

The weak form (2.3) serves as basis for a spatial finite element discretization of the PDE. But in order to be able to compute all quantities, we first discretize the evolving surface itself. We approximate (interpolate) the smooth surface $\Gamma(t)$ by a discrete polygonal surface $\Gamma_h(t)$ homeomorphic to $\Gamma(t)$, where h denotes the grid size. Then

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

is the union of d -dimensional non degenerate simplices T which form an admissible triangulation $\mathcal{T}(t)$. Details of this construction can be found in [2]. We assume that the diameter of each simplex T , $h(T)$, satisfies the bounds $c^{-1}h \leq h(T) \leq ch$ with a positive constant c uniformly for all times. Here $h = \max_{T \in \mathcal{T}} h(T)$.

On the discrete surface Γ_h we use a surface gradient, which has to be understood in a piecewise sense:

$$\nabla_{\Gamma_h} g = \nabla g - \nabla g \cdot n_h n_h.$$

n_h denotes the normal to the discrete surface.

As finite element space on the discrete surface $\Gamma_h(t)$ we choose

$$S_h(t) = \{u_h \in C^0(\Gamma_h(t)) \mid u_h|_T \in \mathbb{P}_1, T \in \mathcal{T}(t)\}.$$

Let $\phi_j(\cdot, t)$ ($j = 1, \dots, N$) be the nodal basis of $S_h(t)$, $\phi_j(a_i(t), t) = \delta_{ji}$, so that

$$S_h(t) = \text{span}\{\phi_1(\cdot, t), \dots, \phi_N(\cdot, t)\}.$$

The vertices $a_j(t)$, $j = 1, \dots, N$ of the simplices are taken to sit on the smooth surface $\Gamma(t)$. The discrete surface has to be evolved by a piecewise linear velocity in order to stay a polygonal surface. We define the discrete velocity of the discrete surface by

$$v_h(x, t) = \sum_{j=1}^N v(a_j(t), t) \phi_j(x, t)$$

Now define an adequate discrete material derivative on the discrete evolving surface,

$$\dot{u}_h = \frac{\partial u_h}{\partial t} + v_h \cdot \nabla u_h. \quad (3.1)$$

Note that there is a slight clash of notation, since the dot is used for continuous and discrete material derivative. But it will always be clear from the context which material derivative is meant.

A very important property of the finite element space is that the (discrete) material derivative of the basis functions vanishes:

$$\dot{\phi}_j = 0. \quad (3.2)$$

We now discretize the PDE spatially by piecewise linear finite elements. For given initial value $u_h(\cdot, 0) = u_{h0} \in S_h(0)$ we solve the system

$$\frac{d}{dt} \int_{\Gamma_h} u_h \varphi_h + \int_{\Gamma_h} \nabla_{\Gamma_h} u_h \cdot \nabla_{\Gamma_h} \varphi_h = \int_{\Gamma_h} u_h \dot{\varphi}_h + \int_{\Gamma_h} f^{-l} \varphi_h \quad \forall \varphi_h \in S_h(t). \quad (3.3)$$

Here by $f^{-l} : \Gamma_h \rightarrow \mathbb{R}$ we understand the extension of the function $f : \Gamma \rightarrow \mathbb{R}$ constantly in normal direction to Γ . For a function $f_h : \Gamma_h \rightarrow \mathbb{R}$, we let $f_h^l : \Gamma \rightarrow \mathbb{R}$ be such that $(f_h^l)^{-l} = f_h$.

Under suitable regularity assumptions an error estimate between continuous solution u and spatially discrete solution u_h was proved in [2]:

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

The work [3] contains an optimal error estimate in the L^2 -norm

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

The discrete form (3.3) of PDE (2.1) is a system of ODEs. Let us derive a standard form for this system. We define the evolving mass matrix $M(t)$ and the stiffness matrix $A(t)$ by

$$M(t)_{ij} = \int_{\Gamma_h(t)} \phi_i(\cdot, t) \phi_j(\cdot, t), \quad A(t)_{ij} = \int_{\Gamma_h(t)} \nabla_{\Gamma_h(t)} \phi_i(\cdot, t) \cdot \nabla_{\Gamma_h(t)} \phi_j(\cdot, t)$$

for $i, j = 1, \dots, N$. The mass matrix is symmetric and positive definite. The stiffness matrix is symmetric and positive semidefinite only, because we are solving on closed surfaces. We denote the discrete solution by

$$u_h(x, t) = \sum_{j=1}^N u_j(t) \phi_j(x, t)$$

and define $u(t) \in \mathbb{R}^N$ as the column vector with entries $u_j(t)$. Then (3.3) can be written as

$$\frac{d}{dt} (M(t)u(t)) + A(t)u(t) = f(t), \quad (3.4)$$

where we use $f = (f_1, \dots, f_N)$ with $f_j = \int_{\Gamma_h} f^{-l} \phi_j$.

For the convenience of the reader we give the arguments for the equivalence of (3.3) and (3.4). The ODE (3.4) follows from (3.3) by choosing $\varphi_h = \phi_j$ for $j = 1, \dots, N$ and using (3.2). For the other direction let $\varphi_h(x, t) = \sum_{j=1}^N \alpha_j(t) \phi_j(x, t)$. Then with (3.2) we have $\dot{\varphi}_h = \sum_{j=1}^N \dot{\alpha}_j \phi_j$ and consequently

$$\begin{aligned} & \frac{d}{dt} \int_{\Gamma_h} u_h \varphi_h + \int_{\Gamma_h} \nabla_{\Gamma_h} u_h \cdot \nabla_{\Gamma_h} \varphi_h - \int_{\Gamma_h} f^{-l} \varphi_h \\ &= \frac{d}{dt} \left(\sum_{j=1}^N \alpha_j \int_{\Gamma_h} u_h \phi_j \right) + \sum_{j=1}^N \alpha_j \int_{\Gamma_h} \nabla_{\Gamma_h} u_h \cdot \nabla_{\Gamma_h} \phi_j - \sum_{j=1}^N \alpha_j \int_{\Gamma_h} f^{-l} \phi_j \\ &= \sum_{j=1}^N \alpha_j \underbrace{\left(\frac{d}{dt} \int_{\Gamma_h} u_h \phi_j + \int_{\Gamma_h} \nabla_{\Gamma_h} u_h \cdot \nabla_{\Gamma_h} \phi_j - \int_{\Gamma_h} f^{-l} \phi_j \right)}_{=0 \text{ by (3.4)}} + \sum_{j=1}^N \dot{\alpha}_j \int_{\Gamma_h} u_h \phi_j \\ &= \int_{\Gamma_h} u_h \sum_{j=1}^N \dot{\alpha}_j \phi_j = \int_{\Gamma_h} u_h \dot{\varphi}_h. \end{aligned}$$

We will need the following formulae for the derivative of surface integrals with respect to a parameter.

LEMMA 3.1 Let $\Gamma_h(t)$, $t \in [0, T]$ be a discrete evolving surface and $w_h(\cdot, t), z_h(\cdot, t) \in S_h(t)$ be given functions. Then

$$\frac{d}{dt} \int_{\Gamma_h} w_h z_h = \int_{\Gamma_h} \dot{w}_h z_h + w_h \dot{z}_h + w_h z_h \nabla_{\Gamma} \cdot v_h. \quad (3.5)$$

With the tensor

$$D(v_h)_{ij} = \delta_{ij} \nabla_{\Gamma_h} \cdot v_h - ((\nabla_{\Gamma_h})_i v_{hj} + (\nabla_{\Gamma_h})_j v_{hi})$$

($i, j = 1, \dots, n$) we have for the derivative of Dirichlet's integral

$$\frac{1}{2} \frac{d}{dt} \int_{\Gamma_h} |\nabla_{\Gamma_h} w_h|^2 = \int_{\Gamma_h} \nabla_{\Gamma_h} w_h \cdot \nabla_{\Gamma_h} \dot{w}_h + \frac{1}{2} \int_{\Gamma_h} D(v_h) \nabla_{\Gamma_h} w_h \cdot \nabla_{\Gamma_h} w_h. \quad (3.6)$$

A proof of this Lemma was given in [2] for smooth surfaces. The proof is easily adapted to evolving discrete surfaces.

4. The ODE system

We consider the large system of ordinary differential equations (3.4) on \mathbb{R}^N , viz.,

$$\frac{d}{dt} (M(t)u(t)) + A(t)u(t) = f(t), \quad u(0) = u_0, \quad (4.1)$$

with symmetric positive definite matrix $M(t)$ and symmetric positive semidefinite matrix $A(t)$. With the finite element method these matrices are sparse.

We work with the norm

$$|w|_t^2 = \langle w | M(t) | w \rangle = w \cdot M(t)w, \quad w \in \mathbb{R}^N,$$

and the semi-norm

$$\|w\|_t^2 = \langle w | A(t) | w \rangle = w \cdot A(t)w, \quad w \in \mathbb{R}^N.$$

LEMMA 4.1 There are constants μ, κ (independent of the discretization parameter h and the length of the time interval T) such that

$$w \cdot (M(s) - M(t))z \leq (e^{\mu(s-t)} - 1) |w|_t |z|_t \quad (4.2)$$

$$w \cdot (A(s) - A(t))z \leq (e^{\kappa(s-t)} - 1) \|w\|_t \|z\|_t \quad (4.3)$$

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

We will apply this lemma with s close to t . Note that then $e^{\mu(s-t)} - 1 \leq 2\mu(s-t)$ and $e^{\kappa(s-t)} - 1 \leq 2\kappa(s-t)$. Apart from the fact that $M(t)$ and $A(t)$ are symmetric positive semi-definite, the inequalities (4.2)-(4.3) are the only properties of the evolving-surface finite-element equations (4.1) that will be used in the stability analysis of their time discretizations.

Proof. For $w, z \in \mathbb{R}^N$ we define the discrete functions $w_h(x, t) = \sum_{j=1}^N w_j \phi_j(x, t)$ and $z_h(x, t) = \sum_{j=1}^N z_j \phi_j(x, t)$. Note that $\dot{w}_h = \dot{z}_h = 0$. Then by the transport formula from Lemma 3.1 we have

$$\begin{aligned} w \cdot (M(s) - M(t))z &= \int_{\Gamma_h(s)} w_h(\cdot, s) z_h(\cdot, s) - \int_{\Gamma_h(t)} w_h(\cdot, t) z_h(\cdot, t) \\ &= \int_t^s \frac{d}{d\sigma} \int_{\Gamma_h(\sigma)} w_h(\cdot, \sigma) z_h(\cdot, \sigma) d\sigma \\ &= \int_t^s \int_{\Gamma_h(\sigma)} w_h(\cdot, \sigma) z_h(\cdot, \sigma) \nabla_{\Gamma_h(\sigma)} \cdot v_h d\sigma \\ &\leq \mu \int_t^s \|w_h\|_{L^2(\Gamma_h(\sigma))} \|z_h\|_{L^2(\Gamma_h(\sigma))} d\sigma \\ &= \mu \int_t^s |w|_\sigma |z|_\sigma d\sigma \end{aligned}$$

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

$$|w|_s^2 \leq |w|_t^2 + \mu \int_t^s |w|_\sigma^2 d\sigma, \quad 0 \leq t \leq s \leq T,$$

and hence the Gronwall inequality yields

$$|w|_s^2 \leq e^{\mu(s-t)} |w|_t^2.$$

Inserting this bound for $|w|_\sigma$ and $|z|_\sigma$ in the above inequality yields the first inequality (4.2).

With Lemma 3.1 we get for the matrix A

$$\begin{aligned} w \cdot (A(s) - A(t))z &= \int_{\Gamma_h(s)} \nabla_{\Gamma_h(s)} w_h(\cdot, s) \cdot \nabla_{\Gamma_h(s)} z_h(\cdot, s) - \int_{\Gamma_h(t)} \nabla_{\Gamma_h(t)} w_h(\cdot, t) \cdot \nabla_{\Gamma_h(t)} z_h(\cdot, t) \\ &= \int_t^s \frac{d}{d\sigma} \int_{\Gamma_h(\sigma)} \nabla_{\Gamma_h(\sigma)} w_h(\cdot, \sigma) \cdot \nabla_{\Gamma_h(\sigma)} z_h(\cdot, \sigma) d\sigma. \end{aligned}$$

Polarization of formula (3.6), keeping in mind that $\dot{w}_h = \dot{z}_h = 0$ here, gives

$$\begin{aligned} & w \cdot (A(s) - A(t)) z \\ &= \int_t^s \int_{\Gamma_h(\sigma)} D(v_h(\cdot, \sigma)) \nabla_{\Gamma_h(\sigma)} w_h(\cdot, \sigma) \cdot \nabla_{\Gamma_h(\sigma)} z_h(\cdot, \sigma) d\sigma \\ &\leq \kappa \int_t^s \|w\|_\sigma \|z\|_\sigma d\sigma \end{aligned}$$

since $\max_{\sigma \in [t, s]} \|D(v_h(\cdot, \sigma))\|_{L^\infty(\Gamma_h(\sigma))}$ is uniformly bounded by a constant κ . Using this inequality together with the Gronwall inequality as above yields (4.3). \square

5. Runge–Kutta time discretization

Method description. We reformulate (4.1) as the system ($\dot{\cdot} = d/dt$)¹

$$\begin{aligned} \dot{y}(t) + A(t)u(t) &= f(t) \\ y(t) &= M(t)u(t) \end{aligned} \tag{5.1}$$

and apply an m -stage implicit RK method in the standard way for differential-algebraic equations [6, 7] (for ease of notation we take constant step size τ , this is not essential): we determine the approximation u_{n+1} to $u(t_{n+1})$ at $t_{n+1} = t_n + \tau$ in a time step starting from u_n via internal stages U_{ni}, Y_{ni} and increments $\dot{U}_{ni}, \dot{Y}_{ni}$ (here the dot is only suggestive notation) by equations of the form (5.1),

$$\begin{aligned} \dot{Y}_{ni} + A_{ni}U_{ni} &= F_{ni} \\ Y_{ni} &= M_{ni}U_{ni} \end{aligned} \tag{5.2}$$

for $i = 1, \dots, m$ with $A_{ni} = A(t_n + c_i\tau)$, $M_{ni} = M(t_n + c_i\tau)$, $F_{ni} = f(t_n + c_i\tau)$, satisfying the RK relations

$$\begin{aligned} u_{n+1} &= u_n + \tau \sum_{j=1}^m b_j \dot{U}_{nj} \\ U_{ni} &= u_n + \tau \sum_{j=1}^m a_{ij} \dot{U}_{nj} \quad (i = 1, \dots, m) \end{aligned}$$

and in the same way

$$\begin{aligned} y_{n+1} &= y_n + \tau \sum_{j=1}^m b_j \dot{Y}_{nj} \\ Y_{ni} &= y_n + \tau \sum_{j=1}^m a_{ij} \dot{Y}_{nj} \quad (i = 1, \dots, m) \end{aligned}$$

¹There should be no confusion about the different uses of the dot notation. The dot represents a material derivative in the PDE context, it represents a time derivative in the ODE context, and it is merely suggestive notation in the Runge–Kutta schemes.

Method assumptions. The method is characterized by its coefficients a_{ij}, b_j, c_i with $0 \leq c_i \leq 1$. We assume that the method has stage order $q \geq 1$ and classical order $p \geq q$. The RK coefficient matrix (a_{ij}) is assumed invertible, and we denote its inverse by (w_{ij}) .

The method is *algebraically stable*: the $m \times m$ matrix

$$(b_i a_{ij} + b_j a_{ji} - b_i b_j) \text{ is positive semi-definite, and all } b_i > 0, \quad (5.3)$$

and it is *stiffly accurate*:

$$c_m = 1 \quad \text{and} \quad b_j = a_{mj} \quad \text{for } j = 1, \dots, m, \quad (5.4)$$

which implies

$$u_{n+1} = U_{nm}, \quad y_{n+1} = Y_{nm}, \quad y_{n+1} = M_{n+1} u_{n+1}$$

with $M_{n+1} = M(t_{n+1})$.

Well-known examples are the collocation methods at Radau nodes, of stage order $q = m$ and classical order $p = 2m - 1$.

6. Defects and errors

Defects. The solution of (4.1) satisfies the RK relations up to a defect (quadrature error)

$$\begin{aligned} u(t_{n+1}) &= u(t_n) + \tau \sum_{j=1}^m b_j \dot{u}(t_n + c_j \tau) + \delta_{n+1} \\ u(t_n + c_i \tau) &= u(t_n) + \tau \sum_{j=1}^m a_{ij} \dot{u}(t_n + c_j \tau) + \Delta_{ni} \quad (i = 1, \dots, m) \end{aligned}$$

and

$$\begin{aligned} y(t_{n+1}) &= y(t_n) + \tau \sum_{j=1}^m b_j \dot{y}(t_n + c_j \tau) + r_{n+1} \\ y(t_n + c_i \tau) &= y(t_n) + \tau \sum_{j=1}^m a_{ij} \dot{y}(t_n + c_j \tau) + R_{ni} \quad (i = 1, \dots, m) \end{aligned}$$

By the assumption of stiff accuracy, we have

$$\delta_{n+1} = \Delta_{nm}, \quad r_{n+1} = R_{nm}.$$

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

$$\begin{aligned} \delta_{n+1} &= O(\tau^{p+1}), \quad \Delta_{ni} = O(\tau^{q+1}) \\ r_{n+1} &= O(\tau^{p+1}), \quad R_{ni} = O(\tau^{q+1}). \end{aligned}$$

Errors. We consider the errors

$$\begin{aligned} e_n &= u_n - u(t_n) \\ E_{ni} &= U_{ni} - u(t_n + c_i \tau) \\ \dot{E}_{ni} &= \dot{U}_{ni} - \dot{u}(t_n + c_i \tau) \end{aligned}$$

and

$$\begin{aligned}\ell_n &= y_n - y(t_n) = M_n e_n \\ L_{ni} &= Y_{ni} - y(t_n + c_i \tau) = M_{ni} E_{ni} \\ \dot{L}_{ni} &= \dot{Y}_{ni} - \dot{y}(t_n + c_i \tau)\end{aligned}$$

Error equations. We subtract to obtain

$$\dot{L}_{ni} + A_{ni} E_{ni} = 0 \quad (6.1)$$

$$L_{ni} = M_{ni} E_{ni} \quad (6.2)$$

and RK relations with defects:

$$e_{n+1} = e_n + \tau \sum_{j=1}^m b_j \dot{E}_{nj} - \delta_{n+1} \quad (6.3)$$

$$E_{ni} = e_n + \tau \sum_{j=1}^m a_{ij} \dot{E}_{nj} - \Delta_{ni} \quad (i = 1, \dots, m) \quad (6.4)$$

and

$$\ell_{n+1} = \ell_n + \tau \sum_{j=1}^m b_j \dot{L}_{nj} - r_{n+1} \quad (6.5)$$

$$L_{ni} = \ell_n + \tau \sum_{j=1}^m a_{ij} \dot{L}_{nj} - R_{ni} \quad (i = 1, \dots, m). \quad (6.6)$$

We note

$$\ell_{n+1} = L_{nm} = M_{nm} E_{nm} = M_{n+1} e_{n+1}. \quad (6.7)$$

Modified error equations. It turns out to be favourable to work with modifications of \dot{E}_{nj} in the stability and error analysis. We set

$$E'_{nj} = \dot{E}_{nj} + \tau^{-1} \sum_{j=1}^m w_{ji} (M_n^{-1} R_{ni} - \Delta_{ni}). \quad (6.8)$$

Then (6.4) becomes

$$E_{ni} = e_n + \tau \sum_{j=1}^m a_{ij} E'_{nj} - D_{ni} \quad \text{with} \quad D_{ni} = M_n^{-1} R_{ni}, \quad (6.9)$$

and, in view of (5.4), Eq. (6.3) turns into

$$e_{n+1} = e_n + \tau \sum_{j=1}^m b_j E'_{nj} - d_{n+1} \quad \text{with} \quad d_{n+1} = M_n^{-1} r_{n+1}. \quad (6.10)$$

With this modification, the defects Δ_{ni} and δ_{n+1} have disappeared from the error equations and the defects in (6.5)-(6.6) and (6.9)-(6.10) are related in a way that is very helpful in the stability analysis.

7. Stability

The following is the technical key result of this paper.

LEMMA 7.1 If the Runge–Kutta method is algebraically stable and stiffly accurate, then there exist $\tau_0 > 0$ depending only on μ, κ of Lemma 4.1 and C_T depending on μ, κ, T such that for $\tau \leq \tau_0$ and $t_n \leq T$, the errors are bounded by

$$|e_n|_{t_n}^2 + \tau \sum_{k=1}^n \|e_k\|_{t_k}^2 \leq C_T \tau \sum_{k=1}^n |d_k/\tau|_{t_k}^2 + C_T \tau \sum_{k=0}^{n-1} \sum_{i=1}^m \left(\|D_{ki}\|_{t_k}^2 + |D_{ki}|_{t_k}^2 \right).$$

Proof. The proof uses algebraic stability and stiff accuracy similarly to the proof of Theorem 1.1 in [11], but here works with the time-dependent norms and the modified error equations of the previous section.

(a) For brevity, we write $|\cdot|_n$ instead of $|\cdot|_{t_n}$. We start from (6.10), take the squared norm at t_{n+1} and estimate the terms in

$$|e_{n+1}|_{n+1}^2 = \left| e_n + \tau \sum_{j=1}^m b_j E'_{nj} \right|_{n+1}^2 - 2 \left\langle e_n + \tau \sum_{j=1}^m b_j E'_{nj} \mid M_{n+1} \mid d_{n+1} \right\rangle + |d_{n+1}|_{n+1}^2. \quad (7.1)$$

Expressing e_n by (6.9), we obtain for the first term

$$\begin{aligned} \left| e_n + \tau \sum_{j=1}^m b_j E'_{nj} \right|_{n+1}^2 &= |e_n|_{n+1}^2 + 2\tau \sum_{j=1}^m b_j \langle E'_{nj} \mid M_{n+1} \mid E_{nj} + D_{nj} \rangle \\ &\quad + \tau^2 \sum_{i=1}^m \sum_{j=1}^m (b_i b_j - b_i a_{ij} - b_j a_{ji}) \langle E'_{ni} \mid M_{n+1} \mid E'_{nj} \rangle, \end{aligned} \quad (7.2)$$

where the last term is non-positive by the assumption of algebraic stability (5.3). In the second and third term we write $M_{n+1} = M_n + (M_{n+1} - M_n)$. By condition (4.2) we have

$$\begin{aligned} |e_n|_{n+1}^2 &= \langle e_n \mid M_{n+1} \mid e_n \rangle = \langle e_n \mid M_n \mid e_n \rangle + \langle e_n \mid M_{n+1} - M_n \mid e_n \rangle \\ &\leq (1 + 2\mu\tau) |e_n|_n^2. \end{aligned} \quad (7.3)$$

In the middle term we write

$$\langle E'_{nj} \mid M_{n+1} \mid E_{nj} + D_{nj} \rangle = \langle E'_{nj} \mid M_n \mid E_{nj} + D_{nj} \rangle + \langle E'_{nj} \mid M_{n+1} - M_n \mid E_{nj} + D_{nj} \rangle \quad (7.4)$$

and estimate the two terms on the right separately.

(b) In the first term we express $M_n E'_{nj}$ in terms of \dot{L}_{nj} as follows. By (6.6) we have

$$\dot{L}_{nj} = \tau^{-1} \sum_{i=1}^m w_{ji} (L_{ni} - \ell_n + R_{ni}).$$

By (6.2) we have $L_{ni} = M_{ni} E_{ni}$ and, using once more (6.9),

$$\ell_n = M_n e_n = M_n E_{ni} - \tau \sum_{k=1}^m a_{ik} M_n E'_{nk} + M_n D_{ni},$$

so that we obtain, recalling $R_{ni} = M_n D_{ni}$,

$$\dot{L}_{nj} = M_n E'_{nj} + \tau^{-1} \sum_{i=1}^m w_{ji} (M_{ni} - M_n) E_{ni}.$$

On the other hand, by (6.1) we have

$$\dot{L}_{nj} = -A_{nj} E_{nj} = -A_n E_{nj} - (A_{nj} - A_n) E_{nj}.$$

Combining these equations yields

$$\begin{aligned} \langle E'_{nj} | M_n | E_{nj} + D_{nj} \rangle &= -\langle E_{nj} | A_n | E_{nj} + D_{nj} \rangle \\ &\quad - \langle E_{nj} | A_{nj} - A_n | E_{nj} + D_{nj} \rangle \\ &\quad - \tau^{-1} \sum_{i=1}^m w_{ji} \langle E_{ni} | M_{ni} - M_n | E_{nj} + D_{nj} \rangle. \end{aligned}$$

These terms are now estimated using the Cauchy-Schwarz inequality, Young's inequality, and (4.2)-(4.3):

$$\begin{aligned} -\langle E_{nj} | A_n | E_{nj} + D_{nj} \rangle &\leq -\|E_{nj}\|_n^2 + \|E_{nj}\|_n \|D_{nj}\|_n \\ &\leq -\frac{3}{4} \|E_{nj}\|_n^2 + \|D_{nj}\|_n^2 \\ -\langle E_{nj} | A_{nj} - A_n | E_{nj} + D_{nj} \rangle &\leq 2\kappa\tau \|E_{nj}\|_n \|E_{nj} + D_{nj}\|_n \\ &\leq 3\kappa\tau \|E_{nj}\|_n^2 + \kappa\tau \|D_{nj}\|_n^2 \\ |\langle E_{ni} | M_{ni} - M_n | E_{nj} + D_{nj} \rangle| &\leq 2\mu\tau |E_{ni}|_n |E_{nj} + D_{nj}|_n \\ &\leq 2\mu\tau |E_{ni}|_n^2 + \mu\tau |E_{nj}|_n^2 + \mu\tau |D_{nj}|_n^2. \end{aligned}$$

Taken all together, the first term on the right-hand side of (7.4) is bounded, for sufficiently small τ , by

$$\begin{aligned} \langle E'_{nj} | M_n | E_{nj} + D_{nj} \rangle &\leq -\frac{2}{3} \|E_{nj}\|_n^2 + C \sum_{i=1}^m |E_{ni}|_n^2 \\ &\quad + C \|D_{nj}\|_n^2 + C |D_{nj}|_n^2. \end{aligned} \tag{7.5}$$

(c) To bound the last term in (7.4), we rewrite (6.9) as

$$E'_{nj} = \tau^{-1} \sum_{i=1}^m w_{ji} (E_{ni} - e_n + D_{ni})$$

and use (4.2) to estimate

$$\langle E'_{nj} | M_{n+1} - M_n | E_{nj} + D_{nj} \rangle \leq C |e_n|_n^2 + C \sum_{i=1}^m |E_{ni}|_n^2 + C \sum_{i=1}^m |D_{ni}|_n^2. \tag{7.6}$$

(d) The second term on the right-hand side of (7.1) is estimated using (5.4) as

$$e_n + \tau \sum_{j=1}^m b_j E'_{nj} = e_n + \tau \sum_{j=1}^m a_{mj} E'_{nj} = E_{nm} + D_{nm} = E_{nm} + d_{n+1}$$

and the Cauchy-Schwarz inequality and (4.2) to obtain

$$\begin{aligned} 2 \langle e_n + \tau \sum_{j=1}^m b_j E'_{nj} \mid M_{n+1} \mid d_{n+1} \rangle &\leq 2 |E_{nm} + d_{n+1}|_{n+1} |d_{n+1}|_{n+1} \\ &\leq \tau(1 + 2\mu\tau) |E_{nm}|_n^2 + (1 + 2\tau)\tau |d_{n+1}/\tau|_{n+1}^2. \end{aligned} \quad (7.7)$$

(e) The above bounds contain terms $|E_{ni}|_n^2$ which we further estimate. With (6.4), we rewrite

$$|E_{ni}|_n^2 = \langle e_n \mid M_n \mid E_{ni} \rangle + \tau \sum_{j=1}^m a_{ij} \langle E'_{nj} \mid M_n \mid E_{ni} \rangle - \langle D_{ni} \mid M_n \mid E_{ni} \rangle.$$

The first term on the right-hand side is estimated as

$$\langle e_n \mid M_n \mid E_{ni} \rangle \leq |e_n|_n |E_{ni}|_n \leq \frac{1}{2}\delta |E_{ni}|_n^2 + \frac{1}{2}\delta^{-1} |e_n|_n^2$$

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

$$-\langle D_{ni} \mid M_n \mid E_{ni} \rangle \leq \frac{1}{2}\delta |E_{ni}|_n^2 + \frac{1}{2}\delta^{-1} |D_{ni}|_n^2.$$

As in part (b), the expressions $\langle E'_{nj} \mid M_n \mid E_{ni} \rangle$ are rewritten as

$$\begin{aligned} \langle E'_{nj} \mid M_n \mid E_{ni} \rangle &= -\langle E_{nj} \mid A_n \mid E_{ni} \rangle - \langle E_{nj} \mid A_{nj} - A_n \mid E_{ni} \rangle \\ &\quad - \tau^{-1} \sum_{k=1}^m w_{jk} \langle E_{nk} \mid M_{nk} - M_n \mid E_{ni} \rangle \end{aligned}$$

and bounded by

$$|\langle E'_{nj} \mid M_n \mid E_{ni} \rangle| \leq C \sum_{k=1}^m \|E_{nk}\|_n^2 + C \sum_{k=1}^m |E_{nk}|_n^2.$$

Hence, choosing δ sufficiently small (but independent of τ), we obtain the bound

$$|E_{ni}|_n^2 \leq C |e_n|_n^2 + C\tau \sum_{k=1}^m \|E_{nk}\|_n^2 + C \sum_{k=1}^m |D_{nk}|^2. \quad (7.8)$$

(f) Combining (7.1)–(7.8), we thus have

$$\begin{aligned} |e_{n+1}|_{n+1}^2 - |e_n|_n^2 + \frac{1}{2}\tau \sum_{j=1}^m b_j \|E_{nj}\|_n^2 &\leq C\tau |e_n|_n^2 + C\tau |d_{n+1}/\tau|_{n+1}^2 \\ &\quad + C\tau \sum_{i=1}^m \left(\|D_{ni}\|_n^2 + |D_{ni}|_n^2 \right). \end{aligned}$$

Summing over n and using a discrete Gronwall inequality finally gives the stated result. \square

8. Error bounds

If it holds that

$$\sup_{0 \leq t \leq T} \left| M(t)^{-1} \frac{d^k(Mu)}{dt^k}(t) \right|_t \leq \alpha \quad \text{for } k = q+1, q+2 \quad (8.1)$$

$$\int_0^T \left\| M(t)^{-1} \frac{d^{q+1}(Mu)}{dt^{q+1}}(t) \right\|_t^2 dt \leq \alpha^2, \quad (8.2)$$

then Lemma 7.1 yields the following error bound of order $q+1$, where q is the stage order.

THEOREM 8.1 Under the regularity conditions (8.1)-(8.2), the error of the algebraically stable and stiffly accurate Runge–Kutta discretization of stage order q and classical order $p \geq q+1$ is bounded by

$$|u_n - u(t_n)|_{t_n} + \left(\tau \sum_{k=1}^n \|u_k - u(t_k)\|_{t_k}^2 \right)^{1/2} \leq C_T \alpha \tau^{q+1}$$

for $t_n = n\tau \leq T$.

Proof. It suffices to note that under conditions (8.1)-(8.2), the Peano representation of the quadrature errors R_{ni} shows that the defects $D_{ni} = M_n^{-1} R_{ni}$ are bounded by

$$\begin{aligned} \sup_{0 \leq n\tau \leq T} |D_{ni}|_{t_n} &\leq C\alpha\tau^{q+1}, & \sup_{0 \leq n\tau \leq T} |d_n|_{t_n} &\leq C\alpha\tau^{q+2}, \\ \sum_{0 \leq n\tau \leq T} \|D_{ni}\|_{t_n}^2 &\leq (C\alpha\tau^{q+1})^2, \end{aligned}$$

and to apply Lemma 7.1. \square

The classical order p is obtained if stronger regularity conditions are satisfied. Suppose that

$$\left\| M(t)^{-1} \frac{d^{k_j-1}}{dt^{k_j-1}} (A(t)M(t)^{-1}) \dots \frac{d^{k_1-1}}{dt^{k_1-1}} (A(t)M(t)^{-1}) \frac{d^l}{dt^l} (M(t)u(t)) \right\|_t \leq \beta$$

$$\text{for all } k_1 \geq 1, \dots, k_j \geq 1 \text{ and } l \geq q+1 \text{ with } k_1 + \dots + k_j + l \leq p, \quad (8.3)$$

and the same bounds in the norm $|\cdot|_t$ for $k_1 + \dots + k_j + l \leq p+1$.

(The 0-th derivative of AM^{-1} is just AM^{-1} itself.) Then, there is the following error bound of full order p .

THEOREM 8.2 Under conditions (8.3), the error of the Runge–Kutta discretization is bounded by

$$|u_n - u(t_n)|_{t_n} + \left(\tau \sum_{k=1}^n \|u_k - u(t_k)\|_{t_k}^2 \right)^{1/2} \leq C_T \beta \tau^p$$

for $t_n = n\tau \leq T$.

Proof. The proof adapts that of Theorem 1 in [12] to the present situation. The trick is to modify the error equations such that they have smaller defects. This will be achieved by an iterative procedure. Add the defect in (6.6) to L_{ni} to obtain

$$L_{ni}^{(1)} = L_{ni} + R_{ni}$$

and define $E_{ni}^{(1)}$ such that

$$L_{ni}^{(1)} = M_{ni} E_{ni}^{(1)}.$$

By (6.2), we thus have

$$E_{ni}^{(1)} = E_{ni} + M_{ni}^{-1} R_{ni}.$$

We define $\dot{L}_{ni}^{(1)}$ such that (6.1) holds for the modified errors:

$$\dot{L}_{ni}^{(1)} = -A_{ni} E_{ni}^{(1)} = \dot{L}_{ni} - A_{ni} M_{ni}^{-1} R_{ni}.$$

We determine $\dot{E}_{ni}^{(1)}$ such that no defect appears in formula (6.4) for the modified errors:

$$\dot{E}_{nj}^{(1)} = E'_{nj} = \dot{E}_{nj} + \tau^{-1} \sum_{i=1}^m w_{ji} (M_{ni}^{-1} R_{ni} - \Delta_{ni}).$$

We then get for these modified errors in the internal stages (but unmodified e_n and ℓ_n) equations (6.3)–(6.6) with modified defects

$$\begin{aligned} d_{n+1}^{(1)} &= M_{n+1}^{-1} r_{n+1}, & D_{ni}^{(1)} &= 0 \\ r_{n+1}^{(1)} &= r_{n+1} - \tau \sum_{j=1}^m b_j A_{nj} M_{nj}^{-1} R_{nj}, & R_{ni}^{(1)} &= -\tau \sum_{j=1}^m a_{ij} A_{nj} M_{nj}^{-1} R_{nj}. \end{aligned}$$

Here we used (5.4) in the formula for $d_{n+1}^{(1)}$, in the form that $\sum_{j=1}^m b_j w_{ji} = 1$ for $i = m$ and 0 else and using (6.7).

The construction is such that the defects $R_{ni}^{(1)}$ in the internal stages carry an additional factor τ compared to R_{nj} , at the price that AM^{-1} is applied to R_{nj} . The relation (6.7) is no longer fully satisfied for the modified errors, but we have

$$e_{n+1} = E_{nm}^{(1)} + d_{n+1}^{(1)}, \quad \ell_{n+1} = L_{nm}^{(1)} - r_{n+1}.$$

By the order conditions for Runge–Kutta methods, the defects d_{n+1}, r_{n+1} and $d_{n+1}^{(1)}, r_{n+1}^{(1)}$ are all $O(\tau^{p+1})$ in the norm $\|\cdot\|_{t_{n+1}}$ under the regularity conditions (8.3). The defects $R_{ni}^{(1)}$ are $O(\tau^{q+2})$, one order higher than R_{ni} .

The construction can now be continued iteratively until, after $p - q$ steps, all defects are of size $O(\tau^{p+1})$. With the stability lemma we then conclude to the full order $O(\tau^p)$ of the errors. We omit the technical details that ensure that condition (8.3) is indeed sufficient to achieve the full order p ; cf. [12] for a related situation. \square

9. Regularity estimates

We show that under suitable conditions on the evolving surfaces the assumptions (8.1) and (8.2) can be fulfilled for the time discretization of (3.3). We do this for $f = 0$.

In the following we denote time derivatives of k -th order by the superscript (k) . We also use this notation for k -th order discrete material derivatives according to (3.1). We omit the omnipresent argument t in all appearing functions and surfaces.

We start with formulae for higher order Leibniz rules.

LEMMA 9.1 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

$$\frac{d^k}{dt^k} \int_{\Gamma_h} f = \int_{\Gamma_h} f^{(k)} + \sum_{l=1}^k \int_{\Gamma_h} g_{kl} f^{(k-l)}. \quad (9.1)$$

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

$$\frac{d^k}{dt^k} \int_{\Gamma_h} \nabla_{\Gamma_h} f \cdot \nabla_{\Gamma_h} \varphi_h = \int_{\Gamma_h} \nabla_{\Gamma_h} f^{(k)} \cdot \nabla_{\Gamma_h} \varphi_h + \sum_{l=1}^k G_{kl} \nabla_{\Gamma_h} f^{(k-l)} \cdot \nabla_{\Gamma_h} \varphi_h \quad (9.2)$$

for any function φ_h with $\dot{\varphi}_h = 0$.

Proof. One easily proves this by induction with the help of the Leibniz rules from Lemma 3.1. The rule for Dirichlet's integral is used in a polarized form. \square

In the following we assume that a and B are sufficiently often continuously differentiable with respect to time. Then g_{kl} and G_{kl} are bounded independently of the grid size h and we can prove the following lemma.

LEMMA 9.2 Let $u_h = \sum_{j=1}^N u_j \phi_j$ be the solution of (3.3). Then

$$M^{-1}(Mu)^{(k)} \cdot (Mu)^{(k)} \leq c \sum_{l=0}^k \|u_h^{(l)}\|_{L^2(\Gamma_h)}^2 \quad (9.3)$$

and

$$M^{-1}(Mu)^{(k)} \cdot AM^{-1}(Mu)^{(k)} \leq c \sum_{l=0}^k (\|u_h^{(l)}\|_{L^2(\Gamma_h)}^2 + \|\nabla_{\Gamma_h} u_h^{(l)}\|_{L^2(\Gamma_h)}^2). \quad (9.4)$$

Proof. We set $w = M^{-1}(Mu)^{(k)}$ and $w_h = \sum_{j=1}^N w_j \phi_j$. We then observe

$$\int_{\Gamma_h} w_h \phi_j = \sum_{k=1}^N w_k \int_{\Gamma_h} \phi_k \phi_j = (Mw)_j = (Mu)_j^{(k)} = \frac{d^k}{dt^k} \int_{\Gamma_h} u_h \phi_j.$$

Then by Lemma 9.1 we have that

$$\int_{\Gamma_h} w_h \varphi_h = \int_{\Gamma_h} u_h^{(k)} \varphi_h + \sum_{l=1}^k \int_{\Gamma_h} g_{kl} u_h^{(k-l)} \varphi_h \quad \forall \varphi_h \in S_h(t)$$

This means that

$$w_h = u_h^{(k)} + \sum_{l=1}^k P_h(g_{kl} u_h^{(k-l)})$$

with the L^2 -projection P_h onto S_h . Here we used the fact that the material derivatives of $u_h \in S_h$ again are elements of S_h , since $\dot{\phi}_i = 0$. Then,

$$\sqrt{w \cdot Mw} = \|w_h\|_{L^2(\Gamma_h)} \leq \|u_h^{(k)}\|_{L^2(\Gamma_h)} + \sum_{l=1}^k \|g_{kl} u_h^{(k-l)}\|_{L^2(\Gamma_h)},$$

which yields (9.3). We write similarly

$$\sqrt{w \cdot Aw} = \|\nabla_{\Gamma_h} w_h\|_{L^2(\Gamma_h)} \leq \|\nabla_{\Gamma_h} u_h^{(k)}\|_{L^2(\Gamma_h)} + \sum_{l=1}^k \|\nabla_{\Gamma_h} P_h(g_{kl} u_h^{(k-l)})\|_{L^2(\Gamma_h)}. \quad (9.5)$$

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 (9.4) for the case $k = 1$ and discuss the general case later. For $k = 1$ we estimate the last term on the right hand side of (9.5) as follows:

$$\begin{aligned} & \|\nabla_{\Gamma_h} P_h(au_h)\|_{L^2(\Gamma_h)} \\ & \leq \|\nabla_{\Gamma_h} P_h(u_h(\nabla_{\Gamma_h} \cdot v_h - (\nabla_{\Gamma} \cdot v)^{-l}))\|_{L^2(\Gamma_h)} \\ & \quad + \|\nabla_{\Gamma_h} (P_h(u_h(\nabla_{\Gamma} \cdot v)^{-l}) - u_h(\nabla_{\Gamma} \cdot v)^{-l})\|_{L^2(\Gamma_h)} \\ & \quad + \|\nabla_{\Gamma_h} (u_h(\nabla_{\Gamma} \cdot v)^{-l})\|_{L^2(\Gamma_h)} \\ & \leq \frac{c}{h} \|P_h(u_h(\nabla_{\Gamma_h} \cdot v_h - (\nabla_{\Gamma} \cdot v)^{-l}))\|_{L^2(\Gamma_h)} \\ & \quad + \frac{c}{h} \|P_h(u_h(\nabla_{\Gamma} \cdot v)^{-l}) - u_h(\nabla_{\Gamma} \cdot v)^{-l}\|_{L^2(\Gamma_h)} \\ & \quad + c \|u_h\|_{L^2(\Gamma_h)} + c \|\nabla_{\Gamma_h} u_h\|_{L^2(\Gamma_h)}. \end{aligned}$$

By interpolation estimates from [2] and since u_h is piecewise linear on Γ_h and v is sufficiently smooth we have that

$$\|P_h(u_h(\nabla_{\Gamma} \cdot v)^{-l}) - u_h(\nabla_{\Gamma} \cdot v)^{-l}\|_{L^2(\Gamma_h)} \leq ch^2 (\|u_h\|_{L^2(\Gamma_h)} + \|\nabla_{\Gamma_h} u_h\|_{L^2(\Gamma_h)}).$$

For the remaining term we observe:

$$\begin{aligned} & \|P_h(u_h(\nabla_{\Gamma_h} \cdot v_h - (\nabla_{\Gamma} \cdot v)^{-l}))\|_{L^2(\Gamma_h)} \\ & \leq \|u_h\|_{L^2(\Gamma_h)} \|\nabla_{\Gamma_h} \cdot v_h - (\nabla_{\Gamma} \cdot v)^{-l}\|_{L^\infty(\Gamma_h)} \leq ch \|u_h\|_{L^2(\Gamma_h)}, \end{aligned}$$

since v_h is the linear interpolant of v^{-l} .

Thus we have proved the estimate

$$\|\nabla_{\Gamma_h} P_h(au_h)\|_{L^2(\Gamma_h)} \leq c (\|u_h\|_{L^2(\Gamma_h)} + \|\nabla_{\Gamma_h} u_h\|_{L^2(\Gamma_h)})$$

and with (9.5) for $k = 1$ we arrive at the inequality

$$\sqrt{w \cdot Aw} \leq \|\nabla_{\Gamma_h} \dot{u}_h\|_{L^2(\Gamma_h)} + c (\|u_h\|_{L^2(\Gamma_h)} + \|\nabla_{\Gamma_h} u_h\|_{L^2(\Gamma_h)}).$$

This gives (9.4) 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 z one has the identity

$$(\nabla_{\Gamma_h} \cdot z)' = \nabla_{\Gamma_h} \cdot \dot{z} - \text{trace}(\mathcal{A} \nabla_{\Gamma_h} z) \quad (9.6)$$

with the matrix $\mathcal{A}_{lr} = (\nabla_{\Gamma_h})_l v_{hr} - \sum_{s=1}^{d+1} n_{hs} n_{hl} (\nabla_{\Gamma_h})_r v_{hs}$ ($l, r = 1, \dots, d+1$). One then has to use this formula for $z = v_h$ and follow the ideas of the case $k = 1$. \square

According to the previous lemma we now have to prove a priori estimates for the material time derivatives of the discrete solution u_h of the problem (3.3).

THEOREM 9.1 Assume that the given evolution of $\Gamma_h(t)$, $t \in [0, T]$, is sufficiently smooth. Then we have the a priori estimate

$$\sup_{(0,T)} \|u_h^{(k)}\|_{L^2(\Gamma_h)}^2 + \int_0^T \|\nabla_{\Gamma_h} u_h^{(k)}\|_{L^2(\Gamma_h)}^2 dt \leq c \sum_{l=0}^k \|u_h^{(l)}(\cdot, 0)\|_{L^2(\Gamma_{h0})}^2. \quad (9.7)$$

Proof. The discrete PDE (3.3) is equivalent to the system

$$\frac{d}{dt} \int_{\Gamma_h} u_h \phi_j + \int_{\Gamma_h} \nabla_{\Gamma_h} u_h \cdot \nabla_{\Gamma_h} \phi_j = 0 \quad j = 1, \dots, N. \quad (9.8)$$

We differentiate this equation k times with respect to time and use Lemma 9.1. Then

$$\begin{aligned} \int_{\Gamma_h} u_h^{(k+1)} \phi_j + \sum_{l=1}^{k+1} g_{k+1,l} u_h^{(k+1-l)} \phi_j \\ + \int_{\Gamma_h} \nabla_{\Gamma_h} u_h^{(k)} \cdot \nabla_{\Gamma_h} \phi_j + \sum_{l=1}^k G_{kl} \nabla_{\Gamma_h} u_h^{(k-l)} \cdot \nabla_{\Gamma_h} \phi_j = 0. \end{aligned}$$

We multiply this equation with $u_j^{(k)}$ and sum over $j = 1, \dots, N$ and get

$$\begin{aligned} \int_{\Gamma_h} u_h^{(k+1)} u_h^{(k)} + \int_{\Gamma_h} |\nabla_{\Gamma_h} u_h^{(k)}|^2 \\ = - \sum_{l=1}^{k+1} \int_{\Gamma_h} g_{k+1,l} u_h^{(k+1-l)} u_h^{(k)} - \sum_{l=1}^k \int_{\Gamma_h} G_{kl} \nabla_{\Gamma_h} u_h^{(k-l)} \cdot \nabla_{\Gamma_h} u_h^{(k)}. \end{aligned}$$

Standard arguments then lead to the estimate

$$\begin{aligned} \frac{d}{dt} \|u_h^{(k)}\|_{L^2(\Gamma_h)}^2 + \|\nabla_{\Gamma_h} u_h^{(k)}\|_{L^2(\Gamma_h)}^2 \\ \leq c \|u_h^{(k)}\|_{L^2(\Gamma_h)}^2 + c \sum_{l=0}^{k-1} \left(\|u_h^{(l)}\|_{L^2(\Gamma_h)}^2 + \|\nabla_{\Gamma_h} u_h^{(l)}\|_{L^2(\Gamma_h)}^2 \right). \end{aligned}$$

From this we get inequality (9.7). \square

COROLLARY 9.1 Under suitable smoothness assumptions on $\Gamma(t)$, $t \in [0, T]$, conditions (8.1) and (8.2) are fulfilled with

$$\alpha = c \sum_{l=0}^k \|u_h^{(l)}(\cdot, 0)\|_{L^2(\Gamma_{h0})}.$$

Proof. This follows by a combination of Lemma 9.2 and Theorem 9.1. \square

Without proof, we expect that condition (8.3) is satisfied for smooth solutions of equations on smooth closed surfaces. As already the case of plane domains shows, condition (8.3) fails to hold uniformly in the mesh size on surfaces with boundary; cf. the discussion of order reduction phenomena in [10, 12, 13].

10. Implementation

Implementation of ESFEM. The implementation of the evolving surface finite element method is analogous to a Cartesian finite element method. The only differences are that the vertices of the elements are $(d + 1)$ -dimensional, i.e., the d -dimensional simplices making up the discrete surface live in \mathbb{R}^{d+1} and that the matrices M and A have to be assembled in each time step anew. See also Section 7.2 in [2]. The program is set up in such a way that for given time t it provides the sparse matrices $M(t)$ and $A(t)$ in suitable form.

Implementation in the RADAU code. We indicate how to implement the method in the code RADAU5 or RADAU of Hairer and Wanner [7, 8]. That code is written for problems of the form

$$B\dot{x} = f(t, x)$$

with a constant, not necessarily invertible square matrix B . Our problem (5.1) is of this form with

$$x = \begin{pmatrix} y \\ u \end{pmatrix}, \quad B = \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix}, \quad f(t, x) = \begin{pmatrix} 0 & -A(t) \\ I & -M(t) \end{pmatrix} \begin{pmatrix} y \\ u \end{pmatrix}.$$

The code requires the user to specify a Jacobian at each step, which here is chosen as

$$J_n = \begin{pmatrix} 0 & -A(t_{n+1}) \\ I & -M(t_{n+1}) \end{pmatrix}.$$

It also requires a routine for solving linear systems with the matrices

$$\tau^{-1}\lambda_i B - J_n = \begin{pmatrix} \tau^{-1}\lambda_i I & A(t_{n+1}) \\ -I & M(t_{n+1}) \end{pmatrix} \quad \text{for } i = 1, \dots, m,$$

where λ_i are the eigenvalues of the inverse coefficient matrix (w_{ij}) (which are real or come in complex conjugate pairs, with positive real part). By straightforward block Gaussian elimination, this reduces to solving linear systems with the m matrices

$$\tau^{-1}\lambda_i M(t_{n+1}) + A(t_{n+1}). \tag{10.1}$$

Building the mass and stiffness matrices and solving linear systems with the matrices (10.1) are the main computational efforts in the method.

Iteration for the internal stages. Let us describe the approach in more detail. The equations (5.2)-(5.3) can be combined into a linear system for the internal stages U_{ni} :

$$M_{ni}U_{ni} + \tau \sum_{j=1}^m a_{ij}A_{nj}U_{nj} = M_n u_n. \tag{10.2}$$

We solve this iteratively. Given an iterate $U_{ni}^{(k)}$ ($i = 1, \dots, m$), we determine

$$U_{ni}^{(k+1)} = U_{ni}^{(k)} + \delta U_{ni}^{(k)}$$

from the equations

$$M_{n+1} \delta U_{ni}^{(k)} + \tau \sum_{j=1}^m a_{ij} A_{n+1} \delta U_{nj}^{(k)} = \rho_{ni}^{(k)}$$

with

$$\rho_{ni}^{(k)} = M_n u_n - M_{ni} U_{ni}^{(k)} - \tau \sum_{j=1}^m a_{ij} A_{nj} U_{nj}^{(k)}.$$

Equivalently, with $\delta U_n^{(k)} = (\delta U_{ni}^{(k)})_{i=1}^m$ and $\mathcal{Q} = (a_{ij})$, this is rewritten as

$$(I_m \otimes M_{n+1} + \tau \mathcal{Q} \otimes A_{n+1}) \delta U_n^{(k)} = \rho_n^{(k)}.$$

If we diagonalize $\mathcal{Q}^{-1} = T \Lambda T^{-1}$ with $\Lambda = \text{diag}(\lambda_i)$ and set

$$\delta V_n^{(k)} = (T^{-1} \otimes I) \delta U_n^{(k)}, \quad \sigma_n^{(k)} = \tau^{-1} (\Lambda T^{-1} \otimes I) \rho_n^{(k)},$$

then the system becomes

$$(\tau^{-1} \Lambda \otimes M_{n+1} + I_m \otimes A_{n+1}) \delta V_n^{(k)} = \sigma_n^{(k)},$$

which decouples into the m equations

$$(\tau^{-1} \lambda_i M_{n+1} + A_{n+1}) \delta V_{ni}^{(k)} = \sigma_{ni}^{(k)} \quad (i = 1, \dots, m).$$

This yields $\delta U_n^{(k)} = (T \otimes I) \delta V_n^{(k)}$ and the new iterate $U_n^{(k+1)} = U_n^{(k)} + \delta U_n^{(k)}$.

Convergence of the iteration. We show that under the given conditions on $M(t)$ and $A(t)$ and on the Runge–Kutta method, the above iteration converges linearly with rate $O(\tau)$. In the following result we denote the iteration errors as $\mathcal{E}_{ni}^{(k)} = U_{ni}^{(k)} - U_{ni}$.

LEMMA 10.1 There exist $\tau_0 > 0$ and C , both depending only on μ, κ of Lemma 4.1, such that for $\tau \leq \tau_0$,

$$\sum_{j=1}^m \left(|\mathcal{E}_{nj}^{(k+1)}|_{t_{n+1}}^2 + \tau \|\mathcal{E}_{nj}^{(k+1)}\|_{t_{n+1}}^2 \right) \leq C \tau^2 \sum_{j=1}^m \left(|\mathcal{E}_{nj}^{(k)}|_{t_{n+1}}^2 + \tau \|\mathcal{E}_{nj}^{(k)}\|_{t_{n+1}}^2 \right).$$

Proof. We find

$$\begin{aligned} M_{n+1} \mathcal{E}_{ni}^{(k+1)} + \tau \sum_{j=1}^m a_{ij} A_{n+1} \mathcal{E}_{nj}^{(k+1)} \\ = (M_{n+1} - M_{ni}) \mathcal{E}_{ni}^{(k)} + \tau \sum_{j=1}^m a_{ij} (A_{n+1} - A_{nj}) \mathcal{E}_{nj}^{(k)}. \end{aligned}$$

We multiply this equation with $b_i \mathcal{E}_{ni}^{(k+1)}$, sum over i and use the algebraic stability condition (5.3) on the left-hand side and conditions (4.2)-(4.3) on the right-hand side to conclude

$$\begin{aligned} & \sum_{i=1}^m b_i |\mathcal{E}_{ni}^{(k+1)}|_{n+1}^2 + \frac{1}{2} \tau \left\| \sum_{i=1}^m b_i \mathcal{E}_{ni}^{(k+1)} \right\|_{n+1}^2 \\ & \leq 2\mu\tau \sum_{i=1}^m |\mathcal{E}_{ni}^{(k+1)}|_{n+1} \cdot |\mathcal{E}_{ni}^{(k)}|_{n+1} + C\kappa\tau^2 \sum_{i=1}^m \sum_{j=1}^m \|\mathcal{E}_{ni}^{(k+1)}\|_{n+1} \cdot \|\mathcal{E}_{nj}^{(k)}\|_{n+1}. \end{aligned}$$

This inequality does not yet bound $\sum_{i=1}^m b_i \|\mathcal{E}_{ni}^{(k+1)}\|_{n+1}^2$. For this purpose we rewrite the error equation equivalently as

$$\begin{aligned} & \tau^{-1} \sum_{j=1}^m w_{ji} M_{n+1} \mathcal{E}_{ni}^{(k+1)} + A_{n+1} \mathcal{E}_{nj}^{(k+1)} \\ & = \tau^{-1} \sum_{j=1}^m w_{ji} (M_{n+1} - M_{ni}) \mathcal{E}_{ni}^{(k)} + (A_{n+1} - A_{nj}) \mathcal{E}_{nj}^{(k)}. \end{aligned}$$

We multiply by $b_j \mathcal{E}_{nj}^{(k+1)}$, sum over j and use the algebraic stability condition (5.3) and the stiff accuracy condition (5.4) on the left-hand side and again conditions (4.2)-(4.3) on the right-hand side to obtain

$$\begin{aligned} & \frac{1}{2} \tau^{-1} |\mathcal{E}_{nm}^{(k+1)}|_{n+1}^2 + \sum_{j=1}^m b_j \|\mathcal{E}_{nj}^{(k+1)}\|_{n+1}^2 \\ & \leq C\mu \sum_{j=1}^m \sum_{i=1}^m |\mathcal{E}_{nj}^{(k+1)}|_{n+1} \cdot |\mathcal{E}_{ni}^{(k)}|_{n+1} + 2\kappa\tau \sum_{j=1}^m \|\mathcal{E}_{nj}^{(k+1)}\|_{n+1} \cdot \|\mathcal{E}_{nj}^{(k)}\|_{n+1}. \end{aligned}$$

Combining the two inequalities and using Young's inequality on the right-hand side yields the result. \square

11. Numerical experiments

We take up Example 7.3 from [2], which is a PDE on a moving surface with time-dependent curvature. The surface is given as the level set

$$\Gamma(t) = \{x \in \mathbb{R}^3 : d(x, t) = 0\} \quad \text{with} \quad d(x, t) = \frac{x_1^2}{a(t)} + x_2^2 + x_3^2 - 1,$$

which is an ellipsoid with time-dependent axis. We have chosen $a(t) = 1 + \frac{1}{4} \sin(t)$. As exact continuous solution, we choose $u(x, t) = e^{-6t} x_1 x_2$ and compute a right-hand side for the PDE from the equation $f = u_t + v \cdot \nabla u + u \nabla_{\Gamma} \cdot v - \Delta_{\Gamma} u$.

In a first numerical experiment we consider the evolving surface finite element equations (3.4) for four spatial refinement levels, with $2^{2\ell+6} + 2$ meshpoints, for $\ell = 1, 2, 3, 4$. We integrate the differential equations in time numerically using the Radau IIA method with three stages with

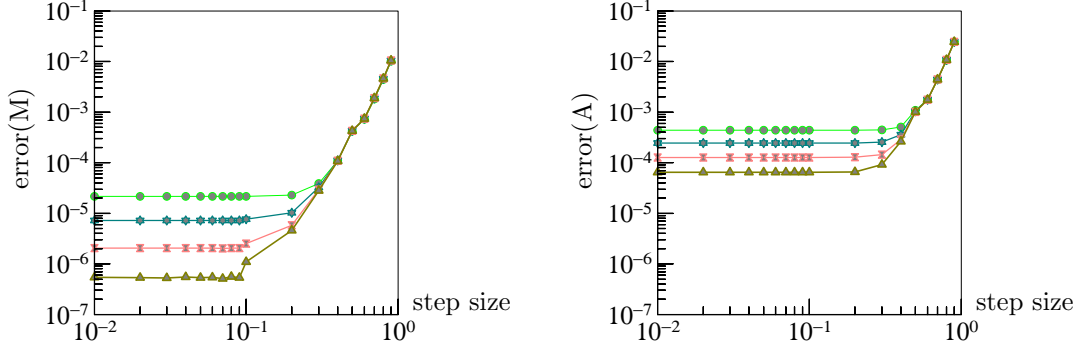


FIG. 1. Errors in L^2 -norm (left) and energy semi-norm (right) vs. time step size for four spatial refinements at $t = 1$.

fixed time step size τ . At time $t = 1$, 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 ,

$$|e|_t = (e \cdot M(t)e)^{1/2} \quad \text{and} \quad \|e\|_t = (e \cdot A(t)e)^{1/2}.$$

In Figure 1 we plot $|e|_t$ and $\|e\|_t$ at $t = 1$ to the left and right, respectively, versus the time step size τ . We observe the full order of temporal convergence $p = 5$ and error independence of the spatial refinement level in the regime where the temporal error dominates the spatial error. In the complementary regime, for smaller time steps, we clearly observe a faster rate of spatial convergence in the L^2 -norm than in the energy seminorm, in accordance with the convergence theory for the evolving surface finite element method in [2, 3]. Higher refinement levels correspond to lower-lying error curves.

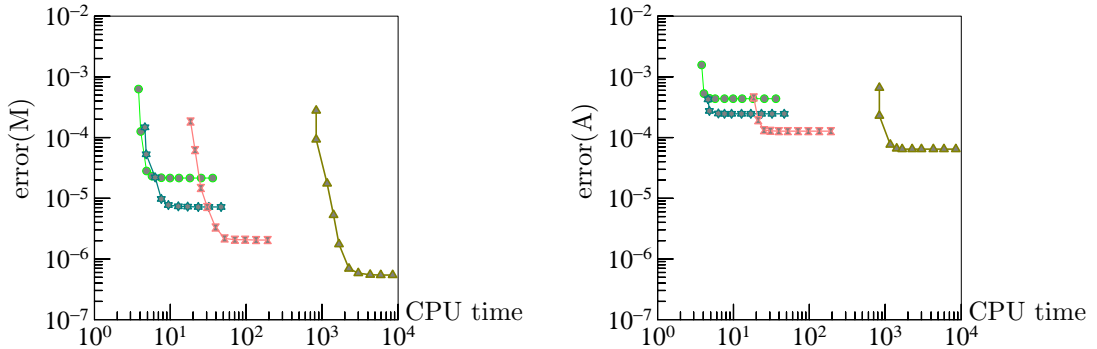


FIG. 2. Errors in L^2 -norm (left) and energy semi-norm (right) vs. CPU time for four spatial refinements and ten tolerances at $t = 1$.

In a second numerical experiment we use the time integrator with variable time steps as provided by the RADAU5 code of [7]. In Figure 2 we plot the errors in the M -norm and A -seminorm versus computing time in seconds on a standard PC for ten local error tolerances ranging from $Atol = Rtol = 10^{-1}$ to $Atol = Rtol = 10^{-10}$. Here, each curve corresponds to the

errors of one spatial mesh for the various tolerance parameters, and higher spatial refinement corresponds to smaller errors.

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