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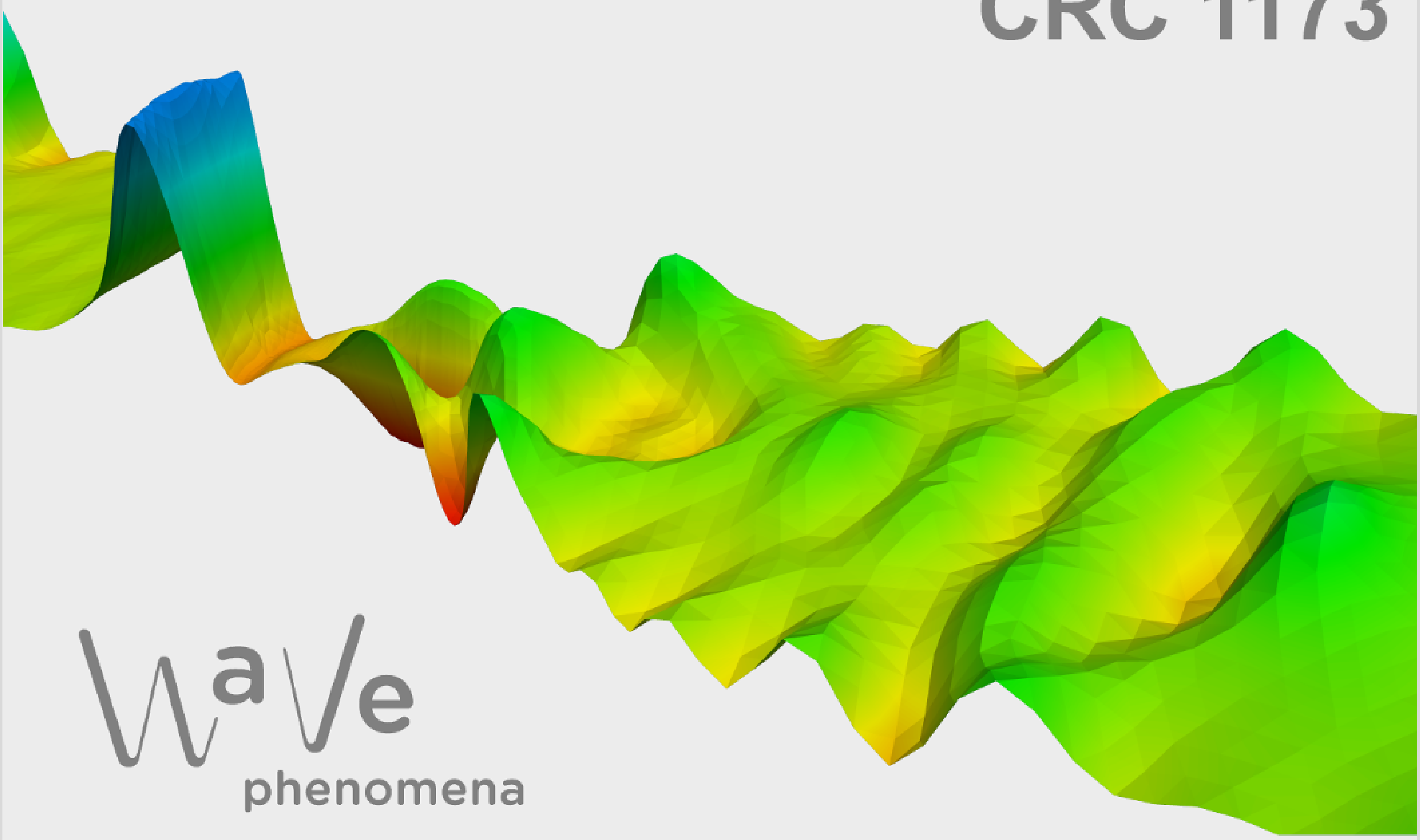

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FULL DISCRETIZATION ERROR ANALYSIS OF EXPONENTIAL INTEGRATORS FOR SEMILINEAR WAVE EQUATIONS

BENJAMIN DÖRICH AND JAN LEIBOLD

ABSTRACT. In this article we prove full discretization error bounds for semilinear second-order evolution equations. We consider exponential integrators in time applied to an abstract nonconforming semi discretization in space. Since the fully discrete schemes involve the spatially discretized semigroup, a crucial point in the error analysis is to eliminate the continuous semigroup in the representation of the exact solution. Hence, we derive a modified variation-of-constants formula driven by the spatially discretized semigroup which holds up to a discretization error. Our main results provide bounds for the full discretization errors for exponential Adams and explicit exponential Runge–Kutta methods. We show convergence with the stiff order of the corresponding exponential integrator in time, and errors stemming from the spatial discretization.

As an application of the abstract theory, we consider an acoustic wave equation with kinetic boundary conditions, for which we also present some numerical experiments to illustrate our results.

1. INTRODUCTION

In the present paper we analyze the full discretization of semilinear second-order evolution equations

$$\begin{aligned} u''(t) + Bu'(t) + Au(t) &= f(t, u(t)), \quad t \in (0, T], \\ u(0) = u^0, \qquad u'(0) &= v^0, \end{aligned} \tag{1.1}$$

posed on a Hilbert space H with unbounded operators A and B and a smooth nonlinearity f. The numerical scheme is obtained by applying exponential Runge–Kutta and multistep methods to the first-order formulation of a spatially discretized version of (1.1).

Equation (1.1) covers a wide range of second-order semilinear wave equations. The most prominent example is the acoustic wave equation subject to homogeneous Dirichlet or Neumann boundary conditions. A more interesting example, however, is the acoustic wave equation with kinetic boundary conditions. This model was derived in [14] for a membrane with a boundary that carries a mass density and is subject to linear tension. We also refer to [33, 34], where analytical wellposedness of such equations was shown and further references are given.

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Kinetic boundary conditions are a special type of dynamic boundary conditions, given by a differential equation on the boundary and usually posed on smooth boundaries. In practice, such boundaries have to be approximated by piecewise polynomials, which leads to nonconforming space discretizations. This makes the error analysis much more involved, since the exact and the numerical solution are defined on different spatial domains. To tackle this difficulty, the so-called *unified error analysis* was introduced in [15] for linear wave-type equations, and extended in [16] to the semilinear case. The unified error analysis is a systematic approach, where an abstract space discretization of (1.1) is considered as an evolution equation on a finite dimensional space. In [15, 16], abstract error bounds were derived, which lead to optimal convergence rates for a large class of equations and corresponding conforming and nonconforming space discretizations.

In this paper, we combine the unified error analysis with exponential integrators. A review on those schemes can, e.g., be found in [19]. Compared to classical numerical integrators, where the fundamental theorem of calculus is used as the starting point for approximations, exponential integrators are based on the variation-of-constants formula. This way, the representation of the solution incorporates the unbounded linear part via semigroup theory, while only the smooth nonlinear part within the integral is approximated.

We focus on two different classes of methods. On the one hand, we consider exponential Adams methods. Here, the nonlinearity is replaced by an interpolation polynomial through preceding approximations and the polynomial is integrated exactly. Such methods were first proposed in [29] and a rigorous error analysis for the time discretization was performed in [7] and [20]. On the other hand, we employ explicit exponential Runge–Kutta methods, first considered in [11, 12, 24]. They extend the classical Runge–Kutta methods by the use of operator-valued coefficients which depend on the linear part of the problem. For the methods considered in this work, error bounds for the spatially continuous case were derived in [18]. In [10], related schemes have been applied to stiff kinetic equations. For the (semi-)linear Schrödinger equation, symmetric but implicit variants of these schemes and their geometric properties were derived in [8].

For a long time, these methods have been regarded as unpractical due to evaluation of a matrix exponential and related matrix functions. However, this view changed when in [17] for the first time an implementation was proposed that was competitive in certain scenarios. For quasilinear Maxwell's equations, the numerical experiments in [31] confirm this computational potential. Further, their efficiency was demonstrated in [26, 28] in the application to molecular dynamics and nonlinear coupled oscillators. Besides the Krylov methods to compute a matrix function applied to a vector, a different approach is considered in [22]. Here, the analytic functions are expressed by the Cauchy integral formula which is discretized such that it remains to evaluate a fixed number of resolvents. Very recently, in [6] novel rational exponential integrators were derived which gain efficiency and accuracy by a parallel-in-time computation of resolvents applied to a vector in order to evaluate the matrix exponential.

So far, the error analysis has mostly been performed for abstract evolution equations or for systems of ordinary differential equations. Concerning the full discretization error analysis involving exponential integrators, we are only aware of the following works. In [5, 9], stochastic parabolic partial differential equations are discretized by the exponential Euler method combined with a spectral method in space. This type of space discretization has very favorable properties in the analysis, however, one needs to know the relevant eigenvalues and eigenvectors of the differential operators exactly. This is for example ensured if one considers periodic boundary conditions and constant coefficients in the differential operator. In this spirit, the very elegant time discretization error analysis of a quasilinear wave equation by trigonometric integrators in [13] is easily extended to a full discretization due to the Fourier spectral methods in space. In [1, 2], exponential splitting methods are applied to parabolic evolution equations and the order reduction induced by the boundary conditions is investigated. For finite difference and spectral discretization, the results are extended to full discretization error bounds.

However, none of these error analyses is applicable to general wave equations with non-constant coefficients on general domains and, in particular, not to unstructured meshes and nonconforming space discretizations. The main contribution of our paper is to fill this gap. We provide full discretization error bounds in terms of the stiff order of the exponential integrator in time and the abstract space discretization error terms from the unified error analysis. Due to the general framework, these bounds apply to a large class of equations and space discretizations, e.g., those considered in [15, 16]. To prove these bounds we have to intertwine the techniques used in the proofs for the time and space discretization, respectively. A crucial difficulty of the error analysis is to come up with a suitable representation of the exact solution involving the discretized semigroup. This is in sharp contrast to spectral space discretizations mentioned above, where the projection onto the finite dimensional space usually commutes with the exact semigroup. Further, this issue has not occurred so far in the analyses of standard implicit time integration methods.

The rest of the paper is structured as follows: In Section 2, we introduce an abstract framework adapted to the first-order formulation of (1.1), and present the abstract space discretization. Further, we collect the properties of the discrete objects in order to perform the error analysis.

The fully discrete schemes are presented in Section 3. We discuss the methods and state our main results for the first-order system. The proofs are given in Section 4. We first derive the defects for the exact solution expressed by a modified variation-of-constants formula and provide bounds on those. From this, the fully discrete errors bounds are established. We then transfer our results in Section 5 to the abstract second-order evolution equation (1.1) to conclude the corresponding novel error bounds.

In Section 6, we discuss a concrete example of a wave equation with kinetic boundary conditions and present numerical experiments to confirm our theoretical findings.

2. General Setting and the unified error analysis

In this section, we introduce the analytical framework for the second-order evolution equation (1.1). Since the exponential integrators considered in this paper are applied to first-order systems, we rewrite (1.1) in a first-order form. For this, we present an abstract space discretization established in [15, 16], where a unified error analysis for space discretizations of linear and semilinear wave-type equations was derived. We recall the setting to keep this presentation self-contained.

2.1. **The continuous second-order problem.** Let V, H be Hilbert spaces and V be densely and continuously embedded in H. We consider the following variational differential equation (2.1) as a prototype for weak formulations of second-order wave equations: seek $u \in C^2([0,T];H) \cap C^1([0,T];V)$ such that

$$\begin{aligned} m\big(u'', v\big) + b\big(u', v\big) + a\big(u, v\big) &= m\big(f(t,u), v\big) \quad \text{for all } v \in V, t \in (0,T], \\ u(0) = u^0, \qquad u'(0) &= v^0. \end{aligned} \tag{2.1}$$

We pose the following assumptions.

Assumption 2.1.

a) The bilinear form m is a scalar product on H with induced norm $\|\cdot\|_m$.
b) $a\colon V \times V \to \mathbb{R}$ is a symmetric bilinear form and there exists a constant $c_G \geq 0$ such that
$$\tilde{a} := a + c_G m$$
is a scalar product on V with induced norm $\|\cdot\|_{\tilde{a}}$.
c) The bilinear form $b\colon V \times H \to \mathbb{R}$ is continuous and there exists a $\beta_{\mathrm{qm}} \geq 0$ such that
$$b\big(v, v\big) + \beta_{\mathrm{qm}} \|v\|_m^2 \geq 0 \quad \text{for all } v \in V.$$
d) The nonlinearity f satisfies $f \in C^1([0,T] \times V; H)$ and is locally Lipschitz-continuous on V with Lipschitz-constant $L_{T,M}$, i.e., for all $t \in [0,T]$ and all $v, w \in V$ with $\|v\|_{\tilde{a}}, \|w\|_{\tilde{a}} \leq M$ it holds
$$\|f(t,v) - f(t,w)\|_m \leq L_{T,M} \|v - w\|_{\tilde{a}}.$$

By the dense and continuous embedding of the Hilbert spaces there exists a constant $C_{H,V} > 0$ such that

$$\|v\|_m \leq C_{H,V} \|v\|_{\tilde{a}} \quad \text{for all } v \in V.$$

We define operators $A\colon D(A) \to H$ and $B\colon V \to H$ induced by the bilinear forms a and b via

$$\begin{aligned} m\big(Av, w\big) &= a\big(v, w\big), \qquad \text{for all } v \in D(A), w \in V, \\ m\big(Bv, w\big) &= b\big(v, w\big), \qquad \text{for all } v \in V, w \in H, \end{aligned}$$

with

$$D(A) = \big\{ v \in V \mid \exists C = C(v) > 0 \text{ such that } \forall w \in V : |a\big(v, w\big)| \leq C \|w\|_m \big\}.$$

By the construction of the operators A and B, a solution of (2.1) additionally satisfies $u \in C([0,T]; D(A))$. Hence, problem (2.1) is equivalent to the evolution equation (1.1). In order to rewrite (1.1) in a first-order formulation, we define $X = V \times H$, $u'(t) = v(t)$ and set

$$x(t) = \begin{bmatrix} u(t) \\ v(t) \end{bmatrix}, \quad S = \begin{bmatrix} 0 & -\mathrm{I} \\ A & B \end{bmatrix}, \quad g\,(t, x) = \begin{bmatrix} 0 \\ f(t,u) \end{bmatrix}, \quad x^0 = \begin{bmatrix} u^0 \\ v^0 \end{bmatrix}. \tag{2.2}$$

Then (1.1) is equivalent to the evolution equation

$$\begin{aligned} x'(t) + Sx(t) &= g(t, x(t)), \qquad t \in (0,T], \\ x(0) &= x^0. \end{aligned} \tag{2.3}$$

2.2. **The continuous first-order problem.** In the following sections, we consider a general system of the form (2.3) on a Hilbert space X with scalar product $p\big(\cdot,\cdot\big)$. In this setting, we derive the fully discrete schemes and perform the error analysis. In Section 5, we transfer these results back to the formulation (1.1).

We pose the following classical assumptions, which are a direct consequence of Assumption 2.1, cf. [16, Sec. 3.2].

Assumption 2.2.

a) The linear operator $S\colon D(S) \to X$ is the generator of a C_0-semigroup with

$$\left\| \mathrm{e}^{-tS} \right\|_{X \leftarrow X} \leq \mathrm{e}^{c_{\mathrm{qm}} t} \tag{2.4}$$

for some $c_{\mathrm{qm}} \geq 0$.

b) The nonlinearity $g \in C^1([0,T] \times X; X)$ is locally Lipschitz continuous w.r.t. the second component with constant $L_{T,M}$.

Assumption 2.2 ensures local wellposedness of (2.3), cf. [30, Thm. 6.1.5].

Lemma 2.3. *If Assumption 2.2 holds true, then (2.3) is locally wellposed, i.e., for every $x^0 \in X$ there exists $t^*\big(x^0\big) > 0$ such that, for all $T < t^*\big(x^0\big)$, (2.3) has a unique solution*

$$x \in C^1\big([0,T]; X\big) \cap C\big([0,T]; D(S)\big).$$

For the rest of the paper we fix some $T < t^*\big(x^0\big)$ in order to obtain uniform bounds of the solution on $[0,T]$.

2.3. **Abstract space discretization.** We now introduce an abstract space discretization of the evolution equation (2.3). We use the setting introduced in [15,16] to analyze nonconforming space discretizations of linear and semilinear wave-type equations.

For this, let $(X_h)_h$ be a family of finite dimensional vector spaces related to a discretization parameter h, e.g., the maximal mesh width of a finite element discretization. In X_h, we seek an approximation x_h to the solution x of (2.3). Let $p_h\big(\cdot,\cdot\big)$ be a scalar product on X_h and let $S_h \in \mathcal{L}(X_h, X_h)$ and $g_h\colon [0,T] \times X_h \to X_h$ be discretizations of S and g, respectively. We impose the following conditions similar to Assumption 2.2.

Assumption 2.4.

a) The linear operator $S_h \in \mathcal{L}(X_h; X_h)$ is the generator of a C_0-semigroup with

$$\left\| \mathrm{e}^{-tS_h} \right\|_{X_h \leftarrow X_h} \leq \mathrm{e}^{\widehat{c}_{\mathrm{qm}} t}. \tag{2.5}$$

b) The nonlinearity $g_h\colon [0,T] \times X_h \to X_h$ is locally Lipschitz continuous w.r.t. the second component with constant $\widehat{L}_{T,M}$, i.e., for all $x_h, y_h \in X_h$ with $\|x_h\|_{X_h}, \|y_h\|_{X_h} \leq M$ and $t \in [0,T]$:

$$\|g_h(t,x_h) - g_h(t,y_h)\|_{X_h} \leq \widehat{L}_{T,M} \|x_h - x_h\|_{X_h}. \tag{2.6}$$

The constants $\widehat{c}_{\mathrm{qm}}$ and $\widehat{L}_{T,M}$ are independent of h.

The discretized evolution equation (2.3) is then of the form

$$\begin{aligned} x_h'(t) + S_h x_h(t) &= g_h(t, x_h(t)), \qquad t \in (0,T], \\ x_h(0) &= x_h^0, \end{aligned} \tag{2.7}$$

$$
\begin{tikzcd}
Z \arrow[r, hook] \arrow[dr, "J_h"'] & X \arrow[d, dashed, "\mathcal{L}_h^*"] \arrow[r, phantom, "\supset"] & \mathcal{L}_h(X_h) \\
 & X_h \arrow[ur, "\mathcal{L}_h"'] &
\end{tikzcd}
$$

FIGURE 1. Overview of spaces and operators, taken from [16, Fig. 3.1].

where $x_h^0 \in X_h$ is an approximation of x^0.

For exponential Runge–Kutta methods of order $p \geq 3$ we require additional regularity of the discretized nonlinearity which is beyond the Lipschitz property given in (2.6).

Assumption 2.5. The nonlinearity g_h is in $C^3([0,T] \times X_h; X_h)$ with derivatives bounded independent of h.

For a concrete example, we comment on this assumption in Remark 6.1.

2.4. **Abstract space discretization errors.** We explicitly allow for nonconforming space discretizations where $X_h \nsubseteq X$. Thus, to relate the continuous and discrete solution, we make the following assumptions:

Assumption 2.6.

a) There exists a *lift operator* $\mathcal{L}_h \colon X_h \to X$ which satisfies

$$\|\mathcal{L}_h y_h\|_X \leq \widehat{C}_X \|y_h\|_{X_h} \qquad \text{for all } y_h \in X_h \tag{2.8}$$

with $\widehat{C}_X$ independent of h.

By $\mathcal{L}_h^* \colon X \to X_h$ we denote the adjoint of the lift operator defined via

$$p_h\big(\mathcal{L}_h^* y, y_h\big) = p\big(y, \mathcal{L}_h y_h\big) \qquad \text{for all } y \in X, y_h \in X_h.$$

b) There exists a Hilbert space Z, which is densely and continuously embedded in X, and a *reference operator* $J_h \in \mathcal{L}(Z, X_h)$ which satisfies

$$\|J_h z\|_{X_h} \leq \widehat{C}_{J_h} \|z\|_Z \qquad \text{for all } z \in Z \tag{2.9}$$

with a constant $\widehat{C}_{J_h}$ independent of h.

The reference operator J_h could, e.g., be an interpolation operator defined on a subspace Z of the continuous functions, and should satisfy $\mathcal{L}_h J_h z \approx z$ for all $z \in Z$. Figure 1 illustrates the relations of the spaces and operators.

In our error analysis, we will bound the space discretization errors in terms of the following quantities:

Definition 2.7 (Space discretization errors)**.**

a) The *linear remainder operator* is defined via

$$R_h := \mathcal{L}_h^* S - S_h J_h \colon D(S) \cap Z \to X_h. \tag{2.10}$$

b) The *nonlinear remainder operator* $r_h \colon [0,T] \times Z \to X_h$ is given by

$$r_h(t,z) := \mathcal{L}_h^* g(t,z) - g_h(t, J_h z). \tag{2.11}$$

c) The space discretization errors are collected in the term

$$E_h(t) = \left\| x_h^0 - J_h x^0 \right\|_{X_h} + t \left\| \Delta_{J_h} x' \right\|_{L^\infty([0,t];X_h)} + t \| R_h x \|_{L^\infty([0,t];X_h)} + t \| r_h(\cdot, x(\cdot)) \|_{L^\infty([0,t];X_h)} \tag{2.12}$$

where $\Delta_{J_h} \coloneqq J_h - \mathcal{L}_h^* \colon Z \to X_h$ is the *reference error*.

Additionally, for our analysis we need the following assumptions on the regularity of the exact solution and the consistency of the discretization.

Assumption 2.8. The solution of (2.3) satisfies $x \in C^1([0,T];Z)$ and the error terms in (2.12) converge to zero, i.e.,

$$E_h(T) \to 0 \quad \text{for} \quad h \to 0.$$

Remark 2.9. The assumptions are satisfied for wave equations with various boundary conditions, in particular of dynamical and Dirichlet type, discretized by non-conforming finite elements, cf. [16, 25]. More details are provided in Sections 5 and 6. A further example covered by the framework, are discontinuous Galerkin methods applied to linear Maxwell's equations, cf. [15].

3. Exponential integrators and main results

In the following we present the fully discrete schemes obtained by applying exponential integrators to the spatially discretized evolution equation (2.7) and state our main results, the full discretization error bounds. We denote by $\tau > 0$ the time step size and set $t_n = n\tau$. Further, we abbreviate

$$t_{n+s} \coloneqq t_n + \tau s, \quad s \in [0,1], \tag{3.1}$$

and denote the fully discrete approximation at time t_n by $x_h^n \approx x(t_n)$. Most exponential integrators are based on the variation-of-constants formula for the solution of (2.7)

$$x_h(t_{n+1}) = \mathrm{e}^{-\tau S_h} x_h(t_n) + \tau \int_0^1 \mathrm{e}^{-(1-s)\tau S_h} g_h(t_{n+s}, x_h(t_{n+s}))\,\mathrm{d}s, \tag{3.2}$$

where only the nonlinearity g_h is approximated. Applying Taylor expansion to $s \mapsto g_h(t_{n+s}, x_h(t_{n+s}))$, the φ-functions given by

$$\varphi_{k+1}(z) = \int_0^1 \mathrm{e}^{(1-s)z} \frac{s^k}{k!}\,\mathrm{d}s, \quad k \ge 0, \tag{3.3}$$

appear naturally. They are analytic in $\mathbb{C}$ and closely related to the exponential function. In order to expand the right-hand side, we assume the following differentiability.

Assumption 3.1. Let $m \ge 1$ and x be the exact solution of (2.3). Then, the differentiability condition

$$s \mapsto g(s, x(s)) \in C^m\big([0,T];X\big)$$

holds.

We start with the prototypical example, namely the exponential Euler method. It is constructed by freezing the right-hand side in (3.2) at the last approximation and is given by

$$x_h^{n+1} = \mathrm{e}^{-\tau S_h} x_h^n + \tau \varphi_1(-\tau S_h) g_h(t_n, x_h^n)\,. \tag{3.4}$$

Concerning the time integration, it is well known that the stiff order of (3.4) is one, cf. [18, Thm. 4.2]. This is actually a special case of Theorem 3.2. Higher order methods can be constructed for example in the following two ways.

3.1. **Exponential Adams methods.** On the one hand, we consider the exponential k-step Adams methods. They were proposed in [29] and time integration error bounds were derived in [20]. The schemes can be expressed as

$$x_h^{n+1} = \mathrm{e}^{-\tau S_h} x_h^n + \tau \int_0^1 \mathrm{e}^{-(1-s)\tau S_h} p_h^{n,k}(t_{n+s})\,\mathrm{d}s, \quad k \geq 1, \tag{3.5}$$

where $p_h^{n,k}$ is the interpolation polynomial through the points

$$\Big(\big(t_{n-k+1}, g_h^{n-k+1}\big), \dots, \big(t_n, g_h^n\big) \Big) \quad \text{with} \quad g_h^j \coloneqq g_h(t_j, x_h^j). \tag{3.6}$$

We note that the integral in (3.5) can also be written as a linear combination of the φ-functions $\varphi_1, \dots, \varphi_k$ applied to g_h^j. The exponential Euler scheme (3.4) is obtained by setting $k = 1$.

Closely related methods, using the variation-of-constants formula (3.2) from t_n to t_{n+k}, have been constructed and analyzed in [7]. We expect that for these methods the results obtained in the following can be achieved fully analogously and, hence, we do not further comment on this.

Theorem 3.2. *Let Assumptions 2.2, 2.4, 2.6, 2.8, and 3.1 for $m = k$ hold. Further, consider the exact solution x of (2.3) and the approximations x_h^n obtained from (3.5). Then, there are $\tau_0, h_0 > 0$ and a constant $C > 0$ such that for all $\tau \leq \tau_0, h \leq h_0$, and $t_k \leq t_n \leq T$ it holds*

$$\begin{aligned} \|\mathcal{L}_h x_h^n - x(t_n)\|_X &\leq \|\big(\mathcal{L}_h J_h - \mathrm{I}\big)x(t_n)\|_X + C\big(\tau^k + E_h(t_n)\big) \\ &\quad + C\sum_{j=1}^{k-1} \|x_h^j - J_h x(t_j)\|_{X_h}, \end{aligned}$$

where C is independent of τ and h, and $E_h(t_n)$ is defined in (2.12).

Remark 3.3.

a) For $k = 2$, an exponential Euler step yields a sufficiently good starting value x_h^1. For $k \geq 3$, we suggest computing the starting values $x_h^j, j = 1, \dots, k-1$, via the starting procedure proposed in [7, 20]. There, one has to solve a nonlinear system of equations which is usually done by fixed point iteration. We expect that by our proofs, one can derive the same error bounds as for the following approximations, but we omit the details here.
b) We note that the constant C can actually be written in the form

$$C = C(t_n) = c_1 t_n \mathrm{e}^{c_2 t_n}$$

with constants $c_1, c_2 > 0$ independent of the time t_n.

TABLE 1. Stiff order conditions for explicit exponential Runge–Kutta methods in (3.7), cf. [18, Table 2]. Here $\mathcal{D}_h$ and $\mathcal{K}_h$ denote arbitrary bounded operators on X_h. The functions ψ_i and $\psi_{k,\ell}$ are defined in (3.8).

Order	Order condition
1	$\psi_1(-\tau S_h) = 0$
2	$\psi_2(-\tau S_h) = 0$
	$\psi_{1,i}(-\tau S_h) = 0$
3	$\psi_3(-\tau S_h) = 0$
	$\sum_{i=1}^{s} b_i(-\tau S_h)\mathcal{D}_h\psi_{2,i}(-\tau S_h) = 0$
4	$\psi_4(-\tau S_h) = 0$
	$\sum_{i=1}^{s} b_i(-\tau S_h)\mathcal{D}_h\psi_{3,i}(-\tau S_h) = 0$
	$\sum_{i=1}^{s} b_i(-\tau S_h)\mathcal{D}_h \sum_{j=2}^{i-1} a_{ij}(-\tau S_h)\mathcal{D}_h\psi_{2,j}(-\tau S_h) = 0$
	$\sum_{i=1}^{s} b_i(-\tau S_h)c_i\mathcal{K}_h\psi_{2,i}(-\tau S_h) = 0$

3.2. **Exponential Runge–Kutta methods.** Further, we consider the class of explicit s-stage exponential Runge–Kutta methods introduced in [12]. Error bounds for the time integration were derived in [18]. Given analytic coefficients satisfying $|a_{ij}(z)|, |b_i(z)| \leq C$ for $\operatorname{Re} z \leq \widehat{c}_{\mathrm{qm}}$, they read

$$\begin{aligned} X_h^{ni} &= \mathrm{e}^{-c_i\tau S_h}x_h^n + \tau\sum_{j=1}^{i-1} a_{ij}(-\tau S_h)g_h(t_{n+c_j}, X_h^{nj}), \quad i = 1,\ldots,s, \\ x_h^{n+1} &= \mathrm{e}^{-\tau S_h}x_h^n + \tau\sum_{i=1}^{s} b_i(-\tau S_h)g_h(t_{n+c_i}, X_h^{ni}). \end{aligned} \tag{3.7}$$

For the error analysis, several order conditions are necessary in order to ensure convergence also in the stiff case. They relate the φ-functions defined in (3.3) to certain combinations of the coefficients a_{ij}, b_i and use the following quantities

$$\psi_j(z) = \varphi_j(z) - \sum_{k=1}^{s} b_k(z)\frac{c_k^{j-1}}{(j-1)!}, \tag{3.8a}$$

$$\psi_{j,i}(z) = \varphi_j(c_i z)c_i^j - \sum_{k=1}^{i-1} a_{ik}(z)\frac{c_k^{j-1}}{(j-1)!}. \tag{3.8b}$$

In Table 1, we collected the order conditions derived in [18]. In particular, we are interested in the methods satisfying the stiff order conditions for $p = 2, 3, 4$. For the methods, which we present in the following, the corresponding order conditions of Table 1 are satisfied for all $h > 0$.

In order to obtain schemes of order $p = 2$ using $s = 2$ stages, they lead to the choices

$$a_{21}(z) = c_2\varphi_1(c_2 z), \quad b_1(z) = \varphi_1(z) - \frac{1}{c_2}\varphi_2(z), \quad b_2(z) = \frac{1}{c_2}\varphi_2(z). \tag{3.9}$$

To obtain order $p = 3$, we can for example use the method (5.16) from [23, eq. (51)]

$$
\begin{array}{c|cccc}
0 & & & & \\
\frac{1}{2} & \frac{1}{2}\varphi_{1,2} & & & \\
\frac{1}{2} & \frac{1}{2}\varphi_{1,2} - \varphi_{2,2} & \varphi_{2,2} & & \\
1 & \varphi_1 - 2\varphi_2 & 0 & 2\varphi_2 & \\
\hline
 & \varphi_1 - 3\varphi_2 + 4\varphi_3 & 2\varphi_2 - 4\varphi_3 & 2\varphi_2 - 4\varphi_3 & -\varphi_2 + 4\varphi_3
\end{array} \tag{3.10}
$$

which satisfies the stiff order conditions up to order $p = 3$ with $\varphi_{j,2} \coloneqq \varphi_j\left(\frac{1}{2}\cdot\right)$. Another example for a method of order $p = 3$ is given in [32, Example 4.5.5]. Using 8 inner stages, a method satisfying the order conditions up to order $p = 4$ is proposed in [27, Sec. 5], but we refrain from stating the coefficients.

For these methods, we derive the following error bounds of optimal order.

Theorem 3.4. *Let $p \in \{2, 3, 4\}$ and let Assumptions 2.2, 2.4, 2.6, 2.8, and 3.1 hold for $m = p$. For $p \in \{3, 4\}$ we additionally require Assumption 2.5. Further, consider the exact solution x of (2.3) and the approximations x_h^n obtained from (3.7) with coefficients satisfying the order conditions of Table 1 up to order p. Then, there are $\tau_0, h_0 > 0$ and a constant $C > 0$ such that for all $\tau \le \tau_0$ and $h \le h_0$ it holds*

$$
\|\mathcal{L}_h x_h^n - x(t_n)\|_X \le \|\big(\mathcal{L}_h J_h - \mathrm{I}\big)x(t_n)\|_X + C\big(\tau^p + E_h(t_n)\big), \quad t_n \le T, \tag{3.11}
$$

where C is independent of τ and h, and $E_h(t_n)$ is defined in (2.12).

Remark 3.5. In the papers [7, 18, 20, 27], a special focus is put on parabolic problems such as the heat equation. When dealing with analytical semigroups the smoothing property can be heavily exploited and the order conditions can be severely relaxed. In this case, second-order convergence is also achieved by

$$
a_{21}(z) = c_2\varphi_1(c_2 z), \quad b_1(z) = \big(1 - \frac{1}{2c_2}\big)\varphi_1(z), \quad b_2(z) = \frac{1}{2c_2}\varphi_1(z), \tag{3.12}
$$

which does not require the evaluation of the φ_2-function compared to (3.9). Furthermore, the parabolic smoothing allows to gain one order in τ for the schemes of order $p = 3$ and $p = 4$ above, cf. [18, Thm. 4.7] and [27, Thm. 4.1].

4. Proofs of the main results

In the following section, we aim to bound the fully discrete error which can be decomposed into

$$
\begin{aligned}
\mathcal{L}_h x_h^n - x(t_n) &= \mathcal{L}_h\big(x_h^n - J_h x(t_n)\big) + \big(\mathcal{L}_h J_h - \mathrm{I}\big)x(t_n) \\
&=: \mathcal{L}_h e_h^n + e_{J_h}^n\,.
\end{aligned} \tag{4.1}
$$

The error $e_{J_h}^n$ is an approximation error of the spatial discretization. It is independent of the time integration method. By (2.8) it holds

$$
\|\mathcal{L}_h x_h^n - x(t_n)\|_X \le \widehat{C}_X \|e_h^n\|_{X_h} + \|e_{J_h}^n\|_X,
$$

and thus it is sufficient to bound the first term. To shorten the notation further, we introduce

$$
\widetilde{x}^{n+s} \coloneqq x(t_{n+s}), \quad \widetilde{g}^{n+s} \coloneqq g(t_{n+s}, \widetilde{x}^{n+s}), \quad \widetilde{g}_h^{n+s} \coloneqq g_h(t_{n+s}, J_h\widetilde{x}^{n+s}) \tag{4.2}
$$

for the exact solution as well as the exact and discretized nonlinearity evaluated at the exact solution.

The first result of this section is concerned with the representation of the exact solution. Simply using the variation-of-constants formula, we are not able to provide suitable bounds of the defect, as we exemplify for the exponential Euler method. We insert $J_h\widetilde{x}^n$ into the numerical scheme (3.4) and obtain the defect

$$\delta^n = J_h\widetilde{x}^{n+1} - \left(\mathrm{e}^{-\tau S_h} J_h\widetilde{x}^n + \tau\varphi_1(-\tau S_h)\widetilde{g}_h^n\right).$$

Expanding $J_h\widetilde{x}^{n+1}$ by the variation-of-constants formula, one readily observes that the defect δ^n contains the term

$$J_h\mathrm{e}^{-\tau S}\widetilde{x}^n - \mathrm{e}^{-\tau S_h}J_h\widetilde{x}^n = \int_0^\tau \mathrm{e}^{-(\tau-s)S_h}\left(S_hJ_h - J_hS\right)\mathrm{e}^{-sS}\widetilde{x}^n\,\mathrm{d}s. \tag{4.3}$$

Writing

$$S_hJ_h - J_hS = (S_hJ_h - \mathcal{L}_h^*S) + (\mathcal{L}_h^* - J_h)S$$

and using R_h and Δ_{J_h} from Definition 2.7, one can bound (4.3) in X_h in terms of

$$\|R_h\mathrm{e}^{-sS}\widetilde{x}^n\|_{X_h} + \|\Delta_{J_h}\mathrm{e}^{-sS}S\widetilde{x}^n\|_{X_h}, \quad s\in[0,\tau]. \tag{4.4}$$

However, suitable bounds on these terms are in general not available, as we explain for the first term in the following counterexample.

Example 4.1. Let $\Omega = (0,1)$, $V = H_0^1(\Omega)$, $H = L^2(\Omega)$, $A = -\Delta$, $B = 0$ in (2.2). Then, $\mathrm{e}^{-\tau S}x^0$ is the solution at time $t = \tau$ of the one-dimensional wave equation

$$u_{tt}(t,\mathbf{x}) - \Delta u(t,\mathbf{x}) = 0, \quad \mathbf{x}\in\Omega,\ t\geq 0, \tag{4.5}$$

subject to homogeneous Dirichlet boundary conditions and initial values u^0, v^0.

The remainder operator R_h applied to $x = [u,v]^\intercal$ contains, among others, interpolation errors of u and v, cf. [15, Lem. 4.7]. Hence, when discretizing with finite elements of order q, a bound for (4.4) of order $\mathcal{O}(h^q)$ requires at least that $\mathrm{e}^{-tS}x^0 \in H^{q+1}(\Omega)\times H^{q+1}(\Omega)$. However, choosing

$$u^0(\mathbf{x}) = u(0,\mathbf{x}) = \mathbf{x}(1-\mathbf{x}), \qquad v^0(\mathbf{x}) = u_t(0,\mathbf{x}) = 0,$$

we note that $u^0, v^0 \in C^\infty(\overline{\Omega})$. Extending the initial values to an odd function on $[-1,1]$ and then periodically to $\mathbb{R}$, the exact solution is given by d'Alembert's formula. Since the extended version of u^0 is not C^2 at $\mathbf{x} = \ell$, $\ell\in\mathbb{Z}$, we obtain that $u(t,\cdot)\notin H^{q+1}(\Omega)$, $q\geq 2$, for almost all $t\geq 0$. ◇

Hence, we take a different approach that only requires regularity of the exact solution x. The crucial point is to write J_hx in a modified variation-of-constants formula that is driven by the discretized operator S_h up to an error covered by (2.12).

Lemma 4.2. *Let Assumptions 2.2, 2.4, and 2.6 hold, and let $x\in C^1\big([0,T];Z\big)$ be the solution of (2.3). Then, we have the representation*

$$J_h\widetilde{x}^{n+1} = \mathrm{e}^{-\tau S_h}J_h\widetilde{x}^n + \tau\int_0^1 \mathrm{e}^{-(1-s)\tau S_h}\mathcal{L}_h^*\widetilde{g}^{n+s}\,\mathrm{d}s + E_{HG}^n(\tau) \tag{4.6}$$

with remainder $E_{HG}^n(\tau)$ bounded by

$$\|E_{HG}^n(\tau)\|_{X_h} \leq \tau\mathrm{e}^{\tau\widehat{c}_{\mathrm{qm}}}\left(\left\|\Delta_{J_h}x'\right\|_{L^\infty([t_n,t_{n+1}];X_h)} + \|R_hx\|_{L^\infty([t_n,t_{n+1}];X_h)}\right), \tag{4.7}$$

where Δ_{J_h} and R_h are given in Definition 2.7.

Proof. We use equation (2.3) to obtain

$$\begin{aligned} J_h x'(t) &= \mathcal{L}_h^* x'(t) + \Delta_{J_h} x'(t) \\ &= -\mathcal{L}_h^* S x(t) + \mathcal{L}_h^* g(t,x(t)) + \Delta_{J_h} x'(t) \\ &= -S_h J_h x(t) + \mathcal{L}_h^* g(t,x(t)) - R_h x(t) + \Delta_{J_h} x'(t). \end{aligned}$$

Applying the variation-of-constants formula and (2.5) yields the assertion. □

The following two subsections treat the classes of exponential integrators separately. However, all the error estimates rely on the representation of the exact solution provided by Lemma 4.2. Throughout, we use a local in time version of $E_h(t)$ defined in (2.12), given by

$$\begin{aligned} \varepsilon_h^n = {} & \|R_h x\|_{L^\infty([t_n,t_{n+1}];X_h)} + \|r_h(\cdot,x(\cdot))\|_{L^\infty([t_n,t_{n+1}];X_h)} \\ & + \left\|\Delta_{J_h} x'\right\|_{L^\infty([t_n,t_{n+1}];X_h)} \end{aligned} \tag{4.8}$$

to account for the spatial defects.

4.1. **Exponential Adams methods.** Using the notation defined in (4.2), for the analysis we introduce the two auxiliary interpolation polynomials $\widetilde{p}_h^{n,k}$ through the discretized nonlinearity evaluated at $J_h x$

$$\Big(\big(t_{n-k+1}, \widetilde{g}_h^{n-k+1}\big), \ldots, \big(t_n, \widetilde{g}_h^n\big)\Big),$$

and $\widetilde{p}^{n,k}$ through the continuous nonlinearity evaluated at exact solution x

$$\Big(\big(t_{n-k+1}, \widetilde{g}^{n-k+1}\big), \ldots, \big(t_n, \widetilde{g}^n\big)\Big).$$

Lemma 4.3. *Under the assumptions of Theorem 3.2, the exact solution satisfies*

$$J_h \widetilde{x}^{n+1} = \mathrm{e}^{-\tau S_h} J_h \widetilde{x}^n + \tau \int_0^1 \mathrm{e}^{-(1-s)\tau S_h} \widetilde{p}_h^{n,k}(t_{n+s})\,\mathrm{d}s + \delta^n, \quad n \geq k, \tag{4.9}$$

where the defect is bounded by

$$\|\delta^n\|_{X_h} \leq C\tau\big(\tau^k + \sum_{j=0}^{k-1} \varepsilon_h^{n-j}\big)$$

with a constant C independent of τ and h, and ε_h^n defined in (4.8).

Proof. Employing (4.6) and (4.9), we obtain

$$\begin{aligned} \delta^n &= \tau \int_0^1 \mathrm{e}^{-(1-s)\tau S_h} \big(\mathcal{L}_h^* \widetilde{g}^{n+s} - \widetilde{p}_h^{n,k}(t_{n+s})\big)\,\mathrm{d}s + E_{\mathrm{HG}}^n(\tau) \\ &= \tau \int_0^1 \mathrm{e}^{-(1-s)\tau S_h} \mathcal{L}_h^* \big(\widetilde{g}^{n+s} - \widetilde{p}^{n,k}(t_{n+s})\big)\,\mathrm{d}s \\ &\quad + \tau \int_0^1 \mathrm{e}^{-(1-s)\tau S_h} \mathcal{L}_h^* \widetilde{p}^{n,k}(t_{n+s}) - \widetilde{p}_h^{n,k}(t_{n+s})\,\mathrm{d}s + E_{\mathrm{HG}}^n(\tau)\,. \end{aligned}$$

The first term is bounded using the standard interpolation bounds and Assumption 3.1. The second term yields a linear combination of the nonlinear remainders

$r_h(t_{n-j}, \widetilde{x}^{n-j})$, $j = 0, \dots, k-1$, given in (2.11), and for the last term we employ the bound (4.7). □

From the bounds on the defects, we conclude our first main result.

Proof of Theorem 3.2. We recall that by (4.1) it is sufficient to bound e_h^n and assume first that the numerical approximations x_h^n are bounded. Subtracting (4.9) from (3.5), we derive the error recursion

$$\begin{aligned} e_h^{n+1} &= \mathrm{e}^{-\tau S_h} e_h^n + \tau \int_0^1 \mathrm{e}^{-(1-s)\tau S_h} \big(p_h^{n,k}(t_{n+s}) - \widetilde{p}_h^{n,k}(t_{n+s}) \big) \, \mathrm{d}s - \delta^n \\ &= \mathrm{e}^{-\tau S_h} e_h^n + \tau \sum_{j=0}^{k-1} L^{n,j}(x_h^{n-j}, \widetilde{x}^{n-j}) - \delta^n, \end{aligned}$$

where by Assumption 2.4 it holds with a constant $C_{\widehat{L}}$ independent of τ and h

$$\| L^{n,j}(x_h^{n-j}, \widetilde{x}^{n-j}) \|_{X_h} \le C_{\widehat{L}} \mathrm{e}^{\widehat{c}_{\mathrm{qm}} \tau} \| e_h^{n-j} \|_{X_h}.$$

Hence, resolving the error recursion and taking norms, we obtain for $n \ge k$

$$\| e_h^n \|_{X_h} \le \mathrm{e}^{\widehat{c}_{\mathrm{qm}} t_n} k \sum_{m=0}^{k-1} \| e_h^m \|_{X_h} + k C_{\widehat{L}} \sum_{m=k}^{n-1} \mathrm{e}^{\widehat{c}_{\mathrm{qm}} (t_n - t_m)} \| e_h^m \|_{X_h} + \mathrm{e}^{\widehat{c}_{\mathrm{qm}} t_n} \sum_{m=1}^{n} \| \delta^m \|_{X_h}.$$

Multiplication with $\mathrm{e}^{-\widehat{c}_{\mathrm{qm}} t_n}$ and the application of a discrete Gronwall lemma yields the desired error bound. By an induction argument, Assumption 2.8 yields the existence of $h_0, \tau_0 > 0$ such that the numerical approximations indeed remain bounded and the claim follows. □

4.2. **Exponential Runge–Kutta methods.** Our error analysis within this section is based on the analysis for the time discretization presented in [18]. In the following, we show how to extend these results in the presence of additional spatial errors. We first insert the reference operator J_h applied to the exact solution x into the numerical scheme and obtain with the defects $\Delta_h^{n,i}$, δ_h^n

$$\begin{aligned} J_h \widetilde{x}^{n+c_i} &= \mathrm{e}^{-c_i \tau S_h} J_h \widetilde{x}^n + \tau \sum_{j=1}^{i-1} a_{ij}(-\tau S_h) \widetilde{g}_h^{n+c_j} + \Delta_h^{n,i}, \\ J_h \widetilde{x}^{n+1} &= \mathrm{e}^{-\tau S_h} J_h \widetilde{x}^n + \tau \sum_{i=1}^{s} b_i(-\tau S_h) \widetilde{g}_h^{n+c_i} + \delta_h^n. \end{aligned} \tag{4.10}$$

Introducing the error of the inner stages $E_h^{ni} = X_h^{ni} - J_h \widetilde{x}^{n+c_i}$, we derive the error recursions

$$\begin{aligned} E_h^{ni} &= \mathrm{e}^{-c_i \tau S_h} e_h^n + \tau \sum_{j=1}^{i-1} a_{ij}(-\tau S_h) \big(g_h(t_{n+c_j}, X_h^{nj}) - \widetilde{g}_h^{n+c_j} \big) - \Delta_h^{n,i}, \\ e_h^{n+1} &= \mathrm{e}^{-\tau S_h} e_h^n + \tau \sum_{i=1}^{s} b_i(-\tau S_h) \big(g_h(t_{n+c_i}, X_h^{ni}) - \widetilde{g}_h^{n+c_i} \big) - \delta_h^n. \end{aligned} \tag{4.11}$$

In the following, we establish bounds on E_h^{ni} and e_h^{n+1}. In large parts, we follow the arguments in [18] and, use the shorthand notation

$$\widetilde{g}^{(j),n} := \frac{\mathrm{d}^{\mathrm{j}}}{\mathrm{d}t^j} g(t, x(t))\Big|_{t=t_n}$$

which is well-defined by Assumption 3.1. As a first result, derive the structure of the defects. This is an extension of [18, Lem. 4.1] incorporating the spatial defects $\Delta_{h,\mathrm{sp}}^{n,i}$, $\delta_{h,\mathrm{sp}}^n$.

Lemma 4.4. *Let Assumptions 2.2, 2.4, 2.6, and 3.1 for $m = p$ hold. The defects can be expressed as*

$$\Delta_h^{n,i} = \Delta_{h,sp}^{n,i} + \Delta_{h,\tau}^{n,i} + \sum_{j=1}^{p-1} \tau^j \psi_{j,i}(-\tau S_h) \mathcal{L}_h^* \widetilde{g}^{(j-1),n},$$
$$\delta_h^n = \delta_{h,sp}^n + \delta_{h,\tau}^n + \sum_{j=1}^{p} \tau^j \psi_j(-\tau S_h) \mathcal{L}_h^* \widetilde{g}^{(j-1),n}.$$

They satisfy

$$\|\Delta_{h,sp}^{n,i}\|_{X_h} + \|\delta_{h,sp}^n\|_{X_h} \le C\tau\, \varepsilon_h^n, \quad \|\Delta_{h,\tau}^{n,i}\|_{X_h} \le C\tau^p, \quad \|\delta_{h,\tau}^n\|_{X_h} \le C\tau^{p+1} \tag{4.12}$$

with constants C independent of τ and h, and ε_h^n defined in (4.8).

Proof. We only prove the claim for δ_h^n since the argument for $\Delta_h^{n,i}$ is easily deduced from it. We obtain from (4.10), Lemma 4.2, and (2.11)

$$\begin{aligned}
\delta_h^n &= J_h \widetilde{x}^{n+1} - \mathrm{e}^{-\tau S_h} J_h \widetilde{x}^n - \tau \sum_{i=1}^{s} b_i(-\tau S_h) \widetilde{g}_h^{n+c_i} \\
&= \tau \Big(\int_0^1 \mathrm{e}^{-(1-s)\tau S_h} \mathcal{L}_h^* \widetilde{g}^{n+s}\, \mathrm{d}s - \sum_{i=1}^{s} b_i(-\tau S_h) \widetilde{g}_h^{n+c_i} \Big) + E_{\mathrm{HG}}^n(\tau) \\
&= \tau \Big(\int_0^1 \mathrm{e}^{-(1-s)\tau S_h} \mathcal{L}_h^* \widetilde{g}^{n+s}\, \mathrm{d}s - \sum_{i=1}^{s} b_i(-\tau S_h) \mathcal{L}_h^* \widetilde{g}^{n+c_i} \Big) \\
&\quad + \tau \sum_{i=1}^{s} b_i(-\tau S_h) r_h(t_{n+c_i}, \widetilde{x}^{n+c_i}) + E_{\mathrm{HG}}^n(\tau).
\end{aligned}$$

The last two terms are collected in $\delta_{h,\mathrm{sp}}^n$ and satisfy (4.12). It remains to study the first difference. Applying Taylor expansion on $\widetilde{g}_h^{n+s}$ and $\widetilde{g}_h^{n+c_i}$, we derive the desired representation and the bounds on the defects follow from Assumption 3.1. ∎

From this we derive the second main result.

Proof of Theorem 3.4. For the sake of readability, we only treat the case of a globally Lipschitz function. The local version is obtained by an induction argument.

(a) We first consider the case $p = 2$. As in [18, Sec. 4.3] we derive from (4.11)

$$\|e_h^{n+1}\|_{X_h} \le C\tau \sum_{j=0}^{n} \|e_h^j\|_{X_h} + C \sum_{j=0}^{n} \Big(\|\delta_{h,\mathrm{sp}}^j\|_{X_h} + \|\delta_{h,\tau}^j\|_{X_h} \Big) + C\tau \sum_{j=0}^{n} \Big(\max_{i=1,\dots,s} \|\Delta_{h,\mathrm{sp}}^{j,i}\|_{X_h} + \max_{i=1,\dots,s} \|\Delta_{h,\tau}^{j,i}\|_{X_h} \Big),$$

where we used Assumption 2.4 and the order conditions in Table 1 and Lemma 4.4 with $p = 2$. The bounds in (4.12) and a discrete Gronwall lemma yield the result.

(b) We now turn to the case $p \in \{3, 4\}$. We follow the steps of [18, Thm. 4.7] and explain the necessary modifications.

(1) Using Assumption 2.5, we obtain the discrete analogue to [18, Lem. 4.4]

$$\begin{aligned} g_h(t_{n+c_j}, X_h^{nj}) - \widetilde{g}_h^{n+c_j} &= \mathcal{D}_h^n E_h^{ni} + c_i \tau \mathcal{K}_h^n E_h^{ni} + Q_h^{ni}, \\ g_h(t_n, x^n) - \widetilde{g}_h^n &= \mathcal{D}_h^n e_h^n + Q_h^n, \end{aligned} \tag{4.13}$$

with the operators

$$\mathcal{D}_h^n := \frac{\partial g_h}{\partial x_h}(t_n, J_h \widetilde{x}^n), \quad \mathcal{K}_h^n := \frac{\partial^2 g_h}{\partial t \, \partial x_h}(t_n, J_h \widetilde{x}^n) + \frac{\partial^2 g_h}{\partial x_h^2}(t_n, J_h \widetilde{x}^n) J_h x'(t_n).$$

In addition, there is a constant $C > 0$ independent of τ and h such that

$$\|Q_h^{ni}\|_{X_h} \le C\big(\tau^2 + \|E_h^{ni}\|_{X_h}\big)\|E_h^{ni}\|_{X_h}, \quad \|Q_h^n\|_{X_h} \le C\|e_h^n\|_{X_h}^2 .$$

(2) We proceed as in [18, Lem. 4.5 and 4.6]. Using (4.13), we inductively eliminate the inner stages in (4.11). Employing the order conditions, which are satisfied up to order p, and Lemma 4.4, leads to the representation of the global error

$$e_h^{n+1} = \mathrm{e}^{-\tau S_h} e_h^n + \tau \mathcal{N}_h^n(e_h^n) e_h^n + \tau\big(\tau^p + \varepsilon_h^n\big)\mathcal{R}_h^n, \tag{4.14}$$

with uniformly bounded operators

$$\|\mathcal{N}_h^n(e_h^n)\|_{X_h \leftarrow X_h}, \|\mathcal{R}_h^n\|_{X_h} \le C.$$

(3) Resolving the error recursion (4.14), using (2.5), and the application of a discrete Gronwall lemma gives the result. $\square$

5. Application to second-order wave-type equations

In this section we explain how our results apply to second-order wave-type equations. For this purpose, we first present an abstract spatial discretization of (1.1) which was introduced in [15, 16]. In these references, it was proven that this discretization fits into the setting of Sections 2.3 and 2.4. We shortly recall the relevant results.

5.1. **Abstract space discretization.**

Let V_h be a finite dimensional vector space. We consider the following discretized version of (2.1) on $(0, T]$

$$\begin{aligned} m_h\big(u_h'', v_h\big) + b_h\big(u_h', v_h\big) + a_h\big(u_h, v_h\big) &= m_h\big(f_h(t, u_h), v_h\big) \quad \text{for all } v_h \in V_h, \\ u_h(0) = u_h^0, \qquad u_h'(0) &= v_h^0. \end{aligned} \tag{5.1}$$

For the discretized quantities we require similar properties as for their continuous counterparts, cf. Assumption 2.1.

Assumption 5.1.

a) The bilinear form $a_h \colon V_h \times V_h \to \mathbb{R}$ is symmetric and there exists a constant $\widehat{c}_G \geq 0$ such that
$$\tilde{a}_h \coloneqq a_h + \widehat{c}_G m_h$$
is a scalar product on V_h with induced norm $\|\cdot\|_{\tilde{a}_h}$.

b) The bilinear form m_h is also a scalar product on V_h. We denote V_h equipped with this scalar product m_h by H_h and the induced norm by $\|\cdot\|_{m_h}$.

c) The bilinear form $b_h \colon V_h \times H_h \to \mathbb{R}$ is bounded independent of h and there exists a $\widehat{\beta}_{\mathrm{qm}} \geq 0$ such that
$$b_h\big(v_h, v_h\big) + \widehat{\beta}_{\mathrm{qm}} \|v_h\|_{m_h}^2 \geq 0 \quad \text{for all } v_h \in V_h.$$

d) The nonlinearity $f_h \colon [0,T] \times V_h \to H_h$ is locally Lipschitz-continuous on V_h with constant $\widehat{L}_{T,M}$.

e) There exists a constant $\widehat{C}_{H,V} > 0$ such that $\|v_h\|_{m_h} \leq \widehat{C}_{H,V} \|v_h\|_{\tilde{a}_h}$ for all $v_h \in V_h$.

All constants in this assumption are independent of h.

Similar to the continuous case, we reformulate (5.1) as an evolution equation. For this purpose, we define $A_h, B_h \in \mathcal{L}(V_h; V_h)$ via
$$m_h\big(A_h v_h, \varphi_h\big) = a_h\big(v_h, \varphi_h\big), \quad m_h\big(B_h v_h, \varphi_h\big) = b_h\big(v_h, \varphi_h\big) \quad \text{for all } v_h, \varphi_h \in V_h.$$
Then, (5.1) is equivalent to
$$\begin{aligned} u_h''(t) + B_h u_h'(t) + A_h u_h(t) &= f_h(t, u_h(t)), \quad t \in (0,T], \\ u_h(0) = u_h^0, \qquad u_h'(0) &= v_h^0. \end{aligned} \tag{5.2}$$

5.2. **Framework for error analysis.** Similar to the first-order case we assume the existence of certain operators that are necessary for the error analysis.

Assumption 5.2.

a) There exists a lift operator $\mathcal{L}_h^V \in \mathcal{L}(V_h; V)$ satisfying
$$\|\mathcal{L}_h^V v_h\|_m \leq \widehat{C}_H \|v_h\|_{m_h}, \qquad \|\mathcal{L}_h^V v_h\|_{\tilde{a}} \leq \widehat{C}_V \|v_h\|_{\tilde{a}_h} \tag{5.3}$$
for all $v_h \in V_h$ with constants $\widehat{C}_H, \widehat{C}_V > 0$ independent of h.

b) There exists an interpolation operator $I_h \colon Z^V \to H_h$ defined on a dense subspace Z^V of V with
$$\|I_h z\|_{m_h} \leq \widehat{C}_{I_h} \|z\|_{Z^V} \quad \text{for all } z \in Z^V \tag{5.4}$$
where the constant $\widehat{C}_{I_h} > 0$ is independent of h.

Under Assumption 5.2, we can define the following operators and quantities that will appear in the latter error bounds.

Definition 5.3.

a) The adjoints of the lift operator $\mathcal{L}_h^{V*} \colon V \to V_h$ and $\mathcal{L}_h^{H*} \colon H \to H_h$ w.r.t. the scalar products in V and H are defined via
$$\begin{aligned} m_h\big(\mathcal{L}_h^{H*} v, w_h\big) &= m\big(v, \mathcal{L}_h^V w_h\big) \quad && \text{for all } v \in H, w_h \in H_h, \\ \tilde{a}_h\big(\mathcal{L}_h^{V*} v, w_h\big) &= \tilde{a}\big(v, \mathcal{L}_h^V w_h\big) && \text{for all } v \in V, w_h \in V_h. \end{aligned}$$

b) Our error bounds rely on the errors in the scalar products that are defined for $v_h, w_h \in V_h$ via

$$\begin{aligned}\Delta m\big(v_h, w_h\big) &\coloneqq m\big(\mathcal{L}_h^V v_h, \mathcal{L}_h^V w_h\big) - m_h\big(v_h, w_h\big),\\ \Delta\tilde{a}\big(v_h, w_h\big) &\coloneqq \tilde{a}\big(\mathcal{L}_h^V v_h, \mathcal{L}_h^V w_h\big) - \tilde{a}_h\big(v_h, w_h\big).\end{aligned}$$

5.3. **Fully discrete error bounds.** In this section we explain how the error bounds from Section 3 translate to the second-order equations considered in this section. In the same way as in (2.2), defining $X_h = V_h \times H_h$ and

$$x_h(t) = \begin{bmatrix} u_h(t) \\ v_h(t) \end{bmatrix}, \quad S_h = \begin{bmatrix} 0 & -\mathrm{I} \\ A_h & B_h \end{bmatrix}, \quad g_h\left(t, x_h\right) = \begin{bmatrix} 0 \\ f_h(t, u_h) \end{bmatrix}, \quad x_h^0 = \begin{bmatrix} u_h^0 \\ v_h^0 \end{bmatrix},$$

the second-order equation (5.2) is equivalent to (2.7).

We now recall the results from [16], which show that the first-order formulations of (1.1) as well as (5.2), respectively, fit in the setting of Section 2. In [16, Sec. 3.2], it was shown that Assumption 5.1 implies Assumption 2.4. We define the first-order reference operator $J_h \colon Z \to X_h$ via

$$J_h \begin{bmatrix} v \\ w \end{bmatrix} \coloneqq \begin{bmatrix} \mathcal{L}_h^{V*} v \\ I_h w \end{bmatrix}$$

on $Z = V \times Z^V \overset{d}{\hookrightarrow} X$. Using this definition, it was shown in the proof of [16, Thm. 3.9] that Assumption 5.2 implies Assumption 2.6 and, that for all $t \in [0, T]$ the error term $E_h(t)$ defined in (2.12) is bounded by $E_h(t) \leq \sum_{i=1}^5 E_i$ with

$$\begin{aligned}
E_1 \coloneqq& \|u_h^0 - \mathcal{L}_h^{V*} u^0\|_{\tilde{a}_h} + \|v_h^0 - I_h v^0\|_{m_h},\\
E_2 \coloneqq& \|\mathcal{L}_h^{H*} f\big(\cdot, u(\cdot)\big) - f_h\big(\cdot, \mathcal{L}_h^{V*} u(\cdot)\big)\|_{L^\infty([0,T];H_h)},\\
E_3 \coloneqq& \|(\mathrm{I} - \mathcal{L}_h^V I_h) u\|_{L^\infty([0,T];V)} + \|(\mathrm{I} - \mathcal{L}_h^V I_h) u'\|_{L^\infty([0,T];V)}\\
&+ \|(\mathrm{I} - \mathcal{L}_h^V I_h) u''\|_{L^\infty([0,T];H)},\\
E_4 \coloneqq& \Big\| \max_{\|\varphi_h\|_{\tilde{a}_h}=1} \Delta\tilde{a}\big(I_h u, \varphi_h\big) \Big\|_{L^\infty(0,t)} + \Big\| \max_{\|\psi_h\|_{m_h}=1} \Delta m\big(I_h u, \psi_h\big) \Big\|_{L^\infty(0,t)}\\
&+ \Big\| \max_{\|\varphi_h\|_{\tilde{a}_h}=1} \Delta\tilde{a}\big(I_h u', \varphi_h\big) \Big\|_{L^\infty(0,t)} + \Big\| \max_{\|\psi_h\|_{m_h}=1} \Delta m\big(I_h u'', \psi_h\big) \Big\|_{L^\infty(0,t)},\\
E_5 \coloneqq& \Big\| \max_{\|\psi_h\|_{m_h}=1} |b\big(u', \mathcal{L}_h^V \psi_h\big) - b_h\big(I_h u', \psi_h\big)| \Big\|_{L^\infty(0,t)}.
\end{aligned} \tag{5.5}$$

Thus, the consistency Assumption 2.8 is implied by the following condition.

Assumption 5.4. The solution of (1.1) satisfies $u \in C^2([0, T]; Z^V)$ and the error terms in (5.5) converge to zero, i.e.,

$$E_i \to 0, \quad \text{for} \quad h \to 0, \quad i = 1, \dots 5.$$

It remains to transfer Assumptions 2.5 and 3.1 into the second-order formulation. The Fréchet differentiability is easily obtained from the following reformulation.

Assumption 5.5. The nonlinearity f_h satisfies $f_h \in C^3([0, T] \times V_h; H_h)$ with derivatives bounded independent of h.

Analogously, Assumption 3.1 takes the following form.

Assumption 5.6. Let $m \geq 1$ and u be the exact solution of (1.1). The the differentiability

$$s \mapsto f(s, x(s)) \in C^m\big([0,T]; H\big)$$

holds.

Employing the above assumptions, we rephrase the main theorems of Section 3 for the second-order wave equation (1.1).

Corollary 5.7. *Let Assumptions 2.1, 5.1, 5.2, 5.4, and 5.6 be satisfied. Then, Theorems 3.2 and 3.4 (for $p = 2$) hold true for the first-order formulation of the second-order wave equation (1.1) with corresponding spatial discretization (5.2). If additionally Assumption 5.5 is satisfied, then Theorem 3.4 holds also true for $p = 3$ and $p = 4$. In particular, we obtain the following two error bounds.*

a) *For the k-step Adams method (3.5), it holds for $t_k \leq t_n \leq T$*

$$\begin{aligned}\|\mathcal{L}_h^V u_h^n - u(t_n)\|_{\tilde{a}} + \|\mathcal{L}_h^V v_h^n - v(t_n)\|_m &\leq C(\tau^k + \sum_{i=1}^{5} E_i) \\ &\quad + C \sum_{j=1}^{k-1} \Big(\|u_h^j - \mathcal{L}_h^{V*} u(t_j)\|_{\tilde{a}_h} + \|v_h^j - I_h v(t_j)\|_{m_h} \Big).\end{aligned}$$

b) *For an exponential Runge–Kutta method (3.7) of order p, it holds for $t_n \leq T$*

$$\|\mathcal{L}_h^V u_h^n - u(t_n)\|_{\tilde{a}} + \|\mathcal{L}_h^V v_h^n - v(t_n)\|_m \leq C(\tau^p + \sum_{i=1}^{5} E_i).$$

We emphasize that this result immediately implies full discretization error bounds for concrete examples if the space discretization admits suitable bounds on the errors E_i. An application is given in the following section.

6. Application: Wave equation with kinetic boundary conditions

In this section, we apply the abstract theory of Section 5 to a semilinear wave equation with kinetic boundary conditions. By this example we illustrate our results and perform some numerical experiments.

6.1. **Continuous equation.** Let $\Omega = B_1(0) \subset \mathbb{R}^2$ be the two-dimensional unit sphere with boundary $\Gamma = \partial\Omega$ and corresponding outer normal vector $\mathbf{n}$. By Δ_Γ we denote the Laplace–Beltrami operator on Γ and consider the wave equation with kinetic boundary conditions and nonlinear forcing terms given by

$$u_{tt} + \big(1 + \mathbf{x} \cdot \nabla\big) u_t - \Delta u = |u|u + \eta_\Omega(t, \mathbf{x}), \qquad \text{for } t \geq 0, \mathbf{x} \in \Omega, \tag{6.1a}$$

$$u_{tt} + \partial_{\mathbf{n}} u - \Delta_\Gamma u = u^3 + \eta_\Gamma(t, \mathbf{x}), \qquad \text{for } t \geq 0, \mathbf{x} \in \Gamma, \tag{6.1b}$$

$$u(0, \mathbf{x}) = u^0(\mathbf{x}), \qquad u_t(0, \mathbf{x}) = v^0(\mathbf{x}), \qquad \text{in } \overline{\Omega} \tag{6.1c}$$

with inhomogeneities η_Ω, η_Γ. In [16, Sec. 2.1], it was shown that a more general version of this equation fits into the setting of Section 2.1 with

$$H = L^2(\Omega) \times L^2(\Gamma), \quad V = H^1(\Omega; \Gamma), \quad Z = D(A) = H^2(\Omega; \Gamma),$$

$$A = \begin{bmatrix} -\Delta & 0 \\ \partial_{\mathbf{n}} & -\Delta_\Gamma \end{bmatrix}, \quad B = \begin{bmatrix} (1 + \mathbf{x} \cdot \nabla) & 0 \\ 0 & 0 \end{bmatrix}, \quad f(t, u) = \begin{bmatrix} |u|u + \eta_\Omega(t, \mathbf{x}) \\ (\gamma u)^3 + \eta_\Gamma(t, \mathbf{x}) \end{bmatrix},$$

where

$$H^k(\Omega;\Gamma) \coloneqq \{v \in H^k(\Omega) \mid \gamma(v) \in H^k(\Gamma)\} \subset H^k(\Omega) \times H^k(\Gamma)$$

and $\gamma\colon H^1(\Omega) \to L^2(\Gamma)$ denotes the trace operator.

6.2. **Discretization.** To discretize (6.1) in space we use the bulk-surface finite element method as presented in [16, Sec. 2.2]. We denote the maximal mesh width by h. This discretization is nonconforming since the computational domain Ω_h does not coincide exactly with Ω. Further, in [16, Sec. 2.2] it was proven, that the discretization fits into the setting of Section 5. Moreover, in the proof of [16, Thm. 2.7] it was shown that, for finite elements of order q, the space discretization error terms from (5.5) are bounded by

$$E_i \leq Ch^q. \tag{6.2}$$

Remark 6.1. Note that compared to [16, Sec. 2.2] the only additional assumptions that we require in Section 5 in order to prove the full discretization bounds are Assumptions 5.5 and 5.6 which correspond to Assumptions 2.5 and 3.1 in the first-order formulation.

a) The proof of the Lipschitz continuity of the discretized nonlinearity f_h in [16, Lem. 2.6] is non-trivial and relies on discrete norms that are equivalent to the L^q norms on the finite elements space. This is necessary to prove that the local Lipschitz constant is independent of h. Similarly, one can prove the differentiability of f_h, and bounds for the derivatives independent of h required in Assumption 5.5. In fact, we can also treat more general nonlinearities in (6.1) if the underlying function and its derivatives satisfy certain growth conditions.
b) Assumption 5.6 is a regularity assumption on the exact solution and was already necessary to prove convergence of the time discretization, cf. [7, 18, 20]. The exact solution in our numerical experiments satisfies this assumption.

6.3. **Numerical results.** We implemented the numerical experiments in `C++` using the finite element library `deal.II` (version 9.2) [3, 4]. The codes to reproduce the experiments are available at https://doi.org/10.5445/IR/1000134973.

The finite element discretization was implemented as described in [25, Ch. 6.5.1]. For the time discretization, we consider the exponential Euler scheme (3.4), the exponential two-step Adams method (3.5) (for $k = 2$), and the exponential trapezoidal rule of order $p = 2$ given by (3.9) with $c_2 = 1$. To evaluate the matrix functions appearing in the exponential integrators, we used a rational Krylov method including mass matrices as described in [21, Alg. 2].

For our computations, we set

$$\begin{aligned}
u^0(\mathbf{x}) &= 0, \qquad v^0(\mathbf{x}) = 2\pi \mathbf{x}_1\mathbf{x}_2, \\
\eta_\Omega(t,\mathbf{x}) &= -\left(4\pi^2 + |\sin(2\pi t)\mathbf{x}_1\mathbf{x}_2|\right)\sin(2\pi t)\mathbf{x}_1\mathbf{x}_2 + 6\pi\cos(2\pi t)\mathbf{x}_1\mathbf{x}_2, \\
\eta_\Gamma(t,\mathbf{x}) &= -4\pi^2\sin(2\pi t)\mathbf{x}_1\mathbf{x}_2 + 6\sin(2\pi t)\mathbf{x}_1\mathbf{x}_2 - \left(\sin(2\pi t)\mathbf{x}_1\mathbf{x}_2\right)^3.
\end{aligned}$$

Then, the exact solution of (6.1) is given by

$$u(t,\mathbf{x}) = \sin(2\pi t)\mathbf{x}_1\mathbf{x}_2.$$

Since the computation of the lift of a finite element function is very laborious, we do not compute the full error $\mathcal{L}_h^V u_h^n - u(t_n)$. Instead, in our numerical examples

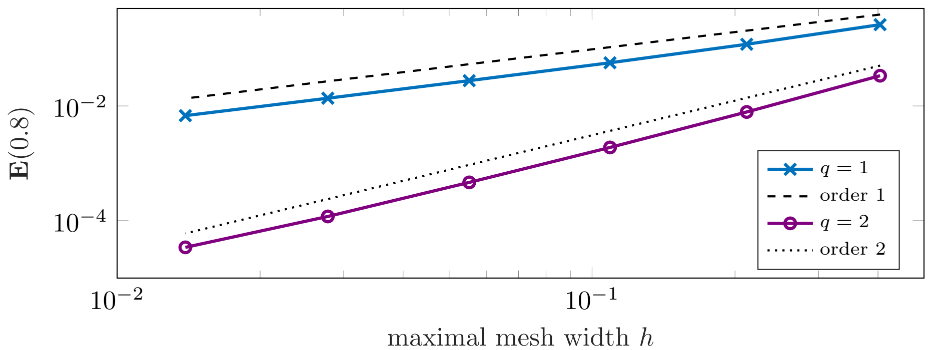

FIGURE 2. Error $\mathbf{E}(0.8)$ of the exponential trapezoidal rule (with time step size $\tau = 5.33 \cdot 10^{-4}$) combined with finite elements of order $q = 1$ and $q = 2$ plotted against the mesh width h.

we consider the error

$$\mathbf{E}(t) \coloneqq \|u_h(t) - u(t)\big|_{\Omega_h}\|_{H^1(\Omega_h;\Gamma_h)} + \|u_h'(t) - u'(t)\big|_{\Omega_h}\|_{L^2(\Omega_h)\times L^2(\Gamma_h)},$$

cf. [25, Ch. 6] for more details. We evaluate the integrals appearing in $\mathbf{E}$ with a quadrature rule of higher order, such that the quadrature error is negligible. The restriction of u to Ω_h is possible since in our case we have $\Omega_h \subset \Omega$.

In Figure 2 the convergence of the error w.r.t. the spatial mesh width h is shown when using the exponential trapezoidal rule. We observe that for finite elements of order q the error converges with order q in space for $q = 1, 2$ as predicted by Corollary 5.7 combined with (6.2).

In Figure 3, we consider the convergence of the error w.r.t. the time step size τ. For all three time discretization schemes we observe the order predicted by Theorems 3.2 and 3.4, respectively, until the error is dominated by the error of the spatial approximation.

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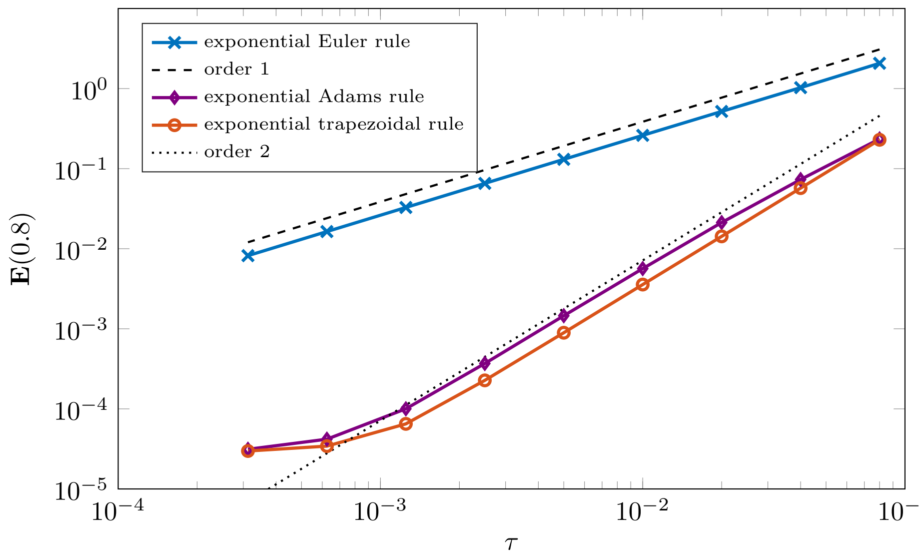

FIGURE 3. Error $\mathbf{E}(0.8)$ of the exponential Euler, the exponential trapezoidal, and the two-step exponential Adams scheme combined with finite elements of order $q = 1$ and $q = 2$ ($h \approx 0.014$) plotted against the time step size τ.

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