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A SPACE-TIME FINITE ELEMENT METHOD FOR THE NONLINEAR SCHRÖDINGER EQUATION: THE CONTINUOUS GALERKIN METHOD*

OHANNES KARAKASHIAN† AND CHARALAMBOS MAKRIDAKIS‡

Abstract. The convergence of a class of continuous Galerkin methods for the nonlinear (cubic) Schrödinger equation is analyzed in this paper. These methods allow variable temporal stepsizes as well as changing of the spatial grid from one time level to the next. We show the existence of the resulting approximations and prove optimal order error estimates in $L^\infty(L^2)$ and in $L^\infty(H^1)$. These estimates are valid under weak restrictions on the space-time mesh. These restrictions are milder if the elliptic projection is used at every time step instead of the L^2 projection. We also give superconvergence results at the temporal nodes t^n.

Key words. continuous Galerkin method, nonlinear Schrödinger equation

AMS subject classifications. 65M60, 65M12

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1. Introduction.

In this work we continue our study of space-time finite element methods for nonlinear problems of nonparabolic character working as a model with the nonlinear Schrödinger equation (NLS)

$$
\begin{aligned}
&u_t = \mathrm{i}\,\Delta u + \mathrm{i}\,\lambda |u|^2 u \quad \text{in } \Omega \times [0,T],\\
&u = 0 \quad \text{on } \partial\Omega \times [0,T],\\
&u(\cdot,0) = u^0 \quad \text{in } \Omega,
\end{aligned}
\tag{1.1}
$$

where Ω is a bounded domain in $\mathbb{R}^2$, u is a complex-valued function defined on $\overline{\Omega} \times [0,T]$, and λ is a real parameter; cf. [S]. We consider a class of methods that is an extension of the continuous Galerkin method. In contrast to previous applications of this method to parabolic and hyperbolic problems, [AM], [BL], [FP], the analysis presented herein allows flexible space-time mesh structures necessary for adaptive computations. In particular, we are able to modify the spatial mesh in time and to prove convergence under mild mesh conditions.

The method. Let $0 = t^0 < t^1 < \cdots < t^N = T$ be a partition of $[0,T]$, and

$$I_n = (t^n, t^{n+1}], \quad k_n = t^{n+1} - t^n.$$

We associate a partition $\mathcal{T}_{hn}$ of Ω and a finite element space S_h^n with each interval I_n:

$$S_h^n = \{\chi \in H_0^1(\Omega) : \chi|_K \in \mathbb{P}_{r-1}(K), K \in \mathcal{T}_{hn}\},$$

where $\mathbb{P}_p(S)$ is the space of polynomials of degree p. We also associate a space S_h^{-1} with $\{t^0\}$, but for simplicity we take $S_h^{-1} = S_h^0$. In the following we shall denote by

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†Department of Mathematics, University of Tennessee, Knoxville, TN 37996 (ohannes@math.utk.edu). The work of this author was partly supported by NSF grant INT-9504845.

‡Department of Mathematics, University of Crete, 71409 Heraklion-Crete, Greece and Institute of Applied and Computational Mathematics, FORTH, 71110 Heraklion-Crete, Greece (makr@sargos.math.uch.gr).The work of this author was sponsored by a research grant from the University of Crete and by the General Secretariat for Research and Technology through PENED-1747.

K a generic element of the partition $\mathcal{T}_{hn}$. Also h_K stands for the diameter of K, and $h_n = \max_{K\in\mathcal{T}_{hn}} h_K$.

For a positive integer q, let $V_q = V_{hk}(q)$ be the space of piecewise polynomial functions $\varphi : \Omega \times (0,T] \to \mathbb{C}$ of the form $\varphi|_{\Omega\times I_n} = \sum_{j=0}^{q} t^j \chi_j(x)\,,\ \chi_j \in S_h^n$. Hence, the functions of V_q are, for each $t \in I_n$, elements of S_h^n and, for each $x \in \Omega$, piecewise polynomial functions of degree q with *possible* discontinuities at the nodes t^n, $n = 0, \ldots, N-1$. Let also $V_q^n = \{\varphi|_{\Omega\times I_n} \ :\ \varphi \in V_q\}$.

The continuous Galerkin (cG) method for (1.1) that we consider is the following: Find $U \in V_q$ satisfying

$$\begin{aligned} &\int_{I_n} \big\{(U_t,\phi) + \mathrm{i}\,(\nabla U,\nabla\phi) - \mathrm{i}\,\lambda\,(|U|^2U,\phi)\big\}\,dt = 0 \quad \forall\phi\in V_{q-1}^n,\\ &\qquad\qquad U^{n+} = \Pi^n U(t^n), \quad n = 0,\ldots,N-1, \end{aligned} \tag{1.2}$$

where $U^0 = u^0$, $v^{n+} = \lim_{t\to t^n+} v(t)$ and Π^n denotes an appropriate projection operator onto S_h^n. We are interested in two particular choices of Π^n, namely, the L^2-projection and the elliptic projection into S_h^n. Note that if $S_h^{n-1} \subset S_h^n$, then $U^{n+} = U(t^n)$, and U is continuous at t^n. In general, however, U might have discontinuities at the time nodes due to the spatial mesh modification with n. It seems that (1.2) is a natural extension of the method analyzed in [AM] for parabolic and in [BL], [FP] for hyperbolic problems in the case where $S_h^n = S_h\ \forall\ n$. The flexibility in the selection of the space-time mesh allowed by (1.2) is the same with that of the discontinuous Galerkin (dG) method analyzed in [EJ1, EJ2, EJ3] and in [KM1]. Further, our convergence results for the cG method parallel those obtained for the dG method in [KM1] for (1.1). The analysis presented in this paper contains interesting similarities but also important differences with that of [KM1]. Note that in a recent paper, Dörfler [Dr] considered a method similar to (1.2) with $q = 1$ for a linear Schrödinger equation and proposed an adaptive algorithm based on a posteriori estimates.

Notation. Let $H^\ell(S)$ be the (complex) Sobolev space of order ℓ, and we denote its norm by $\|\cdot\|_{\ell,S}$ ($\|\cdot\|_\ell$ if $S = \Omega$). Also $(\cdot,\cdot)$ denotes the inner product, and $\|\cdot\|$ denotes the corresponding norm on $L^2(\Omega)$; $\|\cdot\|_\infty$ denotes the norm of $L^\infty(\Omega)$ and $\|\cdot\|_{1,\infty}$ denotes the norm of $W^{1,\infty}(\Omega)$. Also, we shall make frequent use of the following notation: We denote by $|\!|\!|\cdot|\!|\!|_n$ and by $\max_{I_n}\|\cdot\|$ the norms of $L^2(I_n, L^2(\Omega))$ and $C(\bar I_n, L^2(\Omega))$, respectively, i.e.,

$$|\!|\!|v|\!|\!|_n := \Big(\int_{I_n} \|v(t)\|^2 dt\Big)^{1/2}.$$

Also for $s, m = 0, 1, \ldots$ and $v \in H^m(\Omega)$ we let

$$\|h_n^s v\|_{m,h} := \left(\sum_{K\in\mathcal{T}_{hn}} h_K^{2s}\,\|v\|_{m,K}^2\right)^{1/2}.$$

Summary of results. We introduce the modified scheme

$$\begin{aligned} &\int_{I_n} \{(U_t,\phi) + \mathrm{i}\,(\nabla U,\nabla\phi) - \mathrm{i}\,\lambda\,(f(U),\phi)\}\,dt = 0 \quad \forall\phi\in V_{q-1}^n,\\ &\qquad\qquad U^{n+} = \Pi^n U(t^n), \quad n = 0,\ldots,N-1, \end{aligned} \tag{1.3}$$

where $U^0 = u^0$ and $f = f(z)$, $f : \mathbb{C} \to \mathbb{C}$, is an appropriate globally Lipschitz continuous function (cf. section 4) such that $f(z) = |z|^2 z$ in a ball with a radius that depends on the solution u of (1.1). In particular, u is in that ball. As a first step toward proving the convergence of (1.2) to (1.1) we analyze the stability and convergence of (1.3). Sections 2 and 3 are devoted to the analysis of (1.3): In section 2 we establish the existence of a solution of (1.3) by using a crucial stability result which is used throughout the paper. The proofs make use of properties of the Lagrange interpolating polynomials associated with the *Gauss–Legendre* points of each I_n. In section 3 we present the basic error analysis in $L^\infty(L^2(\Omega))$ for (1.3) with $\Pi^n = P^n$, for all n, where P^n is the L^2-projection into S_h^n. The main result of this section can be stated as follows (cf. Theorem 3.1): If u is the solution of (1.1) and $U \in V_q^n$ is the solution of (1.3), then

$$
\begin{aligned}
\max_{t\in[0,T]} \|u(t) - U(t)\| \le C \max_m k_m^{q+1} \max_{I_m} \left(\|u^{(q+1)}\| + \|u^{(q+2)}\| + \|\Delta u^{(q+1)}\|\right) \\
+ C \max_m \max_{I_m} (\|h_m^r u_t\|_{r,h} + \|h_m^r u\|_{r,h}) \\
+ C\mathcal{N}_C \max_m \|J[\omega^m]\|,
\end{aligned} \tag{1.4}
$$

where $\mathcal{N}_C$ denotes the number of times where $S_h^j \ne S_h^{j-1}$, $j = 1, \ldots, N-1$, and $J[\omega^n] = \omega^{n+} - \omega^n = (P_E^n - P_E^{n-1})u(t^n)$ is the jump of the elliptic projection $\omega(t) = P_E^n u(t)$ at t^n. The estimate (1.4) is obviously valid for the corresponding linear problem, i.e., if $f(u) = g(x,t)$. If we do not change the spaces S_h^n too often, (1.4) establishes an optimal-order convergence rate; compare with Dupont [D]. In any case, however, (1.4) guarantees convergence, since $\|J[\omega^m]\|$ is always bounded by $\|h_{m-1}^r u\|_{r,h} + \|h_m^r u\|_{r,h}$. An interesting feature of the proof of (1.4) is the combination of two time interpolating operators and of the corresponding quadrature rules. These are the interpolants at the Gauss–Legendre and at the Lobatto points of each I_n. By using the Gauss–Legendre interpolant we handle the stability of the scheme and by using the Lobatto interpolant we obtain the desired consistency estimate. Together, these lead to the optimal-order error estimate (1.4). Note that in the analysis in [KM1] of the dG method the use of one interpolation operator was sufficient. As in [KM1] the proof makes use of finite element and finite difference techniques, taking full advantage of appropriate energy-type estimates. We refer to [BL], [FP], where a cG method (with $S_h^n = S_h$ for all n) is analyzed for linear second-order hyperbolic problems. See also [EF], [FR].

Section 4 is devoted to $L^\infty(H^1(\Omega))$ estimates. First we complete the convergence analysis of (1.2) in the case where $\Pi^n = P^n\ \forall\ n$. In that case and assuming that for each n, $1 \le n \le N-1$, there holds

$$
\begin{array}{l} S_h^{n-1} \subset S_h^n, \\ \|\nabla P^n v\| \le C_P \|\nabla v\| \quad \forall v \in H_0^1(\Omega) \end{array} \quad \text{or} \quad k_n \ge C_N(k^{2(q+1)} + h^{2r}), \tag{1.5}
$$

we derive optimal order $L^\infty(H^1(\Omega))$ estimates for (1.3), which in view of an inverse inequality imply that the solution U of (1.3) is a solution of (1.2) as well (Theorem 4.1) and thus satisfies the error bound (1.4). Here

$$
k = \max_{0\le n\le N-1} k_n,\ h = \max_{\substack{K\in\mathcal{T}_{hn}\\ 0\le n\le N-1}} h_K,\ \underline{h} = \min_{\substack{K\in\mathcal{T}_{hn}\\ 0\le n\le N-1}} h_K,\ C_N = c|\ln(\underline{h})|. \tag{1.6}
$$

Next we study the convergence of (1.2) in $L^\infty(H^1(\Omega))$ in the case where $\Pi^n = P_E^n\ \forall\ n$. An optimal order convergence result holds in this case as well; cf. Theorem 4.2.

The use of this projection allows us to improve the mesh conditions (1.5) to the sole requirement that S_h^n should satisfy the stability property $\|\nabla P^n v\| \le C_P\|\nabla v\|$ $\forall v \in H_0^1(\Omega)$.

In section 5, we prove a superconvergence result for (1.2) in the case where $\Pi^n = P^n$ for all n. Under the assumptions of sections 3 and 4 and assuming that u has sufficient regularity, we show that

$$\begin{aligned}\|u(t^{n+1}) - U(t^{n+1})\| \le C \max_{m\le n} C_1(m,u)k_m^\sigma + C \max_{m\le n} C_2(m,u)h_m^r \\ + C\mathcal{N}_C(n-1) \max_{m\le n} \|J[\omega^n]\|\,,\end{aligned} \tag{1.7}$$

where $\sigma = 2q$ if Ω is polyhedral and $\sigma = \min\{q+3, 2q\}$ otherwise; $C_1(m,u)$ and $C_2(m,u)$ are constants that depend on m and u but are independent of h and k. The proof is based on an extension of the techniques of [KM1] and [KAD] to the case at hand and relies on a consistency analysis significantly different from that of section 3.

It is to be noted that the constants appearing in the estimates (1.4) and (1.7) are of the form e^{LT}, where L is a (Lipschitz) constant depending on the solution u of (1.1). If u blows up at some finite time $t^* > T$ but close to T, then these estimates obviously lose their effectiveness. However, a finer analysis devoted to numerical blowup for (1.1) can be done to lead to meaningful estimates in this case. These issues will be addressed in a forthcoming paper.

In section 6, we report on numerical computations with $q = 2, 3$ for a model test problem and also provide comparisons with the dG method analyzed in [KM1] as well as some related implicit Runge–Kutta (IRK) methods analyzed in [KAD].

The observations in [KM1] concerning the connection between the dG method and the class of Radau IIA Runge–Kutta methods apply for the cG method with the difference that the Gauss–Legendre IRK methods are now the corresponding class, the link being provided by the Lagrange interpolating polynomials associated with the Gauss–Legendre abscissas; cf. also Hulme [H].

Indeed, replacing the (nonlinear in U) temporal integral $\int_{I_n}(|U|^2U,\phi)dt$ in (1.2) by the q-point Gauss–Legendre quadrature rule yields the q-stage Gauss–Legendre IRK method. Therefore, for the NLS equation, the essential and only difference between any one of these two space-time finite element methods and its IRK counterpart resides in the way in which the nonlinear term is evaluated. An interesting way of looking at this state of affairs is to view the IRK methods as efficient implementations of the space-time finite element methods. Indeed, this observation is supported by the numerical evidence offered in section 6: The dG and cG methods, while more accurate than their respective IRK counterparts, are less efficient due to the extra work required in evaluating the nonlinear temporal integral exactly. Note that this is possible in the case of the NLS equation since that term is polynomial in t on each I_n.

As far as the analysis is concerned, our experience with the cG method parallels and reinforces the observations made in [KM1]. As noted there, the analysis of IRK methods requires considerable machinery consisting of separate sets of conditions for existence, stability, and consistency (cf. [KAD] for details). In particular, the consistency analysis is more reminiscent of the superconvergence techniques encountered in section 5. In contrast, the convergence of the space-time finite element methods studied here and in [KM1] flows directly from the weak formulations and some elementary properties of Lagrange interpolating polynomials.

As a conclusion we believe that our general approach established in [KM1] and in the present paper to two different and important space-time finite element methods for the model problem (1.1) can be used to analyze and/or to construct new and potentially more effective finite element methods for the numerical solution of particular problems within the general class of time dependent PDEs. In [KM2] we analyze the convergence of a cG method with mesh modification for nonlinear second-order hyperbolic problems.

2. Existence. For each $q \geq 1$, consider the Gauss–Legendre integration rule,

$$\int_0^1 g(\tau)d\tau \cong \sum_{j=1}^{q} w_j g(\tau_j), \quad 0 < \tau_1 < \cdots < \tau_q < 1, \tag{2.1}$$

which is *exact for all polynomials of degree* $\leq 2q-1$.

For fixed $q \geq 1$, let $\{\ell_i\}_{i=1}^q$ be the Lagrange polynomials of degree $q-1$ associated with the abscissas $\tau_1, \dots, \tau_q$, i.e.,

$$\ell_i(\tau) = \prod_{\substack{j=1 \\ i \neq j}}^{q} \frac{(\tau - \tau_j)}{(\tau_i - \tau_j)}. \tag{2.2}$$

Using the linear transformation $t = t^n + \tau k_n$ that maps [0,1] onto $\overline{I}_n$, we adapt the quadrature rule (2.1) to the interval $\overline{I}_n$ by defining its abscissas and weights as follows:

$$\begin{aligned} &t^{n,j} = t^n + \tau_j k_n, \quad j = 1, \dots, q, \\ &\ell_{n,i}(t) = \ell_i(\tau), \\ &w_{n,i} = \int_{t^n}^{t^{n+1}} \ell_{n,i}(t)dt = k_n \int_0^1 \ell_i(\tau)d\tau = k_n w_i, \qquad i = 1, \dots, q. \end{aligned} \tag{2.3}$$

We shall also use the Lagrange polynomials $\{\hat{\ell}_i\}_{i=0}^q$ of degree q associated with the $q+1$ points $0 = \tau_0 < \tau_1 < \cdots < \tau_q$,

$$\hat{\ell}_i(\tau) = \prod_{\substack{j=0 \\ j \neq i}}^{q} \frac{(\tau - \tau_j)}{(\tau_i - \tau_j)}.$$

We also let $t^{n,0} = t^n$. Then $U|_{I_n}$ is uniquely determined by the functions $U^{n,j} \in S_h^n$, ($U^{n,j} = U(x, t^{n,j})$) such that

$$U(x,t) = \sum_{j=0}^{q} \hat{\ell}_{n,j}(t) U^{n,j}(x), \quad (x,t) \in \Omega \times I_n. \tag{2.4}$$

It is important to note that $U^{n,0} = U^{n+} = \Pi^n U(t^n)$ and is given. Now, if $\psi = \psi(x), \psi \in S_h^n$, the function $\varphi = \ell_{n,i}\psi$ is an element of V_{q-1}^n. Therefore (1.3) is equivalent to

$$\begin{aligned} \sum_{j=1}^{q} m_{ij}(U^{n,j}, \psi) + \mathrm{i}\, k_n w_i (\nabla U^{n,i}, \nabla \psi) - \mathrm{i}\,\lambda \int_{I_n} \ell_{n,i}(t)(f(U), \psi)dt& \\ = -m_{i0}(U^{n+}, \psi), \quad i = 1, \dots, q, \quad \psi \in S_h^n\,,& \end{aligned} \tag{2.5}$$

with

$$m_{ij} = \int_{I_n} \hat{\ell}'_{n,j}(t)\, \ell_{n,i}(t)dt, \quad i = 1, \ldots, q, \ j = 0, \ldots, q.$$

To establish the existence of U, or equivalently that of $\{U^{n,j}\}_{j=1}^{q}$, it will suffice to show that the $q \times q$ array $\widetilde{\mathcal{M}} = D^{-1/2}\mathcal{M}D^{1/2}$ is positive definite, where $D = \operatorname{diag}\{\tau_1, \ldots, \tau_q\}$ and $\mathcal{M}_{ij} = m_{ij}, \quad i,j = 1, \ldots, q$.

To begin, note that $\hat{\ell}_i(\tau) = \frac{\tau}{\tau_i}\ell_i(\tau), \ i = 1, \ldots, q$, and hence

$$\begin{aligned} m_{ij} &= \int_{t^n}^{t^{n+1}} \hat{\ell}'_{n,j}(t)\ell_{n,i}(t)dt = \int_0^1 \hat{\ell}'_j(\tau)\ell_i(\tau)d\tau \\ &= \int_0^1 \frac{1}{\tau_j}\left[\ell_j(\tau) + \tau\ell'_j(\tau)\right]\ell_i(\tau)d\tau \\ &= \frac{w_i}{\tau_j}\left[\delta_{ij} + \tau_i\ell'_j(\tau_i)\right], \quad i,j = 1, \ldots, q, \end{aligned}$$

in view of the exactness of the Gauss–Legendre quadrature rule on $\mathbb{P}_{2q-1}$. Now consider the $q \times q$ array $\mathcal{N}$ defined by

$$\mathcal{N}_{ij} = w_i\tau_i\ell'_j(\tau_i), \quad i,j = 1, \ldots, q. \tag{2.6}$$

It is clear that

$$\mathcal{M} = (W + \mathcal{N})D^{-1}, \quad W := \operatorname{diag}\{w_1, \ldots, w_q\}, \tag{2.7}$$

and that $\mathcal{N}, \mathcal{M}$ are independent of k_n. It is worth noting that $A \equiv \mathcal{M}^{-1}W$ is the tableau of the q-stage Gauss–Legendre Runge–Kutta method.

LEMMA 2.1. *Let* $\alpha := \frac{1}{2}\min_{j} \frac{w_j}{\tau_j}$. *Then*

$$\mathbf{x}^T\widetilde{\mathcal{M}}\mathbf{x} \geq \alpha|\mathbf{x}|^2 = \alpha\left(\sum_{i=1}^{q} x_i^2\right) \quad \forall \mathbf{x} \in \mathbb{R}^q. \tag{2.8}$$

Proof. Let $\gamma_{ij} = \int_0^1 \tau\ell'_j(\tau)\ell_i(\tau)d\tau, \ i,j = 1, \ldots, q$. Since the quadrature rule (2.1) is exact on $\mathbb{P}_{2q-1}$, it follows that

$$\gamma_{ij} = \sum_{\ell=1}^{q} w_\ell\tau_\ell\ell'_j(\tau_\ell)\ell_i(\tau_\ell) = w_i\tau_i\ell'_j(\tau_i) = \mathcal{N}_{ij}.$$

On the other hand, integrating by parts,

$$\gamma_{ij} = \ell_i(1)\ell_j(1) - \int_0^1 \ell_i(\tau)\ell_j(\tau)d\tau - \int_0^1 \tau\ell_j(\tau)\ell'_i(\tau)d\tau.$$

Thus,

$$\begin{aligned} \gamma_{ij} + \gamma_{ji} = \mathcal{N}_{ij} + \mathcal{N}_{ji} &= \ell_i(1)\ell_j(1) - \int_0^1 \ell_i(\tau)\ell_j(\tau)d\tau \\ &= \ell_i(1)\ell_j(1) - w_j\delta_{ij}. \end{aligned}$$

Now

$$
\begin{aligned}
\mathbf{x}^T\widetilde{\mathcal{M}}\mathbf{x} &= \mathbf{x}^T D^{-1/2}(W+\mathcal{N})D^{-1/2}\mathbf{x}\\
&= \mathbf{x}^T D^{-1/2}\left(W+\frac{1}{2}[\mathcal{N}+\mathcal{N}^T]\right)D^{-1/2}\mathbf{x}\\
&= \sum_{j=1}^{q}\frac{w_j}{\tau_j}x_j^2+\frac{1}{2}\left(\sum_{j=1}^{q}\frac{x_j}{\tau_j^{1/2}}\ell_j(1)\right)^2-\frac{1}{2}\sum_{j=1}^{q}\frac{w_j}{\tau_j}x_j^2,
\end{aligned}
\tag{2.9}
$$

which establishes the required result. □

To prove the existence of U we introduce $\{\widetilde{U}^{n,j}\}_{j=1}^q$, where $\widetilde{U}^{n,j}=\tau_j^{-1/2}U^{n,j}\in S_h^n$. Then

$$
U(x,t)=\sum_{j=1}^{q}\tau_j^{1/2}\hat{\ell}_{n,j}(t)\widetilde{U}^{n,j}(x)+\hat{\ell}_{n,0}(t)U^{n+}(x),\qquad (x,t)\in\Omega\times I_n. \tag{2.10}
$$

To take advantage of the positive definiteness of $\widetilde{\mathcal{M}}$ we choose $\varphi=\tau_i^{-1/2}\ell_{n,i}\psi$ in (1.3), where $\psi\in S_h^n$, and we use (2.10) to obtain (cf. (2.5)) that $\{\widetilde{U}^{n,j}\}_{j=1}^q$ satisfy

$$
\begin{aligned}
\sum_{j=1}^{q}\widetilde{m}_{ij}(\widetilde{U}^{n,j},\psi)+\mathrm{i}\,k_n w_i(\nabla\widetilde{U}^{n,i},\nabla\psi)-\mathrm{i}\,\lambda\int_{I_n}\tau_i^{-1/2}\ell_{n,i}(f(U),\psi)dt&\\
+\tau_i^{-1/2}m_{i0}(U^{n+},\psi)=0,\ \ i=1,\dots,q,\ \psi\in S_h^n.&
\end{aligned}
\tag{2.11}
$$

The proof of existence of U is based on the stability result of Lemma 2.1 and on a variant of Brouwer's fixed point theorem; cf. [Br]. For details see [KM1].

3. Error analysis in $L^\infty(L^2(\Omega))$.

In this section we shall operate under the assumption that $\Pi^n=P^n$, the L^2-projection operator onto S_h^n. As usual we split the error $U-u$ into $(U-W)+(W-u)$, where $W\in V_q$ is an appropriately chosen function, and we estimate $E=U-W$ and $u-W$. We next define W and derive the basic error equation for E:

By P_E^n we denote the elliptic projection operator $P_E^n: H_0^1(\Omega)\to S_h^n$ defined by

$$
(\nabla P_E^n v,\nabla\chi)=(\nabla v,\nabla\chi)\qquad\forall\chi\in S_h^n. \tag{3.1}
$$

We assume that the family of spaces $\{S_h^n\}$ satisfies

$$
\|\nabla(v-P_E^n v)\|\le c\|h_n^{s-1}v\|_{s,h},\qquad v\in H^s\cap H_0^1,\ \ 2\le s\le r, \tag{3.2}
$$

and

$$
\|v-P_E^n v\|\le c\|h_n^{s}v\|_{s,h},\qquad v\in H^s\cap H_0^1,\ \ 2\le s\le r, \tag{3.3}
$$

where c is independent of n. For the validity of (3.2), (3.3) in various cases cf. [BS], [Ci], and [KM1, Remark 3.1].

We now introduce the functions ω,η,

$$
\omega(x,t)=P_E^n u(x,t),\quad \eta=u-\omega,\quad (x,t)\in\Omega\times I_n,\ \ n=0,\dots,N-1. \tag{3.4}
$$

Obviously these functions are continuous with respect to t in each time interval I_n and have jump discontinuities at the points t^n, only if $S_h^{n-1}\neq S_h^n$.

In order to define the function W, we shall resort to a (temporal) interpolation of ω utilizing $q+1$ Lobatto points. The reason for doing so is, first, to ensure that $W(t^{n+1})$ and W^{n+} coincide with $\omega(t^{n+1})$ and ω^{n+}, respectively, and, second, to provide a quadrature rule sufficiently accurate for the estimates to follow. Indeed, consider the $q+1$ roots $0 = \xi_0 < \cdots < \xi_q = 1$ of the polynomial $L(x) = \frac{d^{q-1}}{dx^{q-1}}[x(1-x)]^q$. It is known (cf., e.g., [BS]) that the corresponding Lobatto quadrature rule

$$\int_0^1 g(\tau)\,d\tau \approx \sum_{j=0}^{q} b_j g(\xi_j) \tag{3.5}$$

is exact on $\mathbb{P}_{2q-1}$. As done with the Gauss–Legendre points, we can define the points $\xi^{n,j}$ and the weights $b_{n,j}$ corresponding to the interval I_n. For each $n, 0 \le n \le N-1$, we define $W\big|_{I_n} \in V_q^n$ by

$$W(\xi^{n,j}) = \omega(\xi^{n,j}), \quad j = 0, \ldots, q \quad (W(\xi^{n,0}) = \omega^{n+}). \tag{3.6}$$

We also set $W(t^0) = P_E^0 u^0$.

Standard approximation and stability results for Lagrangian interpolation (cf., e.g., [BS], [Ci]) give

$$\|u - W\|_n \le c k_n^{q+1} \|u^{(q+1)}\|_n + c k_n^{1/2} \max_{I_n} \|h_n^s u\|_{s,h}, \quad 2 \le s \le r, \tag{3.7a}$$

and

$$\max_{I_n} \|u - W\| \le c k_n^{q+1} \max_{I_n} \|u^{(q+1)}\| + c \max_{I_n} \|h_n^s u\|_{s,h}, \qquad 2 \le s \le r. \tag{3.7b}$$

The basic error equation. The function $E = E|_{I_n} = U - W$ satisfies

$$\begin{aligned}
\int_{I_n} \Big\{ (E_t, \phi) + \mathrm{i}\,(\nabla E, \nabla\phi) - \mathrm{i}\,\lambda (f(U) - f(W), \phi) \Big\}\, dt &= -\Big\{ (W(t^{n+1}), \phi(t^{n+1})) \\
&\quad - \int_{I_n} (W, \phi_t)\, dt - (W^{n+}, \phi^{n+}) \Big\} - \mathrm{i} \int_{I_n} (\nabla W, \nabla \phi) \\
&\quad + \mathrm{i}\,\lambda \int_{I_n} (f(W), \phi)\, dt \quad \forall \phi \in V_{q-1}^n,\ n = 0, 1, \ldots, N-1,
\end{aligned} \tag{3.8}$$

where we have integrated by parts the term $\int_{I_n} (W_t, \phi) dt$.

Now let $\phi = \ell_{n,i}\psi$, $\psi \in S_h^n$ in (3.8). In view of the exactness of the Gauss–Legendre and Lobatto quadrature rules on $\mathbb{P}_{2q-1}$ we obtain the *basic error equation* for E (cf. (2.5)),

$$\begin{aligned}
&\sum_{j=0}^{q} m_{ij} (E(t^{n,j}), \psi) + \mathrm{i}\, k_n w_i (\nabla E(t^{n,i}), \nabla \psi) - \mathrm{i}\,\lambda \int_{I_n} \ell_{n,i} (f(U) - f(W), \psi) dt \\
&= -\Big\{ (\omega(t^{n+1}), \ell_{n,i}(t^{n+1})\psi) - \sum_{j=0}^{q} b_{n,j} \ell'_{n,i}(\xi^{n,j}) (\omega(\xi^{n,j}), \psi) - (\omega^{n+}, \ell_{n,i}(t^{n+})\psi) \Big\} \\
&\qquad - \mathrm{i} \sum_{j=0}^{q} b_{n,j} \ell_{n,i}(\xi^{n,j}) (\nabla \omega(\xi^{n,j}), \nabla \psi) + \mathrm{i}\,\lambda \int_{I_n} \ell_{n,i}(t) (f(W), \psi) dt \\
&= (\Theta^{n,i} + A^{n,i} + B^{n,i}, \psi) + \mathrm{i}\,\lambda \int_{I_n} \ell_{n,i}\, (f(W) - f(u), \psi)\, dt, \quad i = 1, \ldots, q,
\end{aligned} \tag{3.9}$$

where

$$
\begin{aligned}
&\Theta^{n,i} := \ell_{n,i}(t^{n+1})\eta(t^{n+1}) - \sum_{j=0}^{q} b_{n,j}\ell'_{n,i}(\xi^{n,j})\eta(\xi^{n,j}) - \ell_{n,i}(t^{n+})\eta^{n+}\\
&A^{n,i} := \sum_{j=0}^{q} b_{n,j}\ell'_{n,i}(\xi^{n,j})u(\xi^{n,j}) - \int_{I_n}\ell'_{n,i}(t)u\,dt \qquad (3.10)\\
&B^{n,i} := \mathrm{i}\sum_{j=0}^{q} b_{n,j}\ell_{n,i}(\xi^{n,j})\Delta u(\xi^{n,j}) - \mathrm{i}\int_{I_n}\ell_{n,i}\Delta u\,dt.
\end{aligned}
$$

Here we used the definition of W and P_E^n and the fact that for any $\phi \in V_{q-1}^n$ there holds

$$
(u(t^{n+1}),\phi(t^{n+1})) - \int_{I_n}(u,\phi_t)dt - (u^{n+},\phi^{n+}) - \mathrm{i}\int_{I_n}(\Delta u,\phi)dt - \mathrm{i}\,\lambda\int_{I_n}(f(u),\phi)dt = 0.
$$

In the convergence proof we also estimate $\widetilde{E}^{n,j} = \tau_j^{-1/2}E(t^{n,j}),\ j = 1,\dots,q$ (cf. (2.11)). Therefore, we write the analogue of (3.9) for $\widetilde{E}^{n,j}$ (note that $E = \sum_{j=0}^{q}\tau_j^{1/2}\hat{\ell}_{n,j}\widetilde{E}^{n,j}$ $+\ \hat{\ell}_{n,0}E^{n+}$ in I_n):

$$
\begin{aligned}
&\sum_{i,j=1}^{q}\widetilde{m}_{ij}(\widetilde{E}^{n,j},\psi) + \mathrm{i}\,k_n w_i(\nabla\widetilde{E}^{n,i},\nabla\psi) - \mathrm{i}\,\lambda\tau_i^{-1/2}\int_{I_n}\ell_{n,i}(f(U)-f(W),\psi)dt\\
&\quad = \tau_i^{-1/2}\Big\{ - m_{i0}(E^{n+},\ell_{n,i}(t^n)\psi) + (\Theta^{n,i} + A^{n,i} + B^{n,i},\psi) \qquad (3.11)\\
&\qquad + \mathrm{i}\,\lambda\int_{I_n}\ell_{n,i}(f(W)-f(u),\psi)\,dt\Big\}, \quad i = 1,\dots,q.
\end{aligned}
$$

Our next task is to bound the terms $\Theta^{n,i}, A^{n,i}$, and $B^{n,i}$. In the following lemma, we derive appropriate estimates for these terms, which allow us to obtain the optimal-order convergence result of our scheme.

LEMMA 3.1. *For any n, $0 \le n \le N-1$, and for $i = 1,\dots,q$ there holds*

$$
\|\Theta^{n,i}\| \le ck_n^{1/2}\Big(\int_{I_n}\|h_n^r u_t\|_{r,h}^2\Big)^{1/2}, \qquad (3.12a)
$$

$$
\|A^{n,i}\| \le ck_n^{q+3/2}\|u^{(q+2)}\|_n, \qquad (3.12b)
$$

$$
\|B^{n,i}\| \le ck_n^{q+3/2}\|\Delta u^{(q+1)}\|_n\,, \qquad (3.12c)
$$

where $\Theta^{n,i}, A^{n,i}$, and $B^{n,i}$ are defined in (3.10).

Proof. Using the Lobatto integration rule we observe that for $i = 1,\dots,q$,

$$
\ell_{n,i}(t^{n+1}) - \sum_{j=0}^{q} b_{n,j}\ell'_{n,i}(\xi^{n,j}) - \ell_{n,i}(t^{n+}) = \ell_{n,i}(t^{n+1}) - \int_{I_n}\ell'_{n,i}(t)dt - \ell_{n,i}(t^{n+}) = 0.
$$

Therefore, there exist constants β_{ij} (independent of n) such that

$$\begin{aligned}\Theta^{n,i} &= \sum_{j=1}^{q} \beta_{ij} \left(\eta(\xi^{n,j}) - \eta(\xi^{n,j-1})\right) \qquad (\eta(\xi^{n,0}) := \eta^{n+}) \\ &= \sum_{j=1}^{q} \beta_{ij} \int_{\xi^{n,j-1}}^{\xi^{n,j}} \eta_t(s) ds\,.\end{aligned}$$

Since $\eta_t = (I - P_E^n)u_t$, (3.3) implies

$$\|\Theta^{n,i}\| \le c \int_{I_n} \|h_n^r u_t\|_{r,h} \le c k_n^{1/2} \Big(\int_{I_n} \|h_n^r u_t\|_{r,h}^2 \Big)^{1/2}. \tag{3.13}$$

Now let $\mathcal{I}_{Lo}^{n,q}$ be the Lagrange interpolation operator at the $q+1$ Lobatto points $t^n = \xi^{n,0} < \cdots < \xi^{n,q} = t^{n+1}$. Using the fact that for each $x \in \Omega$, $\ell_{n,i}\mathcal{I}_{Lo}^{n,q}\Delta u$ is a polynomial of degree $2q-1$ in t we obtain

$$B^{n,i} = \mathrm{i} \sum_{j=0}^{q} b_{n,j} \ell_{n,i}(\xi^{n,j}) (\mathcal{I}_{Lo}^{n,q}\Delta u)(\xi^{n,j}) - \mathrm{i} \int_{I_n} \ell_{n,i} \Delta u\, dt = \mathrm{i} \int_{I_n} \ell_{n,i} (\mathcal{I}_{Lo}^{n,q} - I)\Delta u\, dt.$$

Hence

$$\begin{aligned}\|B^{n,i}\| &\le c \Big(\int_{I_n} |\ell_{n,i}(t)|^2 dt \Big)^{1/2} \|\!|(\mathcal{I}_{Lo}^{n,q} - I)\Delta u\|\!|_n \\ &\le c \Big(k_n \int_0^1 |\ell_i(\tau)|^2 d\tau \Big)^{1/2} c k_n^{q+1} \|\!|\Delta u^{(q+1)}\|\!|_n \\ &\le c k_n^{q+3/2} \|\!|\Delta u^{(q+1)}\|\!|_n\,.\end{aligned} \tag{3.14}$$

We next let $\mathcal{I}_{Lo}^{n,q+1}$ denote the Lagrange interpolation operator at the $q+2$ points of $[t^n, t^{n+1}]$ consisting of the $q+1$ Lobatto points $\xi^{n,0}, \dots, \xi^{n,q}$ and any number in $[t^n, t^{n+1}]$ distinct from the above, e.g., the average of any two consecutive Lobatto points. Then, using the fact that for each $x \in \Omega$, $\ell'_{n,i}\mathcal{I}_{Lo}^{n,q+1}u$ is a polynomial of degree $2q-1$ in t, and the accuracy of the Lobatto integration rule we obtain

$$A^{n,i} = \sum_{j=0}^{q} b_{n,j} \ell'_{n,i}(\xi^{n,j}) (\mathcal{I}_{Lo}^{n,q+1}) u(\xi^{n,j}) - \int_{I_n} \ell'_{n,i} u\, dt = \int_{I_n} \ell'_{n,i} (\mathcal{I}_{Lo}^{n,q+1} - I) u\, dt,$$

and therefore

$$\begin{aligned}\|A^{n,i}\| &\le c \Big(\int_{I_n} |\ell'_{n,i}(t)|^2 dt \Big)^{1/2} \|\!|(\mathcal{I}_{Lo}^{n,q+1} - I) u\|\!|_n \\ &\le c \Big(k_n^{-1} \int_0^1 |\ell'_i(\tau)|^2 d\tau \Big)^{1/2} c k_n^{q+2} \|\!|u^{(q+2)}\|\!|_n \\ &\le c k_n^{q+3/2} \|\!|u^{(q+2)}\|\!|_n\,. \qquad \square\end{aligned} \tag{3.15}$$

At this point, we make the simple but important observation that the L^2-projection operator $P_t^n : \mathbb{P}_q[t^n, t^{n+1}] \to \mathbb{P}_{q-1}[t^n, t^{n+1}]$ coincides with the Lagrange interpolation operator $\mathcal{I}_{GL}^{n,q-1}$ corresponding to the q Gauss–Legendre points $t^{n,1} < \cdots < t^{n,q}$.

Indeed, for $v \in \mathbb{P}_q[t^n, t^{n+1}]$ and any $\phi \in \mathbb{P}^n_{q-1}[t^n, t^{n+1}]$,

$$\int_{I_n} (\mathcal{I}^{n,q-1}_{GL} v)\phi dt = \sum_{j=1}^{q} w_{n,j} (\mathcal{I}^{n,q-1}_{GL} v)(t^{n,j})\phi(t^{n,j}) \\ = \sum_{j=1}^{q} w_{n,j} v(t^{n,j})\phi(t^{n,j}) = \int_{I_n} v\phi dt,$$

again owing to the fact that the q-point Gauss–Legendre quadrature is exact on $\mathbb{P}_{2q-1}$.

We now set $\psi = E(t^{n,i})$ in the ith equation of (3.9) and sum from $i = 1$ to q and take real parts. Note that

$$\mathrm{Re}\ \sum_{i=1}^{q}\sum_{j=0}^{q} m_{ij}(E(t^{n,j}), E(t^{n,i})) = \mathrm{Re}\ \int_{I_n} (E_t, \mathcal{I}^{n,q-1}_{GL} E)dt = \mathrm{Re}\ \int_{I_n} (E_t, E)dt \\ = \frac{1}{2}\|E(t^{n+1})\|^2 - \frac{1}{2}\|E^{n+}\|^2.$$

Thus, ($\mathcal{I}^{n,q-1}_{GL} = P^n_t$)

$$\begin{aligned} \frac{1}{2}\|E(t^{n+1})\|^2 - \frac{1}{2}\|E^{n+}\|^2 = &-\lambda\,\mathrm{Im} \int_{I_n} (f(U) - f(W), P^n_t E)dt \\ &+ \lambda\,\mathrm{Im} \int_{I_n} (f(u) - f(W), P^n_t E)dt \\ &+ \mathrm{Re} \sum_{i=1}^{q} (\Theta^{n,i} + A^{n,i} + B^{n,i}, E(t^{n,i})). \end{aligned} \tag{3.16}$$

Using the properties of f (cf. Lemma 4.1) and (3.7a) we obtain

$$\left| \int_{I_n} (f(U) - f(W), P^n_t E)dt \right| \le c|\!|\!|E|\!|\!|^2_n, \tag{3.17}$$

and

$$\begin{aligned} &\left| \int_{I_n} (f(u) - f(W), P^n_t E)dt \right| \\ &\qquad \le c\left\{ k_n^{q+1}|\!|\!|u^{(q+1)}|\!|\!|_n + k_n^{1/2} \max_{I_n} \|h_n^r u\|_{r,h} \right\} |\!|\!|E|\!|\!|_n. \end{aligned} \tag{3.18}$$

We shall next establish the equivalence of norms

$$C_1 \left\{ k_n \sum_{j=0}^{q} \|v^j\|^2 \right\}^{1/2} \le |\!|\!|v|\!|\!|_n \le C_2 \left\{ k_n \sum_{j=0}^{q} \|v^j\|^2 \right\}^{1/2} \tag{3.19}$$

with $v = \sum_{j=0}^{q} \hat{\ell}_{n,j} v^j \in V^n_q$. The first inequality is a consequence of the inverse property

$$\max_{I_n} |y(t)| \le C_I k_n^{-1/2} \left(\int_{I_n} |y(t)|^2 dt \right)^{1/2} \quad \forall y \in \mathbb{P}_q(I_n), \tag{3.20}$$

while the second follows easily from the fact that $\int_{I_n} \hat{\ell}^2_{n,j}(t)\,dt \le ck_n$. Now using (3.17)–(3.19) and Lemma 3.1, it follows from (3.16) that

$$\|E(t^{n+1})\|^2 \le \|E^{n+}\|^2 + c|\!|\!|E|\!|\!|^2_n + c\,\mathcal{E}_n, \tag{3.21}$$

where $\mathcal{E}_n$ denotes the optimal (consistency) term

$$\mathcal{E}_n = k_n^{2q+2}\left(|\!|\!|u^{(q+1)}|\!|\!|^2_n + |\!|\!|u^{(q+2)}|\!|\!|^2_n + |\!|\!|\Delta u^{(q+1)}|\!|\!|^2_n\right) + \int_{I_n} \|h_n^r u_t\|^2_{r,h} dt + k_n \max_{I_n} \|h_n^r u\|^2_{r,h}.$$

We next consider the term $\|E^{n+}\|$. Note that since $\Pi^n = P^n$ here,

$$E^{n+} = U^{n+} - W^{n+} = P^n E(t^n) - P^n J[\omega^n], \tag{3.22}$$

where $J[\omega^n] = \omega^{n+} - \omega(t^n) = (P_E^n - P_E^{n-1})u(t^n)$ is the "jump" in the elliptic projection of u across t^n. Hence it follows from (3.21) and (3.22) that

$$\|E(t^{n+1})\|^2 \le (1+\beta_n)\|E(t^n)\|^2 + c|\!|\!|E|\!|\!|^2_n + \mathcal{E}_n + M_n\|J[\omega^n]\|^2, \tag{3.23}$$

where M_n is a number depending on n which will be specified in the following discussion and

$$\beta_n = \begin{cases} 0 & \text{if } \ S_h^n = S_h^{n-1}, \\ \frac{1}{M_n - 1} & \text{otherwise}, \end{cases} \qquad n = 1, \dots, N-1. \tag{3.24}$$

An essential step now is the estimation of $|\!|\!|E|\!|\!|_n$ in terms of $\|E(t^n)\|$ and of consistency terms. Indeed, we have the following result.

LEMMA 3.2. *For any n, $1 \le n \le N$, and k_n sufficiently small, there holds*

$$|\!|\!|E|\!|\!|^2_n \le ck_n\Big\{\|E(t^n)\|^2 + k_n\mathcal{E}_n + \|J[\omega^n]\|^2\Big\}. \tag{3.25}$$

Proof. Let $\psi = \widetilde{E}^{n,i}$ in the ith equation of (3.11) and sum from $i = 1$ to q and take real parts. As done in the existence proof, it follows from Lemma 2.1 that

$$\mathrm{Re}\sum_{i,j=1}^q \widetilde{m}_{ij}(\widetilde{E}^{n,j}, \widetilde{E}^{n,i}) \ge \alpha \sum_{j=1}^q \|\widetilde{E}^{n,j}\|^2 .$$

Using (4.3) and the fact that $\int_{I_n} \ell^2_{n,i}(t)dt = w_i k_n$, we obtain

$$\left|\lambda \sum_{i=1}^q \tau_i^{-1/2} \int_{I_n} \ell_{n,i}(f(U) - f(W), \widetilde{E}^{n,i})dt\right| \le ck_n^{1/2}|\!|\!|E|\!|\!|_n \left\{\sum_{i=1}^q \|\widetilde{E}^{n,i}\|^2\right\}^{1/2},$$

$$\left|\lambda \sum_{i=1}^q \tau_i^{-1/2} \int_{I_n} \ell_{n,i}(f(u) - f(W), \widetilde{E}^{n,i})dt\right| \le ck_n^{1/2}|\!|\!|u - W|\!|\!|_n \left\{\sum_{i=1}^q \|\widetilde{E}^{n,i}\|^2\right\}^{1/2}.$$

Thus,

$$\alpha \sum_{j=1}^q \|\widetilde{E}^{n,j}\|^2 \le c\left\{\sum_{j=1}^q \|\widetilde{E}^{n,j}\|^2\right\}^{1/2} \left\{\|E^{n+}\| + ck_n^{1/2}|\!|\!|E|\!|\!|_n + ck_n^{1/2}|\!|\!|u - W|\!|\!|_n + \left(\sum_{i=1}^q \left[\|\Theta^{n,i}\|^2 + \|A^{n,i}\|^2 + \|B^{n,i}\|^2\right]\right)^{1/2}\right\}.$$

The quantities $\sum_{j=1}^{q} \|\widetilde{E}^{n,j}\|^2$ and $\sum_{j=1}^{q} \|E(t^{n,j})\|^2$ are equivalent modulo constants that depend only on the τ_i's. Hence, using (3.19), for k_n sufficiently small we obtain

$$\begin{aligned}\|E\|_n^2 &\le ck_n\|E^{n+}\|^2 + ck_n^2\|u-W\|_n^2 \\ &\quad + ck_n\left(\sum_{i=1}^{q}\left[\|\Theta^{n,i}\|^2 + \|A^{n,i}\|^2 + \|B^{n,i}\|^2\right]\right),\end{aligned}$$

(3.25) now follows from this, (3.22), (3.7a), and Lemma 3.1. ∎

We are now ready to prove the main convergence result for the modified scheme.

THEOREM 3.1. *Let u be the solution of* (1.1). *If U is the solution of* (1.3), *then it satisfies*

$$\begin{aligned}\max_{I_n}\|E\| \le C_n \Bigg\{ &\|h_0^r u^0\|_{r,h} + \left(\sum_{m=0}^{n} k_m^{2q+2}\left(\|u^{(q+1)}\|_m^2 + \|u^{(q+2)}\|_m^2 + \|\Delta u^{(q+1)}\|_m^2\right)\right. \\ &\left. + \sum_{m=0}^{n}\int_{I_m}\|h_m^r u_t\|_{r,h}^2\,dt + \sum_{m=0}^{n} k_m \max_{I_m}\|h_m^r u\|_{r,h}^2\right)^{1/2} \\ &+ \mathcal{N}_C(n-1)\max_{1\le m\le n}\|J[\omega^m]\|\Bigg\},\end{aligned} \tag{3.26}$$

$n = 0,\dots,N-1$; therefore, (1.4) *holds as well. Here $C_n = ce^{ct_n}$, and $\mathcal{N}_C(n)$ denotes the number of times where $S_h^j \ne S_h^{j-1}$, $j = 1,\dots n$.*

Proof. By Lemma 3.2 and (3.23) we obtain

$$\|E(t^{n+1})\|^2 \le (1+\beta_n+ck_n)\,\|E(t^n)\|^2 + c\,\mathcal{E}_n + (ck_n+M_n)\,\|J[\omega^n]\|^2.$$

Therefore,

$$\begin{aligned}\|E(t^{n+1})\|^2 \le \prod_{j=0}^{n}(1+\beta_j+ck_j)\,\|E(t^0)\|^2 + c\sum_{m=0}^{n}\left(\prod_{j=m+1}^{n}(1+\beta_j+ck_j)\right) \\ \times\left(\mathcal{E}_m + (ck_m+M_m)\,\|J[\eta^m]\|^2\right).\end{aligned}$$

The rest of the proof is similar to that of [KM1, Theorem 3.1]. Now fix n and choose $M_m = M = \mathcal{N}_C(n)$, $m = 1,\dots,n$, where $\mathcal{N}_C(n)$ is the number of times where $S_h^j \ne S_h^{j-1}$, $j = 1,\dots,n$ (in the case where $\mathcal{N}_C(n) = 0$ or 1 we take $M = 2$). Then $\beta_j = \beta = \frac{1}{M-1}$ for $S_h^j \ne S_h^{j-1}$ (cf. (3.24)),

$$\begin{aligned}\prod_{j=0}^{n}(1+\beta_j+ck_j) &\le \prod_{\substack{j=0\\ \beta<ck_j}}^{n}(1+2ck_j)\prod_{\substack{j=0\\ \beta\ge ck_j}}^{n}(1+2\beta) \\ &\le \prod_{j=0}^{n}(1+2ck_j)(1+2\beta)^M \le e^{2ct_{n+1}}3e^2.\end{aligned} \tag{3.1}$$

Set $C_n := c\left(3e^{2ct_n+2}\right)^{1/2}$. Then since $J[\omega^0] = 0$ and $E(t^0) = u^0 - P_E^0 u^0$, from (3.3) we obtain

$$\|E(t^{n+1})\| \le C_{n+1}\left\{\|h_0^r u^0\|_{r,h} + \left(\sum_{m=0}^{n}\mathcal{E}_m\right)^{1/2} + \sqrt{M}\left(\sum_{m=1}^{n}\|J[\omega^m]\|^2\right)^{1/2}\right\},$$

where $M = \mathcal{N}_C(n)$. In view of this and Lemma 3.2, we obtain for any $n = 0, \dots, N-1$,

$$\|E\|_n \le C_n k_n^{1/2} \left\{ \|h_0^r u^0\|_{r,h} + \left(\sum_{m=0}^{n-1} \mathcal{E}_m \right)^{1/2} + \sqrt{\mathcal{N}_C(n-1)} \left(\sum_{m=1}^{n} \|J[\omega^m]\|^2 \right)^{1/2} \right\}.$$

Since $E|_{I_n} \in V_q^n$, applying the inverse inequality (3.20) together with the triangle inequality yields (3.26). $\square$

4. $\boldsymbol{H^1}$-estimates. In this section we prove $L^\infty(H^1)$-estimates for the schemes (1.3) and (1.2) under appropriate assumptions on the mesh. First, we state an auxiliary result concerning a concrete choice of the function f used in the modified scheme; for a proof cf. [KM1].

LEMMA 4.1. *Let $M := \sup_{[0,T]} \|u\|_\infty + 1$. Then there exists a function $f : \mathbb{C} \to \mathbb{C}$ such that*

$$f(z) = |z|^2 z \quad \text{if } |z| \le M, \tag{4.1}$$

$$|f(z)| \le c_1 |z|, \quad c_1 > 0 \quad \forall\, z \in \mathbb{C}, \tag{4.2}$$

$$|f(z) - f(w)| \le c_2 |z - w|, \quad c_2 > 0 \quad \forall\, z, w \in \mathbb{C}, \tag{4.3}$$

$$\|\nabla_x (f(v_1) - f(v_2))\| \le c_3 \|\nabla_x (v_1 - v_2)\|, \quad c_3 = c_3(M') > 0, \tag{4.4}$$

where $\|v_1\|_{1,\infty} \le M'$ and $v_2 \in H^1$. $\square$

Our analysis will be based on the following result.

PROPOSITION 4.1. *For a given n, $1 \le n \le N-1$, assume that*

$$\|\nabla P^n v\| \le C_P \|\nabla v\| \quad \forall v \in H_0^1(\Omega), \tag{4.5}$$

where P^n is the L^2-projection onto S_h^n. Then

$$\|\nabla E(t^{n+1})\|^2 \le \|\nabla E^{n+}\|^2 + c k_n \|\nabla E(t^n)\|^2 + c k_n^{2q} \left(\|\nabla u^{(q+1)}\|_n^2 + \|\nabla \Delta u^{(q)}\|^2 dt \right)$$
$$+ c \int_{I_n} \|h_n^{r-1} u_t\|_{r,h}^2 dt + c k_n \max_{I_n} \|h_n^{r-1} u\|_{r,h}^2 + c k_n \|\nabla J[\omega^n]\|^2.$$

Remark 4.1. For a proof of (4.5) in the case of nonuniform meshes, cf. Crouzeix and Thomée [CrT].

Proof. We introduce first the discrete operator $A_h^n : H_0^1(\Omega) \to S_h^n$ defined by

$$(A_h^n v, \chi) = (\nabla v, \nabla \chi) \quad \forall \chi \in S_h^n\,. \tag{4.6}$$

Set $\psi = A_h^n E(t^{n,i})$ in the ith equation of (3.9), sum over i, from $i = 1$ to q, and take real parts. Then, using the fact that the L^2-projection operator $P_t^n : \mathbb{P}_q[t^n, t^{n+1}] \to \mathbb{P}_{q-1}[t^n, t^{n+1}]$ coincides with the Lagrange interpolation operator $\mathcal{I}_{GL}^{n,q-1}$ corresponding to the Gauss–Legendre points $t^{n,1} < \cdots < t^{n,q}$ and the definition of A_h^n we obtain

$$\frac{1}{2}\|\nabla E(t^{n+1})\|^2 - \frac{1}{2}\|\nabla E^{n+}\|^2$$
$$= -\operatorname{Im} \lambda \int_{I_n} (\nabla P^n (f(U) - f(W)) - \nabla P^n (f(u) - f(W)), \nabla \mathcal{I}_{GL}^{n,q-1} E) dt \tag{4.7}$$
$$+ \operatorname{Re} \sum_{i=1}^{q} (\nabla P^n [\Theta^{n,i} + A^{n,i} + B^{n,i}], \nabla E(t^{n,i})).$$

Assume for a moment that the following estimates are valid:

$$\begin{aligned}\Big|\int_{I_n}(\nabla P^n(f(U)-f(W))-\nabla P^n(f(u)-f(W)),\nabla\mathcal{I}_{GL}^{n,q-1}E)dt\Big| &\le c|\!|\!|\nabla E|\!|\!|_n^2\\ &+ck_n^{2(q+1)}|\!|\!|\nabla u^{(q+1)}|\!|\!|_n^2+ck_n\max_{I_n}\|h_n^{r-1}u\|_{r,h}^2,\end{aligned}\tag{4.8a}$$

and

$$\begin{aligned}\Big|\sum_{i=1}^q\Big(\nabla P^n[\Theta^{n,i}+A^{n,i}+B^{n,i}],\nabla E(t^{n,i})\Big)\Big| &\le c|\!|\!|\nabla E|\!|\!|_n^2+c\int_{I_n}\|h_n^{r-1}u\|_{r,h}^2\\ &+ck_n^{2q}\Big(|\!|\!|\nabla u^{(q+1)}|\!|\!|_n^2+\int_{I_n}\|\nabla\Delta u^{(q)}\|^2dt\Big).\end{aligned}\tag{4.8b}$$

Then

$$\begin{aligned}\|\nabla E(t^{n+1})\|^2 &\le \|\nabla E^{n+}\|^2+c|\!|\!|\nabla E|\!|\!|_n^2+ck_n^{2q}\left(|\!|\!|\nabla u^{(q+1)}|\!|\!|_n^2+\int_{I_n}\|\nabla\Delta u^{(q)}\|^2dt\right)\\ &+c\int_{I_n}\|h_n^{r-1}u_t\|_{r,h}^2dt+ck_n\max_{I_n}\|h_n^{r-1}u\|_{r,h}^2.\end{aligned}\tag{4.9}$$

Next, starting from the error equation (3.11) with $\psi=A_h^n\widetilde{E}^{n,i}$ and adapting the proof of Lemma 3.2 we get

$$\begin{aligned}|\!|\!|\nabla E|\!|\!|_n^2 \le ck_n\Bigg\{&\|\nabla E(t^n)\|^2+ck_n^{2q}\left(|\!|\!|\nabla u^{(q+1)}|\!|\!|_n^2+\int_{I_n}\|\nabla\Delta u^{(q)}\|^2dt\right)\\ &+ck_n\left(\int_{I_n}\|h_n^{r-1}u_t\|_{r,h}^2dt+ck_n\max_{I_n}\|h_n^{r-1}u\|_{r,h}^2\right)+\|\nabla J[\omega^n]\|^2\Bigg\}.\end{aligned}\tag{4.10}$$

Combining (4.9) and (4.10) we obtain the desired estimate. It remains to prove (4.8a) and (4.8b). For this, using the fact that $\sup_{[0,T]}\|W\|_{1,\infty}$ is bounded (cf. Remark 4.2, (4.4), and (4.5)), we obtain

$$\Big|\int_{I_n}(\nabla P^n(f(U)-f(W)),\nabla\mathcal{I}_{GL}^{n,q-1}E)dt\Big|\le c|\!|\!|\nabla E|\!|\!||\!|\!|\mathcal{I}_{GL}^{n,q-1}\nabla E|\!|\!|\le c|\!|\!|\nabla E|\!|\!|_n^2\,.$$

As in (3.18),

$$\begin{aligned}\Big|\int_{I_n}(\nabla P^n(f(u)-f(W)),\nabla\mathcal{I}_{GL}^{n,q-1}E)dt\Big| &\le c\Big(\int_{I_n}\|\nabla(u-W)\|^2dt\Big)^{1/2}|\!|\!|\nabla\mathcal{I}_{GL}^{n,q-1}E|\!|\!|_n\\ &\le c\Big(k_n^{q+1}|\!|\!|\nabla u^{(q+1)}|\!|\!|_n+ck_n^{1/2}\max_{I_n}\|h_n^{r-1}u\|_{r,h}\Big)|\!|\!|\nabla E|\!|\!|_n\,.\end{aligned}$$

Similar arguments to those used in the proof of (3.12a), (4.5), and the analogue of (3.19) for ∇E imply

$$\Big|\sum_{i=1}^q\Big(\nabla P^n\Theta^{n,i},\nabla E(t^{n,i})\Big)\Big|\le c\Big(\int_{I_n}\|h_n^{r-1}u_t\|_{r,h}^2\Big)^{1/2}|\!|\!|\nabla E|\!|\!|_n\,.$$

Now $\nabla A^{n,i} = \int_{I_n} \ell'_{n,i}(\mathcal{I}_{Lo}^{n,q+1} - I)\nabla u dt$, and therefore from (4.5) (cf. (3.15)),

$$\left| \sum_{i=1}^{q} \Big(\nabla P^n A^{n,i}, \nabla E(t^{n,i}) \Big) \right| \leq c k_n^q |\!|\!| \nabla u^{(q+1)} |\!|\!|_n |\!|\!| \nabla E |\!|\!|_n .$$

By similar arguments,

$$\left| \sum_{i=1}^{q} \Big(\nabla P^n B^{n,i}, \nabla E(t^{n,i}) \Big) \right| \leq c k_n^q |\!|\!| \nabla \Delta u^{q} |\!|\!|_n |\!|\!| \nabla E |\!|\!|_n$$

and the proof is complete. $\square$

Remark 4.2. It is reasonable to assume that $\sup_{[0,T]} \|W\|_{1,\infty}$ is bounded by a constant independent of h, without the assumption of quasiuniformity; cf. [SW].

The next result establishes the convergence of the nonlinear scheme (1.2) in the case $\Pi^n = P^n$. For the definition of the quantities k, h, $\underline{h}$, and C_N, cf. (1.6).

THEOREM 4.1. *Assume that for each n, $1 \leq n \leq N-1$, there holds*

$$\begin{array}{ll} S_h^{n-1} \subset S_h^n & \\ \|\nabla P^n v\| \leq C_P \|\nabla v\| \quad \forall v \in H_0^1(\Omega) & \end{array} \quad \textit{or} \quad k_n \geq C_N (k^{2(q+1)} + h^{2r}) . \tag{4.1}$$

Then for h and k small enough the solution U of (1.3) *with $\Pi^n = P^n$ is a solution of* (1.2) *as well, which satisfies the error bound of Theorem* 3.1.

Proof. First we need an estimate of the term $\|\nabla E^{n+}\|$ appearing in Proposition 4.1 in the case where $S_h^{n-1} \subset S_h^n$. Note that in this case $U^{n+} = P^n U(t^n) = U(t^n)$ and, therefore,

$$\|\nabla E^{n+}\|^2 = \|\nabla E(t^n)\|^2 + \|\nabla(\omega^n - \omega^{n+})\|^2,$$

where we have used that $(\nabla(\omega^n - \omega^{n+}), \nabla\psi) = 0$ for all $\psi \in S_h^{n-1}$. Therefore, the estimate of Proposition 4.1 implies in this case

$$\begin{aligned} \|\nabla E(t^{n+1})\|^2 \leq (1 + ck_n)\|\nabla E(t^n)\|^2 + ck_n^{2q} \Big(|\!|\!| \nabla u^{(q+1)} |\!|\!|_n^2 + |\!|\!| \nabla \Delta u^{(q)} |\!|\!|_n^2 \Big) \\ + c \int_{I_n} \|h_n^{r-1} u_t\|_{r,h}^2 dt + ck_n \max_{I_n} \|h_n^{r-1} u\|_{r,h}^2 + (1 + ck_n)\|\nabla J[\omega^n]\|^2. \end{aligned} \tag{4.11}$$

The rest of the proof follows the lines of the proof in [KM1, Theorem 4.1]. Indeed, to show the desired result, it suffices to prove

$$\max_{[0,T]} \|E\|_\infty \leq \beta(h, k, \underline{h}), \quad \beta(h, k, \underline{h}) \to 0 \ \text{ as } h, k \to 0. \tag{4.12}$$

We shall use the inequality [Th, p. 67]

$$\max_{I_n} \|E\|_\infty \leq c|\ln(\underline{h})| \max_{I_n} \|\nabla E\| . \tag{4.13}$$

We assume first that for all n up to n_0, $S_h^{n-1} \subseteq S_h^n$, and the hypotheses of Proposition 4.1 are valid. Hence as in the proof of Theorem 3.1 one can show, by using (4.11), that for each n, $0 \le n \le n_0$ there holds

$$\max_{I_n} \|\nabla E\| \le cC_n \Bigg\{ \|h_0^{r-1} u^0\|_{r,h} + \Bigg(\sum_{m=0}^{n} k_m^{2q} \Big(\|\!|\nabla u^{(q+1)}|\!\|_m^2 + \|\!|\nabla \Delta u^q|\!\|_m^2 \Big) \tag{4.14}$$
$$+ \sum_{m=0}^{n} \int_{I_m} \|h_m^{r-1} u_t\|_{r,h}^2 dt + \sum_{m=0}^{n} k_m \max_{I_m} \|h_n^{r-1} u\|_{r,h} \Bigg)^{1/2}$$
$$+ \sqrt{\mathcal{N}_C(n-1)} \max_{1 \le m \le n} |\nabla J[\omega^m]\| \Bigg\}.$$

Hence, up to t^{n_0+1}, (4.12) holds provided $\ln(\underline{h})(h^{r-1} + k^{q-1}) \to 0$ as $h, k \to 0$. At the first time where $S_h^{n-1} \not\subseteq S_h^n$, say, at $n_0 + 1$, set $\psi = E(t^{n,i})$ in (3.9), sum over i, and take imaginary parts. Then using the estimates of Lemma 3.1 and Theorem 3.1 we obtain

$$\|\!|\nabla E|\!\|_{n_0+1} \le c(k^{q+1} + h^r) + c\mathcal{N}_C(n_0) h^r .$$

Hence the inverse inequality (3.20) implies

$$\max_{I_{n_0+1}} \|\nabla E\| \le c k_{n_0+1}^{-1/2} (k^q + h^r) + c k_{n_0+1}^{-1/2} \mathcal{N}_C(n_0) h^r ,$$

which in turn implies inequality (4.12) for the interval I_{n_0+1} in view of our assumption on the mesh in this case. Proceeding in time in a similar fashion we complete the proof. ∎

Next we prove the H^1-convergence of the nonlinear scheme (1.2) in the case $\Pi^n = P_E^n$, without restrictions on the variation of the space-time mesh, except of that required for the validity of (4.5).

THEOREM 4.2. *Assume that* (4.5) *is valid for each* n, $1 \le n \le N-1$. *Then for* h *and* k *small enough the solution* U *of* (1.3) *with* $\Pi^n = P_E^n$, *is a solution of* (1.2) *as well, which satisfies the* H^1 *error bound*

$$\max_{t \in [0,T]} \|\nabla(u(t) - U(t))\| \le C_n \Big\{ \max_m k_m^q \max_{I_m} \Big(\|\nabla u^{(q+1)}\| + \|\nabla \Delta u^{(q)}\| \Big) \tag{4.15}$$
$$+ \max_m \max_{I_m} \big(\|h_m^{r-1} u_t\|_{r,h} + \|h_m^{r-1} u\|_{r,h} \big)$$
$$+ \mathcal{N}_C \max_m \|\nabla J[\omega^m]\| \Big\},$$

where $C_n = ce^{ct_n}$.

Proof. Let $E = U - W$, where U is the solution of (1.3) with $\Pi^n = P_E^n$. As in (3.22),

$$E^{n+} = P_E^n E(t^n) - P_E^n J[\omega^n],$$

and therefore the stability properties of the elliptic projection P_E^n and Proposition 4.1 imply

(4.2)
$$\|\nabla E(t^{n+1})\|^2 \le (1 + \beta_n + ck_n) \|\nabla E(t^n)\|^2 + ck_n^{2q} \Big(\|\!|\nabla u^{(q+1)}|\!\|_n^2 + \|\!|\nabla \Delta u^q|\!\|_n^2 dt \Big)$$
$$+ c \int_{I_n} \|h_n^{r-1} u_t\|_{r,h}^2 dt + ck_n \max_{I_n} \|h_n^{r-1} u\|_{r,h}^2 + (M_n + ck_n) \|\nabla J[\omega^n]\|^2,$$

where β_n and M_n are chosen as in section 3. Hence following the steps of the proof of Theorem 3.1 one can show that the inequality (4.14) holds for each n, $0 \le n \le N-1$ in this case. Therefore, the solution U of (1.3) satisfies the error bound (4.15). Now, in view of (4.13) it is easy to see that the analogue of (4.12) holds in this case as well, and the proof is complete. ∎

5. Superconvergence. In this section we shall prove a superconvergence result at the temporal nodes t^n, $n = 1, \dots, N$; i.e., we shall show that $\|U^n - u(t^n)\| = O(h^r + k^\sigma)$ for some $q < \sigma \le 2q$, the value of the integer σ depending on the domain Ω; cf. (5.6). In order to show that, we shall handle the consistency of the scheme in a different way; cf. [KAD], [KM1]. A central role will be played by the functions $u^{n,1}, \dots, u^{n,q}$, which differ from $u(t^{n,1}), \dots, u(t^{n,q})$, respectively, but satisfy $u^{n,i} = u(t^{n,i}) + O(k_n^{q+1})$. These functions will have the form

$$u^{n,i}(x) = \sum_{\ell=0}^{\sigma} k_n^\ell \alpha_{i\ell}(x), \quad i = 0, \dots, q, \quad u^{n,0} = u(t^n), \tag{5.1}$$

where the functions $\alpha_{i\ell} = \alpha_{i\ell}(x)$ will be specified. At this point, we assume that the latter are smooth and vanish on $\partial\Omega$ and therefore the elliptic projections $P_E^n u^{n,i}$, $i = 0, \dots, q$, are well defined. In this case, the function W,

$$W(t) = \sum_{j=0}^{q} \hat{\ell}_{n,j}(t) W(t^{n,j}) = \sum_{j=0}^{q} \hat{\ell}_{n,j}(t) P_E^n u^{n,j}\,, \quad t \in I_n\,, \quad n = 0, \dots, N-1,$$

is an element of V_q^n. Note that it is different from the corresponding function used in section 3. We shall compare the solution U of (1.3) (which is also a solution of (1.2), in view of the results of section 4) with W.

As motivation for our choice of the $\alpha_{i\ell}$, we begin by letting

$$E = U - W = \sum_{j=0}^{q} \hat{\ell}_{n,j}(t) E(t^{n,j}) = \sum_{j=0}^{q} \hat{\ell}_{n,j}(t) [U(t^{n,j}) - P_E^n u^{n,j}].$$

Then the analogue of (3.9) is

$$\begin{aligned} &\sum_{j=0}^{q} m_{ij} (E(t^{n,j}), \psi) + \mathrm{i}\, k_n w_i (\nabla E(t^{n,i}), \nabla\psi) + \mathrm{i}\,\lambda \int_{I_n} \ell_{n,i}\, (f(U) - f(W), \psi)\, dt \\ &\qquad = (\theta^{n,i}, \psi) - (\rho^{n,i}, \psi) - \mathrm{i}\,\lambda \int_{I_n} \ell_{n,i}\, \left(|\Lambda_q^n|^2 \Lambda_q^n - f(W), \psi\right) dt, \\ &\qquad\quad i = 1, \dots, q \quad \forall \psi \in S_h^n, \end{aligned} \tag{5.2}$$

where

$$\theta^{n,i} = \ell_{n,i}(t^{n+1}) \eta^{n+1} - \sum_{j=1}^{q} w_{n,j} \ell'_{n,i}(t^{n,j}) \eta^{n,j} - \ell_{n,i}(t^n) \eta^{n,0}, \quad i = 1, \dots, q,$$

$$\eta^{n,j} = (I - P_E^n) u^{n,j}, \quad j = 0, \dots, q, \quad \eta^{n+1} = (I - P_E^n) u^{n+1},$$

$$u^{n+1} := \Lambda_q^n(t^{n+1}), \quad \Lambda_q^n(t) := \sum_{j=0}^{q} \hat{\ell}_{n,j}(t) u^{n,j},$$

$$\rho^{n,i} = \ell_{n,i}(t^{n+1})u^{n+1} - \sum_{j=1}^{q} w_{n,j}\ell'_{n,i}(t^{n,j})u^{n,j} - \ell_{n,i}(t^n)u(t^n) \tag{5.1}$$

$$-\mathrm{i}\, k_n w_i \Delta u^{n,i} - \mathrm{i}\,\lambda \int_{I_n} \ell_{n,i}|\Lambda_q^n|^2\Lambda_q^n dt \tag{5.2}$$

$$= \int_{I_n} \ell_{n,i}\left[(\Lambda_q^n)' - \mathrm{i}\,\Delta\Lambda_q^n - \mathrm{i}\,\lambda|\Lambda_q^n|^2\Lambda_q^n\right] dt, \quad i = 1,\dots,q. \tag{5.3}$$

It is clear that $W|_{I_n} = P_E^n \Lambda_q^n$. Also $u^{n,i} = u(t^{n,i}) + O(k_n^{q+1})$ will imply that $\|\Lambda_q^n(t)\|_\infty \le M$, and by Lemma 4.1, $|\Lambda_q^n|^2\Lambda_q^n = f(\Lambda_q^n)$, and therefore the second term of the right-hand side of (5.2) will be easily estimated. We shall concentrate on estimating the consistency terms $\rho^{n,i}$. In particular, we shall define $u^{n,j}$ such that $\rho^{n,i}$ is as small as possible. For this, let $\widetilde{\Lambda}_q^n$, be the function of s, such that $\widetilde{\Lambda}_q^n(s) = \Lambda_q^n(t)$, where $t = t^n + sk_n$, $0 \le s \le 1$, i.e.,

$$\widetilde{\Lambda}_q^n(s) = \sum_{j=0}^{q} \hat{\ell}_j(s)u^{n,j}\,.$$

Note that (for notational simplicity we drop the index n in k_n)

$$\rho^{n,i} = k\int_0^1 \ell_i(s)\left[\frac{1}{k}(\widetilde{\Lambda}_q^n)' - \mathrm{i}\,\Delta\widetilde{\Lambda}_q^n - \mathrm{i}\,\lambda|\widetilde{\Lambda}_q^n|^2\widetilde{\Lambda}_q^n\right] ds, \quad i = 1,\dots,q. \tag{5.3}$$

We begin by setting

$$\alpha_{j0} = u(t^n), \quad j = 0,\dots,q. \tag{5.4}$$

Using (5.1) and (5.4) in (5.3) together with the fact that $\alpha_{0\ell} = 0$ for $\ell \ge 1$, we see that

$$\begin{aligned}\rho^{n,i} = k\sum_{\ell=0}^{\sigma-1} k^\ell &\Bigg\{\sum_{j=1}^{q}\left(\int_0^1 \ell_i(s)\hat{\ell}'_j(s)ds\right)\alpha_{j,\ell+1} - \mathrm{i}\,w_i\Delta\alpha_{i\ell}\\ &-\mathrm{i}\,\lambda\sum_{|m|=\ell}\sum_{j_1,j_2,j_3=0}^{q}\left(\int_0^1 \ell_i(s)\hat{\ell}_{j_1}(s)\hat{\ell}_{j_2}(s)\hat{\ell}_{j_3}(s)ds\right)\alpha_{j_1m_1}\alpha_{j_2m_2}\overline{\alpha}_{j_3m_3}\Bigg\}\\ &- \mathrm{i}\,\lambda k\sum_{\ell=\sigma}^{3\sigma} k^\ell \sum_{\substack{|m|=\ell\\ m_i\le\sigma}}\sum_{j_1,j_2,j_3=0}^{q}\left(\int_0^1 \ell_i(s)\hat{\ell}_{j_1}(s)\hat{\ell}_{j_2}(s)\hat{\ell}_{j_3}(s)ds\right)\alpha_{j_1m_1}\alpha_{j_2m_2}\overline{\alpha}_{j_3m_3}\\ &- \mathrm{i}\,k^{\sigma+1}w_i\Delta\alpha_{i\sigma}, \quad i = 1,\dots,q,\end{aligned}$$

where $m = (m_1, m_2, m_3)$ is a multi-index. Since the last two terms of this equation are of order $k^{\sigma+1}$, defining the $\alpha_{j\ell}$'s recursively by

$$\begin{aligned}&\sum_{j=1}^{q}\left(\int_0^1 \ell_i(s)\hat{\ell}'_j(s)ds\right)\alpha_{j,\ell+1} - \mathrm{i}\,w_i\Delta\alpha_{i\ell}\\ &\quad - \mathrm{i}\,\lambda\sum_{|m|=\ell}\sum_{j_1,j_2,j_3=0}^{q}\left(\int_0^1 \ell_i(s)\hat{\ell}_{j_1}(s)\hat{\ell}_{j_2}(s)\hat{\ell}_{j_3}(s)ds\right)\alpha_{j_1m_1}\alpha_{j_2m_2}\overline{\alpha}_{j_2m_3} = 0,\\ &\qquad i = 1,\dots,q, \quad \ell = 0,\dots,\sigma-1,\end{aligned} \tag{5.5}$$

it follows that $\|\rho^{n,i}\| = O(k^{\sigma+1})$. Obviously we would like to choose σ as large as possible.

Note that $\int_0^1 \ell_i(s)\hat{\ell}_j'(s)ds$ are the elements of the array $\mathcal{M}$, which is invertible; cf. Lemma 2.1. Hence, the functions $\alpha_{j\ell}$ are well defined to a level ℓ limited only by the degree of regularity of $u(t^n)$. We assume this to be sufficiently large. However, a new barrier is presented by the requirement that $u^{n,i}$ and thus $\alpha_{i\ell},\ i=0,\dots,q,\ \ell = 0,\dots,\sigma$ should vanish on $\partial\Omega$. (We recall that this is required in order to define the elliptic projections $P_E^n u^{n,i}$.) This particular requirement determines an upper bound for σ.

In the following we shall show (Propositions 5.1 and 5.2) that if $\alpha_{i\ell}$ are determined by (5.4), (5.5), for $\ell \geq 0$, then

$$u^{n,i} = u(t^{n,i}) + O(k_n^{q+1}),\ i=1,\dots,q, \quad \text{and } u^{n+1} = u(t^{n+1}) + O(k_n^{\sigma+1}),$$

and (Proposition 5.3)

$$u^{n,i}|_{\partial\Omega} = 0, \quad i=0,\dots,q,$$

provided that σ is at most

$$\sigma = \begin{cases} 2q, & \Omega \text{ is polyhedral,} \\ \min\{q+3, 2q\} & \text{otherwise.} \end{cases} \tag{5.6}$$

PROPOSITION 5.1. *Let* $\{\alpha_{i\ell}\}$, $i=0,\dots,q$, $\ell \geq 0$, *be given by* (5.4) *and* (5.5). *Then with* $\partial_t^\ell u$ *denoting* $\frac{\partial^\ell}{\partial t^\ell}\, u|_{t=t^n}$,

$$\alpha_{i\ell} = \frac{\tau_i^\ell}{\ell!}\partial_t^\ell u, \quad i=0,\dots,q, \quad \ell=0,\dots,q, \quad (\tau_0^0 = 1), \tag{5.7a}$$

$$\alpha_{i,q+1} = \begin{cases} 0, & i=0, \\ \left(\displaystyle\sum_{j=1}^{q} \left(\mathcal{M}^{-1}\right)_{ij} w_j \tau_j^q\right) \dfrac{\partial_t^{q+1} u}{q!}, & i=1,\dots,q. \end{cases} \tag{5.7b}$$

Proof. Obviously (5.7a) holds for $\ell = 0$ since in this case it reduces to (5.4). So we assume that it holds up to some $\ell \leq q-1$. Then

$$\Delta\alpha_{i\ell} = \frac{\tau_i^\ell}{\ell!}\partial_t^\ell \Delta u, \quad i=0,\dots,q. \tag{5.8}$$

Also, for any m, $0 \leq m \leq q$,

$$\begin{aligned} \sum_{j=0}^{q} \hat{\ell}_j(s)\alpha_{jm} &= \sum_{j=0}^{q} \hat{\ell}_j(s)\frac{\tau_j^m}{m!}\partial_t^m u \\ &= \frac{\partial_t^m u}{m!}\sum_{j=0}^{q} \hat{\ell}_j(s)\tau_j^m = \frac{s^m}{m!}\partial_t^m u. \end{aligned}$$

Hence, with $m!$ denoting $m_1!m_2!m_3!$, we obtain using the fact that for $\ell \leq q-1$, $s^\ell \ell_i(s) \in \mathbb{P}_{2q-2}$,

$$\begin{aligned}
&\sum_{|m|=\ell} \sum_{j_1,j_2,j_3=0}^{q} \left(\int_0^1 \ell_i(s)\hat{\ell}_{j_1}(s)\hat{\ell}_{j_2}(s)\hat{\ell}_{j_3}(s)\,ds \right) \alpha_{j_1m_1}\alpha_{j_2m_2}\overline{\alpha}_{j_3m_3} \\
&\quad= \sum_{|m|=\ell} \left(\int_0^1 s^\ell \ell_i(s)ds \right) \frac{1}{m!} \partial_t^{m_1} u\, \partial_t^{m_2} u\, \partial_t^{m_3} \overline{u} \qquad (5.9)\\
&\quad= \sum_{|m|=\ell} \frac{w_i\tau_i^\ell}{m!} \partial_t^{m_1} u\, \partial_t^{m_2} u\, \partial_t^{m_3} \overline{u} = \frac{w_i \tau_i^\ell}{\ell!} \partial_t^\ell (|u|^2 u), \quad i=1,\dots,q,
\end{aligned}$$

where we have used Leibniz's formula in the last step.

To establish (5.7a) for $\ell+1$ as well, it suffices, in view of (1.1), (5.8), (5.9), and the invertibility of $\mathcal{M}$, to show that $\sum_{j=1}^q (\int_0^1 \ell_i(s)\hat{\ell}_j'(s)\,ds)\tau_j^{\ell+1} = (\ell+1)w_i\tau_i^\ell$. Indeed, since $\ell+1 \leq q$ and $\tau_0 = 0$,

$$\sum_{j=1}^q \hat{\ell}_j'(s)\tau_j^{\ell+1} = \left(\sum_{j=0}^q \hat{\ell}_j(s)\tau_j^{\ell+1} \right)' = (s^{\ell+1})' = (\ell+1)s^\ell,$$

and we have, using $\ell \leq q-1$ once more,

$$\sum_{j=1}^q \left(\int_0^1 \ell_i(s)\hat{\ell}_j'(s)ds \right) \tau_j^{\ell+1} = (\ell+1)\int_0^1 s^\ell \ell_i(s)ds = (\ell+1)w_i\tau_i^\ell. \qquad \square$$

Having established (5.7a), we see that the proof of (5.7b) is immediate.

This result shows that the $\alpha_{j\ell}$'s are, up to level $\ell = q+1$, scalar multiples of time derivatives of u at $t = t^n$. Hence $\alpha_{j\ell}|_{\partial\Omega} = 0,\ j = 0,\dots,q,\ \ell = 0,\dots,q+1$. Unfortunately this is not the case for $\ell > q+1$ in general. Instead, we have the following result.

PROPOSITION 5.2. *Let* $\{\alpha_{i\ell}\}$, $i = 0,\dots,q$, $\ell \geq 0$, *be given by* (5.4) *and* (5.5). *Then*

$$\sum_{j=0}^q \hat{\ell}_j(1)\alpha_{j\ell} = \frac{\partial_t^\ell u}{\ell!}, \quad \ell = 0,\dots,2q, \tag{5.10}$$

and

$$\sum_{j=1}^q w_j\tau_j^\mu \alpha_{j\ell} = \frac{\partial_t^\ell u}{\ell!(\mu+\ell+1)}, \quad \ell=0,\dots,2q-1, \quad 0 \leq \mu \leq 2q-1-\ell. \tag{5.11}$$

Proof. We begin by showing that by virtue of (5.7a), (5.10) holds for $\ell = 0,\dots,q$ and that (5.11) holds for $\ell = 0,\dots,q,\ 0 \leq \mu \leq 2q-1-\ell$. Indeed, for $0 \leq \ell \leq q$,

$$\sum_{j=0}^q \hat{\ell}_j(1)\alpha_{j\ell} = \sum_{j=0}^q \hat{\ell}_j(1)\frac{\tau_j^\ell}{\ell!}\partial_t^\ell u = \frac{\partial_t^\ell u}{\ell!} s^\ell\big|_{s=1}.$$

Moreover, for $0 \leq \ell \leq q,\ 0 \leq \mu \leq 2q-1-\ell$, from (5.7a) it follows that

$$\sum_{j=1}^q w_j\tau_j^\mu\alpha_{j\ell} = \frac{\partial_t^\ell u}{\ell!}\sum_{j=1}^q w_j\tau_j^{\mu+\ell} = \frac{\partial_t^\ell u}{\ell!}\int_0^1 s^{\mu+\ell}ds = \frac{\partial_t^\ell u}{\ell!(\mu+\ell+1)}; \tag{5.4}$$

i.e., (5.11) also holds for $\ell = 0, \dots, q$. We shall next establish (5.11) and (5.10) together (in that order) by induction on ℓ. So assume that both hold up to ℓ, $q \le \ell \le 2q-2$, and let μ be such that $0 \le \mu \le 2q-2-\ell$. First observe that

$$
\begin{aligned}
&\sum_{i=1}^{q} \tau_i^{\mu} \sum_{j=1}^{q} \left(\int_0^1 \ell_i(s) \hat{\ell}_j'(s) ds \right) \alpha_{j,\ell+1} = \sum_{j=1}^{q} \left(\int_0^1 s^{\mu} \hat{\ell}_j'(s) ds \right) \alpha_{j,\ell+1} \\
&= \sum_{j=1}^{q} \left[s^{\mu} \hat{\ell}_j(s) \Big|_0^1 - \mu \int_0^1 s^{\mu-1} \hat{\ell}_j(s) ds \right] \alpha_{j,\ell+1} = \sum_{j=1}^{q} \left[\hat{\ell}_j(1) - \mu w_j \tau_j^{\mu-1} \right] \alpha_{j,\ell+1}.
\end{aligned} \tag{5.12}
$$

Using the induction hypothesis we have

$$
\sum_{i=1}^{q} w_i \tau_i^{\mu} \Delta \alpha_{i\ell} = \Delta \frac{\partial_t^{\ell} u}{\ell! (\ell + \mu + 1)}. \tag{5.13}
$$

Now let

$$
\begin{aligned}
M^{\ell} &= \{ m = (m_1, m_2, m_3), \quad 0 \le m_i \le \ell, \quad |m| = \ell \}, \\
M_0^{\ell} &= \left\{ m \in M^{\ell}, \quad 0 \le m_i \le q-1, \quad i = 1,2,3 \right\}, \\
M_i^{\ell} &= \left\{ m \in M^{\ell}, \quad q \le m_i \le 2q-2 \right\}, \quad i = 1,2,3.
\end{aligned}
$$

Note that if $m \in M^{\ell}$ is such that for some i, $q \le m_i \le 2q-2$, then the other two components of m are less than or equal to $q-2$. Thus

$$
M_i^{\ell} \cap M_j^{\ell} = \phi \quad \text{if } i \ne j \text{ and } M^{\ell} = \cup_{i=0}^{3} M_i^{\ell}.
$$

Hence, by Proposition 5.1 and since $\mu \le q-2$,

$$
\begin{aligned}
&\sum_{i=1}^{q} \tau_i^{\mu} \sum_{m \in M_0^{\ell}} \sum_{j_1, j_2, j_3 = 0}^{q} \left(\int_0^1 \ell_i(s) \hat{\ell}_{j_1}(s) \hat{\ell}_{j_2}(s) \hat{\ell}_{j_3}(s) ds \right) \alpha_{j_1 m_1} \alpha_{j_2 m_2} \overline{\alpha}_{j_3 m_3} \\
&\qquad = \sum_{m \in M_0^{\ell}} \int_0^1 \left(\sum_{i=1}^{q} \tau_i^{\mu} \ell_i(s) \right) \left(\sum_{j_1=0}^{q} \frac{\tau_{j_1}^{m_1} \partial_t^{m_1} u}{m_1!} \hat{\ell}_{j_1}(s) \right) \left(\sum_{j_2=0}^{q} \frac{\tau_{j_2}^{m_2} \partial_t^{m_2} u}{m_2!} \hat{\ell}_{j_2}(s) \right) \\
&\qquad\qquad \times \left(\sum_{j_3=0}^{q} \frac{\tau_{j_3}^{m_3} \partial_t^{m_3} \overline{u}}{m_3!} \hat{\ell}_{j_3}(s) \right) ds \\
&\qquad = \sum_{m \in M_0^{\ell}} \int_0^1 s^{\mu+\ell} ds \frac{1}{m!} \partial_t^{m_1} u \, \partial_t^{m_2} u \, \partial_t^{m_3} \overline{u} = \frac{\partial_t^{m_1} u \, \partial_t^{m_2} u \, \partial_t^{m_3} \overline{u}}{m! (\mu + \ell + 1)}.
\end{aligned} \tag{5.14}
$$

Similarly, using the induction hypothesis, we obtain

$$
\begin{aligned}
\sum_{i=1}^{q} \tau_i^{\mu} \sum_{m\in M_1^\ell} \sum_{j_1,j_2,j_3=0}^{q} \left(\int_0^1 \ell_i(s)\hat{\ell}_{j_1}(s)\hat{\ell}_{j_2}(s)\hat{\ell}_{j_3}(s)ds\right) \alpha_{j_1m_1}\alpha_{j_2m_2}\overline{\alpha}_{j_3m_3} \\
= \sum_{m\in M_1^\ell} \int_0^1 \left(\sum_i \tau_i^{\mu}\ell_i(s)\right)\left(\sum_{j_1=0}^{q}\hat{\ell}_{j_1}(s)\alpha_{j_1m_1}\right)\left(\sum_{j_2=0}^{q}\frac{\tau_{j_2}^{m_2}\partial_t^{m_2}u}{m_2!}\hat{\ell}_{j_2}(s)\right) \\
\times\left(\sum_{j_3=0}^{q}\frac{\tau_{j_3}^{m_3}\partial_t^{m_3}\overline{u}}{m_3!}\hat{\ell}_{j_3}(s)\right)ds \\
= \sum_{m\in M_1^\ell}\frac{\partial_t^{m_2}u\,\partial_t^{m_3}\overline{u}}{m_2!m_3!}\int_0^1 s^{\mu+m_2+m_3}\sum_{j_1=0}^{q}\hat{\ell}_{j_1}(s)\alpha_{j_1m_1}ds \\
= \sum_{m\in M_1^\ell}\frac{\partial_t^{m_2}u\,\partial_t^{m_3}\overline{u}}{m_2!m_3!}\sum_{j_1=1}^{q} w_{j_1}\tau_{j_1}^{\mu+m_2+m_3}\alpha_{j_1m_1} \\
= \sum_{m\in M_1^\ell}\frac{\partial_t^{m_2}u\,\partial_t^{m_3}\overline{u}}{m_2!m_3!}\,\frac{\partial_t^{m_1}u}{m_1!(\mu+m_2+m_3+m_1+1)} = \sum_{m\in M_1^\ell}\frac{\partial_t^{m_1}u\,\partial_t^{m_2}u\,\partial_t^{m_3}\overline{u}}{m!(\mu+\ell+1)},
\end{aligned}
\tag{5.15}
$$

where we have used the facts that $\mu + m_2 + m_3 + m_1 = \mu + \ell \leq 2q - 2$ and that $\mu + m_2 + m_3 \leq q - 2$.

The sums over M_2^ℓ and M_3^ℓ yield similar expressions; from (5.12)–(5.15) we obtain upon using (1.1),

$$
\sum_{j=1}^{q}\left[\hat{\ell}_j(1) - \mu w_j \tau_j^{\mu-1}\right]\alpha_{j,\ell+1} = \frac{\partial_t^{\ell+1}u}{\ell!(\mu+\ell+1)}.
$$

First, letting $\mu = 0$ in the above shows that (5.10) holds for $\ell + 1$ as well (recall $\alpha_{0\ell} = 0$, $\ell \geq 1$). Now for $1 \leq \mu \leq 2q - 1 - \ell$,

$$
\begin{aligned}
\sum_{j=1}^{q} w_j\tau_j^{\mu-1}\alpha_{j,\ell+1} &= \frac{1}{\mu}\left[\sum_{j=1}^{q}\hat{\ell}_j(1)\alpha_{j,\ell+1} - \frac{\partial_t^{\ell+1}u}{\ell!(\mu+\ell+1)}\right] = \frac{1}{\mu}\left[\frac{\partial_t^{\ell+1}u}{(\ell+1)!} - \frac{\partial_t^{\ell+1}u}{\ell!(\mu+\ell+1)}\right] \\
&= \frac{\partial_t^{\ell+1}u}{(\ell+1)!(\mu+\ell+1)}.
\end{aligned}
$$

This completes the proof of the proposition. $\square$

In choosing the value of σ, we have the following result whose proof is similar to Proposition 4.1 of [KAD] and hence is omitted.

Proposition 5.3. *Assume that the solution u of* (1.1) *is in $C^\mu(\overline{\Omega}\times[0,T])$ for μ sufficiently large. If σ is given by* (5.6), *then*

$$
\alpha_{j\ell}\,|_{\partial\Omega} = 0, \quad j = 0,\dots,q, \quad \ell = 0,\dots,\sigma. \quad \square \tag{5.16}
$$

This result hinges upon proving that if u is sufficiently smooth and that if u^0 satisfies certain compatibility conditions so that (1.1) holds in $\overline{\Omega}\times[0,T]$, then

$$
\Delta^s\partial_t^j u\Big|_{\partial\Omega\times[0,T]} = 0 \text{ for } j \geq 0 \text{ and } \begin{cases} s \geq 0 & \text{if } \Omega \text{ is polyhedral,} \\ s = 0,1,2 & \text{for general } \Omega. \end{cases} \tag{5.17}
$$

Now it follows from (5.10) that $u^{n+1} = \sum_{j=0}^{q} \hat{\ell}_j(1) u^{n,j} = \sum_{\ell=0}^{\sigma} k_n^{\ell} \frac{\partial_t^{\ell}}{\ell!} u$. Hence

$$\|u^{n+1} - u(t^{n+1})\| \leq c k_n^{\sigma+1}. \tag{5.18a}$$

From the definition of the α's through the recurrence relation (5.5) it follows that

$$\max_{1\leq i\leq q} \|\rho^{n,i}\| \leq c k_n^{\sigma+1}, \tag{5.18b}$$

while Proposition 5.1 implies

$$\max_{1\leq i\leq q} \|u(t^{n,i}) - u^{n,i}\| \leq c k_n^{q+1}. \tag{5.18c}$$

We next consider the other terms in (5.2). First, there exist constants $\widetilde{\beta}_{ij}$ such that

$$\begin{aligned} \theta^{n,i} &= \sum_{j=1}^{q+1} \widetilde{\beta}_{ij} (I - P_E^n)(u^{n,j} - u^{n,j-1}) \quad (u^{n,q+1} := u^{n+1}) \\ &= \sum_{j=1}^{q+1} \widetilde{\beta}_{ij} (I - P_E^n) \sum_{\ell=1}^{\sigma} k_n^{\ell} [\alpha_{j,\ell} - \alpha_{j-1,\ell}]. \end{aligned}$$

Hence,

$$\|\theta^{n,i}\| \leq c k_n h_n^r, \quad i = 1, \dots, q. \tag{5.19}$$

It follows from (5.1) and (5.5) that for k_n sufficiently small $\max_{I_n} \|\Lambda_q^n\|_\infty \leq M$. Hence $|\Lambda_q^n|^2 \Lambda_q^n = f(\Lambda_q^n)$. Also, since $W = P_E^n \Lambda_q^n$, we obtain the estimate

$$\int_{I_n} (\,|\Lambda_q^n|^2 \Lambda_q^n - f(W), \phi)\,dt \leq c|\!|\!|\Lambda_q^n - W|\!|\!|_n |\!|\!|\phi|\!|\!|_n \leq c k_n^{1/2} h_n^r |\!|\!|\phi|\!|\!|_n. \tag{5.20}$$

Now putting $\psi = E(t^{n,i})$ in the ith equation of (5.2), summing and taking real parts yields, in view of (3.17), (5.18b), (5.19), and (5.20),

$$\|E(t^{n+1})\|^2 \leq \|E^{n+}\|^2 + c|\!|\!|E|\!|\!|_n^2 + c k_n h_n^{2r} + c k_n^{2\sigma+1}. \tag{5.21}$$

Also, since

$$E^{n+} = P^n[U(t^n) - P_E^n u(t^n)] = P^n[E(t^n) + P_E^{n-1}(u^n - u(t^n)) + (P_E^{n-1} - P_E^n) u(t^n)],$$

it follows from the analogue of (5.18a) for n that

$$\|E^{n+}\| \leq \|E(t^n)\| + c k_{n-1}^{\sigma+1} + \|J[\omega^n]\|. \tag{5.22}$$

Now starting from (5.2) and applying techniques similar to those used in Lemma 3.2, we obtain the estimate

$$|\!|\!|E|\!|\!|_n^2 \leq c k_n \|E^{n+}\|^2 + c k_n^3 h_n^{2r} + c k_n^{2\sigma+3}. \tag{5.23}$$

Thus, using (5.22) and (5.23) in (5.21) yields the superconvergence result.

THEOREM 5.1. *Let u be the solution of* (1.1). *Assume that the hypotheses of Theorem* 4.1 *hold. If U is a solution of* (1.2) *and u is regular enough, then the following estimate holds for n, $n = 1, \dots, N$:*

$$\begin{aligned} \|u(t^n) - U(t^n)\| \leq C \max_{m\leq n-1} C_1(m,u) k_m^{\sigma} + C_n \max_{m\leq n-1} C_2(m,u) h_m^r \\ + C\mathcal{N}_C(n-1) \max_{m\leq n-1} \|J[\omega^n]\|\,, \end{aligned} \tag{5.5}$$

where $C_1(m,u)$ and $C_2(m,u)$ are constants that depend on m and u but are independent of h and k.

6. Numerical results. In this section we report results of some numerical experiments which were designed to validate the convergence results of the cG method as well as the dG method studied in [KM1] and those of IRK methods analyzed in [KAD]. To keep the scope of experiments manageable, we restricted ourselves to the study of the superconvergence estimates. Additionally, we wanted to compare the performance of the four classes of methods by studying the relationship between the errors and CPU times used.

In all the experiments, the errors were computed using the function

$$u(x,t) = Ae^{-i[2\pi mx]}\operatorname{sech}\left[2\pi m\left(x-\frac{1}{2}\right)+8m^2\pi^2 t\right],$$

which is an exact solution to the Cauchy problem for the equation

$$u_t = \mathrm{i}\, u_{xx} + \mathrm{i}\,\lambda |u|^2 u, \tag{6.1}$$

where $\lambda = 8\pi^2 m^2/A^2$. A is the amplitude and m is a frequencylike parameter. Since $|u|$ decays exponentially as a function of x, we found it convenient to solve (6.1) with periodic boundary conditions on $[0,1]$. Thus we took $S_h^n = S_h$ to be the space of 1-periodic smooth splines of degree $r-1 \geq 0$ defined on a uniform partition of $[0,1]$.

We shall next describe the time-stepping procedure $U^n \to U^{n+1}$ in a unified framework for all the four types of methods. For the cG method, this depends on the computation of the quantities $U^{n,1},\dots,U^{n,q}$ defined by (2.4) and which satisfy the coupled system of equations (2.5). Note that the dG method also fits in this framework with

$$m_{ij} = \delta_{iq}\delta_{jq} - w_j \ell_i'(\tau_j),\ i,j=1,\dots,q, \quad \text{and} \quad m_{i0} = -\ell_i(0),\ i=1,\dots,q. \tag{6.2}$$

An important computational consideration is the evaluation of the temporal integral: We evaluate it exactly using a $\tilde{q}$-point Gauss–Legendre quadrature formula with $\tilde{q} = 2q$ for the cG method and $\tilde{q} = 2q-1$ for the dG method.

At this point, it is interesting to note that use of the q-point Gauss–Legendre quadrature formula to evaluate the integral in (2.5) reduces that term to $(|U^{n,i}|^2 U^{n,i},\psi)$. Replacing the integral with this term gives exactly the q-stage Gauss–Legendre IRK method. A similar modification applied to the dG method but using the q-point Radau quadrature formula instead, results in the q-stage Radau IIA IRK method. This illustrates the close relationship between the dG and cG methods and the Radau IIA and Gauss–Legendre IRK methods, respectively: The only difference, at least in the case of the NLS equation, resides in the evaluation of the nonlinear term.

Introducing the operators $L_h, F_h : S_h \to S_h$, given by

$$(L_h\phi,\psi) = (\nabla\phi,\nabla\psi), \quad (F_h(\phi),\psi) = (|\phi|^2\phi,\psi) \quad \forall \psi \in S_h,$$

we write all four methods in the form

$$\begin{aligned}\sum_{j=1}^{q} m_{ij} U^{n,j} + \mathrm{i}\, k_n w_i L_h U^{n,i} &= -m_{i0}U^n \\ &\quad + \mathrm{i}\,\lambda k_n \sum_{m=1}^{\tilde{q}} \tilde{w}_m \ell_i(\tilde{\tau}_m) F_h\left(\sum_{j=1}^{q} \ell_j(\tilde{\tau}_m) U^{n,j}\right),\ i=1,\dots,q.\end{aligned} \tag{6.3}$$

We next show a way to decouple the equations (6.3). As noted earlier in the paper, the array $\mathcal{A} = \mathcal{M}^{-1}W,\ W =$ diag $\{w_1, \dots, w_2\}$ is the tableau of the corresponding IRK method. It is known (cf. [DV]) that $\mathcal{A}$ is diagonalizable: $\mathcal{A} = S^{-1}\Gamma S$. The eigenvalues γ_i are complex with one exception when q is odd. Thus, we rewrite (6.3) in terms of the transformed quantities $\tilde{U}^{n,i} = \sum_{j=1}^{q} S_{ij}U^{n,j}$, as

$$(I + \mathrm{i}\, k\gamma_i L_h)\tilde{U}^{n,i} = \left(\sum_{j=1}^{q} S_{ij}\right) U^n + \mathrm{i}\, k\lambda \sum_{m=1}^{\tilde{q}} b_{im} F_h \left(\sum_{j=1}^{q} c_{mj}\tilde{U}^{n,j}\right),\ i = 1, \dots, q,$$

with

$$b_{im} = \sum_{j=1}^{q} S_{ij}\tilde{w}_m \ell_j(\tilde{\tau}_m), \quad c_{mj} = \sum_{k=1}^{q} S_{kj}^{-1}\ell_k(\tilde{\tau}_m).$$

The unknowns $\tilde{U}^{n,i}$ are approximated by means of the explicit-implicit algorithm

$$(I + \mathrm{i}\, k\gamma_i L_h)\tilde{U}^{n,i}_{\ell+1} = \left(\sum_{j=1}^{q} S_{ij}\right) U^n + \mathrm{i}\, k\lambda \sum_{i=1}^{\tilde{q}} b_{im} F_h \left(\sum_{j=1}^{q} c_{mj}\tilde{U}^{n,j}_{\ell}\right),\ i = 1, \dots, q,$$

$\ell = 0, \dots, \ell^* - 1$. This method was analyzed in [ADK] and is convergent under mild assumptions on k and h.

We next give the values of the various parameters used in the experiments in which a FORTRAN code was run on a 333 MHz DEC Alpha500 workstation. First, we took the amplitude A and the frequency m to be 0.1 and 20, respectively. Also, we integrated the equation over the temporal interval $[0, 0.0003]$, in the span of which the peak of $|u|$ travels about 0.25. Since we are concentrating on the temporal component of the error, we chose the number of spatial subdivisions to be 1500. Combined with high accuracy afforded by the use of quintic splines ($r = 6$), this effectively rendered the spatial component of the error extremely small. At every time step, we used 20 iterations of the explicit-implicit procedure to effectively solve the nonlinear systems of equations. Although somewhat of an overkill, this ensured that the nonlinear equations are always solved exactly.

These parameters being constant throughout the experiments, we executed 8 separate runs for each combination of the values of $N = 20, 30, \dots, 150$, $q = 2, 3$, and each of the four methods. The figures provide a useful summary of these experiments. Figure 1 shows the errors in terms of the number of time steps for all runs. Let us note at this point that in computing the errors we followed a procedure used in [BDKM], which was devised in order to capture numerically the asymptotic convergence rates over a greater range of the values of N by further eliminating the spatial errors. This simply consisted in reporting the error as $\|U^N - U^{300}\|$ instead of $\|U^N - u(., 0.0003)\|$. The use of the reference run U^{300} instead of the exact value has the interesting effect of cancelling out the spatial component of the error and is effective especially for large values of N.

Figure 1 confirms the asymptotic rates of convergence for all methods concerned. Another interesting fact that emerges is that the space-time methods are more accurate, albeit only slightly, than their Runge–Kutta counterparts.

A different picture emerges from Figure 2, where the CPU times (in seconds) are mapped in terms of the errors. In each case, the Runge–Kutta method is shown to be

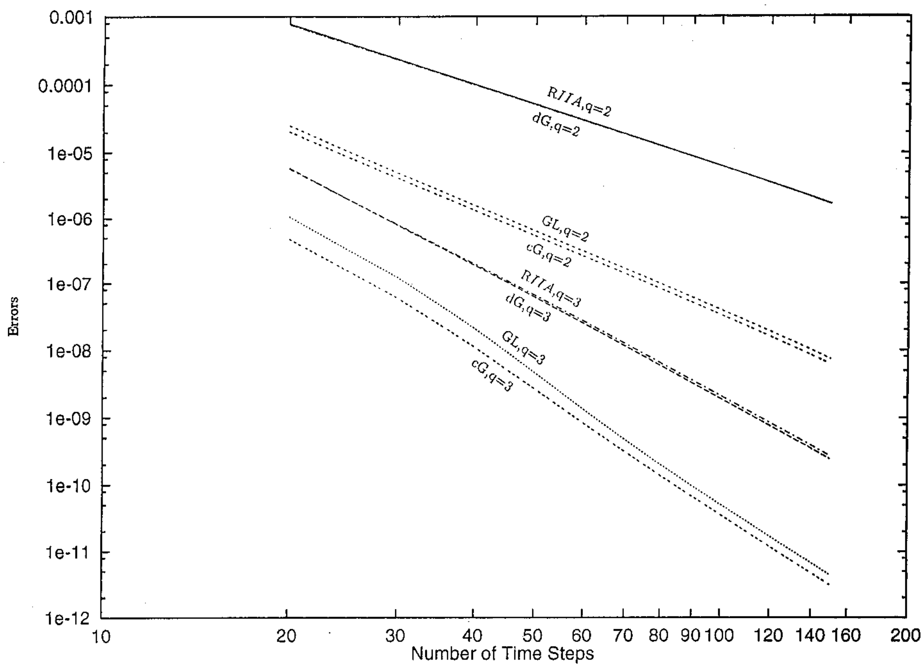
0.001
0.0001
1e-05
1e-06
1e-07
1e-08
1e-09
1e-10
1e-11
1e-12
Errors
10
20
30
40
50
60
70
80
90
100
120
140
160
200
Number of Time Steps
RIIA,q=2
dG,q=2
GL,q=2
cG,q=2
RIIA,q=3
dG,q=3
GL,q=3
cG,q=3

FIG. 1.

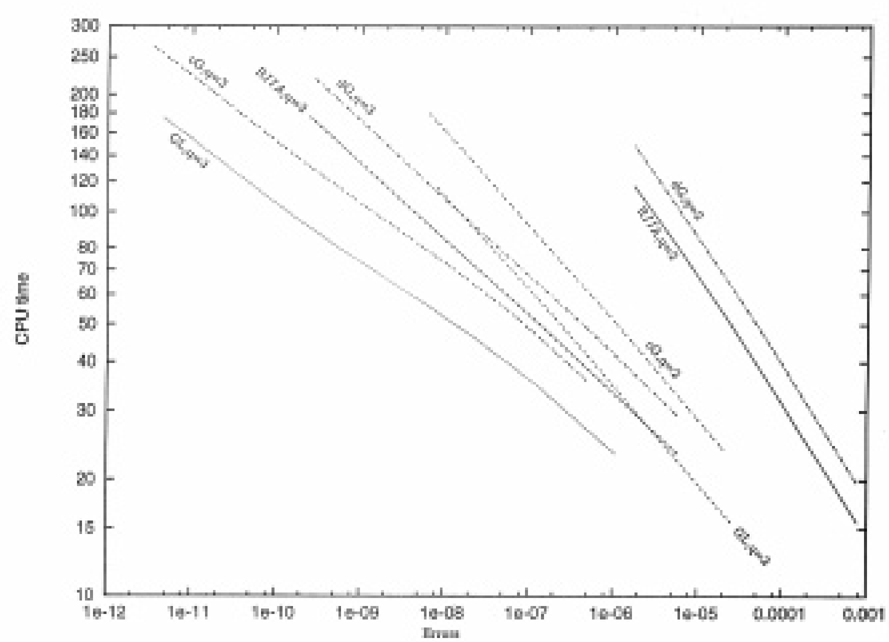
300
250
200
180
160
140
120
100
80
70
60
50
40
30
20
15
10
CPU time
1e-12
1e-11
1e-10
1e-09
1e-08
1e-07
1e-06
1e-05
0.0001
0.001
Errors

FIG. 2.

more efficient than its space-time counterpart. This is a consequence of the fact that while the latter are only slightly more accurate in absolute terms, they are significantly (up to 50%) more time consuming, due to the cost of the exact integration of the nonlinear term. In a sense, one could say that a Runge–Kutta method constitutes an effective way of implementing a space-time finite element method! We should keep in mind that this is the case only when time stepping is done. With nonstructured meshes, it is not clear what relationship, if any, exists between the two methods.

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