ERROR ESTIMATES FOR FINITE ELEMENT METHODS FOR A WIDE–ANGLE PARABOLIC EQUATION

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Abstract. We consider a model initial– and boundary–value problem for the third–order wide–angle parabolic approximation of underwater acoustics with depth– and range–dependent coefficients. We discretize the problem in the depth variable by the standard Galerkin finite element method and prove optimal–order L^2–error estimates for the ensuing continuous–in–range semidiscrete approximation. The associated o.d.e. systems are then discretized in range, first by a second–order accurate Crank–Nicolson type method, and then by the fourth–order, two–stage Gauss–Legendre, implicit Runge–Kutta scheme. We show that both these fully discrete methods are unconditionally stable and possess L^2–error estimates of optimal rates.

Dedicated to Professor Robert Vichnevetsky on the occasion of his 65^{th} birthday.

1. Introduction

We shall study Galerkin finite element methods for approximating the solution of the following model initial– and boundary–value problem for a complex *Sobolev type* partial differential equation: Let $R > 0$ and $z_{\max} > 0$ be given and let I be the interval $(0, z_{\max})$. We seek a complex–valued function $u = u(z, r)$, $(z, r) \in \bar{I} \times [0, R]$, satisfying

$$\begin{aligned} &\big[1 + \sigma(\beta(z,r) + \mathrm{i}\nu(z,r))\big]u_r + \alpha\sigma u_{zzr} \\ &\qquad = \mathrm{i}\alpha u_{zz} + \mathrm{i}\big[\beta(z,r) + \mathrm{i}\nu(z,r)\big]u, \qquad \text{in } \bar{I} \times [0, R], \end{aligned} \tag{1.1}$$

$$u(0, r) = u(z_{\max}, r) = 0, \qquad 0 \le r \le R, \tag{1.2}$$

$$u(z, 0) = u^0(z), \qquad z \in I. \tag{1.3}$$

Here α and σ are real constants with $\alpha \neq 0$, and β and ν are smooth, real–valued functions on $\bar{I} \times [0, R]$. We shall assume that ν is nonnegative and that u^0 is a given, suitably smooth, complex–valued function on $\bar{I}$. The p.d.e. (1.1) is written in the form

$$(1 + \alpha\sigma\mathcal{R})u_r = \mathrm{i}\alpha\mathcal{R}u, \tag{1.4}$$

where $\mathcal{R}v = v_{zz} + \alpha^{-1}[\beta(z, r) + \mathrm{i}\nu(z, r)]v$.

The third–order p.d.e. (1.1) occurs in problems of wave propagation as a *wide–angle*, *parabolic* approximation to the Helmholtz equation in cylindrical coordinates in the absence of azimuthal dependence. In particular, we have in mind its application in the area of underwater acoustics, [12], [14], where u is the value at depth z and range r of a field variable generated by a harmonic point source in a single layer (water) of

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depth $z_{\max}$ with pressure release conditions at the surface and at the bottom. (For simplicity, we shall analyze in detail the single–layer case. In the companion paper [5] we have indicated how our results extend to more general *interface* problems with multiple horizontal layers.) In (1.3) the initial value $u^0(z)$ models the effect of the source at $r = 0$, while the particular form of (1.1) emerges as an approximation to a pseudodifferential expression in which $\sqrt{1+x}$ is approximated near $x = 0$ by a rational function with linear numerator and denominator of the form $(1+px)/(1+qx)$, $p \neq q$. The choice $p = 3/4$, $q = 1/4$, [9], corresponds to the (1,1)–Padé approximant of $\sqrt{1+x}$, whereas putting $p = 1/2$, $q = 0$ yields the linear Taylor polynomial of $\sqrt{1+x}$ around $x = 0$ and corresponds to the *standard*, [20], parabolic approximation. In this physical context the constants in (1.1) are given by the formulas $\alpha = (p-q)/k_0$ and $\sigma = q/((p-q)k_0)$, where $k_0 = 2\pi f/c_0$, f is the frequency of the source, and c_0 a constant reference sound speed. In addition, $\beta(z,r) = k_0(p-q)((c_0/c(z,r))^2 - 1)$, where $c(z,r)$ is the range–dependent sound speed of the medium, and $\nu(z,r) \geq 0$ is an empirically determined dissipation coefficient of the form $\nu(z,r) = k_0(p-q)\theta(z,r)$, where $\theta(z,r)$ incorporates various loss terms. We refer the reader to [12], [14], [17], [10], for discussions of the justification of (1.1) as a wide–angle modification of the standard parabolic equation. (The latter corresponds to $\sigma = 0$; here we shall assume that $\sigma \neq 0$ and indeed that $\alpha\sigma = q/k_0^2 > 0$.)

The existence, uniqueness and regularity of solutions of initial– and boundary–value problems such as the one given by (1.1)–(1.3) have been investigated in a more general context by Lagnese, [16], who shows that if $-1/\alpha\sigma$ is not an eigenvalue of the operator $\mathcal{R}$ for any $r \in [0,R]$, then, existence, uniqueness and regularity of solutions follow under standard hypotheses such as sufficient smoothness of the coefficients of (1.1) and the initial value u^0.

In the specific case of the p.d.e. (1.1) posed under the initial and boundary conditions (1.2)–(1.3) the following facts are proved with energy techniques by the authors in [5]:

(*i*) If for each $r \in [0,R], \nu$ is positive at least on a nonempty subinterval of I, then the operator $1 + \alpha\sigma\mathcal{R}$ in (1.4) (acting, say, on $\mathrm{C}^2(\bar{I})$ functions that vanish at 0 and $z_{\max}$) is invertible and the problem (1.1)–(1.3) is well–posed.

(*ii*) If $\nu = 0$ and $1 + \sigma\beta(z,r) < \alpha\sigma(\pi/z_{\max})^2$ for $(z,r) \in \bar{I} \times [0,R]$, then $1 + \alpha\sigma\mathcal{R}$ is invertible and the problem (1.1)–(1.3) is well–posed.

(*iii*) If (1.1)–(1.3) has a solution, then

$$\int_0^{z_{\max}} |u(z,r)|^2\,dz \leq \int_0^{z_{\max}} |u(z,t)|^2\,dz, \quad 0 \leq t \leq r \leq R, \tag{1.5}$$

with *equality* if $\nu = 0$.

In what follows we shall assume that the data of (1.1)–(1.3) are such that the problem possesses a unique solution which is smooth enough for the purposes of its numerical approximation.

In section 2 below we analyze the standard Galerkin discretization of (1.1)–(1.3) with respect to the depth variable (semidiscretization), and prove that its error is of optimal order of accuracy in L^2. In section 3 we discretize the problem in r as well using a Crank–Nicolson scheme, for which we also prove an L^2 optimal rate result for the error. A more accurate scheme for range–stepping (of fourth–order of accuracy in r) is analyzed in section 4. It is based on the two–stage implicit Runge–Kutta method of Gauss–Legendre type; issues of its efficient implementation are discussed in section 5.

In [15] and [5] various numerical experiments with finite element methods (such as the ones analyzed herein) were presented, indeed in the presence of interfaces. For finite element computations for the third–order wide–angle equation analyzed here and some of its higher order extensions with a scheme that uses piecewise linear elements in the depth variable and an ADI–Crank–Nicolson range–stepping we refer the reader to the work of Collins, [10], [11]. For computations with and error analysis of *finite difference* methods cf. e.g. [12], [14], [17], [8], [19], [2] and [6].

The following notation will be used in the sequel. For (complex–valued) $f, g \in L^2 = L^2(I)$, we let

$$(f, g) = \int_I f(z)\overline{g(z)}\, dz,$$

where an overbar denotes complex conjugation. The associated L^2 norm will be denoted by $\|\cdot\|$. For integer $s \geq 1$, $H^s = H^s(I)$ will denote the usual, complex Sobolev (Hilbert) spaces with corresponding norms $\|\cdot\|_s$. We let $H_0^1 = H_0^1(I) = \{v \in H^1(I) : v(0) = v(z_{\max}) = 0\}$ and by $|\cdot|_\infty$ we denote the norm of $L^\infty(I)$.

2. Semidiscretization

In this section we shall analyze the (standard) Galerkin semidiscrete approximation of the solution of (1.1)–(1.3). To this effect we discretize the problem in z as follows: For an integer M let $\{z_0, z_1, \dots, z_M\}$ be a (not necessarily uniform) partition of $\bar{I}$ such that $z_0 = 0$ and $z_M = z_{\max}$, and put $e_i = (z_{i-1}, z_i)$, $h_i = z_i - z_{i-1}$ and $h = \max_{1\leq i\leq M} h_i$. Then, for integer $s \geq 2$, define

$$\begin{aligned}\mathcal{X}_h =&\{\chi : \chi \in C^{s-2}(\bar{I}) \text{ complex–valued}, \chi|_{\bar{e}_i} \in P_{s-1},\\ &i = 1, \dots, M, \text{ and } \chi(0) = \chi(z_{\max}) = 0\},\end{aligned}$$

where P_j are the polynomials of degree at most j. $\mathcal{X}_h$ is a family of finite–dimensional subspaces of H_0^1, that satisfies the following approximation property: Given $v \in H^s \cap H_0^1$, there exists an element $v_I \in \mathcal{X}_h$ (the interpolant of v) such that

$$\|v - v_I\| + h\|v - v_I\|_1 \leq ch^j\|v\|_j, \quad 1 \leq j \leq s, \tag{2.1}$$

for some constant c independent of h and v.

Define now the *semidiscrete approximation* of the solution u of (1.1)–(1.3) in $\mathcal{X}X_h$ as the map $u_h : [0, R] \to \mathcal{X}_h$ satisfying

$$\begin{aligned}&([1 + \sigma(\beta(r) + \mathrm{i}\nu(r))]u_{hr}, \chi) - \alpha\sigma\mathcal{B}(u_{hr}, \chi) =\\ &\quad - \mathrm{i}\alpha\mathcal{B}(u_h, \chi) + \mathrm{i}([\beta(r) + \mathrm{i}\nu(r)]u_h, \chi), \quad \forall\chi \in \mathcal{X}_h,\\ &u_h(0) = u_h^0,\end{aligned} \tag{2.2}$$

where, for $\varphi, \chi \in H^1(I)$, $\mathcal{B}(\varphi, \chi) = (\varphi', \chi')$, and where $\beta(r) = \beta(\cdot, r)$ etc.. We assume that $u^0 \in H^s \cap H_0^1$, and $u_h^0 \in \mathcal{X}_h$ is an approximation to u^0 such that

$$\|u^0 - u_h^0\| \le ch^s \|u^0\|_s. \tag{2.3}$$

E.g. $u_h^0 = \mathcal{P}u^0$, where $\mathcal{P}$ is the L^2 projection operator onto $\mathcal{X}_h$.

Introducing on $\mathcal{X}_h$ the linear operators $\mathcal{D}_h$, $\mathcal{B}_h(r)$, $\mathcal{B}_h(r)$ and $\mathcal{L}_h(r)$, $0 \le r \le R$, defined for $\varphi, \chi \in \mathcal{X}_h$ by

$$\begin{aligned} &(\mathcal{D}_h\varphi, \chi) = -\mathcal{B}(\varphi, \chi),\\ &(\mathcal{B}_h(r)\varphi, \chi) = (\beta(r)\varphi, \chi),\\ &(\mathcal{N}_h(r)\varphi, \chi) = (\nu(r)\varphi, \chi),\\ &\mathcal{L}_h(r) = \alpha\mathcal{D}_h + \mathcal{B}_h(r) + \mathrm{i}\mathcal{N}_h(r), \end{aligned} \tag{2.4}$$

we may rewrite (2.2) as

$$(1 + \alpha\sigma\mathcal{R}_h(r))u_{hr} = \mathrm{i}\mathcal{L}_h(r)u_h, \quad 0 \le r \le R, \quad u_h(0) = u_h^0, \tag{2.5}$$

where $\mathcal{R}_h = \alpha^{-1}\mathcal{L}_h$.

If we assume that $-1/\alpha\sigma$ is not an eigenvalue of the operator $\mathcal{R} = \mathcal{R}(r)$ defined after (1.4), then, for h sufficiently small, the operator $1 + \alpha\sigma\mathcal{R}_h(r)$ is invertible on $\mathcal{X}_h$, i.e. the o.d.e. initial–value problem (2.5) has a unique solution. This may be proved by a duality argument in the standard manner, cf. [18]; here we outline the proof for the reader's convenience.

Given $r \in [0, R]$, let $v_h \in \mathcal{X}_h$ be a solution of the homogeneous linear system $(1 + \alpha\sigma\mathcal{R}_h(r))v_h = 0$, i.e. let

$$([1 + \sigma(\beta + \mathrm{i}\nu)]v_h, \varphi) - \alpha\sigma(v_h', \varphi') = 0, \quad \forall\varphi \in \mathcal{X}_h. \tag{2.6}$$

Putting $\varphi = v_h$ and taking real and imaginary parts in the above we obtain, respectively,

$$\|v_h\|^2 + \sigma(\beta v_h, v_h) - \alpha\sigma\|v_h'\|^2 = 0, \tag{2.7}$$

$$(\nu v_h, v_h) = 0. \tag{2.8}$$

If $\nu(z, r) > 0$ for $z \in \bar{I}$, then (2.8) gives $v_h = 0$ and the proof is ended. Otherwise, (2.7) yields

$$\|v_h'\| \le c\|v_h\|, \tag{2.9}$$

for some constant c. Consider now the indefinite, inhomogeneous elliptic problem $(1 + \alpha\sigma\mathcal{R}^*(r))w = v_h$, i.e.

$$([1 + \sigma(\beta - \mathrm{i}\nu)]w, \varphi) - \alpha\sigma(w', \varphi') = (v_h, \varphi), \quad \forall\varphi \in H_0^1, \tag{2.10}$$

which, by our assumption, has a unique solution w that can be shown to satisfy, cf. [1], [16],

$$\|w\|_2 \le c\|v_h\|. \tag{2.11}$$

Taking $\varphi = v_h$ in (2.10), letting $w_I \in \mathcal{X}_h$ be the interpolant of w and using (2.6) yields

$$\|v_h\|^2 = ([1+\sigma(\beta - \mathrm{i}\nu)](w-w_I), v_h) - \alpha\sigma(w' - w_I', v_h'),$$

from which, in view of (2.1), (2.11) and the Poincaré inequality, we obtain

$$\begin{aligned}\|v_h\|^2 &\le c\|w-w_I\|\,\|v_h\| + \alpha\sigma\|w'-w_I'\|\,\|v_h'\|\\ &\le ch^2\|w\|_2\,\|v_h\| + ch\|w\|_2\,\|v_h'\|\\ &\le ch\|v_h\|\,\|v_h'\|.\end{aligned}$$

Hence

$$\|v_h\| \le ch\|v_h'\|,$$

which, when combined with (2.9), yields, for h sufficiently small, $v_h = 0$, q.e.d..

Using a straightforward energy technique one may show, cf. section 2 of [5], that the $L^2(I)$ norm of $u_h(\cdot, r)$ is a non–increasing function of r. Specifically we have

$$\|u_h(r)\| \le \|u_h(t)\|, \quad \text{for } 0 \le t \le r \le R,$$

which holds as an *equality* in the nondissipative case $\nu = 0$.

We proceed now to show an optimal–rate L^2 estimate for the error of the semidiscrete approximation. In the sequel we shall frequently use an *elliptic projection* operator $\mathcal{P}_1 : H_0^1 \to \mathcal{X}_h$, defined by

$$\mathcal{B}(\mathcal{P}_1 v, \chi) = \mathcal{B}(v, \chi), \quad \forall \chi \in \mathcal{X}_h. \tag{2.12}$$

It is well–known that, under our hypotheses,

$$\|v - \mathcal{P}_1 v\| + h\|v - \mathcal{P}_1 v\|_1 \le ch^j\|v\|_j, \quad 1 \le j \le s, \tag{2.13}$$

for $v \in H^s \cap H_0^1$.

Theorem 2.1. *Let u and u_h be the solutions of* (1.1)–(1.3) *and* (2.2)*, respectively, with u_h^0 chosen so that* (2.3) *is satisfied. Then for u sufficiently smooth, there exists a constant $c = c(u, R)$ such that*

$$\max_{0\le r\le R} \|u(r) - u_h(r)\| \le ch^s. \tag{2.14}$$

Proof. We write $u_h - u = (u_h - \mathcal{P}_1 u) + (\mathcal{P}_1 u - u) =: \vartheta + \varrho$. By (2.13)

$$\|\varrho(r)\| \le ch^s\|u(r)\|_s. \tag{2.15}$$

Since $(\mathcal{P}_1 u)_r = \mathcal{P}_1 u_r$, ϑ satisfies

$$\begin{aligned}&([1+\sigma(\beta(r)+\mathrm{i}\nu(r))]\vartheta_r, \chi) - \alpha\sigma\mathcal{B}(\vartheta_r, \chi)\\ &\qquad + \mathrm{i}\alpha\mathcal{B}(\vartheta, \chi) - \mathrm{i}((\beta(r)+\mathrm{i}\nu(r))\vartheta, \chi) = (\omega, \chi),\end{aligned}$$

for $\chi \in \mathcal{X}_h$, with $\omega = -[1+\sigma(\beta(r)+\mathrm{i}\nu(r))]\varrho_r + i(\beta(r)+\mathrm{i}\nu(r))\varrho$. Taking $\chi = \vartheta$ and then real parts we have

$$\begin{aligned}&\mathrm{Re}((1+\sigma\beta(r))\vartheta_r, \vartheta) - \sigma\,\mathrm{Im}(\nu(r)\vartheta_r, \vartheta)\\ &\qquad - \alpha\sigma\,\mathrm{Re}\,\mathcal{B}(\vartheta_r, \vartheta) + (\nu(r)\vartheta, \vartheta) = \mathrm{Re}(\omega, \vartheta).\end{aligned} \tag{2.16}$$

For $\chi = \vartheta_r$ taking imaginary parts we have

$$\begin{aligned} \sigma(\nu(r)\vartheta_r, \vartheta_r) + \alpha \operatorname{Re} \mathcal{B}(\vartheta, \vartheta_r) - \operatorname{Re}(\beta(r)\vartheta, \vartheta_r) \\ + \operatorname{Im}(\nu(r)\vartheta, \vartheta_r) = \operatorname{Im}(\omega, \vartheta_r). \end{aligned} \tag{2.17}$$

Multiplying (2.17) by σ and adding the resulting equation to (2.16) we get

$$\begin{aligned} \frac{1}{2}\frac{d}{dr}\|\vartheta\|^2 &= \operatorname{Re}(\vartheta_r, \vartheta) \\ &= -\sigma^2(\nu\vartheta_r, \vartheta_r) - (\nu\vartheta, \vartheta) + 2\sigma \operatorname{Im}(\nu\vartheta_r, \vartheta) + \operatorname{Re}(\omega, \vartheta) + \sigma \operatorname{Im}(\omega, \vartheta_r) \\ &\le \operatorname{Re}(\omega, \vartheta) + \sigma \operatorname{Im}(\omega, \vartheta_r) \\ &= \operatorname{Re}(\omega, \vartheta) + \sigma \operatorname{Im}\{\frac{d}{dr}(\omega, \vartheta) - (\omega_r, \vartheta)\}. \end{aligned}$$

Integrating both sides with respect to r and using the Cauchy–Schwarz and the arithmetic–geometric mean inequalities we have

$$\|\vartheta(r)\|^2 \le c(\mathcal{A} + \int_0^r \|\vartheta(t)\|^2\, dt), \tag{2.18}$$

where

$$\mathcal{A} = \|\vartheta(0)\|^2 + \|\omega(0)\|^2 + \|\omega(r)\|^2 + \int_0^r (\|\omega(t)\|^2 + \|\omega_r(t)\|^2)\, dt.$$

Using (2.3), (2.13) and (2.15) it is easily seen that $\mathcal{A} \le c(u, R)h^{2s}$. Then (2.18) and Gronwall's lemma imply that

$$\max_{0\le r\le R} \|\vartheta(r)\| \le ch^s.$$

Therefore (2.14) is proved in view of (2.15). □

3. Crank–Nicolson fully discrete scheme

Let $k > 0$ be a constant range step, such that $R = Nk$ for some integer N. For $0 \le n \le N$, we shall approximate $u^n = u(\cdot, r^n)$, where $r^n = nk$, by $U^n \in \mathcal{X}_h$ which is required to satisfy the following Crank–Nicolson type scheme:

$$\begin{aligned} &([1 + \sigma(\beta^{n-1/2} + \mathrm{i}\nu^{n-1/2})]\partial_r U^n, \chi) - \alpha\sigma\mathcal{B}(\partial_r U^n, \chi) \\ &\quad + \mathrm{i}\alpha\mathcal{B}(U^{n-1/2}, \chi) - \mathrm{i}((\beta^{n-1/2} + \mathrm{i}\nu^{n-1/2})U^{n-1/2}, \chi) = 0, \\ &\quad \forall \chi \in \mathcal{X}_h, \quad 1 \le n \le N, \\ &U^0 = u_h^0, \end{aligned} \tag{3.1}$$

where $U^{n-1/2} = (U^n + U^{n-1})/2$ and $\partial_r U^n = (U^n - U^{n-1})/k$, $r^{n-1/2} = r^{n-1} + k/2$, $\beta^{n-1/2} = \beta(\cdot, r^{n-1/2})$, $\nu^{n-1/2} = \nu(\cdot, r^{n-1/2})$ and $u_h^0 \in \mathcal{X}_h$ is chosen to satisfy (2.3).

It is not hard to see that if U^n satisfies (3.1) then

$$\|U^n\| \le \|U^{n-1}\|, \qquad 1 \le n \le N, \tag{3.2}$$

with *equality* if $\nu = 0$. In fact, putting $\chi = U^{n-1/2}$ in (3.1) and taking real parts we have

$$\begin{aligned}
&\|U^n\|^2 - \|U^{n-1}\|^2 + 2k(\nu^{n-1/2}U^{n-1/2}, U^{n-1/2}) \\
&\quad - \alpha\sigma\{\mathcal{B}(U^n, U^n) - \mathcal{B}(U^{n-1}, U^{n-1})\} - 2\sigma\,\mathrm{Im}(\nu^{n-1/2}U^n, U^{n-1}) \\
&\quad + \sigma\{(\beta^{n-1/2}U^n, U^n) - (\beta^{n-1/2}U^{n-1}, U^{n-1})\} = 0.
\end{aligned} \tag{3.3}$$

On the other hand, putting $\chi = \partial_r U^n$ in (3.1), taking imaginary parts, and multiplying by σ we obtain

$$\begin{aligned}
&2k\sigma^2(\nu^{n-1/2}\partial_r U^n, \partial_r U^n) - 2\sigma\,\mathrm{Im}(\nu^{n-1/2}U^n, U^{n-1}) \\
&\quad - \sigma\{(\beta^{n-1/2}U^n, U^n) - (\beta^{n-1/2}U^{n-1}, U^{n-1})\} \\
&\quad + \alpha\sigma\{\mathcal{B}(U^n, U^n) - \mathcal{B}(U^{n-1}, U^{n-1})\} = 0.
\end{aligned} \tag{3.4}$$

Adding (3.3) and (3.4), we obtain (3.2), with equality if $\nu = 0$.

The existence and uniqueness of the solution of the linear system of equations represented by (3.1) for $0 \le n \le N$ follows from (3.2). Thus, the existence and uniqueness of this fully discrete approximation does not depend on the invertibility of $1 + \alpha\sigma\mathcal{R}_h$; this is due to the artificial $O(k)$ 'absorption' term introduced in the elliptic operator by the Crank–Nicolson range discretization. Throughout the rest of this work we shall denote by D differentiation with respect to z, with $D^j v = \partial^j v/\partial z^j$, while $v^{(j)}$ will denote the j^{th} derivative $\partial^j v/\partial r^j$ with respect to the range variable.

Theorem 3.1. *Let U^n and $u^n = u(\cdot, r^n)$ be the solutions of* (3.1) *and* (1.1)–(1.3), *respectively, and u_h^0 be suitably chosen to satisfy* (2.3). *Then, for $0 \le n \le N$, we have*

$$\|U^n - u^n\| \le c(u, R)(h^s + k^2). \tag{3.5}$$

Proof. We write $U^n - u^n = (U^n - \mathcal{P}_1 u^n) + (\mathcal{P}_1 u^n - u^n) =: \vartheta^n + \varrho^n$. From (2.1)

$$\|\varrho^n\| \le ch^s\|u^n\|_s.$$

There remains to estimate ϑ^n. For $1 \le n \le N$, we have for $\chi \in \mathcal{X}_h$

$$\begin{aligned}
&([1 + \sigma(\beta^{n-1/2} + \mathrm{i}\nu^{n-1/2})]\partial_r\vartheta^n, \chi) - \alpha\sigma\mathcal{B}(\partial_r\vartheta^n, \chi) \\
&\quad + \mathrm{i}\alpha\mathcal{B}(\vartheta^{n-1/2}, \chi) - \mathrm{i}((\beta^{n-1/2} + \mathrm{i}\nu^{n-1/2})\vartheta^{n-1/2}, \chi) = (\omega^n, \chi),
\end{aligned} \tag{3.6}$$

where we define $\omega^n = \sum_{j=1}^6 \omega_j^n$, with

$$\begin{aligned}
\omega_1^n &= -[1+\sigma(\beta^{n-1/2}+\mathrm{i}\nu^{n-1/2})](\mathcal{P}_1 - I)\partial_r u^n,\\
\omega_2^n &= -[1+\sigma(\beta^{n-1/2}+\mathrm{i}\nu^{n-1/2})](\partial_r u^n - u_r^{n-1/2}),\\
\omega_3^n &= -\alpha\sigma D^2(\partial_r u^n - u_r^{n-1/2}),\\
\omega_4^n &= \mathrm{i}\alpha D^2(\frac{u^n+u^{n-1}}{2} - u^{n-1/2}),\\
\omega_5^n &= \frac{\mathrm{i}}{2}(\beta^{n-1/2}+\mathrm{i}\nu^{n-1/2})(\mathcal{P}_1 - I)(u^n+u^{n-1}),\\
\omega_6^n &= \mathrm{i}(\beta^{n-1/2}+\mathrm{i}\nu^{n-1/2})(\frac{u^n+u^{n-1}}{2} - u^{n-1/2}).
\end{aligned}$$

As has been done in the analogous context during the proof of (3.2), putting $\chi = \vartheta^{n-1/2}$ in equation (3.6) and taking real parts, and then taking $\chi = \sigma\partial_r\vartheta^n$ and imaginary parts, and finally adding the resulting equations yields

$$\|\vartheta^n\|^2 - \|\vartheta^{n-1}\|^2 \le 2k\{\mathrm{Re}(\omega^n, \vartheta^{n-1/2}) + \sigma\,\mathrm{Im}(\omega^n, \partial_r\vartheta^n)\}.$$

Therefore

$$\begin{aligned}
\|\vartheta^n\|^2 - \|\vartheta^0\|^2 &\le 2k\Big\{\mathrm{Re}\sum_{j=1}^n(\omega^j, \vartheta^{j-1/2}) + \sigma\,\mathrm{Im}\sum_{j=1}^n(\omega^j, \partial_r\vartheta^j)\Big\}\\
&= 2k\,\mathrm{Re}\sum_{j=1}^n(\omega^j, \vartheta^{j-1/2}) - 2k\sigma\,\mathrm{Im}\sum_{j=2}^n(\partial_r\omega^j, \vartheta^{j-1})\\
&\quad + 2\sigma\,\mathrm{Im}\{(\omega^n, \vartheta^n) - (\omega^1, \vartheta^0)\},
\end{aligned}$$

which implies

$$\begin{aligned}
\|\vartheta^n\|^2 &\le c(\|\omega^1\|^2 + \|\vartheta^0\|^2 + \|\omega^n\|^2) + \\
&ck(\sum_{j=1}^n\|\omega^j\|^2 + \sum_{j=2}^n\|\partial_r\omega^j\|^2) + \frac{k}{2R}\sum_{j=1}^n\|\vartheta^j\|^2.
\end{aligned} \tag{3.7}$$

We estimate next the ω_i^j and $\partial_r\omega_i^j$, $1 \le i \le 6$. For simplicity, we let $g^{j-1/2} = \beta^{j-1/2} + \mathrm{i}\nu^{j-1/2}$. From (2.13) and the Cauchy–Schwarz inequality we obtain

$$\|\omega_1^j\|^2 \le \frac{ch^{2s}}{k}\int_{r^{j-1}}^{r^j}\|u_r(r)\|_s^2\,dr.$$

By Taylor's theorem

$$\partial_r\omega_1^j = -\frac{1+\sigma g^{j-1/2}}{k}(\mathcal{P}_1 - I)\partial_r(u^j - u^{j-1}) - [\sigma g_r^{j-1/2} + O(k)](\mathcal{P}_1 - I)\partial_r u^{j-1}.$$

Since

$$\partial_r(u^j - u^{j-1}) = -\frac{1}{k}\Big\{\int_{r^{j-1}}^{r^j}(r - r^j)u^{(2)}(r)\,dr - \int_{r^{j-2}}^{r^{j-1}}(r - r^{j-2})u^{(2)}(r)\,dr\Big\},$$

an application of the Cauchy–Schwarz inequality gives

$$\|\partial_r \omega_1^j\|^2 \le \frac{ch^{2s}}{k}\int_{r^{j-2}}^{r^j} (\|u^{(2)}(r)\|_s^2 + \|u_r(r)\|_s^2)\,dr.$$

Next, since

$$\partial_r u^j - u_r^{j-1/2} = \frac{1}{2k}\Big\{\int_{r^{j-1}}^{r^{j-1/2}} (r-r^{j-1})^2 u^{(3)}(r)\,dr + \int_{r^{j-1/2}}^{r^j} (r-r^j)^2 u^{(3)}(r)\,dr\Big\},$$

we obtain

$$\|\omega_2^j\|^2 \le ck^3 \int_{r^{j-1}}^{r^j} \|u^{(3)}(r)\|^2 dr.$$

In order to derive a bound for $\partial_r\omega_2^j$, we write $\omega_2^j = (1+\sigma g^{j-1/2})\tilde\omega_2^j$, where

$$\tilde\omega_2^j = \frac{1}{6k}\Big\{\int_{r^{j-1}}^{r^{j-1/2}} (r-r^{j-1})^3 u^{(4)}(r)\,dr + \int_{r^{j-1/2}}^{r^j} (r-r^j)^3 u^{(4)}(r)\,dr\Big\} - \frac{k^2}{24}u^{(3)j-1/2}.$$

Then

$$\partial_r\omega_2^j = \frac{1+\sigma g^{j-1/2}}{k}(\tilde\omega_2^j - \tilde\omega_2^{j-1}) + [\sigma g_r^{j-1/2} + O(k)]\tilde\omega_2^{j-1},$$

and therefore

$$\|\partial_r\omega_2^j\|^2 \le ck^3\int_{r^{j-2}}^{r^j} \|u^{(4)}(r)\|^2\,dr + ck^4\big(|u^{(3)j-3/2}|_\infty^2 + k\int_{r^{j-2}}^{r^{j-1}} \|u^{(4)}(r)\|^2\,dr\big).$$

Analogously, we obtain

$$\|\omega_3^j\|^2 \le ck^3\int_{r^{j-1}}^{r^j} \|D^2u^{(3)}(r)\|^2\,dr,$$

and

$$\|\partial_r\omega_3^j\|^2 \le ck^3\int_{r^{j-2}}^{r^j} \|D^2u^{(4)}(r)\|^2 dr.$$

Using integration by parts we have

$$\begin{aligned} u^{j-1/2} - \frac{u^j + u^{j-1}}{2} &= \frac{1}{2}\Big\{\int_{r^{j-1}}^{r^{j-1/2}} (r^{j-1}-r)u^{(2)}(r)\,dr + \int_{r^{j-1/2}}^{r^j} (r-r^j)u^{(2)}(r)\,dr\Big\} \\ &= \frac{1}{4}\Big\{\int_{r^{j-1}}^{r^{j-1/2}} (r^{j-1}-r)^2 u^{(3)}(r)\,dr \\ &\quad - \int_{r^{j-1/2}}^{r^j} (r-r^j)^2 u^{(3)}(r)\,dr - \frac{k^2}{2}u^{(2)j-1/2}\Big\}, \end{aligned}$$

which implies

$$\|\omega_4^j\|^2 \le ck^3\int_{r^{j-1}}^{r^j} \|D^2u^{(2)}(r)\|^2 dr,$$

and

$$\|\partial_r\omega_4^j\|^2 \le ck^3\int_{r^{j-2}}^{r^j} \|D^2u^{(3)}(r)\|^2 dr.$$

We also have

$$\|\omega_5^j\|^2 \le ch^{2s}(\|u^0\|_s^2 + \int_0^{r^j} \|u_r(r)\|_s^2\, dr).$$

Since

$$\partial_r \omega_5^j = \frac{ig^{j-1/2}}{2k}(\mathcal{P}_1 - I)(u^j - u^{j-2}) + \frac{\mathrm{i}}{2}[g_r^{j-1/2} + O(k)](\mathcal{P}_1 - I)(u^{j-1} + u^{j-2}),$$

we obtain

$$\|\partial_r \omega_5^j\| \le \frac{ch^s}{k}\int_{r^{j-2}}^{r^j} \|u_r(r)\|_s\, dr + ch^s\Big\{\|u^0\|_s + \int_0^{r^{j-1}} \|u_r(r)\|_s\, dr\Big\},$$

i.e.

$$\|\partial_r \omega_5^j\|^2 \le \frac{ch^{2s}}{k}\int_{r^{j-2}}^{r^j} \|u_r(r)\|_s^2\, dr + ch^{2s}.$$

Further

$$\|\omega_6^j\|^2 \le ck^3 \int_{r^{j-1}}^{r^j} \|u^{(2)}(r)\|^2\, dr,$$

and (with a similar argument as that for ω_4^j)

$$\|\partial_r \omega_6^j\|^2 \le ck^3 \int_{r^{j-2}}^{r^j} \|u^{(3)}(r)\|^2\, dr + ck^4\big(|u^{(2)j-3/2}|_\infty^2 + k\int_{r^{j-2}}^{r^{j-1}} \|u^{(3)}(r)\|^2\, dr\big).$$

Putting all these results together in (3.7), since $\|\vartheta^0\| \le ch^s$, we have

$$\|\vartheta^n\|^2 \le c(u,R)(k^2 + h^s)^2 + \frac{k}{2R}\sum_{j=1}^n \|\vartheta^j\|^2.$$

Therefore

$$\max_{0\le j\le N} \|\vartheta^j\|^2 \le c(u,R)(k^2 + h^s)^2 + \frac{1}{2}\max_{0\le j\le N} \|\vartheta^j\|^2,$$

i.e. $\|\vartheta^n\| \le c(u,R)(k^2 + h^s)$, $0 \le n \le N$, and (3.5) is proved. $\square$

4. A fourth–order Runge–Kutta scheme

In this section we shall discretize the o.d.e. system (2.5) by a higher–order accurate range discretization scheme, namely the two–stage Gauss–Legendre, implicit Runge–Kutta method of fourth–order accuracy, [13], [2], [3], [15].

Arguing as in section 2, we may suppose that $1 + \alpha\sigma\mathcal{R}_h$ is invertible. Then, for purposes of error estimation only we write (2.5) as

$$u_{hr} = \mathrm{i}\mathcal{F}_h(r)u_h, \quad 0 \le r \le R, \quad u_h(0) = u_h^0, \tag{4.1}$$

where the linear operator $\mathcal{F}_h(r) : \mathcal{X}_h \to \mathcal{X}_h$, $0 \le r \le R$, is defined by

$$\mathcal{F}_h(r) = (1 + \alpha\sigma\mathcal{R}_h(r))^{-1}\mathcal{L}_h(r). \tag{4.2}$$

We now discretize (4.1) by the two–stage Gauss–Legendre method. We seek $U^n \in \mathcal{X}_h$, $0 \le n \le N$, approximating $u^n = u(\cdot, r^n)$, and $U^{n,m} \in \mathcal{X}_h$, $0 \le n \le N-1$, $m = 1, 2$, satisfying

$$\begin{aligned} &U^0 = u_h^0, \\ &\text{for } n = 0, \dots, N-1: \\ &U^{n,m} = U^n + \mathrm{i}k \sum_{j=1}^{2} a_{mj} \mathcal{F}_h^{n,j} U^{n,j}, \quad m = 1, 2, \\ &U^{n+1} = U^n + \mathrm{i}k \sum_{j=1}^{2} b_j \mathcal{F}_h^{n,j} U^{n,j}, \end{aligned} \tag{4.3}$$

where $r^{n,j} = r^n + \tau_j k$ and $\mathcal{F}_h^{n,j} = \mathcal{F}_h(r^{n,j})$. The constants appropriate for the two–stage Gauss–Legendre method are $a_{11} = a_{22} = 1/4$, $a_{12} = 1/4 - \sqrt{3}/6$, $a_{21} = 1/4 + \sqrt{3}/6$, $\tau_1 = 1/2 - \sqrt{3}/6$, $\tau_2 = 1/2 + \sqrt{3}/6$, and $b_1 = b_2 = 1/2$. We also assume henceforth that $U^0 = u_h^0$ has been chosen so that (2.3) is satisfied. In the next section we shall spell out an efficient algorithm implementing the scheme (4.3) in a way that does not require computing the operator $\mathcal{F}_h$, i.e. finding the inverse of $1 + \alpha\sigma\mathcal{R}_h$. For the purposes of the theoretical analysis of the scheme we retain (4.3) and write it compactly in the form

$$\boldsymbol{U}^n = U^n \boldsymbol{e} + \mathrm{i}kA\boldsymbol{F}_h^n \boldsymbol{U}^n, \tag{4.4}$$

$$U^{n+1} = U^n + \mathrm{i}kb^T \boldsymbol{F}_h^n \boldsymbol{U}^n, \tag{4.5}$$

where $\boldsymbol{U}^n = (U^{n,1}, U^{n,2})^T \in (\mathcal{X}_h)^2$ and $\mathcal{F}_h^n : (\mathcal{X}_h)^2 \to (\mathcal{X}_h)^2$ is the diagonal operator defined by

$$\boldsymbol{F}_h^n \boldsymbol{V} = (\mathcal{F}_h^{n,1} V^1, \mathcal{F}_h^{n,2} V^2)^T \quad \text{for } \boldsymbol{V} = (V^1, V^2)^T \in (\mathcal{X}_h)^2.$$

In our notation $b^T \boldsymbol{V} = \sum_{i=1}^2 b_i V^i$, $A\boldsymbol{V}$ is the element of $(\mathcal{X}_h)^2$ defined by $(A\boldsymbol{V})_i = \sum_{j=1}^2 a_{ij} V^j$, for $\boldsymbol{V} \in (\mathcal{X}_h)^2$, and finally $U\boldsymbol{e} = (U, U)^T \in (\mathcal{X}_h)^2$, for $U \in \mathcal{X}_h$, i.e. $\boldsymbol{e} = (1, 1)^T$.

In the analysis that follows we shall frequently refer to estimates from [3] in which the analogous problem is analyzed in the case of the standard parabolic approximation. For example, a straightforward computation shows that $\mathrm{Im}(\mathcal{F}_h\varphi, \varphi) \ge 0$, $\forall \varphi \in \mathcal{X}_h$, $0 \le r \le R$, with equality if $\nu = 0$. Hence, we can apply Lemmata 2.1 and 2.2 of [3] and deduce that, given $U^n \in \mathcal{X}_h$, the linear system (4.4) has a unique solution $\boldsymbol{U}^n = (U^{n,1}, U^{n,2})^T \in (\mathcal{X}_h)^2$ which satisfies $\max_{i=1,2} \|U^{n,i}\| \le c\|U^n\|$. Moreover $\|U^n\| \le \|U^{n-1}\|$, $1 \le n \le N$, (with equality if $\nu = 0$). Hence, the scheme (4.4)–(4.5) is unconditionally stable and in fact *conservative* in the L^2 sense in the absence of dissipation.

In the sequel we shall study the consistency and convergence of the scheme (4.3) under the assumption that $(1 + \alpha\sigma\mathcal{R}_h)^{-1}$ exists and is bounded in L^2, uniformly in h and r. This holds again if h is sufficiently small in general, and $-1/\alpha\sigma$ is not an eigenvalue of the operator $\mathcal{R} = \mathcal{R}(r)$ for any $r \in [0, R]$. To see this, given $\varphi \in \mathcal{X}_h$ let $\psi \in \mathcal{X}_h$ solve the problem

$$(1 + \alpha\sigma\mathcal{R}_h)\psi = \varphi, \tag{4.6}$$

where the r–dependence of $\mathcal{R}_h$ (and ψ) is suppressed in the notation. If $\nu(z, r) > 0$ on $\bar{I} \times [0, R]$, taking in (4.6) L^2–inner products of both sides with ψ and then imaginary parts yields

$$\sigma(\nu\psi, \psi) = \mathrm{Im}(\varphi, \psi) \leq \|\varphi\| \, \|\psi\|,$$

from which

$$\|\psi\| \leq c\|\varphi\|, \tag{4.7}$$

for some constant c independent of h and r. If ν is not strictly positive, consider the inhomogeneous indefinite elliptic problem

$$(1 + \alpha\sigma\mathcal{R})w = \varphi, \tag{4.8}$$

for which, cf. section 2, we may assume that

$$\|w\|_2 \leq c\|\varphi\|. \tag{4.9}$$

Since ψ is the Galerkin approximation of w in $\mathcal{X}_h$, it can be seen, cf. [18], that e.g. $\|w - \psi\|_1 \leq ch\|w\|_2$, for h sufficiently small. Therefore, by (4.9) $\|\psi\|_1 \leq \|w\|_1 + ch\|w\|_2 \leq c\|\varphi\|$, for some constant c independent of h and r, implying that (4.7) holds again; (4.7) obviously implies the desired estimate $\|(1 + \alpha\sigma\mathcal{R}_h)^{-1}\| \leq c$, where $\|\cdot\|$ denotes the L^2 induced operator norm on $\mathcal{X}_h$.

For the solution $u(r)$ of (1.1)–(1.3) we denote by $W = W(r) \in \mathcal{X}_h$, $0 \leq r \leq R$, its elliptic projection, i.e. let $W(r) = \mathcal{P}_1 u(r)$.

Let $W^n = W(r^n)$ and consider the following auxiliary problem: Suppose $V^{n,m}$, $1 \leq n \leq N - 1$, $m = 1, 2$, and V^n, $0 \leq n \leq N$, are defined in $\mathcal{X}_h$ by

$$\begin{aligned} &V^0 = W^0, \\ &\text{for } n = 0, \dots, N-1: \\ &V^{n,m} = W^n + \mathrm{i}k \sum_{j=1}^{2} a_{mj} \mathcal{F}_h^{n,j} V^{n,j}, \quad m = 1, 2, \\ &V^{n+1} = W^n + \mathrm{i}k \sum_{j=1}^{2} b_j \mathcal{F}_h^{n,j} V^{n,j}. \end{aligned} \tag{4.10}$$

The following *consistency* result is the main ingredient of our convergence proof.

Proposition 4.1. *Assume that the solution u of* (1.1)–(1.3) *is sufficiently smooth. Then there exists a constant c such that*

$$\max_{0 \leq n \leq N} \|V^n - W^n\| \leq ck(k^4 + h^s). \tag{4.11}$$

Proof. We follow the steps of proof and the notation of Proposition 3.1 of [3]. Let $\tau_{i0} = 1$, $\tau_{ij} = \sum_{m=1}^{2} a_{im}\tau_{m,j-1}$, $j \ge 1$, $i = 1, 2$; then $\tau_{ij} = (\tau_i)^j/j!$, $0 \le j \le 2$, $i = 1, 2$. Let $0 \le n \le N-1$ be given. Set $\Lambda_m W^n = \sum_{j=0}^{4} \tau_{mj} k^j W^{(j)n}$, $e^{n,m} = V^{n,m} - \Lambda_m W^n$, $m = 1, 2$. Then one can easily obtain, cf. [3],

$$\|V^{n+1} - W^{n+1}\| \le ck^5 + \|b^T A^{-1}\boldsymbol{e}^n\|,$$

where $\boldsymbol{e}^n = (e^{n,1}, e^{n,2})^T \in (\mathcal{X}_h)^2$. It remains to prove that

$$\|b^T A^{-1}\boldsymbol{e}^n\| \le ck(k^4 + h^s). \tag{4.12}$$

Using (4.10) we have

$$e^{n,j} = E^{n,j} + \mathrm{i}k \sum_{m=1}^{2} a_{jm} \mathcal{F}_h^{n,m} e^{n,m}, \quad j = 1, 2, \tag{4.13}$$

where

$$E^{n,j} = -\Lambda_j W^n + W^n + \mathrm{i}k \sum_{d=1}^{2} a_{jd} \mathcal{F}_h^{n,d} \Lambda_d W^n, \quad j = 1, 2.$$

By Lemma 2.1 of [3] it suffices to estimate $E^{n,j}$. In fact

$$E^{n,j} = \tilde{I}_1^{n,j} + \tilde{I}_2^{n,j} + O(k^5), \quad j = 1, 2,$$

where

$$\tilde{I}_1^{n,j} := -\sum_{m=1}^{4} \tau_{jm} k^m (W^{(m)n} - \mathrm{i}\mathcal{F}_h^n W^{(m-1)n}),$$
$$\tilde{I}_2^{n,j} := \mathrm{i} \sum_{d=1}^{2} a_{jd} (\mathcal{F}_h^{n,d} - \mathcal{F}_h^n)(\sum_{m=0}^{3} \tau_{dm} k^{m+1} W^{(m)n}).$$

Define $\mathcal{G}_h(r) : \mathcal{X}_h \to \mathcal{X}_h$, $0 \le r \le R$, as $\mathcal{G}_h(r) = \mathcal{B}_h(r) + \mathrm{i}\mathcal{N}_h(r)$. Using (4.2) and (2.4) we obtain

$$\begin{aligned} W^{(m)n} - \mathrm{i}\mathcal{F}_h^n W^{(m-1)n} = (1 + \alpha\sigma\mathcal{R}_h^n)^{-1}\{&(W_r^n + \alpha\sigma\mathcal{D}_h W_r^n - \mathrm{i}\alpha\mathcal{D}_h W^n)^{(m-1)} \\ &- \mathcal{G}_h^n(\mathrm{i}W^n - \sigma W_r^n)^{(m-1)}\}. \end{aligned} \tag{4.14}$$

Since $(\mathcal{D}_h W, \chi) = (D^2 u, \chi)$, $\forall \chi \in \mathcal{X}_h$, we have for $0 \le r \le R$,

$$\begin{aligned} &(W_r + \alpha\sigma\mathcal{D}_h W_r - \mathrm{i}\alpha\mathcal{D}_h W, \chi) = \\ &(\mathcal{P}\Psi, \chi) + ((\beta(r) + \mathrm{i}\nu(r))(\mathrm{i}W - \sigma W_r), \chi), \quad \forall \chi \in \mathcal{X}_h, \end{aligned}$$

where $\Psi(r) = [1 + \sigma(\beta(r) + \mathrm{i}\nu(r))](W_r - u_r) - \mathrm{i}(\beta(r) + \mathrm{i}\nu(r))(W - u)$. Therefore, for $0 \le r \le R$,

$$W_r + \sigma\mathcal{D}_h W_r - \mathrm{i}\mathcal{D}_h W = \mathcal{P}\Psi + \mathcal{G}_h(r)(\mathrm{i}W - \sigma W_r). \tag{4.15}$$

In view of (2.13), we have $\Psi^{(j)} = O(h^s)$, $j \ge 0$. Hence

$$(1 + \alpha\sigma\mathcal{R}_h)W_r = \mathrm{i}\mathcal{L}_h W + O(h^s), \tag{4.16}$$

where the remainder terms are understood in the L^2 norm. Using (4.14) and (4.15) we obtain (note the analogy with relation (3.27) of [3])

$$\begin{aligned}\tilde{I}_1^{n,j} =& -(1+\alpha\sigma\mathcal{R}_h^n)^{-1}\sum_{m=1}^{4}\tau_{jm}k^m\{[\mathcal{G}_h^n(\mathrm{i}W^n-\sigma W_r^n)]^{(m-1)}\\ &-\mathcal{G}_h^n(\mathrm{i}W^n-\sigma W_r^n)^{(m-1)}\}+O(kh^s).\end{aligned}$$

Since

$$\begin{aligned}&\mathcal{F}_h^{n,d}-\mathcal{F}_h^n-(1+\alpha\sigma\mathcal{R}_h^n)^{-1}(\mathcal{L}_h^{n,d}-\mathcal{L}_h^n)=\\ &\sigma(1+\alpha\sigma\mathcal{R}_h^n)^{-1}(\mathcal{L}_h^n-\mathcal{L}_h^{n,d})(1+\alpha\sigma\mathcal{R}_h^{n,d})^{-1}\mathcal{L}_h^{n,d},\end{aligned}$$

we can write

$$\tilde{I}_2^{n,j}=\Omega_1^{n,j}+\Omega_2^{n,j},$$

with

$$\Omega_1^{n,j}=(1+\alpha\sigma\mathcal{R}_h^n)^{-1}\sum_{d=1}^{2}a_{jd}(\mathcal{L}_h^{n,d}-\mathcal{L}_h^n)\Big\{\sum_{m=0}^{3}\tau_{dm}k^{m+1}(\mathrm{i}W^{(m)n})\Big\},$$

and

$$\begin{aligned}\Omega_2^{n,j}=&-\mathrm{i}\sigma(1+\alpha\sigma\mathcal{R}_h^n)^{-1}\Big\{\sum_{d=1}^{2}a_{jd}(\mathcal{L}_h^{n,d}-\mathcal{L}_h^n)\\ &(1+\alpha\sigma\mathcal{R}_h^{n,d})^{-1}\mathcal{L}_h^{n,d}(\sum_{m=0}^{3}\tau_{dm}k^{m+1}W^{(m)n})\Big\}.\end{aligned}$$

However

$$\sum_{m=0}^{3}\tau_{dm}k^{m+1}W^{(m)n}=kW^{n,d}+A^{n,d},$$

where

$$A^{n,d}=k\Big\{-\frac{1}{2}\int_{r^n}^{r^{n,d}}(r^{n,d}-r)^2W^{(3)}(r)dr+\tau_{d3}k^3W^{(3)n}\Big\}.$$

Hence,

$$\begin{aligned}\Omega_2^{n,j}=&-\mathrm{i}k\sigma(1+\alpha\sigma\mathcal{R}_h^n)^{-1}\sum_{d=1}^{2}a_{jd}(\mathcal{L}_h^{n,d}-\mathcal{L}_h^n)(1+\alpha\sigma\mathcal{R}_h^{n,d})^{-1}\mathcal{L}_h^{n,d}W^{n,d}\\ &-\mathrm{i}\sigma(1+\alpha\sigma\mathcal{R}_h^n)^{-1}\sum_{d=1}^{2}a_{jd}(\mathcal{L}_h^{n,d}-\mathcal{L}_h^n)(1+\alpha\sigma\mathcal{R}_h^{n,d})^{-1}\mathcal{L}_h^{n,d}A^{n,d}.\end{aligned}$$

It can be proved (in a manner analogous to the proof of the estimate (3.5) of [3]), that

$$\|\mathcal{L}_h^{(\ell)}(r)W^{(j)}(t)\|\le c,\quad r,t\in[0,R],\quad \ell,j\ge 0, \tag{4.17}$$

which implies that $\mathcal{L}_h^{n,d}A^{n,d}=O(k^4)$. Then (4.16) and Taylor's theorem yield

$$\Omega_2^{n,j}=-k\sigma(1+\alpha\sigma\mathcal{R}_h^n)^{-1}\sum_{d=1}^{2}a_{jd}(\mathcal{L}_h^{n,d}-\mathcal{L}_h^n)W_r^{n,d}+O(k(h^s+k^4)).$$

Moreover,

$$W_r^{n,d} = \sum_{m=0}^{3} \tau_{dm} k^m W_r^{(m)n} + B^{n,d},$$

where

$$B^{n,d} = \frac{1}{2}\int_{r^n}^{r^{n,d}} (r^{n,d} - r)^2 W_r^{(3)}(r)\,dr - \tau_{d3} k^3 W_r^{(3)n}.$$

Again (4.17) and Taylor's theorem imply

$$(1 + \alpha\sigma\mathcal{R}_h^n)^{-1} \sum_{d=1}^{2} a_{jd} (\mathcal{L}_h^{n,d} - \mathcal{L}_h^n) B^{n,d} = O(k^4).$$

Therefore

$$\Omega_2^{n,j} = (1 + \alpha\sigma\mathcal{R}_h^n)^{-1} \sum_{d=1}^{2} a_{jd} (\mathcal{L}_h^{n,d} - \mathcal{L}_h^n) \Big\{ \sum_{m=0}^{3} \tau_{dm} k^{m+1} (-\sigma W_r^{(m)n}) \Big\} + O(kh^s + k^5),$$

implying (note the analogy with relation (3.28) of [3])

$$\begin{aligned}\tilde{I}_2^{n,j} =& (1 + \alpha\sigma\mathcal{R}_h^n)^{-1} \sum_{d=1}^{2} a_{jd} (\mathcal{L}_h^{n,d} - \mathcal{L}_h^n) \\ & \Big\{ \sum_{m=0}^{3} \tau_{dm} k^{m+1} (\mathrm{i}W^n - \sigma W_r^n)^{(m)} \Big\} + O(k(h^s + k^4)).\end{aligned}$$

Now, set $Z = \mathrm{i}W - \sigma W_r, 0 \le r \le R$. Then

$$\tilde{I}_1^{n,j} + \tilde{I}_2^{n,j} = (1 + \alpha\sigma\mathcal{R}_h^n)^{-1} (I_1^{n,j} + I_2^{n,j}) + O(k(h^s + k^4)),$$

with

$$I_1^{n,j} = -\sum_{d=2}^{4} k^d \Big[\sum_{m=1}^{d-1} \gamma_j^{m,d} \frac{\mathcal{G}_h^{(d-m)n} Z^{(m-1)n}}{(d-m)!} \Big],$$

and

$$I_2^{n,j} = \sum_{d=2}^{4} k^d \Big[\sum_{m=1}^{d-1} \delta_j^{m,d} \frac{\mathcal{G}_h^{(d-m)n} Z^{(m-1)n}}{(d-m)!} \Big],$$

where we have set, for $2 \le d \le 4$, $1 \le m \le d-1$, $j = 1, 2$,

$$\gamma_j^{m,d} = \tau_{jd} \frac{(d-1)!}{(m-1)!}, \qquad \delta_j^{m,d} = \sum_{\ell=1}^{2} a_{j\ell} \tau_\ell^{d-m} \tau_{\ell,m-1},$$

(cf. (3.31)–(3.35) in Proposition 3.1 of [3]). Therefore

$$E^{n,j} = \sum_{d=2}^{4} k^d \Big[\sum_{m=1}^{d-1} (\delta_j^{m,d} - \gamma_j^{m,d}) \mathcal{G}_h^{(d-m)n} \frac{Z^{(m-1)n}}{(d-m)!} \Big] + O(k(k^4 + h^s)).$$

Since $\gamma_j^{m,d} = \delta_j^{m,d}, 1 \le m \le d-1, d = 1, 2, 3,$ (cf. Proposition 3.1 of [3]) we conclude that

$$E^{n,j} = \varphi^{n,j} + O(k(k^4 + h^s)), \quad j = 1, 2,$$

where we have put

$$\varphi^{n,j} = k^4 \Big[\sum_{m=1}^{3} (\delta_j^{m,4} - \gamma_j^{m,4}) \frac{\mathcal{G}_h^{(4-m)n} Z^{(m-1)n}}{(4-m)!} \Big].$$

Since $\delta_j^{m,4} - \gamma_j^{m,4} \neq 0$, we have $\varphi^{n,j} = O(k^4)$. Define now $\tilde{e}^{n,j} = e^{n,j} - \varphi^{n,j}$, $\tilde{E}^{n,j} = E^{n,j} - \varphi^{n,j}$, $j = 1, 2$. Then (4.13) is equivalently written as

$$\tilde{e}^{n,j} = \Big(\tilde{E}^{n,j} + \mathrm{i}k \sum_{d=1}^{2} a_{jd} \mathcal{L}_h^{n,d} \varphi^{n,d} \Big) + \mathrm{i}k \sum_{d=1}^{2} a_{jd} \mathcal{L}_h^{n,d} \tilde{e}^{n,d}.$$

Since $\tilde{E}^{n,j} = O(k(k^4 + h^s))$ and (4.17) imply $\|\mathcal{L}_h^{n,j} \varphi^{n,j}\| \leq ck^4$, by Lemma 2.1 of [3] we have $\tilde{e}^{n,j} = O(k(k^4 + h^s))$. Therefore

$$b^T A^{-1} \boldsymbol{e}^n = O(k(k^4 + h^s)) + b^T A^{-1} \boldsymbol{\varphi}^n,$$

where $\boldsymbol{\varphi}^n = (\varphi^{n,1}, \varphi^{n,2})^T \in (\mathcal{X}_h)^2$. By Lemma 3.1 of [3] we further have $b^T A^{-1}(\delta^{m,4} - \gamma^{m,4}) = 0$, $m = 1, 2, 3$, where $\gamma^{m,4} = (\gamma_1^{m,4}, \gamma_2^{m,4})^T, \delta^{m,4} = (\delta_1^{m,4}, \delta_2^{m,4})^T$, i.e. $b^T A^{-1} \boldsymbol{\varphi}^n = 0$, which proves (4.12). □

The following theorem is an immediate consequence of the *stability* of the scheme (4.3) and the *consistency* result just proved.

Theorem 4.1. *Assume that the solution u of* (1.1)–(1.3) *is sufficiently smooth. Then there exists a constant c such that*

$$\max_{0 \leq n \leq N} \|U^n - u^n\| \leq c(k^4 + h^s).$$

Proof. Define $V^{n,m}$, V^n by (4.10) and let $\varepsilon^{n,m} = U^{n,m} - V^{n,m}$, $\varepsilon^n = U^n - V^n$ and $\zeta^n = U^n - W^n$. Then, (4.3) and (4.10) give

$$\varepsilon^{n,m} = \zeta^n + \mathrm{i}k \sum_{j=1}^{2} a_{mj} \mathcal{F}_h^{n,j} \varepsilon^{n,j}, \quad m = 1, 2,$$

$$\varepsilon^{n+1} = \zeta^n + \mathrm{i}k \sum_{j=1}^{2} b_j \mathcal{L}_h^{n,j} \varepsilon^{n,j}.$$

As in the stability proof (cf. Lemma 2.2 of [3]), we have that $\|\varepsilon^{n+1}\| \leq \|\zeta^n\|$. Hence $\|\zeta^{n+1}\| \leq \|\zeta^n\| + \|V^{n+1} - W^{n+1}\|$, which, in view of (4.11), (2.1) and (2.3) yields $\|\zeta^n\| \leq c(k^4 + h^s)$. The result follows in view of (2.13). □

Remark 4.1. The ideas of the convergence proof just concluded do not change appreciably if one discretizes the problem in the range variable using the general *q–stage* Gauss–Legendre scheme. The resulting methods are unconditionally stable (conservative if $\nu = 0$) and can be shown to satisfy the error estimate $\max_{0 \leq n \leq N} \|U^n - u^n\| \leq c(k^{\min(2q, q+2)} + h^s)$. For details cf. [3], [15].

5. Efficient implementation of the Runge–Kutta scheme

In this section we shall study the efficient implementation of the fully discrete scheme (4.3), following [15]. Let $J = \dim \mathcal{X}_h$. The vector $\boldsymbol{U}^n = (U^{n,1}, U^{n,2})^T$ is the solution of the $2J \times 2J$ (complex) linear system represented by the equation

$$\boldsymbol{T}^n \boldsymbol{U}^n = U^n \boldsymbol{e}, \tag{5.1}$$

where

$$\begin{aligned} \boldsymbol{T}^n &= \boldsymbol{T}^n(r^{n,1}, r^{n,2}) \\ &= \begin{pmatrix} 1 - \mathrm{i}a_{11}k(1+\alpha\sigma\mathcal{R}_h^{n,1})^{-1}\mathcal{L}_h^{n,1} & -\mathrm{i}a_{12}k(1+\alpha\sigma\mathcal{R}_h^{n,2})^{-1}\mathcal{L}_h^{n,2} \\ -\mathrm{i}a_{21}k(1+\alpha\sigma\mathcal{R}_h^{n,1})^{-1}\mathcal{L}_h^{n,1} & 1 - \mathrm{i}a_{22}k(1+\alpha\sigma\mathcal{R}_h^{n,2})^{-1}\mathcal{L}_h^{n,2} \end{pmatrix}. \end{aligned}$$

We shall decouple (5.1) using the solution technique of [15], cf. also [2], [3], which is based on an idea from [7] and may be summarized as follows: write (5.1) as

$$\boldsymbol{T}^{*n} \boldsymbol{U}^n = (\boldsymbol{T}^{*n} - \boldsymbol{T}^n)\boldsymbol{U}^n + U^n \boldsymbol{e}, \tag{5.2}$$

with $\boldsymbol{T}^{*n} = \boldsymbol{T}^n(r^{*n}, r^{*n})$, $r^{*n} = r^n + k/2$, and solve (5.2) by a simple iterative method suggested by its form. Denoting by j_n, $0 \le n \le N$, the number of iterations performed at each range step to solve (5.2) (in practice $j_n = 1$ or $j_n = 2$), we compute approximations $U_{j_n}^n$ to U^n by the following algorithm:

$$\begin{aligned} & U_{j_0}^0 = U^0. \\ & \text{for } n = 0, \ldots, N-1: \\ & \quad \text{compute suitable } U_0^{n,1}, U_0^{n,2}, \\ & \quad\quad \text{for } j = 0, \ldots, j_{n+1}-1: \\ & \quad\quad\quad \boldsymbol{T}^{*n}\boldsymbol{U}_{j+1}^n = (\boldsymbol{T}^{*n} - \boldsymbol{T}^n)\boldsymbol{U}_j^n + U_{j_n}^n \boldsymbol{e}, \\ & \quad U_{j_{n+1}}^{n+1} = U_{j_n}^n + \sqrt{3}(U_{j_{n+1}}^{n,2} - U_{j_{n+1}}^{n,1}). \end{aligned} \tag{5.3}$$

Each system in the inner (j) loop of (5.3) is of the form $\boldsymbol{T}^{*n}\boldsymbol{V} = \tilde{\boldsymbol{Z}}$, where $\boldsymbol{V} = (V_1, V_2)^T$, $\tilde{\boldsymbol{Z}} = (\tilde{Z}_1, \tilde{Z}_2)^T \in (\mathcal{X}_h)^2$. Because the operators in the entries of $\boldsymbol{T}^{*n}$ commute now, we may compute the V_i, $i = 1, 2$, as solutions of the two (uncoupled) $J \times J$ complex linear systems

$$\begin{aligned} \tilde{\mathcal{H}}^n \tilde{\mathcal{K}}^n V_1 &= \tilde{Z}_1 + \mathrm{i}k(1+\alpha\sigma\mathcal{R}_h^{*n})^{-1}\mathcal{L}_h^{*n}(a_{12}\tilde{Z}_2 - a_{22}\tilde{Z}_1), \\ \tilde{\mathcal{H}}^n \tilde{\mathcal{K}}^n V_2 &= \tilde{Z}_2 + \mathrm{i}k(1+\alpha\sigma\mathcal{R}_h^{*n})^{-1}\mathcal{L}_h^{*n}(a_{21}\tilde{Z}_1 - a_{11}\tilde{Z}_2), \end{aligned}$$

where

$$\begin{aligned} \tilde{\mathcal{H}}^n &= (1+\alpha\sigma\mathcal{R}_h^{*n})^{-1}\mathcal{H}^n, \quad \tilde{\mathcal{K}}^n = (1+\alpha\sigma\mathcal{R}_h^{*n})^{-1}\mathcal{K}^n, \\ \mathcal{H}^n &= 1 + (\sigma - \mathrm{i}k\mu)\mathcal{L}_h^{*n}, \quad \mathcal{K}^n = 1 + (\sigma - \mathrm{i}k\bar{\mu})\mathcal{L}_h^{*n}, \end{aligned}$$

and $\mu = 1/4 - \mathrm{i}\sqrt{3}/12$. It can be proved that $\mathcal{H}^n$ and $\mathcal{K}^n$ are invertible, cf. [15]. By (5.2) the right–hand side is

$$\tilde{\boldsymbol{Z}} = \begin{pmatrix} (1+\alpha\sigma\mathcal{R}_h^{*n})^{-1} & 0 \\ 0 & (1+\alpha\sigma\mathcal{R}_h^{*n})^{-1} \end{pmatrix} \boldsymbol{Z},$$

where $\mathcal{Z} = (Z_1, Z_2)^T \in (\mathcal{X}_h)^2$ is given by

$$\begin{aligned} Z_m = \mathrm{i}k\big\{&a_{m1}[(1+\alpha\sigma\mathcal{R}_h^{*n})(1+\alpha\sigma\mathcal{R}_h^{n,1})^{-1}\mathcal{L}_n^{n,1} - \mathcal{L}_h^{*n}]U^{n,1} \\ &+ a_{m2}[(1+\alpha\sigma\mathcal{R}_h^{*n})(1+\alpha\sigma\mathcal{R}_h^{n,2})^{-1}\mathcal{L}_n^{n,2} - \mathcal{L}_h^{*n}]U^{n,2}\big\} \\ &+ (1+\alpha\sigma\mathcal{R}_h^{*n})U^n, \qquad m = 1,2. \end{aligned}$$

Since $\mathrm{i}k(1+\alpha\sigma\mathcal{R}_h^{*n})^{-1}\mathcal{L}_h^{*n} = -2\mathrm{i}\sqrt{3}(\tilde{\mathcal{H}}^n - \tilde{\mathcal{K}}^n)$, we deduce

$$\begin{aligned} V_1 &= (\mathcal{K}^n)^{-1}(1+\alpha\sigma\mathcal{R}_h^{*n})(\mathcal{H}^n)^{-1}Z_1 - 2\mathrm{i}\sqrt{3}[(\mathcal{K}^n)^{-1} - (\mathcal{H}^n)^{-1}](a_{12}Z_2 - a_{22}Z_1), \\ V_2 &= (\mathcal{K}^n)^{-1}(1+\alpha\sigma\mathcal{R}_h^{*n})(\mathcal{H}^n)^{-1}Z_2 - 2\mathrm{i}\sqrt{3}[(\mathcal{K}^n)^{-1} - (\mathcal{H}^n)^{-1}](a_{21}Z_1 - a_{11}Z_2). \end{aligned}$$

We see then that computing $\boldsymbol{V}$, given $\boldsymbol{Z}$, reduces to solving a number of complex linear systems with operators $\mathcal{H}^n$ and $\mathcal{K}^n$. At the matrix–vector level the corresponding $J\times J$ matrices will be sparse if a finite element basis is chosen for $\mathcal{X}_h$. The computational costs for solving the systems consist of the LU–decomposition of the complex matrices representing $\mathcal{H}^n$ and $\mathcal{K}^n$, four backsolves to compute

$$(\mathcal{K}^n)^{-1}Z_i, \quad (\mathcal{H}^n)^{-1}Z_i, \quad i = 1,2,$$

two matrix–vector multiplications to construct

$$(1+\alpha\sigma\mathcal{R}_h^{*n})(\mathcal{H}^n)^{-1}Z_i, \quad i = 1,2,$$

and two backsolves to compute

$$(\mathcal{K}^n)^{-1}(1+\alpha\sigma\mathcal{R}_h^{*n})(\mathcal{H}^n)^{-1}Z_i, \quad i = 1,2.$$

In addition, the computational cost to form Z_1 and Z_2 consists of the LU–decomposition of the complex matrices representing $1+\alpha\sigma\mathcal{R}_h^{n,i}$, $i = 1,2$, four matrix–vector multiplications to construct $\mathcal{L}_h^{*n}U^{n,i}$, $\mathcal{L}_h^{n,i}U^{n,i}$, $i = 1,2$, two backsolves to compute $(1+\alpha\sigma\mathcal{R}_h^{n,i})^{-1}\mathcal{L}_h^{n,i}U^{n,i}$, $i = 1,2$, and three matrix–vector multiplications to construct

$$(1+\alpha\sigma\mathcal{R}_h^{*n})U^n, \quad (1+\alpha\sigma\mathcal{R}_h^{*n})(1+\alpha\sigma\mathcal{R}_h^{n,i})^{-1}\mathcal{L}_h^{n,i}U^{n,i}, \quad i = 1,2.$$

When $j = j_{n+1} - 1$ in the inner loop of (5.3) a further simplification reduces by half the computational cost of the last iteration. Since, eventually, only $U_{j_{n+1}}^{n,2} - U_{j_{n+1}}^{n,1}$ is required, it is not hard to see that one needs to compute

$$\begin{aligned} V_2 - V_1 =& (1+\alpha\sigma\mathcal{R}_h^{*n})^{-1}(Z_2 - Z_1) \\ &- 2\mathrm{i}\sqrt{3}[(\mathcal{K}^n)^{-1} - (\mathcal{H}^n)^{-1}]\big\{[\frac{1}{2} - \frac{\mathrm{i}k}{12}\mathcal{L}_h^{*n}(1+\alpha\sigma\mathcal{R}_h^{*n})^{-1}](Z_2 - Z_1) \\ &+ (a_{21}+a_{22})Z_1 - (a_{11}+a_{12})Z_2\big\}, \end{aligned}$$

at a computational cost of three backsolves and a matrix–vector multiplication.

In practice we usually choose $j_n = 2$. The starting values $U_0^{n,1}$ and $U_0^{n,2}$, as well as few of the initial approximations $U_{j_n}^n$, for $0 \le n \le n_0$ (usually $n_0 = 4$) in (5.3), are determined by polynomial extrapolation from previously computed values, cf. [3] and [15] for details. The reader will duly notice the abundant natural parallelicity on two processors of many of the computational tasks outlined above.

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