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SEMIDISCRETE AND SINGLE STEP FULLY DISCRETE APPROXIMATIONS FOR SECOND ORDER HYPERBOLIC EQUATIONS (*)

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Abstract — *Finite element approximations are analysed, for initial boundary value problems for second order hyperbolic equations. For both semidiscrete and fully discrete schemas, optimal order rate of convergence estimates in L^2 are derived, using L^2 projections of the initial data as starting values.*

A new class of single step fully discrete schemes is developed, which are high order accurate in time. The schemes are constructed from a class of rational approximations to e^{-z} , analytic in neighbourhoods of the imaginary axis. The approximations require the solution of 2s linear systems at each time step, with the same real matrix, to yield convergence rate k^s , where k is the time step and s is an arbitrary positive integer.

Résumé — *On étudie des approximations par éléments finis de problèmes aux limites, avec conditions initiales, pour des équations hyperboliques du second ordre utilisant les projections L^2 des données initiales comme valeurs de départ, on obtient des estimations d'ordre optimal du taux de convergence, pour les schémas semi-discretisés et pour les schémas complètement discretisés.*

On introduit une nouvelle famille de schémas complètement discrétisés à un pas, d'une précision d'ordre élevée en temps. On obtient ces schémas à partir d'une famille d'approximations rationnelles de e^{-z} , analytiques dans des voisinages de l'axe imaginaire. Ces approximations nécessitent la solution de 2s systèmes linéaires à chaque pas de temps, correspondant à une même matrice réelle, et conduisant à un taux de convergence en k^s , où k est le pas de temps et s un nombre entier positif arbitraire.

1. INTRODUCTION

1.1. Notation

We consider approximating the solution of the following initial boundary value problem. Let Ω be a bounded domain in \mathbb{R}^N , with smooth boundary $\partial\Omega$ and let $0 < t^* < \infty$ be fixed. A function $u : (0, t^*] \rightarrow \mathbb{R}^1$ is sought which satisfies

$$\left. \begin{aligned} u_{tt} + \mathcal{L}u &= 0 & \text{in } \Omega \times (0, t^*], \\ u &= 0 & \text{on } \partial\Omega \times (0, t^*], \\ u(0) &= u^0 & \text{in } \Omega, \\ u_t(0) &= u_t^0 & \text{in } \Omega, \end{aligned} \right\} \quad (1.1)$$

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u^0 and u_t^0 are given functions, and \mathcal{L} denotes the second order elliptic operator

$$\mathcal{L}u = - \sum_{i,j=1}^N \frac{\partial}{\partial x_i} \left(a_{ij}(x) \frac{\partial u}{\partial x_j} \right) + a_0(x)u,$$

with $a_{ij} = a_{ji} \in C^\infty(\bar{\Omega})$, $i, j = 1, 2, \dots, N$; $a_0 \in C^\infty(\bar{\Omega})$ and $a_0 \geq 0$ on Ω .

\mathcal{L} is assumed to satisfy the uniform ellipticity condition

$$\sum_{i,j=1}^N a_{ij}(x) \xi_i \xi_j \geq \alpha \sum_{i=1}^N \xi_i^2, \quad (1.2)$$

for all $x \in \bar{\Omega}$ and for all $(\xi_1, \dots, \xi_N) \in \mathbb{R}^N$, for some constant $\alpha > 0$.

The following notation will be used throughout. For $s \geq 0$, $H^s(\Omega)$ will denote the Sobolev space of order s , of real valued functions on Ω . The norm on $H^s(\Omega)$ we denote by $\|\cdot\|_{H^s(\Omega)}$. In particular, the inner product on $L^2(\Omega) = H^0(\Omega)$ we denote by (\cdot, \cdot) , and the associated norm by $\|\cdot\|$.

We introduce certain subspaces of the Sobolev space $H^s(\Omega)$, denoted by $\dot{H}^s(\Omega)$. In order to define $\dot{H}^s(\Omega)$, we first note that there exists a sequence $\{\lambda_j\}_{j \geq 1}$ in non decreasing order of real positive eigenvalues of the operator \mathcal{L} , and a corresponding sequence of eigenfunctions $\{\varphi_j\}_{j \geq 1} \subset C^\infty(\Omega)$, satisfying

$$\left. \begin{aligned} \mathcal{L}\varphi_j &= \lambda_j \varphi_j && \text{in } \Omega, \\ \varphi_j &= 0 && \text{on } \partial\Omega. \end{aligned} \right\} \quad (1.3)$$

The set $\{\varphi_j\}_{j \geq 1}$ is complete in $L^2(\Omega)$, and may be chosen orthonormal. Define for $s \geq 0$, the space

$$\dot{H}^s(\Omega) = \{v : \|v\|_s = \left(\sum_{j=1}^{\infty} |(v, \varphi_j)|^2 \lambda_j^s \right)^{\frac{1}{2}} < \infty \}.$$

Then $\dot{H}^0(\Omega) = L^2(\Omega)$, and it may be shown, [7], that

$$\dot{H}^s(\Omega) = \{v \in H^s(\Omega) : \mathcal{L}^j v = 0 \text{ on } \partial\Omega, j < s/2\},$$

and that on $\dot{H}^s(\Omega)$, the norms $\|\cdot\|_s$ and $\|\cdot\|_{H^s(\Omega)}$ are equivalent.

For $s < 0$, $\dot{H}^s(\Omega)$ is defined as the dual of $\dot{H}^{-s}(\Omega)$ with respect to $L^2(\Omega)$.

The norm on $\dot{H}^{-s}(\Omega)$ is given by

$$\|v\|_{-s} = \left(\sum_{j=1}^{\infty} |(v, \varphi_j)|^2 \lambda_j^{-s} \right)^{\frac{1}{2}}, \quad s \geq 0.$$

The solution of (1.1) is formally given by

$$u(t) = \sum_{j=1}^{\infty} [(u^0, \varphi_j) \cos \lambda_j^{\frac{1}{2}} t + \lambda_j^{-\frac{1}{2}} (u_t^0, \varphi_j) \sin \lambda_j^{\frac{1}{2}} t] \varphi_j,$$

for $t \geq 0$, from which it follows that for $0 \leq t \leq t^*$,

$$\|u(t)\|_s^2 + \|u_t(t)\|_{s-1}^2 = \|u^0\|_s^2 + \|u_t^0\|_{s-1}^2, \quad \text{for all } s \geq 0 \quad (1.4)$$

In Section 2, we derive the estimates for semidiscrete approximations

$$\sup_{0 \leq t \leq t^*} \|u(t) - u_h(t)\| \leq C(t^*)h^r [\|u^0\|_{r+1} + \|u_t^0\|_r], \quad (1.5)$$

using standard finite element spaces of piecewise polynomial functions of degree $r-1$, $r \geq 2$. The estimates are obtained with L^2 projections of the initial data as starting values. These estimates were in essence derived prior to this work by the first author in [3, 4], using a special manipulation of an energy formulation. Here (1.5) is obtained via a reformulation of (1.1) and the semidiscrete approximation as appropriate first order systems.

We note also that Dupont [9] and Crouzeix [8], have obtained L^2 estimates, however the choice of stating values yield unnaturally higher smoothness assumptions on the solution.

1.2. Summary of the results

In Section 3, we consider single step fully discrete approximations via rational approximations to e^{-z} . The rational functions are required to satisfy

$$|r_v(iy) - e^{-iy}| \leq C_v |y|^{v+1}, \quad |y| \leq \sigma, \quad (1.6)$$

for constants $C_v < \infty$, $\sigma > 0$ and $v \geq 1$.

In addition such rational functions are divided into two classes, according to either

$$|r_v(iy)| \leq 1 \quad \text{for all real } y, \quad (1.7)$$

or

$$|r_v(iy)| \leq 1 \quad \text{for } |y| \leq \alpha, \quad (1.8)$$

for some constant $\alpha > 0$. The functions satisfying (1.7) we designate as Class *I-I*, and those satisfying (1.8) as Class *I-II*.

For schemes defined by rational functions of Class *I-I*, we obtain estimates

$$\max \|W_1^n - u(nk)\| = C(t^*) \{ h^r [\|u^0\|_{r+1} + \|u_t^0\|_r] + k^v [\|u^0\|_{v+1} + \|u_t^0\|_v] \}, \quad (1.9)$$

where k denotes the discrete time step and W_1^n , the approximation at the time level $t = nk$.

For Class *I-II* schemes, we obtain the same estimate conditionally. That is, provided $k \leq C\alpha h$, for a constant C depending on inverse properties of the finite element space. Class *I-I* schemes are unconditionally stable and convergent.

Again the estimates (1.9) are obtained using L^2 projections of the initial data as starting values.

Another development of this paper is the construction of a family of rational functions $\{r_s(z)\}_{s \geq 1}$ of class I , which is done in Section 4. Briefly, for each integer $s \geq 1$, and any given real number $x > 0$, we establish the existence of a sequence of polynomials $\{\beta_n^{(s)}\}_{n=0}^\infty$ with real coefficients, where β_n is of degree at most n , such that

$$(1 - x^2 z^2)^s e^{-z} = \sum_{n=0}^{\infty} \beta_n^{(s)}(x) z^n, \quad (1.10)$$

for all z

For $s = 1, 2, \dots$, we then define the rational function

$$r_s(z) = \sum_{n=0}^{2s} \beta_n^{(s)}(x) z^n / (1 - x^2 z^2)^s,$$

for $|\operatorname{Re}(z)| < \frac{1}{x}$. r_s is analytic in a neighbourhood of the imaginary axis, and has poles at $z = \pm \frac{1}{x}$ on the real line. r_s will satisfy (1.6) with $v = 2s$, and we show that there exists a real number $x^{(s)} > 0$ such that for the choice $x \geq x^{(s)}$, r_s satisfies (1.7).

This family of rational functions provides schemes of arbitrary accuracy in time, i.e. we have (1.9) with $v = 2s$. In analogy with the work of Nørsett [12], and Thomée and the present authors in [5], for parabolic equations, the resulting scheme for r_s requires the solution of $2s$ linear systems with the same real matrix at each time level.

Other examples of Class I rational functions are provided by Padé approximations, in particular, the diagonal and first two lower codiagonal entries. In general, the use of Padé approximations requires the solution of complex linear systems, in contrast

A table of the polynomials $\{\beta_n^{(s)}\}_{n=0}^{2s}$ and a convenient choice of the parameter $x^{(s)}$ is given for $s = 1, \dots, 5$ in the Appendix.

Crouzeix [8] has also analysed high order in time, single step, fully discrete approximations. There, the choice of starting values is motivated by [9].

Throughout the paper, C will denote a general constant, not necessarily the same in any two places.

2. SEMIDISCRETE APPROXIMATIONS

We introduce the solution operator T of the associated elliptic boundary value problem $T: L^2(\Omega) \rightarrow L^2(\Omega)$ is defined by

$$a(Tf, v) = (f, v), \quad \text{for all } v \in \dot{H}^1(\Omega), \quad \text{for given } f \in L^2(\Omega), \quad (2.1)$$

where $a(., .)$ denotes the bilinear form

$$a(\omega, v) = \int_{\Omega} \left\{ \sum_{i,j=1}^N a_{ij} \frac{\partial \omega}{\partial x_i} \frac{\partial v}{\partial x_j} \right\} dx, \quad \text{for } \omega, v \in H^1(\Omega). \quad (2.1. a)$$

T has a discrete spectrum of real positive eigenvalues $\{\mu_j\}_{j \geq 1}$, where $\mu_j = \lambda_j^{-1}$ with λ_j given by (1.3). Now let \mathbb{L}^2 denote the space $L^2(\Omega) \times L^2(\Omega)$ and define the operator $J : \mathbb{L}^2 \rightarrow \mathbb{L}^2$ by

$$J = \begin{pmatrix} 0 & T \\ -I & 0 \end{pmatrix}$$

We now reformulate (1.1) in terms of the operator J as follows. Let

$$U(t) = \begin{pmatrix} u(t) \\ u_t(t) \end{pmatrix}, \quad U^0 = \begin{pmatrix} u^0 \\ u_t^0 \end{pmatrix}.$$

Then, (1.1) is equivalent to

$$\left. \begin{aligned} JU_t + U &= 0, & t > 0 \\ U(0) &= U^0. \end{aligned} \right\} \quad (2.2)$$

Now, let $0 < h < 1$ be a parameter, and $\{T_h\}_{0 < h \leq 1}$ a family of finite dimensional operators approximating the operator T . In particular, let

$$\{S_h^r(\Omega)\}_{0 < h \leq 1} \subset \dot{H}^1(\Omega)$$

be a standard finite element space of piecewise polynomial functions of degree $r - 1$, with the approximation property

$$\inf_{\chi \in S_h^r(\Omega)} \{ \|\omega - \chi\| + h \|\omega - \chi\|_1 \} \leq Ch^s \|\omega\|_{H^s(\Omega)},$$

for all $\omega \in H^1(\Omega) \cap H^s(\Omega)$, for some constant C independent of h , $1 \leq s \leq r$. The operators $T_h : L^2(\Omega) \rightarrow S_h^r(\Omega)$ are defined by

$$a(T_h f, \chi) = (f, \chi), \quad \text{for all } \chi \in S_h^r(\Omega), \quad \text{for given } f \in L^2(\Omega). \quad (2.4)$$

The family $\{T_h\}_{0 < h \leq 1}$ has the following properties:

T_h is symmetric, positive semidefinite on $L^2(\Omega)$, and positive definite on $S_h^r(\Omega)$ (2.5)

$$\|(T - T_h)f\| \leq Ch^s \|f\|_{s-2}, \quad \text{for all } f \in H^{s-2}(\Omega), \quad 1 \leq s \leq r, \quad (2.6)$$

for some constant C independent of h .

T_h has a discrete spectrum of eigenvalues $\{0\} \cup \{\mu_1^h, \mu_2^h, \dots, \mu_M^h\}$, in non-increasing order, for some integer $M = M(h)$. Furthermore, there exists an $h_0 > 0$ such that for $h \leq h_0$, $\mu_1^h \leq A$, for some constant $A > 0$. (2.7)

Proofs of (2.5)-(2.7) may be found in [1] and [6].

The semidiscrete approximation for the solution u of (1.1) is defined as the mapping $u^h[0, t^*] \rightarrow S_h^r(\Omega)$ satisfying

$$\left. \begin{aligned} T_h u_{tt}^h + u^h &= 0, & 0 < t \leq t^*, \\ u^h(0) &= P u^0, \\ u_t^h(0) &= P u_t^0, \end{aligned} \right\} \quad (2.8)$$

where P denotes the $L^2(\Omega)$ projection operator onto $S_h^r(\Omega)$. Using (2.1) it is easily seen that (2.8) is equivalent to the definition of the standard semidiscrete approximation, in variational form, using $L^2(\Omega)$ projections of u^0 and u_t^0 as starting values, as given for example in [3]. For the subsequent analysis, we now reformulate (2.8) as a first order system, in analogy with (2.2). Set

$$V(t) = \begin{pmatrix} u^h(t) \\ u_t^h(t) \end{pmatrix} \quad t \geq 0;$$

then (2.8) is equivalent to

$$\left. \begin{aligned} J_h V_t + V &= 0, & 0 < t \leq t^*, \\ V(0) &= P U^0, \end{aligned} \right\} \quad (2.9)$$

where

$$J_h = \begin{pmatrix} 0 & T_h \\ -I & 0 \end{pmatrix} : \mathbb{L}^2 \rightarrow S_h^r(\Omega) \times L^2(\Omega),$$

and P denotes the \mathbb{L}^2 projection operator onto $S_h^r(\Omega) \times S_h^r(\Omega)$.

We define a form $((\cdot, \cdot))$ on \mathbb{L}^2 by

$$((\Phi, \Psi)) = (\phi_1, \psi_1) + (T_h \phi_2, \psi_2), \quad (2.10)$$

for

$$\Phi = \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} \quad \text{and} \quad \Psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \in \mathbb{L}^2.$$

The associated seminorm which we denote by $||| \cdot |||$ is given by

$$||| \Phi ||| = ((\Phi, \Phi))^{\frac{1}{2}}. \quad (2.11)$$

We note that

$$((J_h \Phi, \Phi)) = 0, \quad \Phi \in \mathbb{L}^2. \quad (2.12)$$

The following theorem gives estimates in $L^2(\Omega)$ for the error $u(t) - u^h(t)$.

THEOREM 2.1 : *Let u be the solution of (1.1) and let u^h be the semidiscrete approximation defined by (2.8), or equivalently (2.9). Suppose that $u^0 \in \dot{H}^{r+1}(\Omega)$ and $u_t^0 \in \dot{H}^r(\Omega)$. Then there exists a constant $C = C_r(t^*)$, such that*

$$\sup_{0 \leq t \leq t^*} \|u(t) - u^h(t)\| \leq C h^r [\|u^0\|_{r+1} + \|u_t^0\|_r]. \quad (2.13)$$

Proof : Set $E = U - V$, where U is defined by (2.2) and V by (2.9). Then

$$J_h E_t + E = (J_h - J)U_t, \quad 0 < t \leq t^*, \quad (2.14)$$

$$E(0) = (I - P)U^0. \quad (2.15)$$

Setting $\rho = (J_h - J)U_t$ (2.14) gives

$$((J_h E_t, E_t)) + ((E, E_t)) = ((\rho, E_t)),$$

and so, by (2.12),

$$\frac{1}{2} \frac{d}{dt} ||| E(t) |||^2 = \frac{d}{dt} ((\rho(t), E(t))) - ((\rho_t(t), E(t))).$$

Integrating this last equation, we get

$$||| E(t) |||^2 = ||| E(0) |||^2 + 2((\rho(t), E(t))) - 2((\rho(0), E(0))) - 2 \int_0^t ((\rho_t(\tau), E(\tau))) d\tau. \quad (2.16)$$

From (2.4), it follows that $T_h P = T_h$ on $L^2(\Omega)$. Hence, from (2.15), and (2.11),

$$||| E(0) ||| = || u^0 - Pu^0 ||, \quad (2.17)$$

and

$$\begin{aligned} ((\rho(0), E(0))) &= ((T_h - T)u_t(0), u^0 - Pu^0) = -(Tu_t(0), u^0 - Pu^0) \\ &= (u^0, u^0 - Pu^0) = || u^0 - Pu^0 ||^2. \end{aligned} \quad (2.18)$$

Using (2.17) and (2.18) in (2.16),

$$\begin{aligned} ||| E(t) |||^2 &= 2((\rho(t), E(t))) - || u^0 - Pu^0 ||^2 - 2 \int_0^t ((\rho_t(\tau), E(\tau))) d\tau \\ &\leq 2((\rho(t), E(t))) - 2 \int_0^t ((\rho_t(\tau), E(\tau))) d\tau \\ &\leq \frac{1}{4} ||| E(t) |||^2 + 4 ||| \rho(t) |||^2 + 4t^* \int_0^{t^*} ||| \rho_t(\tau) |||^2 d\tau + \frac{1}{4} \sup_{0 \leq \tau \leq t^*} ||| E(\tau) |||^2. \end{aligned}$$

Hence

$$\sup_{0 \leq t \leq t^*} ||| E(t) |||^2 \leq C \left\{ \sup_{0 \leq t \leq t^*} ||| \rho(t) |||^2 + \int_0^{t^*} ||| \rho_t(\tau) |||^2 d\tau \right\}. \quad (2.19)$$

Now, from (2.2), (2.6), and (1.4),

$$\begin{aligned} ||| \rho(t) ||| &= || (T_h - T)u_t(t) || = || (T_h - T)\mathcal{L}u(t) || \\ &\leq Ch^r || u(t) ||_r \leq Ch^r [|| u^0 ||_r + || u_t^0 ||_{r-1}]. \end{aligned} \quad (2.20)$$

Similarly (2.2), (2.6) and (1.4) give

$$\begin{aligned} \int_0^t ||| \rho_t(\tau) |||^2 d\tau &= \int_0^{t^*} || (T_h - T)u_{tt}(\tau) ||^2 d\tau = \int_0^{t^*} || (T_h - T)\mathcal{L}u_t(\tau) ||^2 d\tau \\ &\leq Ch^{2r} \sup_{0 \leq t \leq t^*} || u_t(t) ||_r^2 \leq Ch^{2r} [|| u^0 ||_{r+1} + || u_t^0 ||_r]^2. \end{aligned} \quad (2.21)$$

Hence, using (2.20) and (2.21) in (2.19), we obtain

$$\sup_{0 \leq t \leq t^*} ||| E(t) ||| \leq Ch^r [||u^0||_{r+1} + ||u_t^0||_r].$$

The result of the theorem now follows.

REMARK : We point out that from the above theorem, it easily follows that the optimal rate of convergence $O(h^r)$ in $L^2(\Omega)$ is obtained using any choice of starting values of $u^h(0)$ and $u_t^h(0) \in S_h^r(\Omega)$ satisfying

$$||u^0 - u^h(0)|| = O(h^r)$$

and

$$||u_t^0 - u_t^h(0)|| = O(h^r).$$

3. SINGLE STEP FULLY DISCRETE APPROXIMATIONS

In this section, we define and analyse fully discrete schemes obtained from rational approximations to e^{-z} .

Let r be a complex valued rational function defined for the complex variable z , satisfying

$$|r(iy) - e^{-iy}| \leq C |y|^{v+1}, \quad |y| \leq \sigma, \quad (3.1)$$

for constants $0 < C < \infty$, $\sigma > 0$ and $v > 0$.

DÉFINITION 3.1 : r satisfying (3.1) is said to be of Class $i-I$ if

$$|r(iy)| \leq 1, \quad \text{for all real } y. \quad (3.2)$$

r satisfying (3.1) is said to be of Class $i-II$ if, for some constant $\alpha > 0$,

$$|r(iy)| \leq 1, \quad \text{for all real } y, \text{ with } |y| \leq \alpha. \quad (3.3)$$

Clearly, rational functions of Class $i-I$ are also of Class $i-II$. However a distinction is made since Class $i-I$ functions will yield schemes which are unconditionally stable and convergent. The schemes are defined as follows.

The solution of (2.9) is given by

$$V(t) = e^{-kJ_k^{-1}t} P U^0, \quad t \geq 0, \quad (3.4)$$

and hence for $k > 0$, the proposed discrete time step,

$$V(t+k) = e^{-kJ_k^{-1}t} V(t), \quad t \geq 0. \quad (3.5)$$

Now let $r(z) = D^{-1}(z)N(z)$, where D and N are minimal degree polynomials.

The fully discrete approximation to (1.1), derived from (3.5) we denote by $\{W^n\}_{n \geq 0} \subset S_h^r(\Omega) \times S_h^r(\Omega)$, and is defined by

$$\left. \begin{aligned} W^{n+1} &= D^{-1}(kJ_h^{-1})N(kJ_h^{-1})W^n, \quad n = 0, 1, \dots, \\ W^0 &= PU^0. \end{aligned} \right\} \quad (3.6)$$

We derive estimates for $\|u(nk) - W_1^n\|$ by comparing W^n with the semi-discrete approximation $V(nk)$, $n=0, 1, \dots$. To this end, we define the function

$$F_n(z) = r^n(z) - e^{-nz}, \quad n = 0, 1, \dots \quad (3.7)$$

From (3.6), (3.7) and (3.7), it follows that

$$W^n - V(nk) = F_n(kJ_h^{-1})PU^0. \quad (3.8)$$

The following simple result will be needed.

LEMMA 3.1 : *Let r be of Class i-II. Then, there exists a constant $C^* < \infty$ such that*

$$|r^n(iy) - e^{-ny}| \leq nC^* |y|^l, \quad (3.9)$$

for $|y| \leq \alpha$ and $1 \leq l \leq v+1$, $n = 1, 2, \dots$.

Proof Let $\sigma^* = \min(\sigma, 1)$. Then (3.1) holds with σ replaced by σ^* . Hence

$$|r(iy) - e^{-iy}| \leq C |y|^l, \quad |y| \leq \sigma^*, \quad (3.10)$$

for $1 \leq l \leq v+1$.

Now, if $\sigma^* < \alpha$, from (3.3), for $\sigma^* < |y| \leq \alpha$, and any integer $1 \leq l \leq v+1$,

$$|r(iy) - e^{-iy}| \leq 2 = 2 |y|^l \left(\frac{\sigma^*}{|y|} \right)^l \left(\frac{1}{\sigma^*} \right)^l \leq 2 |y|^l (\sigma^*)^{-(v+1)} = C^* |y|^l, \quad (3.11)$$

with $C^* < \infty$. Hence, from (3.10) and (3.11), we have for some $C^* < \infty$,

$$|r(iy) - e^{-iy}| \leq C^* |y|^l, \quad |y| \leq \alpha, \quad (3.12)$$

for $1 \leq l \leq v+1$.

Now for an integer $n \geq 1$,

$$r^n(iy) - e^{-ny} = (r(iy) - e^{-iy}) \sum_{j=0}^{n-1} r^j(iy) e^{-i(n-j-1)y} \quad (3.13)$$

Hence, using (3.12) and (3.3) in (3.13), we get for $|y| \leq \alpha$,

$$|r^n(iy) - e^{-ny}| \leq |r(iy) - e^{-iy}| \sum_{j=0}^{n-1} |r^j(iy)|^j \leq nC^* |y|^l, \quad 1 \leq l \leq v+1.$$

It is clear that, by choosing $\alpha = \infty$, (3.9) holds for Class i-I.

Let μ_1^h, \dots, μ_M^h , be the set of nonzero eigenvalues of T_h with corresponding eigenfunctions $\psi_1^h, \dots, \psi_M^h$, chosen orthonormal in $L^2(\Omega)$, i. e.

$$T_h \psi_j^h = \mu_j^h \psi_j^h,$$

and

$$(\psi_i^h, \psi_j^h) = \delta_{ij}, \quad i, j = 1, 2, \dots, M.$$

Now let S_h denote the space $S_h^r(\Omega) \times S_h^r(\Omega)$, furnished with the inner product $((\cdot, \cdot))$ and norm $||| \cdot |||$.

It is easily shown that the operator $J_h: S_h \rightarrow S_h$ possesses a corresponding set of purely imaginary eigenvalues $\{\eta_j\}_{j=-M}^M$, given by

$$\begin{aligned} \eta_j &= i(\mu_j^h)^{\frac{1}{2}} \\ \eta_{-j} &= -i(\mu_j^h)^{\frac{1}{2}}, \quad j = 1, 2, \dots, M, \end{aligned}$$

and corresponding eigenvectors $\{\Phi_j\}_{j=-M}^M$, given by

$$\begin{aligned} \Phi_j &= \frac{1}{\sqrt{2}} \begin{pmatrix} \psi_j^h \\ i(\mu_j^h)^{-\frac{1}{2}} \psi_j^h \end{pmatrix} \\ \Phi_{-j} &= \frac{1}{\sqrt{2}} \begin{pmatrix} \psi_j^h \\ -i(\mu_j^h)^{-\frac{1}{2}} \psi_j^h \end{pmatrix}, \quad j = 1, 2, \dots, M. \end{aligned}$$

Since we shall subsequently work with complex valued functions, the previously defined inner product $((\cdot, \cdot))$ of (2.10) is naturally extended to

$$((\Phi, \Psi)) = (\phi_1, \bar{\psi}_1) + (T_h \phi_2, \bar{\psi}_2), \quad \text{on } S_h,$$

where in general $\bar{\phi}$ denotes the complex conjugate of ϕ . Since $\{\Psi_j^h\}_{j=1}^M$ is an orthonormal basis for $S_h^r(\Omega)$, it is easily seen that $\{\Phi_j\}_{j=-M}^M$ forms a complete orthonormal set in S_h , with respect to the above inner product $((\cdot, \cdot))$.

Hence, for any $Z \in \mathbb{L}^2$, we have

$$PZ = \sum_{j=-M}^M ((Z, \Phi_j)) \Phi_j, \quad (3.14)$$

and

$$||| PZ ||| = \left(\sum_{j=-M}^M |((Z, \Phi_j))|^2 \right)^{\frac{1}{2}} \leq ||| Z |||. \quad (3.15)$$

LEMMA 3.2: *Let r be a rational function of Class i-I. Then, there exists a constant C , such that for $Z \in \mathbb{L}^2$, and $nk = t \leq t^*$*

$$||| F_n(kJ_h^{-1})J_h^t Z ||| \leq Ck^{l-1} ||| Z |||, \quad (3.16)$$

$1 \leq l \leq v + 1$.

Proof: From (3.14), it follows that

$$F_n(kJ_h^{-1})J_h^t Z = \sum_{j=-M}^M F_n(k\eta_j^{-1})\eta_j^t ((Z, \Phi_j)) \Phi_j,$$

and so from (3.9) and (3.15), for $1 \leq l \leq v+1$,

$$\begin{aligned} ||| F_n(kJ_h^{-1})J_h^l Z ||| &= \left(\sum_{j=-M}^M |F_n(k\eta_j^{-1})|^2 |\eta_j|^{2l} |((Z, \Phi_j))^2| \right)^{\frac{1}{2}} \\ &\leq \left(\sum_{j=-M}^M n^2 C^{*2} k^{2l} |\eta_j|^{-2l} |\eta_j|^{2l} |((Z, \Phi_j))^2| \right)^{\frac{1}{2}} \\ &= n C^* k^l \left(\sum_{j=-M}^M |((Z, \Phi_j))^2| \right)^{\frac{1}{2}} \leq t^* C^* k^{l-1} ||| Z |||, \end{aligned} \quad (3.17)$$

which gives (3.16).

LEMMA 3.3: Let r be a rational function of Class i-II. Suppose that the operator T_h is such that

$$\mu_M^h \geq C_1 h^2, \quad (3.18)$$

for some constant $C_1 > 0$, independent of h . Then, for k chosen such that

$$k \leq \alpha C_1^{\frac{1}{2}} h, \quad (3.19)$$

there exists a constant C such that, for $Z \in \mathbb{L}^2$,

$$||| F_n(kJ_h^{-1})J_h^l Z ||| \leq C k^{l-1} ||| Z ||| \quad (3.20)$$

for $1 \leq l \leq v+1$.

Proof: From (3.18),

$$\max_{-M \leq j \leq M} |\eta_j|^{-1} = (\mu_M^h)^{-\frac{1}{2}} \leq C_1^{-\frac{1}{2}} h^{-1}.$$

Hence, with (3.19) satisfied, we have

$$k |\eta_j|^{-1} \leq \alpha.$$

With the above inequality and (3.9),

$$|F_n(k\eta_j^{-1})| \leq C^* n k^l |\eta_j|^{-l}, \quad (3.21)$$

for $1 \leq l \leq v+1$. Now using (3.21), the result follows by the same argument as (3.17).

We remark that a sufficient condition for the assumption (3.18) to hold is that the spaces $S_h^r(\Omega)$ possess an inverse property

$$|| \chi ||_1 \leq C h^{-1} || \chi ||, \quad \text{for all } \chi \in S_h^r(\Omega), \quad (3.22)$$

for some constant C independent of h .

We note also the following stability result for the schemes defined by (3.6).

If r is of Class i-I, then for $Z \in \mathbb{L}^2$,

$$||| F_n(kJ_h^{-1})Z ||| \leq C ||| Z |||, \quad n = 0, 1, \dots, \quad (3.23)$$

and

$$||| W^n ||| \leq ||| U^0 |||. \quad (3.23 a)$$

If r is of Class $i-II$ with (3.22) and (3.19) satisfied, then (3.23 a) holds.

Before proceeding to the derivation of the error estimates, we define the following auxiliary functions.

Let Q be the smallest integer such that

$$k\lambda_j^{\frac{1}{2}} > 1, \quad \text{for } j \geq Q.$$

For given $v \in L^2(\Omega)$, we define

$$V^{(k)} = \sum_{j=1}^{Q-1} (v, \varphi_j) \varphi_j.$$

Then $V^{(k)} \in C^\infty(\Omega)$ and satisfies

$$\|V^{(k)}\|_s \leq \|V\|_s, \quad (3.24)$$

and

$$\|V - V^{(k)}\|_{-p} \leq k^{s+p} \|V\|_s, \quad \text{for all } s \geq 0, p \geq 0. \quad (3.25)$$

Also, for any $m \geq 0$,

$$\|V^{(k)}\|_{r+m} \leq k^{-m} \|V\|_r. \quad (3.26)$$

Define

$$U^{0(k)} = \begin{pmatrix} u^{0(k)} \\ u_t^{0(k)} \end{pmatrix}. \quad (3.27)$$

THEOREM 3.1: Let u be the solution of (1.1), and let r be of Class $i-I$. Let $\{W^n\}_{n \geq 0}$ be the sequence of approximations defined by (3.6). Then there exists a constant $C = C(r, v, t^*)$ such that

$$\sup_{0 \leq n \leq [t^*/k]} \|W_1^n - u(nk)\| \leq C \{ h^r [\|u^0\|_{r+1} + \|u_t^0\|_r] + k^v [\|u^0\|_{v+1} + \|u_t^0\|_v] \}. \quad (3.28)$$

Proof: Define the operator $\Lambda = H^2(\Omega) \times L^2(\Omega) \rightarrow \mathbb{L}^2$ by

$$\Lambda = \begin{pmatrix} 0 & \perp I \\ \mathcal{L} & 0 \end{pmatrix}$$

It is easily shown that in \dot{H}^v

$$F_n(kJ_h^{-1}) = \sum_{l=0}^v F_n(kJ_h^{-1}) J_h^l (J - J_h) \Lambda^{l+1} + F_n(kJ_h^{-1}) J_h^{v+1} \Lambda^{v+1}. \quad (3.29)$$

From (3.8) and (3.29),

$$\begin{aligned} V(nk) - W^n &= F_n(kJ_h^{-1})(U^0 - U^{0(k)}) + \sum_{l=0}^v F_n(kJ_h^{-1}) J_h^l (J - J_h) \Lambda^{l+1} U^{0(k)} \\ &\quad + F_n(kJ_h^{-1}) J_h^{v+1} \Lambda^{v+1} U^{0(k)}. \end{aligned} \quad (3.30)$$

Thus, from (3.30),

$$\begin{aligned} ||| V(nk) - W^n ||| &\leq ||| F_n(kJ_h^{-1})(U^0 - U^{0(k)}) ||| + ||| F_n(kJ_h^{-1})(J - J_h)\Lambda U^{0(k)} ||| \\ &+ \sum_{i=0}^v ||| F_n(kJ_h^{-1})J_h^i(J - J_h)\Lambda^{i+1}U^{0(k)} ||| + ||| F_n(kJ_h^{-1})J_h^{v+1}\Lambda^{v+1}U^{0(k)} |||. \end{aligned} \quad (3.31)$$

Now, from (3.23), (3.24), (3.25) and (3.6),

$$\begin{aligned} ||| F_n(kJ_h^{-1})(U^0 - U^{0(k)}) |||^2 &\leq ||| U^0 - U^{0(k)} |||^2 \\ &= C \{ || u^0 - u^{0(k)} ||^2 + (T_h[u_t^0 - u_t^{0(k)}], u_t^0 - u_t^{0(k)}) \} \\ &= C \{ || u^0 - u^{0(k)} ||^2 + ((T_h - T)[u_t^0 - u_t^{0(k)}], u_t^0 - u_t^{0(k)}) \\ &\quad + (T[u_t^0 - u_t^{0(k)}], u_t^0 - u_t^{0(k)}) \} \\ &\leq C \{ || u^0 - u^{0(k)} ||^2 + || (T_h - T)[u_t^0 - u_t^{0(k)}] || || u_t^0 - u_t^{0(k)} || \\ &\quad + || T[u_t^0 - u_t^{0(k)}] ||_1 || u_t^0 - u_t^{0(k)} ||_{-1} \} \\ &\leq C \{ k^{2v} || u^0 ||_v^2 + h^r || u_t^0 ||_{r-2} k^v || u_t^0 ||_v + k^{2v} || u_t^0 ||_{v-1}^2 \} \\ &\leq C \{ k^v [|| u^0 ||_v + || u_t^0 ||_v] + h^r || u_t^0 ||_{r-2} \}^2 \end{aligned} \quad (3.32)$$

Also, from (3.23) and (2.6),

$$||| F_n(kJ_h^{-1})(J - J_h)\Lambda U^{0(k)} ||| \leq C || (T - T_h)\mathcal{L}u^{0(k)} || \leq Ch^r || u^0 ||_r. \quad (3.33)$$

Now, from (3.16) of Lemma 3.2,

$$\sum_{l=1}^v ||| F_n(kJ_h^{-1})J_h^l(J - J_h)\Lambda^{l+1}U^{0(k)} ||| \leq C \sum_{l=1}^v k^{l-1} ||| (J - J_h)\Lambda^{l+1}U^{0(k)} |||. \quad (3.34)$$

For $l+1$ even, we have

$$\Lambda^{l+1} = (-1)^{\frac{l+1}{2}} \begin{pmatrix} \mathcal{L}^{\frac{l+1}{2}} & 0 \\ 0 & \mathcal{L}^{\frac{l+1}{2}} \end{pmatrix}, \quad (3.35)$$

and for $l+1$ odd,

$$\Lambda^{l+1} = (-1)^{\frac{l}{2}} \begin{pmatrix} 0 & -\mathcal{L}^{\frac{l}{2}} \\ \mathcal{L}^{\frac{l}{2}+1} & 0 \end{pmatrix}. \quad (3.36)$$

Thus a simple computation using (3.35) and (3.36) yields

$$||| (J - J_h)\Lambda^{l+1}U^{0(k)} ||| = \begin{cases} || (T - T_h)\mathcal{L}^{\frac{l+1}{2}} u_t^{0(k)} ||, & l+1 \text{ even}, \\ || (T - T_h)\mathcal{L}^{\frac{l}{2}+1} u_t^{0(k)} ||, & l+1 \text{ odd}. \end{cases} \quad (3.37)$$

Hence, from (3.37), (2.6) and (3.26), for $l+1$ even,

$$||| (J - J_h)\Lambda^{l+1}U^{0(k)} ||| \leq Ch^r || u_t^{0(k)} ||_{r-1+l} \leq Ch^r k^{-(l-1)} || u_t^0 ||_r, \quad (3.38)$$

and for $l + 1$ odd,

$$||| (J - J_h) \Lambda^{l+1} U^{0(k)} ||| \leq Ch^r \|u^{0(k)}\|_{r+l} \leq Ch^r k^{-(l-1)} \|u^0\|_{r+1}. \quad (3.39)$$

Also, from (3.16), (3.35), (3.24), (3.26) and (2.6), for $v + 1$ even

$$\begin{aligned} & ||| F_n(kJ_h^{-1})J_h^{v+1}\Lambda^{v+1}U^{0(k)} |||^2 \\ & \leq Ck^{2v} ||| \Lambda^{v+1}U^{0(k)} |||^2 = Ck^{2v} \{ \|\mathcal{L}^{\frac{v+1}{2}} u^{0(k)}\|^2 + (T_h \mathcal{L}^{\frac{v+1}{2}} u_t^{0(k)}, \mathcal{L}^{\frac{v+1}{2}} u_t^{0(k)}) \} \\ & \leq Ck^{2v} \{ \|u^0\|_{v+1}^2 + ([T_h - T] \mathcal{L}^{\frac{v+1}{2}} u_t^{0(k)}, \mathcal{L}^{\frac{v+1}{2}} u_t^{0(k)}) + (T \mathcal{L}^{\frac{v+1}{2}} u_t^{0(k)}, \mathcal{L}^{\frac{v+1}{2}} u_t^{0(k)}) \} \\ & \leq Ck^{2v} \{ \|u^0\|_{v+1}^2 + h^r \|u_t^{0(k)}\|_{v+r-1} \|u_t^{0(k)}\|_{v+1} + \|u_t^0\|_v^2 \} \\ & \leq Ck^{2v} \{ \|u^0\|_{v+1}^2 + h^r k^{-v} \|u_t^0\|_r \|u_t^0\|_v + \|u_t^0\|_v^2 \} \\ & \leq C \{ k^{2v} [\|u^0\|_{v+1}^2 + \|u_t^0\|_v^2] + h^{2r} \|u_t^0\|_r^2 \}. \end{aligned} \quad (3.40)$$

Similarly, from (3.16), (3.36), (3.24), (3.26) and (2.6), for $v + 1$ odd,

$$\begin{aligned} & ||| F_n(kJ_h^{-1})J_h^{v+1}\Lambda^{v+1}U^{0(k)} ||| \\ & \leq Ck^{2v} ||| \Lambda^{v+1}U^{0(k)} ||| = Ck^{2v} \|\mathcal{L}^2 u_t^{0(k)}\|^2 + (T_h \mathcal{L}^{\frac{v}{2}+1} u^{0(k)}, \mathcal{L}^{\frac{v}{2}+1} u^{0(k)}) \\ & \leq Ck^{2v} \{ \|u_t^0\|^2 + ([T_h - T] \mathcal{L}^{\frac{v}{2}+1} u^{0(k)}, \mathcal{L}^{\frac{v}{2}+1} u^{0(k)}) + (T \mathcal{L}^{\frac{v}{2}+1} u^{0(k)}, \mathcal{L}^{\frac{v}{2}+1} u^{0(k)}) \} \\ & \leq Ck^{2v} \{ \|u_t^0\|_v^2 + h^r \|u^{0(k)}\|_{r+v} \|u^{0(k)}\|_{v+2} + \|u^0\|_{v+1}^2 \} \\ & \leq Ck^{2v} \{ \|u_t^0\|_v^2 + h^r k^{-v} \|u^0\|_{r+1} \|u^0\|_{v+1} + \|u^0\|_{v+1}^2 \} \\ & \leq C \{ k^{2v} [\|u^0\|_{v+1}^2 + \|u_t^0\|_v^2] + h^{2r} \|u^0\|_{r+1}^2 \}. \end{aligned} \quad (3.41)$$

Combining the inequalities (3.38), (3.39) in (3.34), we obtain

$$\sum_{l=1}^v ||| F_n(kJ_h^{-1})J_h^l(J - J_h)\Lambda^{l+1}U^{0(k)} ||| \leq Ch^r [\|u^0\|_{r+1} + \|u_t^0\|_r]. \quad (3.42)$$

Now combining (3.32), (3.33), (3.42), (3.40) and (3.41), in (3.31), we obtain

$$||| V(nk) - W^n ||| \leq C \{ h^r [\|u^0\|_{r+1} + \|u_t^0\|_r] + k^v [\|u^0\|_{v+1} + \|u_t^0\|_v] \}. \quad (3.43)$$

The result of the theorem now follows from (3.43) and (2.13) of Theorem 2.1.

We have thus established the unconditional convergence with optimal accuracy for schemes defined by Class *i-I* rational functions. For Class *i-II* functions, the same estimate (3.28) holds however, conditionally.

THEOREM 3.2: *Let u be the solution of (1.1), and let r be of Class *i-II*. Let $\{W^n\}_{n \geq 0}$ be the sequence of approximations defined by (3.6). Suppose that the spaces $S_h^r(\Omega)$ satisfy an inverse property (3.22) and that k and h are related by (3.19). Then, the error estimate (3.28) holds.*

Proof : The result is obtained via the same argument used in Theorem 3.1, with the exception that the results of Lemma 3.3 are used instead of those of Lemma 3.2. The proof is thus omitted.

REMARK : We point out that with the results of the above theorems, the optimal rate of convergence $O(h^r + k^v)$ is obtained with any starting values $W_1^0, W_2^0 \in S_h^r(\Omega)$ satisfying

$$\|W_1^0 - u^0\| = O(h^r),$$

and

$$\|W_2^0 - u_t^0\| = O(h^r).$$

4. RATIONAL APPROXIMATIONS OF $e^{t\tau}$

In this section, we give examples of rational functions yielding the results of Section 3. Particularly, we construct below a family of Class i -I.

4.1. A family of Class i -I

Let s be a positive integer, and $y > 0$ a real parameter, and consider the complex valued function $g(\tau) = e^{y\tau}(1 - \tau^2)^s$, defined for complex τ . g is analytic, and so there exist functions $\alpha_n^{(s)}(y)$, $n = 0, 1, \dots$, such that

$$e^{y\tau}(1 - \tau^2)^s = \sum_{n=0}^{\infty} \alpha_n^{(s)}(y) \tau^n, \quad \text{for all } \tau. \quad (4.1)$$

It follows easily that the functions $\alpha_n^{(s)}$ must satisfy

$$\alpha_0^{(s)}(y) = 1 \quad (4.2)$$

$$\alpha_n^{(s)'}(y) = \alpha_{n-1}^{(s)}(y), \quad n = 1, 2, \dots, \quad (4.3)$$

where

$$\begin{aligned} \alpha_n^{(s)'}(y) &= \frac{d}{dy} \alpha_n^{(s)}(y), \\ \alpha_{2n}^{(s)}(0) &= \begin{cases} (-1)^n \binom{s}{n}, & n = 0, 1, \dots, s, \\ 0, & n > s, \end{cases} \\ \alpha_{2n+1}^{(s)}(0) &= 0, \quad n = 0, 1, \dots \end{aligned} \quad (4.4)$$

It is clear from (4.2)-(4.5) that $\alpha_n^{(s)}$ is a polynomial of degree n , in the real variable y . The set $\{\alpha_n^{(s)}\}_{n \geq 0}$ also has the following properties.

LEMMA 4.1 : Let $s \geq 1$ be an integer. Then, there exists a real number $y^{(s)} > 0$ such that for $0 < y \leq y^{(s)}$

$$(-1)^n \alpha_{2n}^{(s)}(y) \geq 0, \quad n = 0, 1, \dots, s, \quad (4.6)$$

$$(-1)^n \alpha_{2n}^{(s)'}(y) \leq 0, \quad n = 1, 2, \dots, s, \quad (4.7)$$

and

$$(-1)^s \alpha_{2s}^{(s)}(y) < 1. \quad (4.8)$$

Proof : From (4.4) and (4.3),

$$(-1)^n \alpha_{2n}^{(s)}(y) = (-1)^n \alpha_{2n}^{(s)}(0) + (-1)^n \int_0^y \alpha_{2n}^{(s)'}(\mu) d\mu = \binom{s}{n} + (-1)^n \int_0^y \alpha_{2n}^{(s)'}(\mu) d\mu \quad (4.9)$$

Hence choosing $y_n^{(s)} > 0$ such that

$$\left| \int_0^{y_n^{(s)}} \alpha_{2n}^{(s)'}(\mu) d\mu \right| < \frac{1}{2} \binom{s}{n},$$

and

$$y^{(s)} = \min_{1 \leq n \leq s} y_n^{(s)},$$

the result (4.6) follows.

Also, from (4.3), (4.4) and (4.6), for $0 < y \leq y^{(s)}$,

$$\begin{aligned} (-1)^n \alpha_{2n}^{(s)'}(y) &= (-1)^n \alpha_{2n}^{(s)'}(0) + (-1)^n \int_0^y \alpha_{2n}^{(s)''}(\mu) d\mu \\ &= - \int_0^y (-1)^{n-1} \alpha_{2(n-1)}^{(s)}(\mu) d\mu \leq 0, \end{aligned}$$

which gives (4.7).

For $n = s$ in (4.9), for $0 \leq y \leq y^{(s)}$,

$$(-1)^n \alpha_{2s}^{(s)}(y) = 1 + (-1)^s \int_0^y \alpha_{2s}^{(s)'}(\mu) d\mu < 1,$$

by virtue of (4.7), which gives (4.8).

LEMMA 4.2: Let $R_s(y, \tau)$ be the complex valued function

$$R_s(y, \tau) = \sum_{n=0}^{2s} \alpha_n^{(s)}(y) \tau^n / (1 - \tau^2)^s, \quad (4.10)$$

defined for $|\operatorname{Re} \tau| < 1$. And let $y^{(s)}$ be chosen as in Lemma 4.1. Then

$$|R_s(y, i\xi)| \leq 1, \quad (4.11)$$

for $0 < y \leq y^{(s)}$, for all real ξ .

Proof : Define the functions

$$f(y, \tau) = \sum_{n=0}^{2s} \alpha_n^{(s)}(y) \tau^n, \quad (4.12)$$

and

$$F(y, \xi) = f(y, i\xi) f(y, -i\xi). \quad (4.13)$$

Then, from (4.10), we have

$$|R(y, i\xi)|^2 = F(y, \xi) / (i + \xi^2)^{2s}. \quad (4.14)$$

From (4.1) and (4.12),

$$f(0, \tau) = (1 - \tau^2)^s,$$

and so, with (4.14),

$$|R(0, i\xi)|^2 = 1. \quad (4.15)$$

We now show that $\frac{\partial F}{\partial y}(y, \xi) \leq 0$ for $0 < y \leq y^{(s)}$.

From (4.12) and (4.2) and (4.3),

$$\frac{\partial f}{\partial y}(y, \tau) = \sum_{n=1}^{2s} \alpha_{n-1}^{(s)}(y) \tau^n = \tau \sum_{n=0}^{2s} \alpha_n^{(s)}(y) \tau^n - \alpha_{2s}^{(s)}(y) \tau^{2s+1} = \tau f(y, \tau) - \alpha_{2s}^{(s)}(y) \tau^{2s+1}. \quad (4.16)$$

Now, from (4.13), (4.16),

$$\begin{aligned} \frac{\partial F}{\partial y}(y, \xi) &= 2Re \left\{ \frac{\partial f}{\partial y}(y, i\xi) f(y, -i\xi) \right\} \\ &= 2Re \{ [(i\xi) f(y, i\xi) - (i\xi)^{2s+1} \alpha_{2s}^{(s)}(y)] f(y, -i\xi) \} \\ &= -2Re \{ (i\xi)^{2s+1} \alpha_{2s}^{(s)}(y) f(y, -i\xi) \} = -2\alpha_{2s}^{(s)}(y) Re \{ (i\xi)^{2s+1} \sum_{n=0}^{2s} \alpha_{2n}^{(s)}(y) (-i\xi)^n \} \\ &= 2\alpha_{2s}^{(s)}(y) \sum_{n=0}^{s-1} \alpha_{2n+1}^{(s)}(y) (-1)^{n+s+1} \xi^{2(n+s+1)} = 2\alpha_{2s}^{(s)}(y) \sum_{m=s+1}^{2s} \alpha_{2(m-s)-1}^{(s)}(y) (-1)^m \xi^{2m} \\ &= 2(-1)^s \alpha_{2s}^{(s)}(y) \sum_{m=s+1}^{2s} (-1)^{m-s} \alpha_{2(m-s)}^{(s)'}(y) \xi^{2m} \leq 0, \end{aligned} \quad (4.17)$$

for $0 < y \leq y^{(s)}$, by virtue of (4.6) and (4.7). (4.11) now follows from (4.14), (4.15) and (4.17).

We now define the polynomials

$$\beta_n^{(s)}(x) = (-1)^n x^n \alpha_n^{(s)}\left(\frac{1}{x}\right), \quad n = 0, 1, \dots, \quad (4.18)$$

for real $x > 0$.

Making the change of variables $x = \frac{1}{y}$, $z = -\tau y$ in (4.1), we obtain

$$e^{-z}(1 - x^2 z^2)^s = \sum_{n=0}^{\infty} \beta_n^{(s)}(x) z^n, \quad (4.19)$$

valid for all $x > 0$ and for all z , $s = 1, 2, \dots$.

We now define the family of rational functions $\{r_s\}_{s \geq 1}$ by

$$r_s(z) = \sum_{n=0}^{2s} \beta_n^{(s)}(x) z^n / (1 - x^2 z^2)^s, \quad (4.20)$$

for $|Rez| < 1/x$.

From (4.19) it follows that there exists a constant $C_s(x)$ such that

$$|e^{-i\xi} - r_s(i\xi)| \leq C_s(x) |\xi|^{2s+1}, \quad (4.21)$$

for all real ξ , with $|\xi| \leq 1$.

Also, from the definition (4.20) and Lemma 4.2, it follows that for given $s \geq 1$, there exists an $x^{(s)} > 0$ such that

$$|r_s(i\xi)| \leq 1, \quad (4.22)$$

for all real ξ , for the choice $x \geq x^{(s)}$.

The above results we summarize in the following theorem.

THEOREM 4.1: *For each integer $s \geq 1$, there exists a set of polynomials $\{\beta_n^{(s)}\}_{n \geq 1}$ with real coefficients, with $\beta_n^{(s)}$ having degree at most n , $n = 0, 1, \dots$, such that*

$$e^{-z}(1 - x^2 z^2)^s = \sum_{n=0}^{\infty} \beta_n^{(s)}(x) z^n,$$

for all real x , and for all z .

If for $x > 0$, r_s denotes the rational function

$$r_s(z) = \sum_{n=0}^{2s} \beta_n^{(s)}(x) z^n / (1 - x^2 z^2)^s, \quad (4.20)$$

defined for $|\operatorname{Re} z| < 1/x$, then there exists constants $x^{(s)} > 0$ and $C_s(x)$ such that for $x^{(s)} < x < \infty$,

$$|r_s(i\xi) - e^{-i\xi}| \leq C_s(x) |\xi|^{2s+1}, \quad \text{for } |\xi| \leq 1, \quad (4.21)$$

and

$$|r_s(i\xi)| \leq 1, \quad \text{for all real } \xi.$$

A table of the polynomials $\beta_n^{(s)}$, $n = 0, 1, \dots, 2s$, for $s = 1, \dots, 5$ along with convenient choices of the parameter $x^{(s)}$ is given in the Appendix.

By virtue of the results (4.21), (4.22) and Theorem 3.1, the fully discrete schemes defined by (3.1) using the rational functions r_s of (4.20) yield the stability (3.23 a) and the rate of convergence estimates (3.28), with $v = 2s$.

We now examine the computational steps involved in using the rational functions r_s . In this case (3.6) is equivalent to

$$\begin{aligned} & (-1)^s \begin{pmatrix} T_h + x^2 k^2 I & 0 \\ 0 & T_h + x^2 k^2 I \end{pmatrix}^s \begin{pmatrix} W_1^{n+1} \\ W_2^{n+1} \end{pmatrix} \\ &= \begin{pmatrix} \sum_{j=0}^s (-1)^{s-j} k^{2j} T_h^{s-j} [\tilde{\beta}_{2j}^{(s)}(x) W_1^n - k \tilde{\beta}_{2j+1}^{(s)}(x) W_2^n] \\ \sum_{j=0}^s (-1)^{s-j} k^{2j-1} T_h^{s-j} [k \tilde{\beta}_{2j}^{(s)}(x) W_2^n - \tilde{\beta}_{2j-1}^{(s)}(x) W_1^n] \end{pmatrix} \end{aligned}$$

with $\tilde{\beta}_{-1}^{(s)} = 0$, $\tilde{\beta}_{2s+1}^{(s)} = 0$, and $\tilde{\beta}_n^{(s)} = \beta_n^{(s)}$, $n = 0, 1, \dots, s$.

The above equations thus uncouple, into

$$(T_h + x^2 k^2 I)^s W_1^{n+1} = \sum_{j=0}^s (-1)^j k^{2j} T_h^{s-j} [\tilde{\beta}_{2j}^{(s)}(x) W_1^n - k \beta_{2j+1}^{(s)}(x) W_2^n], \quad (4.23)$$

$$(T_h + x^2 k^2 I)^s W_2^{n+1} = \sum_{j=0}^s (-1)^j k^{2j-1} T_h^{s-j} [k \tilde{\beta}_{2j}^{(s)}(x) W_2^n - \tilde{\beta}_{2j-1}^{(s)}(x) W_1^n], \quad (4.24)$$

It is now easily seen that each of the above equations is equivalent to s systems of linear algebraic equations. As an example, we outline the computational steps for the case $s = 2$. From (4.23) and (4.24), for $s = 2$, we have

$$(T_h + k^2 x^2 I)^2 W_1^{n+1} = T_h^2 [\beta_0^{(2)}(x) W_1^n - k \beta_1^{(2)}(x) W_2^n] - k T_h [k \beta_2^{(2)}(x) W_1^n - k^2 \rho_3^{(2)}(x) W_2^n] + \beta_4^{(2)}(x) k^4 W_1^n, \quad (4.25)$$

$$(T_h + k^2 x^2 I)^2 W_2^{n+1} = T_h^2 \beta_0^{(2)}(x) W_2^n + k T_h [\beta_1^{(2)}(x) W_1^n - k \beta_2^{(2)}(x) W_2^n] + k^4 \beta_4^{(2)}(x) W_2^n - k^3 \beta_3^{(2)}(x) W_1^n. \quad (4.26)$$

Set $A_h = T_h + x^2 k^2 I$, and $Z = W_1^{n+1} - \frac{\beta_4^{(2)}(x)}{x^4} W_1^n$. Then (4.25) becomes

$$A_h^2 Z = T_h^2 \left[\left(\beta_0^{(2)}(x) - \frac{\beta_4^{(2)}(x)}{x^4} \right) W_1^n - k \beta_1^{(2)}(x) W_2^n \right] + k T_h \left[k^2 \beta_3^{(2)}(x) W_2^n - \left(\beta_2^{(2)}(x) + 2k \frac{\beta_4^{(2)}(x)}{x^2} \right) W_1^n \right],$$

or

$$A_h T_h^{-1} A_h Z = T_h \left[\left(\beta_0^{(2)}(x) - \frac{\beta_4^{(2)}(x)}{x^4} \right) W_1^n - k \beta_1^{(2)}(x) W_2^n \right] + k \left[k^2 \beta_3^{(2)}(x) W_2^n - \left(\beta_2^{(2)}(x) + 2k \frac{\beta_4^{(2)}(x)}{x^2} \right) W_1^n \right].$$

Now set $Y = T_h^{-1} A_h Z$. Then Y is obtained as the solution of

$$(Y, \chi) + x^2 k^2 a(Y, \chi) = \left[\beta_0^{(2)}(x) - \frac{\beta_4^{(2)}(x)}{x^4} \right] (W_1^n, \chi) - k \beta_1^{(2)}(x) (W_2^n, \chi) + k^3 \beta_3^{(2)}(x) a(W_2^n, \chi) - \left[\beta_2^{(2)}(x) + 2k \frac{\beta_4^{(2)}(x)}{x^2} \right] a(W_1^n, \chi),$$

for all $\chi \in S_h^*(\Omega)$. Z in turn is obtained as the solution of

$$(Z, \chi) + x^2 k^2 a(Z, \chi) = (Y, \chi), \quad \chi \in S_h^*(\Omega).$$

Finally

$$W_1^{n+1} = Z + \frac{\beta_4^{(2)}(x)}{x^4} W_1^n.$$

W_2^{n+1} may be solved for similarly, the whole procedure thus requiring 4 linear systems to be solved at each time level.

For the above scheme ($s = 2$), we thus have the error bounds (3.28) with $v = 4$.

4.2. Other Class i -I schemes

In [5] and [12] the following rational approximations are discussed. For any real $b > 0$, it is shown that

$$e^{-z} = 1 - \sum_{n=0}^{\infty} P_n(b) \left(\frac{z}{1+bz} \right)^{n+1}, \quad (4.27)$$

for $\operatorname{Re} z > -1/2b$. Here $P_n(b)$ is a polynomial of degree n , given by

$$P_n(b) = \frac{b^n L_n^{(1)}(1/b)}{(n+1)}, \quad n = 0, 1, \dots,$$

where $L_n^{(1)}$ denotes the Laguerre polynomials of order 1, of degree n . Using (4.27) the rational functions R_v are defined by

$$R_v(z) = 1 - \sum_{n=0}^{v-2} P_n(b) \left(\frac{z}{1+bz} \right)^{n+1},$$

$\operatorname{Re}(z) > -1/2b$, $v \geq 2$, where $b > 0$ will be a parameter chosen to give R_v certain desired properties. In particular, Nørsett [12] shows that for $v = 2, 3$, $b = b_{v-1}$, where b_{v-1} denotes the smallest zero of $L_{v-1}^{(1)}$, R_v satisfies (3.1) and (3.2). For $v = 4$, with the choice of b as the next to smallest root of $L_{v-1}^{(1)} = L_3^{(1)}$, R_v satisfies (3.1) and (3.2). See [12] for details.

Padé approximations.

The general entry of the Padé table is given by

$$r_{p,q}(z) = N_{p,q}(z)/D_{p,q}(z), \quad \text{where,} \quad p \geq 0, \quad q \geq 0,$$

and

$$N_{p,q}(z) = \sum_{j=0}^q \frac{(p+q-j)! q!}{(p+q)! j! (q-j)!} (-1)^j z^j,$$

and

$$D_{p,q}(z) = \sum_{j=0}^p \frac{(p+q-j)! p!}{(p+q)! j! (p-j)!} z^j.$$

It is known that $r_{p,q}$ satisfies (3.1) with $v = p + q$. (3.2) is satisfied by $r_{p,q}$ for $p \geq 1$ and $p-2 \leq q \leq p$. In fact $|r_{p,q}(iy)| = 1$ for all real y . A partial table is contained in [13].

Using the rational functions $r_{p,q}(z)$ in (3.6), we thus have estimates (3.28) with $v = p + q$, $p = 1, 2, \dots$, $p-2 \leq q \leq p$. The estimate (3.28) for

$p = q = 1$ was prior to this work derived by the first author [3]. Crouzeix [8] also derives error estimates for schemes defined by Padé approximations, using different techniques for starting values.

5. NONSTANDARD METHODS

In this section, we point out that certain nonstandard Galerkin methods proposed for approximating solutions of the associated Dirichlet problem, provide discrete solution operators T_h which satisfy the conditions (2.5)-(2.7). These methods thus fit into the framework of this study. In particular, the three methods reviewed below have been proposed with the aim of relaxing the restriction of having the subspaces $S_h^r(\Omega)$ satisfy the boundary conditions.

5.1. Nitsche's method [10]

Spaces $S_h^r(\Omega) \subset H^1(\Omega)$ of continuous piecewise polynomial functions of degree $r - 1$, for $r \geq 2$ are used. The spaces are required to satisfy

$$\inf_{\chi \in S_h^r(\Omega)} \{ \|V - \chi\| + h \|V - \chi\|_{H^1(\Omega)} + h^{\frac{1}{2}} \|V - \chi\|_{L^2(\partial\Omega)} + h^{\frac{1}{2}} \|V - \chi\|_{H^1(\partial\Omega)} \} \leq Ch^s \|V\|_s \quad (5.1)$$

for $2 \leq s \leq r$, for some constant C .

In addition, the following inverse property is required

$$\left\| \frac{\partial \chi}{\partial n} \right\|_{L^2(\partial\Omega)} \leq C_1 h^{-\frac{1}{2}} \|\chi\|_{H^1(\Omega)}, \quad (5.2)$$

for all $\chi \in S_h^r(\Omega)$, for some constant C_1 .

The nonstandard bilinear form $N_h^r(\cdot, \cdot): H^2(\Omega) \times S_h^r(\Omega) \rightarrow \mathbb{R}^1$ is used,

$$N_h^r(\varphi, \psi) = a(\varphi, \psi) - \int_{\partial\Omega} \left(\varphi \frac{\partial \psi}{\partial n} + \psi \frac{\partial \varphi}{\partial n} - \gamma h^{-1} \varphi \psi \right) d\sigma, \quad (5.3)$$

where $a(\cdot, \cdot)$ is defined by (2.1) a , and $\gamma > 0$, is a specific constant. Nitsche [10] shows that with the assumption (5.2) and γ chosen sufficiently large with respect to C_1 , N_h^r is positive definite on S_h^r . The discrete solutions operator T_h is now defined by

$$N_h^r(T_h f, \chi) = (f, \chi), \quad (5.4)$$

for all $\chi \in S_h^r(\Omega)$, for given $f \in L^2(\Omega)$.

5.2. Nearly zero boundary conditions

A second nonstandard method due to Nitsche [11] uses the spaces $S_h^r(\Omega)$ of 5.1, with the additional assumption of « nearly zero » boundary conditions

$$\|\chi\|_{L^2(\partial\Omega)} \leq C_0 h^{\frac{1}{2}} \|\chi\|_{H^1(\Omega)}, \quad (5.5)$$

for all $\chi \in S_h^r(\Omega)$, for some constant C_0 .

The bilinear form $N_h^0(\gamma = 0)$ is used. With (5.2) and (5.5), and C_0, C_1 sufficiently small, N_h^0 is positive definite on $S_h^r(\Omega)$. The discrete solution operator, T_h , is defined by

$$N_h(T_h f, \chi) = (f, \chi), \quad (5.6)$$

for all $\chi \in S_h^r(\Omega)$, for given $f \in L^2(\Omega)$.

5.3. A Lagrange multiplier method of Babuška

In [2] Babuška proposes the following method. Subspaces $S_h^r(\Omega) \subset H^1(\Omega)$ are chosen satisfying

$$\inf_{\chi \in S_h^r(\Omega)} \{ \|V - \chi\| + h \|V - \chi\|_{H^1(\Omega)} \} \leq Ch^s \|V\|_s,$$

for all $V \in H^s(\Omega)$, for some constant C , $1 \leq s \leq r$.

In addition subspaces $S_\mu(\partial\Omega) \subset H^1(\partial\Omega)$ are employed, satisfying

$$\inf_{\chi \in S_\mu(\partial\Omega)} \{ \mu^{\frac{1}{2}} \|\lambda - \chi\|_{H^{\frac{1}{2}}(\partial\Omega)} + \mu^{-\frac{1}{2}} \|\lambda - \chi\|_{H^{-\frac{1}{2}}(\partial\Omega)} \} \leq C\mu^s \|\lambda\|_{H^s(\partial\Omega)},$$

for all $\lambda \in H^s(\partial\Omega)$, for $\frac{1}{2} \leq s \leq r - \frac{3}{2}$.

Also an inverse property is required,

$$\|\chi\|_{H^1(\partial\Omega)} \leq C\mu^{-1} \|\chi\|_{L^2(\partial\Omega)}, \quad \chi \in S_\mu(\partial\Omega).$$

Babuška shows that for the ratio h/μ sufficiently small, the form $a(\cdot, \cdot)$ is positive definite on the subspace

$$S_h = \left\{ V \in S_h^r(\Omega) : \int_{\partial\Omega} V \lambda d\sigma = 0, \text{ or all } \lambda \in S_\mu(\partial\Omega) \right\}.$$

The discrete solution operator T_h in this case is defined by

$$a(T_h f, \chi) = (f, \chi), \quad (5.7)$$

for all $\chi \in S_h$, for given $f \in L^2(\partial\Omega)$.

For proofs that the operators T_h defined by (5.4), (5.6) and (5.7) satisfy the properties (2.5)-(2.7) required in this work, see [1] and [6].

APPENDIX

The following is a tabulation of the polynomials $\{\beta_n^{(s)}(x)\}_{n=0}^{2s}$, for $s = 1, \dots, 5$. For each $s \geq 1$, a convenient choice of the parameter $x^{(s)}$ is as follows.

Examining the details of Lemma 4.1, we have merely to consider the behavior of the polynomials

$$P_{2n}^{(s)}(y) = (-1)^n \alpha_{2n}^{(s)}(y), \quad n = 1, 2, \dots, s.$$

We first note that from (4.2)-(4.5),

$$P_2^{(s)}(y) = s - \frac{1}{2}y^2, \quad s \geq 1,$$

and hence $P_2^{(s)}$ always has a real positive zero. In general, for $n \geq 1$, if $P_{2n}^{(s)}$ has a real positive zero, we set $Y_n^{(s)}$ to be the smallest positive zero otherwise we set $Y_n^{(s)} = \infty$.

We then choose $y^{(s)} = \min_{1 \leq n \leq s} y_n^{(s)}$, and $x^{(s)} = [y^{(s)}]^{-1}$. The procedure is clearly well defined and yields $x^{(s)}$ with $0 < x^{(s)} < \infty$.

Now since

$$P_{2n}^{(s)}(y) = (-1)^n y^{2n} \beta_{2n}^{(s)}\left(\frac{1}{y}\right), \quad n = 1, \dots, s,$$

the above procedure is equivalent to a root finding procedure on the polynomials $\{\beta_{2n}^{(s)}\}_{n=1}^s$ viz. For each $n \geq 1$ if $\beta_{2n}^{(s)}$ has a real positive zero, we set $x_n^{(s)}$ to be the largest positive zero of $\beta_{2n}^{(s)}$; otherwise we set $x_n^{(s)} = 0$. We now choose

$$x^{(s)} = \max_{1 \leq n \leq s} x_n^{(s)}.$$

Hence, with an efficient root finding algorithm, the parameters $x^{(s)}$ are easily obtained from the polynomials $\{\beta_{2n}^{(s)}\}_{n=1}^s$.

The tables are constructed simply from the formulae (4.2)-(4.5), and the relation (4.18).

$s = 1, v = 2$
$\beta_0^{(1)}(x) = 1$ $\beta_1^{(1)}(x) = -1$ $\beta_2^{(1)}(x) = \frac{1}{2} - x^2$
$s = 2, v = 4$
$\beta_0^{(2)}(x) = 1$ $\beta_1^{(2)}(x) = -1$ $\beta_2^{(2)}(x) = \frac{1}{2} - 2x^2$ $\beta_3^{(2)}(x) = -\frac{1}{6} + 2x^2$ $\beta_4^{(2)}(x) = \frac{1}{24} - x^2 + x^4$

$$s = 3, v = 6$$

$$\beta_0^{(3)}(x) = 1$$

$$\beta_1^{(3)}(x) = -1$$

$$\beta_2^{(3)}(x) = \frac{1}{2} - 3x^2$$

$$\beta_3^{(3)}(x) = -\frac{1}{6} + 3x^2$$

$$\beta_4^{(3)}(x) = \frac{1}{24} - \frac{3}{2}x^2 + 3x^4$$

$$\beta_5^{(3)}(x) = -\frac{1}{120} + \frac{1}{2}x^2 - 3x^4$$

$$\beta_6^{(3)}(x) = \frac{1}{720} - \frac{1}{8}x^2 + \frac{3}{2}x^4 - x^6$$

$$s = 4, v = 8$$

$$\beta_0^{(4)}(x) = 1$$

$$\beta_1^{(4)}(x) = -1$$

$$\beta_2^{(4)}(x) = \frac{1}{2} - 4x^2$$

$$\beta_3^{(4)}(x) = -\frac{1}{6} + 4x^2$$

$$\beta_4^{(4)}(x) = \frac{1}{24} - 2x^2 + 6x^4$$

$$\beta_5^{(4)}(x) = -\frac{1}{120} + \frac{3}{2}x^2 - 6x^4$$

$$\beta_6^{(4)}(x) = \frac{1}{720} - \frac{3}{8}x^2 + 3x^4 - 4x^6$$

$$\beta_7^{(4)}(x) = -\frac{1}{5040} + \frac{3}{40}x^2 - x^4 + 4x^6$$

$$\beta_8^{(4)}(x) = \frac{1}{40320} - \frac{1}{80}x^2 + \frac{1}{4}x^4 - 2x^6 + x^8$$

$$s = 5, v = 10$$

$$\beta_0^{(5)}(x) = 1$$

$$\beta_1^{(5)}(x) = -1$$

$$\beta_2^{(5)}(x) = \frac{1}{2} - 5x^2$$

$$\beta_3^{(5)}(x) = -\frac{1}{6} + 5x^2$$

$$s = 5, v = 10$$

$$\beta_4^{(5)}(x) = \frac{1}{24} - \frac{5}{2}x^2 + 10x^4$$

$$\beta_5^{(5)}(x) = -\frac{1}{120} + \frac{5}{6}x^2 - 10x^4$$

$$\beta_6^{(5)}(x) = \frac{1}{720} - \frac{5}{24}x^2 + 5x^4 - 10x^6$$

$$\beta_7^{(5)}(x) = -\frac{1}{5040} + \frac{1}{24}x^2 - \frac{5}{3}x^4 + 10x^6$$

$$\beta_8^{(5)}(x) = \frac{1}{40320} - \frac{1}{144}x^2 + \frac{5}{12}x^4 - 5x^6 + 5x^8$$

$$\beta_9^{(5)}(x) = -\frac{1}{362880} + \frac{1}{1008}x^2 - \frac{1}{12}x^4 + \frac{5}{3}x^6 - 5x^8$$

$$\beta_{10}^{(5)}(x) = \frac{1}{3628800} - \frac{1}{8064}x^2 + \frac{1}{72}x^4 - \frac{5}{12}x^6 + \frac{5}{2}x^8 - x^{10}$$

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