# Garth A. Baker <br> James H. Bramble <br> Semidiscrete and single step fully discrete approximations for second order hyperbolic equations 

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# SEMIDISCRETE AND SINGLE STEP FULLY DISCRETE APPROXIMATIONS FOR SECOND ORDER HYPERBOLIC EQUATIONS 

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#### Abstract

Finite element approximattons 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 mittal 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 ratıonal approximations to $e^{-z}$, analytic in neighbourhoods of the imaginary axis The approximations require the solution of 2 s linear systems at each time step, with the same real matrix, to yield conver gence rate $k^{s}$, where $k$ is the time step and sis an arbitrary positive integer


Résumé - On étudıe des approxımatıons par éléments fints de problemes aux limites, avec conditions initıales, pour des équatıons hyperboliques du second ordre utilisant les projections $L^{2}$ des données intiales comme valeurs de départ, on obtıent des estımatıons d'ordre optımal du taux de convergence, pour les schémas semi-discrétisés et pour les schemas complètement discrétisés

On introduıt une nouvelle famille de schémas complètement discrétises à un pas, d'une précision d'ordre élevée en temps On obtıent ces schémas à par tır d'une famille d'approxımations ratıonnelles de $e^{-z}$, analytıques dans des voısinages de l'axe imagınaıre Ces approxımations nécessitent la solution de $2 s$ systèmes linéarres à chaque pas de temps, correspondant à une même matrice réelle, et conduisant à un taux de convergence en $k^{s}$, ou $k$ est le pas de temps et $s$ un nombre entier positvf arbitraire

## 1. INTRODUCTION

### 1.1. Notation

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

$$
\left.\begin{array}{rl}
u_{t t}+\mathscr{L} u & =0 \quad \text { in } \quad \Omega \times\left(0, t^{*}\right]  \tag{1.1}\\
u & =0 \quad \text { on } \quad \partial \Omega \times\left(0, t^{*}\right] \\
u(0) & =u^{0} \quad \text { in } \quad \Omega \\
u_{t}(0) & =u_{t}^{0} \quad \text { in } \quad \Omega,
\end{array}\right\}
$$

[^0]$u^{0}$ and $u_{t}^{0}$ are given functions, and $\mathscr{L}$ denotes the second order elliptic operator
$$
\mathscr{L} u=-\sum_{i, j=1}^{N} \frac{\partial}{\partial x_{i}}\left(a_{\imath j}(x) \frac{\partial u}{\partial x_{J}}\right)+a_{0}(x) u
$$
with $a_{i j}=a_{\jmath t} \in C^{\infty}(\bar{\Omega}), i, j=1,2, \ldots, N ; a_{0} \in C^{\infty}(\bar{\Omega})$ and $a_{0} \geqslant 0$ on $\Omega$.
$\mathscr{L}$ is assumed to satisfy the unform ellipticity condition
\[

$$
\begin{equation*}
\sum_{i, j=1}^{N} a_{i \jmath}(x) \xi_{i} \xi_{\jmath} \geqslant \alpha \sum_{i=1}^{N} \xi_{i}^{2}, \tag{1.2}
\end{equation*}
$$

\]

for all $x \in \bar{\Omega}$ and for all $\left(\xi_{1}, \ldots, \xi_{N}\right) \in \mathbb{R}^{N}$, for some constant $\alpha>0$.
The following notation will be used throughout. For $s \geqslant 0, H^{s}(\Omega)$ will denote the Sobolev space of order $s$, of real valued functions on $\Omega$. The norm on $H^{s}(\Omega)$ we denote by $\|.\|_{H^{s}(\Omega)}$. In particular, the inner product on $L^{2}(\Omega)=H^{0}(\Omega)$ we denote by (., .), and the associated norm by \|. \|.

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 $\left\{\lambda_{J}\right\}_{J \geqslant 1}$ in non decreasing order of real positive ergenvalues of the operator $\mathscr{L}$, and a corresponding sequence of eigenfunctions $\left\{\varphi_{J}\right\}_{J \geqslant 1} \subset C^{\infty}(\Omega)$, satisfying

$$
\left.\begin{array}{l}
\mathscr{L} \varphi_{J}=\lambda_{J} \varphi_{J} \quad \text { in } \quad \Omega  \tag{1.3}\\
\varphi_{J}=0 \quad \text { on } \quad \partial \Omega
\end{array}\right\}
$$

The set $\left\{\varphi_{J}\right\}_{, \geqslant 1}$ is complete in $L^{2}(\Omega)$, and may be chosen orthonormal.
Define for $s \geqslant 0$, the space

$$
\dot{H}^{s}(\Omega)=\left\{v:\|v\|_{s}=\left(\sum_{j=1}^{\infty}\left|\left(v, \varphi_{j}\right)\right|^{2} \lambda_{j}^{s}\right)^{\frac{1}{2}}<\infty\right\}
$$

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

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

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

$$
\|v\|_{-s}=\left(\sum_{j=1}^{\infty}\left|\left(v, \varphi_{J}\right)\right|^{2} \lambda_{J}^{-s}\right)^{\frac{1}{2}}, \quad s \geqslant 0 .
$$

The solution of (1.1) is formally given by

$$
u(t)=\sum_{J=1}^{\infty}\left[\left(u^{0}, \varphi_{J}\right) \cos \lambda_{J}^{\frac{1}{2}} t+\lambda_{J}^{\frac{1}{2}}\left(u_{t}^{0}, \varphi_{J}\right) \sin \lambda_{J}^{\frac{1}{2}} t\right] \varphi_{J}
$$

for $t \geqslant 0$, from which it follows that for $0 \leqslant t \leqslant t^{*}$,
$\|u(t)\|_{s}^{2}+\left\|u_{t}(t)\right\|_{s \quad 1}^{2}=\left\|u^{0}\right\|_{s}^{2}+\left\|u_{t}^{0}\right\|_{s-1}^{2}, \quad$ for all $s \geqslant 0$
In Section 2, we derive the estımates for semidiscrete approximations

$$
\begin{equation*}
\sup _{o \leqslant t \leqslant t^{*}}\left\|u(t)-u_{h}(t)\right\| \leqslant C\left(t^{*}\right) h^{r}\left[\left\|u^{0}\right\|_{r+1}+\left\|u_{t}^{0}\right\|_{r}\right] \tag{array}
\end{equation*}
$$

using standard finite element spaces of piecewise polynomial functions of degree $r-1, r \geqslant 2$ The estımates 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 (15) 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 $L^{2}$ estımates, however the choice of stating valves 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

$$
\begin{equation*}
\left|r_{v}(\imath y)-e^{-\imath y}\right| \leqslant C_{v}|y|^{v+1}, \quad|y| \leqslant \sigma \tag{array}
\end{equation*}
$$

for constants $C_{v}<\infty, \sigma>0$ and $v \geqslant 1$
In addition such rational functions are divided into two classes, according to either
or

$$
\begin{array}{ll}
\left|r_{v}(l y)\right| \leqslant 1 & \text { for all real } y \\
\left|r_{v}(l y)\right| \leqslant 1 & \text { for }|y| \leqslant \alpha \tag{array}
\end{array}
$$

for some constant $\alpha>0$ The functions satisfying (17) we designate as Class $i-I$, and those satisfying (18) as Class $i-I I$

For schemes defined by rational functions of Class $l-I$, we obtain estımates

$$
\begin{align*}
\max \left\|W_{1}^{n}-u(n k)\right\|=C\left(t^{*}\right)\left\{h ^ { r } \left[\left\|u^{0}\right\|_{r+1}\right.\right. & \left.+\left\|u_{t}^{0}\right\|_{r}\right] \\
& \left.+k^{v}\left[\left\|u^{0}\right\|_{v+1}+\left\|u_{t}^{0}\right\|_{v}\right]\right\} \tag{19}
\end{align*}
$$

where $k$ denotes the discrete time step and $W_{1}^{n}$, the approximation at the time level $t=n k$

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

Again the estimates (19) are obtained using $L^{2}$ projections of the initial data as starting values
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Another development of this paper is the construction of a family of rational functions $\left\{r_{s}(z)\right\}_{s \geq 1}$ of class $i-I$, which is done in Section 4 Briefly, for each integer $s \geqslant 1$, and any given real number $x>0$, we establish the existence of a sequence of polynomials $\left\{\beta_{n}^{(s)}\right\}_{n=0}^{\infty}$ with real coefficients, where $\beta_{n}$ is of degree at most $n$, such that

$$
\begin{equation*}
\left(1-x^{2} z^{2}\right)^{s} e^{-z}=\sum_{n=0}^{\infty} \beta_{n}^{(s)}(x) z^{n}, \tag{array}
\end{equation*}
$$

for all $z$
For $s=1,2$, , we then define the rational function

$$
r_{s}(z)=\sum_{n=0}^{2 s} \beta_{n}^{(s)}(x) z^{n} /\left(1-x^{2} z^{2}\right)^{s}
$$

for $|\operatorname{Re}(z)|<\frac{1}{x} \quad r_{s}$ 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 (16) with $v=2 s$, and we show that there exists a real number $x^{(s)}>0$ such that for the choice $x \geqq x^{(s)}, r_{s}$ satısfies (17)

This famıly of rational functions provides schemes of arbitrary accuracy in time, 1 e we have (19) with $v=2 s$ 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 $2 s$ linear systems with the same real matrix at each time level

Other examples of Class $i-I$ rational functions are provided by Pade 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 $\left\{\beta_{n}^{s}\right\}_{n=0}^{2 s}$ and a convenient choice of the parameter $x^{(s)}$ is given for $s=1, \quad, 5$ 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

$$
\begin{equation*}
a(T f, v)=(f, v), \quad \text { for all } v \in \dot{H}^{1}(\Omega), \text { for given } f \in L^{2}(\Omega) \tag{array}
\end{equation*}
$$

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

$$
\begin{equation*}
a(\omega, v)=\int_{\Omega}\left\{\sum_{\imath, j=1}^{N} a_{\imath} \frac{\partial \omega}{\partial x_{\imath}} \frac{\partial v}{\partial x_{j}}\right\} d x, \quad \text { for } \quad \omega, v \in H^{1}(\Omega) . \tag{2.1.a}
\end{equation*}
$$

$T$ has a discrete spectrum of real positive eigenvalues $\left\{\mu_{j}\right\}_{j \geqslant 1}$, where $\mu_{J}=\lambda_{j}^{-1}$ with $\lambda_{J}$ 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

$$
J=\left(\begin{array}{rr}
0 & T \\
-I & 0
\end{array}\right)
$$

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

$$
U(t)=\binom{u(t)}{u_{t}(t)}, \quad U^{0}=\binom{u^{0}}{u_{t}^{0}} .
$$

Then, (1.1) is equivalent to

$$
\left.\begin{array}{rlr}
J U_{t}+U & =0, \quad t>0  \tag{2.2}\\
U(0) & =U^{0} . &
\end{array}\right\}
$$

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

$$
\left\{S_{h}^{r}(\Omega)\right\}_{0<h \leqslant 1} \subset \dot{H}^{1}(\Omega)
$$

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

$$
\inf _{\in S_{h}^{S}(\Omega)}\left\{\|\omega-\chi\|+h\|\omega-\chi\|_{1}\right\} \leqslant C h^{s}\|\omega\|_{\mathbf{H}^{s}(\Omega)}
$$

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

$$
\begin{equation*}
a\left(T_{h} f, \chi\right)=(f, \chi), \quad \text { for all } \quad \chi \in S_{h}^{r}(\Omega), \text { for given } f \in L^{2}(\Omega) \tag{2.4}
\end{equation*}
$$

The family $\left\{T_{h}\right\}_{0<h \leqslant 1}$ has the following properties:
$T_{h}$ is symmetric, positive semidefinite on $L^{2}(\Omega)$, and positive definite on $S_{h}^{r}(\Omega)$ (2.5)

$$
\begin{equation*}
\left\|\left(T-T_{h}\right) f\right\| \leqslant C h^{s}\|f\|_{s-2}, \quad \text { for all } \quad f \in H^{s-2}(\Omega), 1 \leqslant s \leqslant r \tag{2.6}
\end{equation*}
$$

for some constant $C$ independent of $h$.
$T_{h}$ has a discrete spectrum of eigenvalues $\{0\} \cup\left\{\mu_{1}^{h}, \mu_{2}^{h}, \ldots, \mu_{M}^{h}\right\}$, in nonincreasing order, for some integer $M=M(h)$. Furthermore, there exists an $h_{0}>0$ such that for $h \leqslant h_{0}, \mu_{1}^{h} \leqslant A$, for some constant $A>0$.

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 $u^{h}\left[0, t^{*}\right] \rightarrow S_{h}^{r}(\Omega)$ satisfying

$$
\left.\begin{array}{rl}
T_{h} u_{t t}^{h}+u^{h} & =0, \quad 0<t \leqslant t^{*}  \tag{2.8}\\
u^{h}(0) & =P u^{0}, \\
u_{t}^{h}(0) & =P u_{t}^{0},
\end{array}\right\}
$$

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

$$
V(t)=\binom{u^{h}(t)}{u_{t}^{h}(t)} \quad t \geqslant 0 ;
$$

then (2.8) is equivalent to

$$
\left.\begin{array}{rl}
J_{h} V_{t}+V & =0, \quad 0<t \leqslant t^{*}  \tag{2.9}\\
V(0) & =P U^{0},
\end{array}\right\}
$$

where

$$
J_{h}=\left(\begin{array}{rr}
0 & T_{h} \\
-I & 0
\end{array}\right): \mathbb{L}^{2} \rightarrow S_{h}^{r}(\Omega) \times L^{2}(\Omega),
$$

and $P$ denotes the $\mathbb{L}^{2}$ projection operator onto $S_{h}^{r}(\Omega) \times S_{h}^{r}(\Omega)$.
We define a form ((.)) on $\mathbb{L}^{2}$ by

$$
\begin{equation*}
((\Phi, \Psi))=\left(\phi_{1}, \psi_{1}\right)+\left(T_{h} \phi_{2}, \psi_{2}\right) \tag{2.10}
\end{equation*}
$$

for

$$
\Phi=\binom{\phi_{1}}{\phi_{2}} \quad \text { and } \quad \Psi=\binom{\psi_{1}}{\psi_{2}} \in \mathbb{L}^{2}
$$

The associated seminorm which we denote by ||| . ||| is given by

$$
\begin{equation*}
\||\Phi|\|=((\Phi, \Phi))^{\frac{1}{2}} \tag{2.11}
\end{equation*}
$$

We note that

$$
\begin{equation*}
\left(\left(J_{h} \Phi, \Phi\right)\right)=0, \quad \Phi \in \mathbb{L}^{2} . \tag{2.12}
\end{equation*}
$$

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 $C=C_{r}\left(t^{*}\right)$, such that

$$
\begin{equation*}
\sup _{0 \leqslant t \leqslant t^{*}}\left\|u(t)-u^{h}(t)\right\| \leqslant C h^{r}\left[\left\|u^{0}\right\|_{r+1}+\left\|u_{t}^{0}\right\|_{r}\right] \tag{2.13}
\end{equation*}
$$

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

$$
\begin{gather*}
J_{h} E_{t}+E=\left(J_{h}-J\right) U_{t}, \quad 0<t \leqslant t^{*},  \tag{2.14}\\
E(0)=(I-P) U^{0} . \tag{2.15}
\end{gather*}
$$

Setting $\rho=\left(J_{h}-J\right) U_{t}(2.14)$ gives

$$
\left(\left(J_{h} E_{t}, E_{t}\right)\right)+\left(\left(E, E_{t}\right)\right)=\left(\left(\rho, E_{t}\right)\right)
$$

and so, by (2.12),

$$
\frac{1}{2} \frac{d}{d t}\|E(t)\| \|^{2}=\frac{d}{d t}((\rho(t), E(t)))-\left(\left(\rho_{t}(t), E(t)\right)\right)
$$

Integrating this last equation, we get
$\||E(t)|\|^{2}=\||E(0)|\|^{2}+2((\rho(t), E(t)))-2((\rho(0), E(0)))-2 \int_{0}^{t}\left(\left(\rho_{t}(\tau), E(\tau)\right)\right) d \tau$.
From (2.4), it follows that $T_{h} P=T_{h}$ on $L^{2}(\Omega)$. Hence, from (2.15), and (2.11),

$$
\begin{equation*}
\|E(0)\|\|=\| u^{0}-P u^{0} \| \tag{2.17}
\end{equation*}
$$

and

$$
\begin{align*}
&((\rho(0), E(0)))=\left(\left[T_{h}-T\right] u_{t t}(0), u^{0}-P u^{0}\right)=-\left(T u_{t t}(0), u^{0}-P u^{0}\right) \\
&=\left(u^{0}, u^{0}-P u^{0}\right)=\left\|u^{0}-P u^{0}\right\|^{2} \tag{2.18}
\end{align*}
$$

Using (2.17) and (2.18) in (2.16),
$\|E(t)\|\left\|^{2}=2((\rho(t), E(t)))-\right\| u^{0}-P u^{0} \|^{2}-2 \int_{0}^{t}\left(\left(\rho_{t}(\tau), E(\tau)\right)\right) d \tau$
$\leqslant 2((\rho(t), E(t)))-2 \int_{0}^{t}\left(\left(\rho_{t}(\tau), E(\tau)\right)\right) d \tau$
$\leqslant \frac{1}{4}\| \| E(t)\| \|^{2}+4\| \| \rho(t)\| \|^{2}+4 t^{*} \int_{0}^{t^{*}}\left|\left\|\left|\rho_{t}(\tau)\left\|\left.\right|^{2} d \tau+\frac{1}{4} \sup _{0 \leqslant \tau \leqslant t^{*}}\left|\|E(\tau) \mid\| \|^{2}\right.\right.\right.\right.\right.$.
Hence

$$
\begin{equation*}
\sup _{0 \leqslant t \leqslant t^{*}}\|\mid E(t)\| \|^{2} \leqslant C\left\{\sup _{0 \leqslant t \leqslant t^{*}}\left|\|\rho(t)\|\left\|^{2}+\int_{0}^{t^{*}}\right\|\right| \rho_{t}(\tau) \|\left.\right|^{2} d \tau\right\} \tag{2.19}
\end{equation*}
$$

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

$$
\begin{align*}
\|\rho(t)\|\|=\|\left(T_{h}-T\right) u_{t t}(t) \| & =\left\|\left(T_{h}-T\right) \mathscr{L} u(t)\right\| \\
& \leqslant C h^{r}\|u(t)\|_{r} \leqslant C h^{r}\left[\left\|u^{0}\right\|_{r}+\left\|u_{t}^{0}\right\|_{r-1}\right] . \tag{2.20}
\end{align*}
$$

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

$$
\begin{align*}
\int_{0}^{t}\left\|\rho_{t}(t)\right\|^{2} d \tau & =\int_{0}^{t^{*}}\left\|\left(T_{h}-T\right) u_{t t t}(\tau)\right\|^{2} d \tau=\int_{0}^{t^{*}}\left\|\left(T_{h}-T\right) \mathscr{L} u_{t}(\tau)\right\|^{2} d \tau \\
& \leqslant C h^{2 r} \sup _{0 \leqslant t \leqslant t^{*}}\left\|u_{t}(t)\right\|_{r}^{2} \leqslant C h^{2 r}\left[\left\|u^{0}\right\|_{r+1}+\left\|u_{t}^{0}\right\|_{r}\right]^{2} \tag{2.21}
\end{align*}
$$

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

$$
\sup _{0 \leqslant t \leqslant t^{*}}\|E(t)\| \| \leqslant C h^{r}\left[\left\|u^{0}\right\|_{r+1}+\left\|u_{t}^{0}\right\|_{r}\right] .
$$

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 $0\left(h^{r}\right)$ 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

$$
\left\|u^{0}-u^{h}(0)\right\|=0\left(h^{r}\right)
$$

and

$$
\left\|u_{t}^{0}-u_{t}^{h}(0)\right\|=0\left(h^{r}\right)
$$

## 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

$$
\begin{equation*}
\left|r(i y)-e^{-i y}\right| \leqslant C|y|^{v+1}, \quad|y| \leqslant \sigma, \tag{3.1}
\end{equation*}
$$

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

$$
\begin{equation*}
|r(i y)| \leqslant 1, \quad \text { for all real } y . \tag{3.2}
\end{equation*}
$$

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

$$
\begin{equation*}
|r(i y)| \leqslant 1, \quad \text { for all real } y, \text { with }|y| \leqslant \alpha . \tag{3.3}
\end{equation*}
$$

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

The solution of (2.9) is given by

$$
\begin{equation*}
V(t)=e^{-k J_{n}^{-1}} P U^{0}, \quad t \geqslant 0 \tag{3.4}
\end{equation*}
$$

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

$$
\begin{equation*}
V(t+k)=e^{-k J_{K}^{-1}} V(t), \quad t \geqslant 0 . \tag{3.5}
\end{equation*}
$$

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

The fully discrete approxımation to (1.1), derived from (3.5) we denote by $\left\{W^{n}\right\}_{n \geqslant 0} \subset S_{h}^{r}(\Omega) \times S_{h}^{r}(\Omega)$, and is defined by

$$
\left.\begin{array}{l}
W^{n+1}=D^{-1}\left(k J_{h}^{-1}\right) N\left(k J_{h}^{-1}\right) W^{n}, \quad n=0,1, \ldots,  \tag{3.6}\\
W^{0}=P U^{0}
\end{array}\right\}
$$

We derive estimates for $\left\|u(n k)-W_{1}^{n}\right\|$ by comparing $W^{n}$ with the semidiscrete approxımation $V(n k), n=0,1, \ldots$ To this end, we define the function

$$
\begin{equation*}
F_{n}(z)=r^{n}(z)-e^{-n z}, \quad n=0,1, \ldots \tag{3.7}
\end{equation*}
$$

From (384), (3.6) and (3.7), it follows that

$$
\begin{equation*}
W^{n}-V(n k)=F_{n}\left(k J_{h}^{-1}\right) P U^{0} \tag{3.8}
\end{equation*}
$$

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

$$
\begin{equation*}
\left|r^{n}(i y)-e^{-i n y}\right| \leqslant n C^{*}|y|^{l} \tag{3.9}
\end{equation*}
$$

for $|y| \leqslant \alpha$ and $1 \leqslant l \leqslant v+1, n=1,2, \ldots,$.
Proof Let $\sigma^{*}=\min (\sigma, 1)$. Then (3.1) holds with $\sigma$ replaced by $\sigma^{*}$. Hence

$$
\begin{equation*}
\left|r(i y)-e^{-\iota y}\right| \leqslant C|y|^{l}, \quad|y| \leqslant \sigma^{*} \tag{3.10}
\end{equation*}
$$

for $1 \leqslant 1 \leqslant v+1$.
Now, if $\sigma^{*}<\alpha$, from (3.3), for $\sigma^{*}<|y| \leqslant \alpha$, and any integer $1 \leqslant l \leqslant v+1$, $\left|r(i y)-e^{-\imath y}\right| \leqslant 2=2|y|^{l}\left(\frac{\sigma^{*}}{|y|}\right)^{l}\left(\frac{1}{\sigma^{*}}\right)^{l} \leqslant 2|y|^{l}\left(\sigma^{*}\right)^{-(v+1)}=C^{*}|y|^{l}$,
with $C^{*}<\infty$. Hence, from (3.10) and (3.11), we have for some $C^{*}<\infty$,

$$
\begin{equation*}
\left|r(i y)-e^{-\imath y}\right| \leqslant C^{*}|y|^{l}, \quad|y| \leqslant \alpha \tag{3.12}
\end{equation*}
$$

for $1 \leqslant l \leqslant v+1$.
Now for an integer $n \geqslant 1$,

$$
\begin{equation*}
r^{n}(i y)-e^{-i n y}=\left(r(i y)-e^{-i y}\right) \sum_{j=0}^{n-1} r^{J}(l y) e^{-l(n-j-1) y} \tag{3.13}
\end{equation*}
$$

Hence, using (3.12) and (3.3) in (3.13), we get for $|y| \leqslant \alpha$, $\left|r^{n}(i y)-e^{-i n y}\right| \leqslant\left|r(i y)-e^{-i y}\right| \sum_{j=0}^{n-1}|r(i y)|^{j} \leqslant n C^{*}|y|^{l}, \quad 1 \leqslant l \leqslant v+1$.

It is clear that, by choosing $\alpha=\infty,(3.9)$ holds for Class $i-I$.
Let $\mu_{1}^{h}, \ldots, \mu_{M}^{h}$, be the set of nonzero eigenvalues of $T_{h}$ with corresponding eigenfunctions $\psi_{1}^{h}, \ldots, \psi_{M}^{h}$, chosen orthonormal in $L^{2}(\Omega)$, i. e.

$$
T_{h} \psi_{j}^{h}=\mu_{j}^{h} \psi_{j}^{h}
$$

and

$$
\left(\psi_{\imath}^{h}, \psi_{j}^{h}\right)=\delta_{\imath \jmath}, \quad i, j=1,2, \ldots, M
$$

Now let $S_{h}$ denote the space $S_{h}^{r}(\Omega) \times S_{h}^{r}(\Omega)$, furnished with the inner product ((.,.)) and norm III . |II.

It is easily shown that the operator $J_{h}: S_{h} \rightarrow S_{h}$ posseses a corresponding set of purely imaginary eigenvalues $\left\{\eta_{J}\right\}_{j=-M}^{M}$, given by

$$
\begin{aligned}
\eta_{J} & =i\left(\mu_{J}^{h}\right)^{\frac{1}{2}} \\
\eta_{-J} & =-i\left(\mu_{J}^{h}\right)^{\frac{1}{2}}, \quad j=1,2, \ldots, M
\end{aligned}
$$

and corresponding eigenvectors $\left\{\Phi_{J}\right\}_{J=-M}^{M}$, given by

$$
\begin{aligned}
\Phi_{J} & =\frac{1}{\sqrt{2}}\binom{\psi_{J}^{h}}{i\left(\mu_{J}^{h}\right)^{-\frac{1}{2}} \psi_{J}^{h}} \\
\Phi_{-J} & =\frac{1}{\sqrt{2}}\binom{\psi_{J}^{h}}{-i\left(\mu_{J}^{h}\right)^{-\frac{1}{2}} \psi_{J}^{h}}, \quad j=1,2, \ldots, M
\end{aligned}
$$

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

$$
((\Phi, \Psi))=\left(\varphi_{1}, \bar{\Psi}_{1}\right)+\left(T_{h} \varphi_{2}, \bar{\psi}_{2}\right), \quad \text { on } \quad S_{n},
$$

where in general $\bar{\varphi}$ denotes the complex conjugate of $\varphi$. Since $\left\{\Psi_{j}^{h}\right\}_{J=1}^{M}$ is an orthonormal basis for $S_{n}^{r}(\Omega)$, it is easily seen that $\left\{\Phi_{j}\right\}_{j=-M}^{M}$ forms a complete orthonormal set in $S_{h}$, with respect to the above inner product ((. . .)).

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

$$
\begin{equation*}
P Z=\sum_{j=-M}^{M}\left(\left(Z, \Phi_{j}\right)\right) \Phi_{J} \tag{3.14}
\end{equation*}
$$

and

$$
\begin{equation*}
\|\mid P Z\|\left\|=\left(\sum_{j=-M}^{M}\left|\left(\left(Z, \Phi_{j}\right)\right)\right|^{2}\right)^{\frac{1}{2}} \leqslant\right\|\|Z\| \tag{3.15}
\end{equation*}
$$

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 $n k=t \leqslant t^{*}$

$$
\begin{equation*}
\left\|\mid F_{n}\left(k J_{h}^{-1}\right) J_{h}^{l} Z\right\| \leqslant C k^{l-1}\|Z\|, \tag{3.16}
\end{equation*}
$$

$1 \leqslant l \leqslant v+1$.
Proof : From (3.14), it follows that

$$
F_{n}\left(k J_{h}^{-1}\right) J_{h}^{l} Z=\sum_{J=-M}^{M} F_{n}\left(k \eta_{J}^{-1}\right) \eta_{J}^{l}\left(\left(Z, \Phi_{j}\right)\right) \Phi
$$

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

$$
\begin{align*}
\left\|\left\|F_{n}\left(k J_{h}^{-1}\right) J_{h}^{l} Z\right\|\right\| & =\left(\sum_{J=-M}^{M}\left|F_{n}\left(k \eta_{J}^{-1}\right)\right|^{2}\left|\eta_{J}\right|^{2 l}\left|\left(\left(Z, \Phi_{J}\right)\right)\right|^{2}\right)^{\frac{1}{2}} \\
& \leqslant\left(\sum_{J=-M}^{M} n^{2} C^{* 2} k^{2 l}\left|\eta_{J}\right|^{-2 l}\left|\eta_{J}\right|^{2 l}\left|\left(\left(Z, \Phi_{J}\right)\right)\right|^{2}\right)^{\frac{1}{2}}  \tag{3.17}\\
& =n C^{*} k^{l}\left(\sum_{J=-M}^{M}\left|\left(\left(Z, \Phi_{J}\right)\right)\right|^{2}\right)^{\frac{1}{2}} \leqslant t^{*} C^{*} k^{l-1}|\|Z \mid\|,
\end{align*}
$$

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

$$
\begin{equation*}
\mu_{M}^{h} \geqq C_{1} h^{2} \tag{3.18}
\end{equation*}
$$

for some constant $C_{1}>0$, independent of $h$. Then, for $k$ chosen such that

$$
\begin{equation*}
k \leqslant \alpha C_{1}^{\frac{1}{1}} h, \tag{3.19}
\end{equation*}
$$

there exists a constant $C$ such that, for $Z \in \mathbb{1}^{2}$,

$$
\begin{equation*}
\left\|\left\|F_{n}\left(k J_{h}^{-1}\right) J_{h}^{l} Z\right\|\right\| \leqslant C k^{l-1} \mid\|Z\| \| \tag{3.20}
\end{equation*}
$$

for $1 \leqslant l \leqslant v+1$.
Proof: From (3.18),

$$
\max _{-M \leqslant J \leqslant M}\left|\eta_{J}\right|^{-1}=\left(\mu_{M}^{h}\right)^{-\frac{1}{2}} \leqslant C_{1}^{-\frac{1}{2}} h^{-1} .
$$

Hence, with (3.19) satisfied, we have

$$
k\left|\eta_{J}\right|^{-1} \leqslant \alpha
$$

With the above inequality and (3.9),

$$
\begin{equation*}
\left|F_{n}\left(k \eta_{J}^{-1}\right)\right| \leqslant C^{*} n k^{l}\left|\eta_{J}\right|^{-l} \tag{3.21}
\end{equation*}
$$

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

$$
\begin{equation*}
\|\chi\|_{1} \leqslant C h^{-1}\|\chi\|, \quad \text { for all } \quad \chi \in S_{h}^{r}(\Omega) \tag{3.22}
\end{equation*}
$$

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 $Z \in \mathbb{L}^{2}$,

$$
\begin{equation*}
\left\|\left\|F_{n}\left(k J_{h}^{-1}\right) Z\right\|\right\| \leqslant C\| \| Z\| \|, \quad n=0,1, \ldots \tag{3.23}
\end{equation*}
$$

and

$$
\begin{equation*}
\left\|\left\|W^{h}\right\|\right\| \leqslant\left\|U^{0}\right\| \| \tag{3.23a}
\end{equation*}
$$

If $r$ is of Class $i$-II with (3.22) and (3.19) satisfied, then (3.23a) holds.
Before proceeding to the derivation of the error estimates, we define the following auxiliary functions.

Let $Q$ be the smallest integer such that

$$
k \lambda_{j}^{\frac{1}{2}}>1, \quad \text { for } \quad j \geqslant Q
$$

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

$$
V^{(k)}=\sum_{J=1}^{Q-1}\left(v, \varphi_{j}\right) \varphi_{J} .
$$

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

$$
\begin{equation*}
\left\|V^{(k)}\right\|_{s} \leqslant\|V\|_{s} \tag{3.24}
\end{equation*}
$$

and

$$
\begin{equation*}
\left\|V-V^{(k)}\right\|_{-p} \leqslant k^{s+p}\|V\|_{s}, \quad \text { for all } \quad s \geqslant 0, p \geqslant 0 \tag{3.25}
\end{equation*}
$$

Also, for any $m \geqslant 0$,

$$
\begin{equation*}
\left\|V^{(k)}\right\|_{r+m} \leqslant k^{-m}\|V\|_{r} . \tag{3.26}
\end{equation*}
$$

Define

$$
\begin{equation*}
U^{0(k)}=\binom{u^{0(k)}}{u_{t}^{0(k)}} . \tag{3.27}
\end{equation*}
$$

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

$$
\begin{align*}
\sup _{0 \leqslant n \leqslant\left[t^{*} / k\right]}\left\|W_{1}^{n}-u(n k)\right\| \leqslant C\left\{h ^ { r } \left[\left\|u^{0}\right\|_{r+1}\right.\right. & \left.+\left\|u_{t}^{0}\right\|_{r}\right] \\
& \left.+k^{v}\left[\left\|u^{0}\right\|_{v+1}+\left\|u_{t}^{0}\right\|_{v}\right]\right\} \tag{3.28}
\end{align*}
$$

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

$$
\Lambda=\left(\begin{array}{rr}
0 & -I \\
\mathscr{L} & 0
\end{array}\right)
$$

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

$$
\begin{equation*}
F_{n}\left(k J_{h}^{-1}\right)=\sum_{l=0}^{v} F_{n}\left(k J_{h}^{-1}\right) J_{h}^{l}\left(J-J_{h}\right) \Lambda^{l+1}+F_{n}\left(k J_{h}^{-1}\right) J_{h}^{v+1} \Lambda^{v+1} \tag{3.29}
\end{equation*}
$$

From (3.8) and (3.29),

$$
\begin{align*}
& V(n k)-W^{n}=F_{n}\left(k J_{h}^{-1}\right)\left(U^{0}-U^{0(k)}\right)+ \sum_{l=0}^{v} \\
& F_{n}\left(k J_{h}^{-1}\right) J_{h}^{l}\left(J-J_{h}\right) \Lambda^{l+1} U^{0(k)}  \tag{3.30}\\
&+F_{n}\left(k J_{h}^{-1}\right) J_{h}^{v+1} \Lambda^{v+1} U^{0(k)}
\end{align*}
$$

Thus, from (3.30),
$\left|\left|\left|V(n k)-W^{n}\right|\|\leqslant\| F_{n}\left(k J_{h}^{-1}\right)\left(U^{0}-U^{0(k)}\right)\| \|+\left\|\left|F_{n}\left(k J_{h}^{-1}\right)\left(J-J_{h}\right) \Lambda U^{0(k)}\right|\right\|\right.\right.$

$$
+\sum_{l=0}^{\nu}\| \| F_{n}\left(k J_{h}^{-1}\right) J_{h}^{l}\left(J-J_{h}\right) \Lambda^{l+1} U^{0(k)}\| \|+\left\|\mid F_{n}\left(k J_{h}^{-1}\right) J_{h}^{\nu+1} \Lambda^{\nu+1} U^{0(k)}\right\| \| .
$$

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

$$
\begin{align*}
& \left\|\left\|F_{n}\left(k J_{h}^{-1}\right)\left(U^{0}-U^{0(k)}\right)\right\|\right\|^{2} \leqslant\| \| U^{0}-U^{0(k)}\| \|^{2} \\
& =C\left\{\left\|u^{0}-u^{0(k)}\right\|^{2}+\left(T_{h}\left[u_{t}^{0}-u_{t}^{0(k)}\right], u_{t}^{0}-u_{t}^{0(k)}\right)\right\} \\
& =C\left\{\left\|u^{0}-u^{0(k)}\right\|^{2}+\left(\left(T_{h}-T\right)\left[u_{t}^{0}-u_{t}^{0(k)}\right], u_{t}^{0}-u_{t}^{0(k)}\right)\right. \\
& \left.+\left(T\left[u_{t}^{0}-u_{t}^{0(k)}\right], u_{t}^{0}-u_{t^{0}}^{0(k)}\right)\right\} \\
& \leqslant C\left\{\left\|u^{0}-u^{0(k)}\right\|^{2}+\left\|\left(T_{h}-T\right)\left[u_{t}^{0}-u_{t}^{0(k)}\right]\right\|\left\|u_{t}^{0}-u_{t}^{0(k)}\right\|\right. \\
& \left.+\left\|T\left[u_{t}^{0}-u_{t}^{0(k)}\right]\right\|_{1}\left\|u_{t}^{0}-u_{t}^{0(k)}\right\|_{-1}\right\} \\
& \leqslant C\left\{k^{2 v}\left\|u^{0}\right\|_{v}^{2}+{ }^{\circ} h^{r}\left\|u_{t}^{0}\right\|_{r-2} k^{v}\left\|u_{t}^{0}\right\|_{v}+k^{2 v}\left\|u_{t}^{0}\right\|_{v-1}^{2}\right\} \\
& \leqslant C\left\{k^{v}\left[\left\|u^{0}\right\|_{v}+\left\|u_{t}^{0}\right\|_{v}\right]+h^{r}\left\|u_{t}^{0}\right\|_{r-2}\right\}^{2} \tag{3.32}
\end{align*}
$$

Also, from (3.23) and (2.6),
$\left\|\left|\left\|F_{n}\left(k J_{h}^{-1}\right)\left(J-J_{h}\right) \Lambda U^{0(k)} \mid\right\| \leqslant C\left\|\left(T-T_{h}\right) \mathscr{L} u^{0(k)}\right\| \leqslant C h^{r}\left\|u^{0}\right\|_{r}\right.\right.$.
Now, from (3.16) of Lemma 3.2,

$$
\begin{equation*}
\sum_{l=1}^{v}\left|\left\|\left|F_{n}\left(k J_{h}^{-1}\right) J_{h}^{l}\left(J-J_{h}\right) \Lambda^{l+1} U^{0(k)}\right|\right\|\right| \leqslant C \sum_{l=1}^{v} k^{l-1}\| \|\left(J-J_{h}\right) \Lambda^{l+1} U^{0(k)}\| \| \tag{3.34}
\end{equation*}
$$

For $l+1$ even, we have

$$
\Lambda^{l+1}=(-1)^{\frac{l+1}{2}}\left(\begin{array}{cc}
\mathscr{L}^{\frac{l+1}{2}} & 0  \tag{3.35}\\
0 & \mathscr{L}^{\frac{l+1}{2}}
\end{array}\right)
$$

and for $l+1$ odd,

$$
\Lambda^{l+1}=(-1)^{\frac{l}{2}}\left(\begin{array}{cc}
0 & -\mathscr{L}^{\frac{l}{2}}  \tag{3.36}\\
\mathscr{L}^{\frac{l}{2}+1} & 0
\end{array}\right)
$$

Thus a simple computation using (3.351 and (3.36) yields
$\left\|\left(J-J_{h}\right) \Lambda^{l+1} U^{0(k)}\right\| \|=\left\{\begin{array}{lll}\left\|\left(T-T_{h}\right) \mathscr{L}^{\frac{l+1}{2}} u_{t}^{0(k)}\right\|, & l+1 & \text { even }, \\ \left\|\left(T-T_{h}\right) \mathscr{L}^{\frac{l}{2}+1} u^{0(k)}\right\|, & l+1 & \text { odd } .\end{array}\right.$
Hence, from (3.37), (2.6) and (3.26), for $l+1$ even,

$$
\begin{equation*}
\left\|\left\|\left(J-J_{h}\right) \Lambda^{l+1} U^{0(k)}\right\|\right\| \leqslant C h^{r}\left\|u_{t}^{o(k)}\right\|_{r-1+l} \leqslant C h^{r} k^{-(l-1)}\left\|u_{t}^{0}\right\|_{r} \tag{3.38}
\end{equation*}
$$

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and for $l+1$ odd,

$$
\begin{equation*}
\left\|\left\|\left(J-J_{h}\right) \Lambda^{l+1} U^{0(k)}\right\|\right\| \leqslant C h^{r}\left\|u^{0(k)}\right\|_{r+l} \leqslant C h^{r} k^{-(l-1)}\left\|u^{0}\right\|_{r+1} \tag{3.39}
\end{equation*}
$$

Also, from (3.16), (3.35), (3.24), (3.26) and (2.6), for $v+1$ even
$\left\|\left|F_{n}\left(k J_{h}^{-1}\right) J_{h}^{v+i} \Lambda^{v+1} U^{0(k)} \|\right|^{2}\right.$
$\leqslant C k^{2 v}\left\|\mid \Lambda^{v+1} U^{0(k)}\right\| \|^{2}=C k^{2 v}\left\{\left\|\mathscr{L}^{\frac{v+1}{2}} u^{0(k)}\right\|^{2}+\left(T_{h} \mathscr{L}^{\frac{v+1}{2}} u_{t}^{0(k)}, \mathscr{L}^{\frac{v+1}{2}} u_{t}^{0(k)}\right)\right\}$
$\leqslant C k^{2 v}\left\{\left\|u^{0}\right\|_{v+1}^{2}+\left(\left[T_{h}-T\right] \mathscr{L}^{\frac{v+1}{2}} u_{t}^{o(k)}, \mathscr{L}^{\frac{v+1}{2}} u_{t}^{0(k)}\right)+\left(T \mathscr{L}^{\frac{v+1}{2}} u_{t}^{0(k)}, \mathscr{L}^{\frac{v+1}{2}} u_{t}^{0(k)}\right)\right\}$
$\leqslant C k^{2 v}\left\{\left\|u^{0}\right\|_{v+1}^{2}+h^{r}\left\|u_{t}^{0(k)}\right\|_{v+r-1}\left\|u_{t}^{0(k)}\right\|_{v+1}+\left\|u_{t}^{0}\right\|_{v}^{2}\right\}$
$\leqslant C k^{2 v}\left\{\left\|u^{0}\right\|_{v+1}^{2}+h^{r} k^{-v}\left\|u_{t}^{0}\right\|_{v}\left\|u_{t}^{0}\right\|_{v}+\left\|u_{t}^{0}\right\|_{v}^{2}\right\}$
$\leqslant C\left\{k^{2 v}\left[\left\|u^{0}\right\|_{v+1}^{2}+\left\|u_{t}^{0}\right\|_{v}^{2}\right]+h^{2 r}\left\|u_{t}^{0}\right\|_{r}^{2}\right\}$.
Similarly, from (3.16), (3.36), (3.24), (3.26) and (2.6), for $v+1$ odd,
$\left|\left|\left|F_{n}\left(k J_{h}^{-1}\right) J_{h}^{v+1} \Lambda^{v+1} U^{0(k)}\right| \|\right.\right.$
$\leqslant C k^{2 v}\left\|\mid \Lambda^{v+1} U^{0(k)}\right\|\left\|=C k^{2 v}\right\| \mathscr{L}^{2} u_{t}^{0(k)} \|^{2}+\left(T_{h} \mathscr{L}^{\frac{v}{2}+1} u^{0(k)}, \mathscr{L}^{\frac{v}{2}+1} u^{0(k)}\right)$
$\leqslant C k^{2 v}\left\{\left\|u_{t}^{0}\right\|^{2}+\left(\left[T_{h}-T\right] \mathscr{L}^{\frac{v}{2}+1} u^{0(k)}, \mathscr{L}^{\frac{v}{2}+1} u^{0(k)}\right)+\left(T \mathscr{L}^{\frac{v}{2}+1} u^{0(k)}, \mathscr{L}^{\frac{v}{2}+1} u^{0(k)}\right)\right\}$
$\leqslant C k^{2 v}\left\{\left\|u_{t}^{0}\right\|_{v}^{2}+h^{r}\left\|u^{0(k)}\right\|_{r+v}\left\|u^{0(k)}\right\|_{v+2}+\left\|u^{0}\right\|_{v+1}^{2}\right\}$
$\leqslant C k^{2 v}\left\{\left\|u_{t}^{0}\right\|_{v}^{2}+h^{r} k^{-v}\left\|u^{0}\right\|_{r+1}\left\|u^{0}\right\|_{v+1}+\left\|u^{0}\right\|_{v+1}^{2}\right\}$
$\leqslant C\left\{k^{2 v}\left[\left\|u^{0}\right\|_{v+1}^{2}+\left\|u_{t}^{0}\right\|_{v}^{2}\right]+h^{2 r}\left\|u^{0}\right\|_{r+1}^{2}\right\}$.
Combining the inequalities (3.38), (3.39) in (3.34), we obtain

$$
\begin{equation*}
\sum_{l=1}^{v}\| \| F_{n}\left(k J_{h}^{-1}\right) J_{h}^{l}\left(J-J_{h}\right) \Lambda^{l+1} U^{0(k)}\| \| \leqslant C h^{r}\left[\left\|u^{0}\right\|_{r+1}+\left\|u_{t}^{0}\right\|_{r}\right] \tag{3.42}
\end{equation*}
$$

Now combining (3.32), (3.33), (3.42), (3.40) and (3.41), in (3.31), we obtain |||V(nk) $-W^{n}\| \| \leqslant\left\{h^{r}\left[\left\|u^{0}\right\|_{r+1}+\left\|u_{t}^{0}\right\|_{r}\right]+k^{v}\left[\left\|u^{0}\right\|_{v+1}+\left\|u_{t}^{0}\right\|_{v}\right]\right\}$.

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 $i-I I$ 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 $\left\{W^{n}\right\}_{n \geqslant 0}$ 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 omited.

Remark: We point out that with the results of the above theorems, the optimal rate of convergence $0\left(h^{r}+k^{v}\right)$ is obtained with any starting values $W_{1}^{0}, W_{2}^{0} \in S_{h}^{r}(\Omega)$ satisfying
and

$$
\left\|W_{1}^{0}-u^{0}\right\|=0\left(h^{r}\right)
$$

$$
\left\|W_{2}^{0}-u_{t}^{0}\right\|=0\left(h^{r}\right)
$$

## 4. RATIONAL APPROXIMATIONS OF $e^{t y}$

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

### 4.1. A family of Class $\boldsymbol{i}-\boldsymbol{I}$

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

$$
\begin{equation*}
e^{y \tau}\left(1-\tau^{2}\right)^{s}=\sum_{n=0}^{\infty} \alpha_{n}^{(s)}(y) \tau^{n}, \quad \text { for all } \tau \tag{4.1}
\end{equation*}
$$

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

$$
\begin{align*}
\alpha_{0}^{(s)}(y) & =1  \tag{4.2}\\
\alpha_{n}^{(s)^{\prime}}(y) & =\alpha_{n-1}^{(s)}(y), \quad n=1,2, \ldots \tag{4.3}
\end{align*}
$$

where

$$
\begin{align*}
\alpha_{n}^{(s)^{\prime}}(y) & =\frac{d}{d y} \alpha_{n}^{(s)}(y), \\
\alpha_{2 n}^{(s)}(0) & = \begin{cases}(-1)^{n}\binom{s}{n}, \quad n=0,1, \ldots, s . \\
0, & n>s,\end{cases}  \tag{4.4}\\
\alpha_{2 n+1}^{(s)}(0) & =0, \quad n=0,1, \ldots
\end{align*}
$$

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 $\left\{\alpha_{n}^{(s)}\right\}_{n \geqslant 0}^{y}$ also has the following properties.

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

$$
\begin{array}{ll}
(-1)^{n} \alpha_{2 n}^{(s)}(y) \geqslant 0, & n=0,1, \ldots, s \\
(-1)^{n} \alpha_{2 n}^{(s)}(y) \leqslant 0, & n=1,2, \ldots, s \tag{4.7}
\end{array}
$$

and

$$
\begin{equation*}
(-1)^{s} \alpha_{2 s}^{(s)}(y)<1 \tag{4.8}
\end{equation*}
$$

Proof : From (4.4) and (4.3),
$(-1)^{n} \alpha_{2 n}^{(s)}(y)=(-1)^{n} \alpha_{2 n}^{(s)}(0)+(-1)^{n} \int_{0}^{y} \alpha_{2 n}^{(s)^{\prime}}(\mu) d \mu=\binom{s}{n}+(-1)^{n} \int_{0}^{y} \alpha_{2 n}^{(s)^{\prime}}(\mu) d \mu$
Hence choosing $\mathrm{y}_{n}^{(s)}>0$ such that

$$
\left|\int_{0}^{y_{n}^{(s)}} \alpha_{2 n}^{\left(s s^{\prime}\right.}(\mu) d \mu\right|<\frac{1}{2}\binom{s}{n}
$$

and

$$
y^{(s)}=\min _{1 \leqslant n \leqslant s} y_{n}^{(s)}
$$

the result (4.6) follows.
Also, from (4.3), (4.4) and (4.6), for $0<y \leqslant y^{(s)}$,
$(-1)^{n} \alpha_{2 n}^{(s)^{\prime}}(y)=(-1)^{n} \alpha_{2 n}^{(s)^{\prime}}(0)+(-1)^{n} \int_{0}^{y} \alpha_{2 n}^{(s)^{\prime \prime}}(\mu) d \mu$

$$
=-\int_{0}^{y}(-1)^{n-1} \alpha_{2(n-1)}^{(s)}(\mu) d \mu \leqslant 0,
$$

which gives (4.7).
For $n=s$ in (4.9), for $0 \leqslant y \leqslant y^{(s)}$,

$$
(-1)^{n} \alpha_{2 s}^{(s)}(y)=1+(-1)^{s} \int_{0}^{y} \alpha_{2 s}^{(s)^{\prime}}(\mu) d \mu<1
$$

by virtue of (4.7), which gives (4.8).
Lemma 4.2: Let $R_{s}(y, \tau)$ be the complex valued function

$$
\begin{equation*}
R_{s}(y, \tau)=\sum_{n=0}^{2 s} \alpha_{n}^{(s)}(y) \tau^{n} /\left(1-\tau^{2}\right)^{s}, \tag{4.10}
\end{equation*}
$$

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

$$
\begin{equation*}
\left|R_{s}(y, i \xi)\right| \leqslant 1 \tag{4.11}
\end{equation*}
$$

for $0<y \leqslant y^{(s)}$, for all real $\xi$.
Proof: Define the functions

$$
\begin{equation*}
f(y, \tau)=\sum_{n=0}^{2 s} \alpha_{n}^{(s)}(y) \tau^{n} \tag{4.12}
\end{equation*}
$$

and

$$
\begin{equation*}
F(y, \xi)=f(y, i \xi) f(y,-i \xi) \tag{4.13}
\end{equation*}
$$

Then, from (4.10), we have

$$
\begin{equation*}
|R(y, i \xi)|^{2}=F(y, \xi) /\left(i+\xi^{2}\right)^{2 s} . \tag{4.14}
\end{equation*}
$$

From (4.1) and (4.12),

$$
f(0, \tau)=\left(1-\tau^{2}\right)^{s}
$$

and so, with (4.14),

$$
\begin{equation*}
|R(0, i \xi)|^{2}=1 \tag{4.15}
\end{equation*}
$$

We now show that $\frac{\partial F}{\partial y}(y, \xi) \leqslant 0$ for $0<y \leqslant y^{(s)}$.
From (4.12) and (4.2) and (4.3),

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

Now, from (4.13), (4.16),
$\frac{\partial F}{\partial y}(y, \xi)=2 \operatorname{Re}\left\{\frac{\partial f}{\partial y}(y, i \xi) f(y,-i \xi)\right\}$
$=2 \operatorname{Re}\left\{\left[(i \xi) f(y, i \xi)-(i \xi)^{2 s+1} \alpha_{2}^{(s)}(y)\right] f(y,-i \xi)\right\}$
$=-2 \operatorname{Re}\left\{(i \xi)^{2 s+1} \alpha_{2 s}^{(s)}(y) f(y,-i \xi)\right\}=-2 \alpha_{2 s}^{(s)}(y) \operatorname{Re}\left\{(i \xi)^{2 s+1} \sum_{n=0}^{2 s} \alpha_{2 n}^{(s)}(y)(-i \xi)^{n}\right\}$
$=2 \alpha_{2 s}^{(s)}(y) \sum_{n=0}^{s-1} \alpha_{2 n+1}^{(s)}(y)(-1)^{n+s+1} \xi^{2(n+s+1)}=2 \alpha_{2 s}^{(s)}(y) \sum_{m=s+1}^{2 s} \alpha_{2(m-s)-1}^{(s)}(y)(-1)^{m} \xi^{2 m}$
$=2(-1)^{s} \alpha_{2 s}^{(s)}(y) \sum_{m=s+1}^{2 s}(-1)^{m-s} \alpha_{2(m-s)}^{(s)^{\prime}}(y) \xi^{2 m} \leqslant 0$,
for $0<y \leqq y^{(s)}$, 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

$$
\begin{equation*}
\beta_{n}^{(s)}(x)=(-1)^{n} x^{n} \alpha_{n}^{(s)}\left(\frac{1}{x}\right), \quad n=0,1, \ldots \tag{4.18}
\end{equation*}
$$

for real $x>0$.
Making the change of variables $x=\frac{1}{y}, \overline{z=}-\tau y$ in (4.1), we obtain

$$
\begin{equation*}
e^{-z}\left(1-x^{2} z^{2}\right)^{s}=\sum_{n=0}^{\infty} \beta_{n}^{(s)}(x) z^{n}, \tag{4.19}
\end{equation*}
$$

valid for all $x>0$ and for all $z, s=1,2, \ldots$.
We now define the family of rational functions $\left\{r_{s}\right\}_{s \geqslant 1}$ by

$$
\begin{equation*}
r_{s}(z)=\sum_{n=0}^{2 s} \beta_{n}^{(s)}(x) z^{n} /\left(1-x^{2} z^{2}\right)^{s} \tag{4.20}
\end{equation*}
$$

for $|\operatorname{Rez}|<1 / x$.
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From (4.19) it follows that there exists a constant $C_{s}(x)$ such that

$$
\begin{equation*}
\left|e^{-\imath \xi}-r_{s}(i \xi)\right| \leqslant C_{s}(x)|\xi|^{2 s+1} \tag{4.21}
\end{equation*}
$$

for all real $\xi$, with $|\xi| \leqslant 1$.
Also, from the definition (4.20) and Lemma 4.2, it follows that for given $s \geqslant 1$, there exists an $x^{(s)}>0$ such that

$$
\begin{equation*}
\left|r_{s}(i \xi)\right| \leqslant 1 \tag{4.22}
\end{equation*}
$$

for all real $\xi$, for the choice $x \geqslant x^{(s)}$.
The above results we summarize in the following theorem.
Theorem 4.1: For each integer $s \geqslant 1$, there exists a set of polynomials $\left\{\beta_{n}^{(s)}\right\}_{n \geqslant 1}$ with real coefficients, with $\beta_{n}^{(s)}$ having degree at most $n, n=0,1, \ldots$, such that

$$
e^{-z}\left(1-x^{2} z^{2}\right)^{s}=\sum_{n=0}^{\infty} \beta_{n}^{(s)}(x) z^{n}
$$

for all real $x$, and for all $z$.
If for $x>0, r_{s}$ denotes the rational function

$$
\begin{equation*}
r_{s}(z)=\sum_{n=0}^{2 s} \beta_{n}^{(s)}(x) z^{n} /\left(1-x^{2} z^{2}\right)^{s} \tag{4.20}
\end{equation*}
$$

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

$$
\begin{equation*}
\left|r_{s}(i \xi)-e^{-\imath \xi}\right| \leqslant C_{s}(x)|\xi|^{2 s+1}, \quad \text { for } \quad|\xi| \leqslant 1 \tag{4.21}
\end{equation*}
$$

and

$$
\left|r_{s}(i \xi)\right| \leqslant 1, \quad \text { for all real } \xi
$$

A table of the polynomials $\beta^{(n)}, n=0,1, \ldots, 2 s$, for $s=1, \ldots, 5$ 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 $v=2 s$.

We now examine the computational steps involved in using the rational functions $r_{s}$. In this case (3.6) is equivalent to

$$
\left.\begin{array}{rl}
(-1)^{s}\left(\begin{array}{cc}
T_{h}+x^{2} k^{2} I & 0 \\
0 & T_{h}
\end{array}\right) x^{2} k^{2} I
\end{array}\right)^{s}\binom{W_{1}^{n+1}}{W_{2}^{n+1}} .
$$

with $\widetilde{\beta}_{-1}^{(s)}=0, \widetilde{\beta}_{2 s+1}^{(s)}=0$, and $\widetilde{\beta}_{n}^{(s)}=\beta_{n}^{(s)}, n=0,1, \ldots, s$.

The above equations thus uncouple, into

$$
\begin{align*}
& \left(T_{h}+x^{2} k^{2} I\right)^{s} W_{1}^{n+1}=\sum_{J=0}^{s}(-1)^{J} k^{2 J} T_{h}^{s-J}\left[\tilde{\beta}_{2 J}^{(s)}(x) W_{1}^{n}-k \beta_{2 J+1}^{(s)}(x) W_{2}^{n}\right]  \tag{4.23}\\
& \left(T_{h}+x^{2} k^{2} I\right)^{s} W_{2}^{n+1}=\sum_{J=0}^{s}(-1)^{J} k^{2 J-1} T_{h}^{s-J}\left[k \tilde{\beta}_{2 J}^{(s)}(x) W_{2}^{n}-\widetilde{\beta}_{2 J-1}^{(s)}(x) W_{1}^{n}\right] \tag{4.24}
\end{align*}
$$

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

$$
\begin{align*}
\left(T_{h}+k^{2} x^{2} I\right)^{2} W_{1}^{n+1} & =T_{h}^{2}\left[\beta_{0}^{(2)}(x) W_{1}^{n}-k \beta_{1}^{(2)}(x) W_{2}^{n}\right] \\
& -k T_{h}\left[k \beta_{2}^{(2)}(x) W_{1}^{n}-k^{2} \rho_{3}^{(2)}(x) W_{2}^{n}\right]+\beta_{4}^{(2)}(x) k^{4} W_{1}^{n} \tag{4.25}
\end{align*}
$$

$$
\begin{align*}
\left(T_{h}+k^{2} x^{2} I\right)^{2} W_{2}^{n+1}=T_{h}^{2} \beta_{0}^{(2)}(x) W_{2}^{n}+ & k T_{h}\left[\beta_{1}^{(2)}(x) W_{1}^{n}-k \beta_{2}^{(2)}(x) W_{2}^{n}\right] \\
& +k^{4} \beta_{4}^{(2)}(x) W_{2}^{n}-k^{3} \beta_{3}^{(2)}(x) W_{1}^{n} \tag{4.26}
\end{align*}
$$

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
$A_{h}^{2} Z=T_{h}^{2}\left[\left(\beta_{0}^{(2)}(x)-\frac{\beta_{4}^{(2)}(x)}{x^{4}}\right) W_{1}^{n}-k \beta_{1}^{(2)}(x) W_{2}^{n}\right]$

$$
+k T_{h}\left[k^{2} \beta_{3}^{(2)}(x) W_{2}^{n}-\left(\beta_{2}^{(2)}(x)+2 k \frac{\beta_{4}^{(2)}(x)}{x^{2}}\right) W_{1}^{n}\right]
$$

or

$$
\begin{aligned}
& A_{h} T_{h}^{-1} A_{h} Z=T_{h}\left[\left(\beta_{0}^{(2)}(x)-\frac{\beta_{4}^{(2)}(x)}{x^{4}}\right) W_{1}^{n}-k \beta_{1}^{(2)}(x) W_{2}^{n}\right] \\
&+k {\left[k^{2} \beta_{3}^{(2)}(x) W_{2}^{n}-\left(\beta_{2}^{(2)}(x)+2 k \frac{\beta_{4}^{(2)}(x)}{x^{2}}\right) W_{1}^{n}\right] . }
\end{aligned}
$$

Now set $Y=T_{h}^{-1} A_{h} Z$. Then $Y$ is obtained as the solution of

$$
\begin{aligned}
(Y, \chi)+x^{2} k^{2} a(Y, \chi)=[ & \left.\beta_{0}^{(2)}(x)-\frac{\beta_{4}^{(2)}(x)}{x^{4}}\right]\left(W_{1}^{n}, \chi\right)-k \beta_{1}^{(2)}(x)\left(W_{2}^{n}, \chi\right) \\
& +k^{3} \beta_{3}^{(2)}(x) a\left(W_{2}^{n}, \chi\right)-\left[\beta_{2}^{(2)}(x)+2 k \frac{\beta_{4}^{(2)}(x)}{x^{2}}\right] a\left(W_{1}^{n}, \chi\right)
\end{aligned}
$$

for all $\chi \in S_{h}^{r}(\Omega) . Z$ in turn is obtained as the solution of

$$
(Z, \chi)+x^{2} k^{2} a(Z, \chi)=(Y, \chi), \quad \chi \in S_{h}^{r}(\Omega)
$$

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

$$
\begin{equation*}
e^{-\dot{z}}=1-\sum_{n=0}^{\infty} P_{n}(b)\left(\frac{z}{1+b z}\right)^{n+1} \tag{4.27}
\end{equation*}
$$

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

$$
P_{n}(b)=\frac{b^{n} L_{n}^{(1)}(1 / b)}{(n+1)}, \quad n=0,1, \ldots
$$

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

$$
R_{v}(z)=1-\sum_{n=0}^{v-2} P_{n}(b)\left(\frac{z}{1+b z}\right)^{n+1}
$$

$\operatorname{Re}(z)>-1 / 2 b, v \geqslant 2$, 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 $L_{v-1}^{(1)}=L_{4}^{(1)}, R_{v}$ satisfies (3.1) and (3.2). See [12] for details.

Padé approximations.
The general entry of the Pade table is given by

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

and

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

and

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

It is known that $r_{p, q}$ satisfies (3.1) with $v=p+q$. (3.2) is satisfied by $r_{p, q}$ for $p \geqslant 1$ and $p-2 \leqslant q \leqslant p$. In fact $\left|r_{p, q}(i y)\right|=1$ 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 $v=p+q, \quad p=1,2, \ldots, p-2 \leqslant q \leqslant p$. 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 $r \geqslant 2$ are used. The spaces are required to satisfy

$$
\begin{align*}
& \inf _{\chi \in S^{r}(\Omega)}\left\{\|V-\chi\|+h\|V-\chi\|_{H^{1}(\Omega)}+h^{\frac{1}{2}}\|V-\chi\|_{L^{2}(\partial \Omega)}\right. \\
& \left.+h^{\frac{3}{2}}\|V-\chi\|_{H^{1}(\partial \Omega)}\right\} \leqslant C h^{s}\|V\|_{s} \tag{5.1}
\end{align*}
$$

for $2 \leqslant s \leqslant r$, for some constant $\mathbf{C}$.
In addition, the following inverse property is required

$$
\begin{equation*}
\left\|\frac{\partial \chi}{\partial n}\right\|_{L^{2}(\partial \Omega)} \leqslant C_{1} h^{-\frac{1}{2}}\|\chi\|_{H^{1}(\Omega)} \tag{5.2}
\end{equation*}
$$

for all $\chi \in S_{h}^{r}(\Omega)$, for some constant $C_{1}$.
The nonstandard bilinear form $N_{h}^{\gamma}(.,):. H^{2}(\Omega) \times S_{h}^{r}(\Omega) \rightarrow \mathbb{R}^{1}$ is used,

$$
\begin{equation*}
N_{h}^{\gamma}(\varphi, \psi)=a(\varphi, \psi)-\int_{\partial \Omega}\left(\varphi \frac{\partial \psi}{\partial n}+\psi \frac{\partial \varphi}{\partial n}-\gamma h^{-1} \varphi \psi\right) d \sigma \tag{5.3}
\end{equation*}
$$

where $a(.,$.$) is defined by (2.1a), and \gamma>0$, is a specific constant. Nitsche [10] shows that with the assumption (5.2) and $\gamma^{\circ}$ chosen sufficiently large with respect to $C_{1}, N_{h}^{\gamma}$ is positive definite on $S_{h}^{r}$. The discrete solutions operator $T_{h}$ is now defined by

$$
\begin{equation*}
N_{h}^{\gamma}\left(T_{h} f, \chi\right)=(f, \chi) \tag{5.4}
\end{equation*}
$$

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

$$
\begin{equation*}
\|\chi\|_{L^{2}(\partial \Omega)} \leqslant C_{0} h^{\frac{1}{2}}\|\chi\|_{H^{1}(\Omega)}, \tag{5.5}
\end{equation*}
$$

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

$$
\begin{equation*}
N_{h}\left(T_{h} f, \chi\right)=(f, \chi), \tag{5.6}
\end{equation*}
$$

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

$$
\inf _{\chi \in S_{h}^{r}(\Omega)}\left\{\|V-\chi\|+h\|V-\chi\|_{H^{1}(\Omega)}\right\} \leqslant C h^{s}\|V\|_{s}
$$

for all $V \in H^{s}(\Omega)$, for some constant $C, 1 \leqslant s \leqslant r$.
In addition subspaces $S_{\mu}(\partial \Omega) \subset H^{1}(\partial \Omega)$ are employed, satisfying

$$
\inf _{\chi \in S_{\mu}(\partial \Omega)}\left\{\mu^{\frac{1}{2}}\|\lambda-\chi\|_{H_{\frac{1}{2}}(\partial \Omega)}+\mu^{-\frac{1}{2}}\|\lambda-\chi\|_{H-\frac{1}{2}(\partial \Omega)}\right\} \leqslant C \mu^{s}\|\lambda\|_{H^{s}(\partial \Omega)},
$$

for all $\lambda \in H^{s}(\partial \Omega)$, for $\frac{1}{2} \leqslant s \leqslant r-\frac{3}{2}$.
Also an inverse property is required,

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

Babuška shows that for the ratio $h / \mu$ sufficiently small, the form $a(.$, .) 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

$$
\begin{equation*}
a\left(T_{h} f, \chi\right)=(f, \chi) \tag{5.7}
\end{equation*}
$$

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 $\left\{\beta_{n}^{(s)}(x)\right\}_{n=0}^{2 s}$, for $s=1, \ldots, 5$. For each $s \geqslant 1$, a convenient choice of the parameter $x^{(s)}$ is as follows.

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

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

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

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

and hence $P_{2}^{(s)}$ always has a real positive zero. In general, for $n \geqslant 1$, if $P_{2 n}^{(s)}$ 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 $y^{(s)}=\min _{1 \leqslant n \leqslant s} y_{n}^{(s)}$, and $x^{(s)}=\left[y^{(s)}\right]^{-1}$. The procedure is clearly well defined and yields $x^{(s)}$ with $0<x^{(s)}<\infty$.

Now since

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

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

$$
x^{(s)}=\max _{1 \leqslant n \leqslant s} x_{n}^{(s)}
$$

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

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

| $s=1, v=2$ |
| :--- |
| $\beta_{1}^{(1)}(x)=1$ |
| $\beta_{1}^{(1)}(x)=-1$ |
| $\beta_{2}^{(1)}(x)=\frac{1}{2}-x^{2}$ |
| $s=2, v=4$ |
| $\beta_{0}^{(2)}(x)=1$ |
| $\beta_{1}^{(2)}(x)=-1$ |
| $\beta_{2}^{(2)}(x)=\frac{1}{2}-2 x^{2}$ |
| $\beta_{3}^{(2)}(x)=-\frac{1}{6}+2 x^{2}$ |
| $\beta_{4}^{(2)}(x)=\frac{1}{24}-x^{2}+x^{4}$ |

$$
s=3, v=6
$$

$$
\beta_{0}^{(3)}(x)=1
$$

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

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

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

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

$$
\beta_{5}^{(3)}(x)=-\frac{1}{120}+\frac{1}{2} x^{2}-3 x^{4}
$$

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

$$
s=4, v=8
$$

$$
\beta_{0}^{(4)}(x)=1
$$

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

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

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

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

$$
\beta_{5}^{(4)}(x)=-\frac{1}{120}+\frac{3}{2} x^{2}-6 x^{4}
$$

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

$$
\beta_{7}^{(4)}(x)=-\frac{1}{5040}+\frac{3}{40} x^{2}-x^{4}+4 x^{6}
$$

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

$$
s=5, v=10
$$

$$
\beta_{0}^{(s)}(x)=1
$$

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

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

$$
\beta_{3}^{(5)}(x)=-\frac{1}{6}+5 x^{2}
$$

$$
\begin{aligned}
s=5, v= & 10 \\
\beta_{4}^{(5)}(x) & =\frac{1}{24}-\frac{5}{2} x^{2}+10 x^{4} \\
\beta_{5}^{(5)}(x) & =-\frac{1}{120}+\frac{5}{6} x^{2}-10 x^{4} \\
\beta_{6}^{(5)}(x) & =\frac{1}{720}-\frac{5}{24} x^{2}+5 x^{4}-10 x^{6} \\
\beta_{7}^{(5)}(x) & =-\frac{1}{5040}+\frac{1}{24} x^{2}-\frac{5}{3} x^{4}+10 x^{6} \\
\beta_{8}^{(5)}(x) & =\frac{1}{40320}-\frac{1}{144} x^{2}+\frac{5}{12} x^{4}-5 x^{6}+5 x^{8} \\
\beta_{9}^{(5)}(x) & =-\frac{1}{362880}+\frac{1}{1008} x^{2}-\frac{1}{12} x^{4}+\frac{5}{3} x^{6}-5 x^{8} \\
\beta_{10}^{(5)}(x) & =\frac{1}{3628800}-\frac{1}{8064} x^{2}+\frac{1}{72} x^{4}-\frac{5}{12} x^{6}+\frac{5}{2} x^{6}+x^{8}-x^{10}
\end{aligned}
$$

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