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HIGH ORDER ACCURATE TWO-STEP APPROXIMATIONS FOR HYPERBOLIC EQUATIONS (*)

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Abstract. — *A new class of two-step fully discrete approximation methods of arbitrary accuracy in time is developed for the initial-boundary value problem for second-order hyperbolic equations. The schemes are derived from the explicit second-order character of the equation, as opposed to previously developed high order accurate schemes based on a first-order system formulation. Optimal order rate of convergence estimates are derived for the error of the full discretizations in L^2 and in L^∞. For a given accuracy these schemes provide approximations to the solution with approximately half the computational work required for a single-step method of the same accuracy.*

Résumé. — *On propose dans ce travail une nouvelle classe de schémas à deux pas pour la résolution numérique des équations hyperboliques du second ordre. Les schémas sont basés sur certaines approximations rationnelles de cos z, et sont réalisés par une relation récursive naturelle pour les équations du second ordre. En comparaison avec les schémas à un pas connus, on obtient la même précision optimale dans L^∞ et L^2, avec moitié moins de calculs.*

1. INTRODUCTION

In [3] a class of approximation schemes is developed for second-order evolution equations in Hilbert space of the form

$$v_{tt}+A\,v=0, \qquad 0<t\leqq t^*,$$
$$v(0)=v^0,$$
$$v_t(0)=v_t^0,$$

where $0<t^*<\infty$ is given and A is a self-adjoint, positive definite, possibly unbounded linear operator. For a chosen constant $k>0$, the relation

$$v(t+2k)-2\cos(k\,A^{1/2})\,v(t+k)+v(t)=0, \qquad 0\leqq t\leqq t^*-2k,$$

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is approximated by the difference equation

$$\omega^{n+2}-2r(kA^{1/2})\omega^{n+1}+\omega^{n}=0, \qquad 0\leqq n\leqq[t^*/k]-2, \tag{1.1}$$

where r is a rational function which satisfies $r(\tau)=\cos\tau+O(\tau^{\nu+2})$ as $\tau\to 0$ for some even integer $\nu\geqq 2$. (1.1) is initialized by $\omega^0=v^0$ and a convenient choice of ω^1 depending on r. Under suitable conditions on r, ω^n approximates $u(nk)$ to $O(k^\nu)$ accuracy.

In this work we analyze the application of the above approximation method to initial-boundary value problems for second-order hyperbolic equations, in which case time and space discretizations are coupled. The problem of interest is the initial-boundary value problem

$$\left.\begin{aligned} u_{tt}=-Lu\equiv \sum_{i,j=1}^{N}\frac{\partial}{\partial x_i}\left(a_{ij}(x)\frac{\partial u}{\partial x_j}\right)-a_0(x)u \quad &\text{in } \Omega\times(0,t^*],\\ u=0 \quad \text{on } \partial\Omega\times(0,t^*],&\\ u(0)=u^0 \quad \text{in } \Omega,&\\ u_t(0)=u_t^0 \quad \text{in } \Omega,&\end{aligned}\right\} \tag{1.2}$$

where Ω is a bounded domain in $\mathbf{R}^N$ with C^∞ boundary $\partial\Omega$ and u^0, u_t^0 are given functions. The operator L is assumed to satisfy the uniform ellipticity condition

$$\sum_{i,j=1}^{N} a_{ij}(x)\xi_i\xi_j\geqq d\sum_{i=1}^{N}\xi_i^2,$$

for some constant $d>0$, for all $x\in\overline{\Omega}$ and all $(\xi_1,\xi_2,\ldots,\xi_N)\in\mathbf{R}^N$ and its coefficients are such that $a_{ij}=a_{ji}\in C^\infty(\overline{\Omega})$, $1\leqq i,j\leqq N$ and $a_0\in C^\infty(\overline{\Omega})$ with $a_0\geqq 0$ in $\overline{\Omega}$.

In the remainder of this section we introduce the notation to be used, which will enable us to define the fully discrete approximations and to state the convergence results. Sections 2 and 3 are devoted to the proofs of the convergence in $L^2(\Omega)$ and $L^\infty(\Omega)$, respectively. In section 4 we provide a family of schemes giving arbitrary accuracy in time, using the rational approximations of [3].

For integer $m\geqq 0$ and $1\leqq p\leqq\infty$, $W_p^m=W_p^m(\Omega)$ will denote the Sobolev space of (classes of) functions on Ω, having distributional derivatives of orders up to m in $L^p=L^p(\Omega)$. In particular, in the customary fashion, for $p=2$ we shall write $H^m=W_2^m$ and we denote the norm on H^m by $\|.\|_{H^m}$. The norm on L^∞ we denote by $\|.\|_{L^\infty}$. The inner product on L^2 we denote by $(.,.)$ and its norm simply by $\|.\|$.

Let $\{\lambda_j\}_{j\geq 1}$ denote the eigenvalues, in nondecreasing order, of the elliptic operator L and $\{\varphi_j\}_{j\geq 1}$ the set of corresponding eigenfunctions, a complete orthonormal set in L^2, with $\varphi_j=0$ on $\partial\Omega$.

For $s\geqq 0$ we consider the spaces

$$\dot{H}^s=\{v\in L^2 : \|v\|_s=(\sum_j \lambda_j^s|(v, \varphi_j)|^2)^{1/2}<\infty\}.$$

For integer $s\geqq 0$ it is known that

$$\dot{H}^s=\{v\in H^s : L^j v=0 \text{ on } \partial\Omega \text{ for integer } j<[s/2]\}$$

and that on $\dot{H}^s$ the norms $\|.\|_s$ and $\|.\|_{H^s}$ are equivalent. For $s\geqq 0$ $\dot{H}^{-s}$ will denote the dual of $\dot{H}^s$ with respect to L^2. It is easily seen that the induced norm on $\dot{H}^{-s}$ is given by

$$\|v\|_{-s}=(\sum_j \lambda_j^{-s}|(v, \varphi_j)|^2)^{1/2}, \qquad s\geqq 0.$$

We shall work with the solution operator $T : L^2 \to \dot{H}^2$ of the associated elliptic boundary value problem, defined by

$$a(Tf, v)=(f, v), \qquad \forall v\in \dot{H}^1, \quad \text{given} \quad f\in L^2,$$

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

$$a(v, w)=\int_\Omega\left(\sum_{i,j=1}^{N} a_{ij}\frac{\partial v}{\partial x_i}\frac{\partial w}{\partial x_j}+a_0 vw\right)dx, \qquad v, w\in H^1.$$

For the space discretization of (1.2) we assume the existence, for $0<h\leqq 1$, of a family of finite dimensional subspaces of L^2, which we denote by $S_h=S_h(\Omega)$, and a corresponding family of finite dimensional operators $T_h : L^2 \to S_h$, which possess the following properties:

T_h is self-adjoint, positive semidefinite on L^2

and positive definite on S_h, (1.3)

there exists an integer $r\geqq 2$ and a constant C such that

$$\|(T_h-T)f\|\leqq C h^s\|f\|_{s-2}, \qquad \forall f\in \dot{H}^{s-2}, \quad 1\leqq s\leqq r, \tag{1.4}$$

T_h has eigenvalues $\{0, \mu_1^h, \ldots, \mu_M^h\}$ in nondecreasing order, for some integer $M=M(h)$. Moreover there exists an $h_0>0$ such that for $h\leqq h_0$, there exists a constant A, independent of h, such that $\mu_M^h\leqq A$. (1.5)

It is well-known, for example for the standard Galerkin method, [4], in the context of finite element approximations, where $S_h \subset \dot{H}^1$ and T_h is defined by

$$a(T_h f, \chi) = (f, \chi), \qquad \forall \chi \in S_h, \tag{1.6}$$

that the properties (1.3)-(1.5) hold.

Following [1], the semidiscrete approximation to (1.2) is defined as the map $u^h : [0, t^*] \to S_h$ satisfying

$$\left.\begin{aligned} &T_h u_{tt}^h + u^h = 0, \qquad 0 < t \leqq t^*,\\ &u^h(0) \quad \text{given in } S_h,\\ &u_t^h(0) \text{ given in } S_h. \end{aligned}\right\} \tag{1.7}$$

In [1, 2], optimal-order rate of convergence estimates for $\sup\limits_{0 \leqq t \leqq t^*} \| u^h(t) - u(t) \|$ and $\sup\limits_{0 \leqq t \leqq t^*} \| u^h(t) - u(t) \|_{L^\infty}$ have been derived.

In order to obtain fully discrete schemes, we discretize (1.7) with respect to time according to (1.1). To this end we introduce the operator $L_h = P T_h^{-1} : S_h \to S_h$, where P is the L^2-projection operator onto S_h, and observe that, from (1.7), for any chosen time step $k > 0$,

$$u^h(t+2k) - 2 \cos (k L_h^{1/2}) u^h(t+k) + u^h(t) = 0, \qquad 0 \leqq t \leqq t^* - 2k. \tag{1.8}$$

We now seek a sequence of approximations $\{\omega^n\}_{n \geqq 0} \subset S_h$, where ω^n will approximate $u(nk)$. Let r be a real rational function of the real variable τ such that there exist constants $\sigma > 0$, $C < \infty$ and an even integer $\nu \geqq 2$ such that

$$|r(\tau) - \cos \tau| \leqq C \tau^{\nu+2}, \qquad 0 \leqq \tau \leqq \sigma. \tag{1.9}$$

With appropriate choices of the initial values ω^0 and ω^1 in S_h we define the sequence of approximations ω^n by

$$\omega^{n+2} - 2 r(k L_h^{1/2}) \omega^{n+1} + \omega^n = 0, \qquad 0 \leqq n \leqq [t^*/k] - 2. \tag{1.10}$$

For convergence results we shall work with the following:

DEFINITION I: The rational approximation r is defined to be *of class C-I* if r satisfies (1.9) and there exists a constant $\varkappa > 0$ such that

$$|r(\tau)| \leqq 1 \qquad \text{for} \quad 0 \leqq \tau \leqq \varkappa. \tag{1.11}$$

DEFINITION II: The rational approximation r is defined to be *of class C-II* if r satisfies (1.9) and

$$|r(\tau)| \leqq 1 \quad \text{for all } \tau \geqq 0. \tag{1.12}$$

Clearly every class C-II function is of class C-I. We make the distinction since the use of class C-II rational functions in (1.10) yields *unconditionally convergent* schemes, whereas with C-I functions the schemes are *conditionally convergent*.

There remains the choice of the initial values ω^0 and ω^1 in order to apply (1.10). These will be chosen in a specific way and will be directly computable from the initial data u^0, u_t^0 of (1.2). Since our error estimation techniques rely on comparisons with the semidiscrete approximation (1.7), our choice of ω^0 and ω^1 will be lucid when made through the choice of $u^h(0)$, $u_t^h(0)$ of (1.7), bearing in mind that we require ω^0 to approximate $u(0)=u^0$, and ω^1 to approximate $u(k)$.

To this end, we set $\mathscr{S}_h=S_h\times S_h$ and define

$$\mathscr{L}_h=\begin{pmatrix}0 & -I\\ L_h & 0\end{pmatrix}: \mathscr{S}_h\to\mathscr{S}_h,$$

$$U^h(t)=[u^h(t),\ u_t^h(t)]^T, \qquad 0\leqq t\leqq t^*,$$

and rewrite (1.7) as

$$U_t^h+\mathscr{L}_h U^h=0, \qquad 0\leqq t\leqq t^*, \tag{1.13}$$

where $U^h(0)=[u^h(0),\ u_t^h(0)]^T$ is to be chosen.

We shall also use the operators

$$\mathscr{T}_h=\begin{pmatrix}0 & T_h\\ -I & 0\end{pmatrix}, \qquad \mathscr{L}=\begin{pmatrix}0 & -I\\ L & 0\end{pmatrix}.$$

In general, we shall choose

$$U^h(0)=\mathscr{T}_h^{2s+1}\mathscr{L}^{2s+1}[u^0,\ u_t^0]^T=[T_h^{s+1}L^{s+1}u^0,\ T_h^s L^s u_t^0]^T, \tag{1.14}$$

for some integer $s\geqq 0$. For $s=0$ we interpret $T_h^s L^s u_t^0$ as Pu_t^0. For the optimal L^2-convergence of our scheme we choose $s=0$ in (1.14) and for L^∞-convergence s will depend on N, as will be seen precisely below. We note that the computation of $U^h(0)$ from (1.14) will require the solution of $2s+1$ linear systems of equations of size $\dim S_h\times\dim S_h$ (elliptic projections) with the same real matrix.

Now ω^0 and ω^1 will be obtained from $U^h(0)$ as follows. We choose

$$\omega^0=u^h(0)=T_h^{s+1}L^{s+1}u^0. \tag{1.15}$$

A convenient choice of ω^1 will be to use a single-step procedure, following [1], over *one time step*. We select a rational function $\tilde r$ of the complex variable $z=x+iy$ satisfying for some constants $\sigma_1>0$ and $C<\infty$,

$$|\tilde r(iy)-e^{-iy}|\leqq C|y|^{\nu+1}, \quad \text{all real } y: \quad |y|\leqq\sigma_1. \tag{1.16}$$

and

$$|\tilde{r}(iy)| \leqq C \quad \text{for all real } y. \tag{1.17}$$

We then define $W=[W_1, W_2]^T \in \mathcal{S}_h$ by

$$W=\tilde{r}(k\mathcal{L}_h)\, U^h(0) \tag{1.18}$$

and we set

$$\omega^1 = W_1. \tag{1.19}$$

It will be seen in section 4 that, with the particular choice of rational functions r to be used in (1.10), the computation of ω^n for $n \geqq 2$ will require the solution of a fixed number (depending on ν) of linear systems of equations at each time step with a fixed real matrix. It will also be seen, using the results of [1], that the rational function $\tilde{r}$ needed for the computation of ω^1 from (1.18), (1.19) may be chosen compatible with r, so that the *same real matrix* is used to obtain ω^1 by solving a fixed number of linear systems.

In section 2 we analyze the convergence of the approximation in L^2. We prove in theorem 2.1 that, if r is of class C-II, $\tilde{r}$ satisfies (1.16) and (1.17), ω^0 is given by (1.15) with $s=0$ and ω^1 is chosen by (1.18), (1.19), then there exists a constant $C = C(t^*)$ such that

$$\max_{0 \leqq n \leqq [t^*/k]} \| \omega^n - u(nk) \| \leqq C\,[h^r (\| u^0 \|_{r+2} + \| u_t^0 \|_{r+1}) + k^\nu (\| u^0 \|_{\nu+2} + \| u_t^0 \|_{\nu+2})]. \tag{1.20}$$

In theorem 2.2 it is seen that if r is of class C-I, $\tilde{r}$ satisfies (1.16), (1.17) and ω^0, ω^1 are chosen as in the above announcement of theorem 2.1, then, if T_h has the property that

$$\mu_1^h \geqq C_1 h^2, \tag{1.21}$$

the estimate (1.20) holds, provided

$$k/h \leqq \varkappa\, C_1^{1/2}, \tag{1.22}$$

with $\varkappa$ as in (1.11).

For example, in the case of the standard Galerkin method (1.6), an *inverse assumption* of the form

$$\| \chi \|_1 \leqq C h^{-1} \| \chi \|, \qquad \forall \chi \in S_h,$$

implies (1.21).

The analysis of convergence in L^∞ of the approximation scheme, done in section 3, is based on L^∞-estimates for the approximation of the associated Dirichlet problem. Such estimates are conveniently stated, following [4], as follows. In addition to (1.3)-(1.5) we require

$$\left.\begin{aligned} \| T_h v \|_{L^\infty} &\leqq C \| T v \|_{W^1_\infty}, \\ \| T_h v \| &\leqq C \| T v \|_1, \\ \| (T_h - T) v \|_{L^\infty} &\leqq \gamma(h) \| T v \|_{W^r_\infty}, \end{aligned}\right\} \tag{1.23}$$

for some constant C, where typically for Galerkin methods $\gamma(h) = C h^r$, if $r > 2$; $\gamma(h) = C h^2 \ln h^{-1}$, if $r = 2$. For the derivation of (1.23) we refer to [4] and the references cited therein.

In addition let J_0 be a positive integer such that for some $h_0 > 0$, for all $0 < h \leqq h_0$:

$$\sum_j (\mu_j^h)^{J_0} \leqq C < \infty, \tag{1.24}$$

for some constant C independent of h. It is shown in [2] that in the case of the standard Galerkin method (1.6) we may choose $J_0 = N$. As noted in [2] and the references cited therein, the existence of such a J_0 will depend on the fact that the spectrum of L_h approximates that of L and on known estimates for the asymptotic distribution of the eigenvalues of L.

In theorem 3.1 we prove that if r is of class C-II and $\tilde{r}$ satisfies (1.16), (1.17) and if $U^h(0)$ is chosen by (1.14) with $s \geqq [N/2] + J_0 + 1$ and in turn ω^0 by (1.15) and ω^1 by (1.18), (1.19), then we have for some constant $C = C(t^*)$:

$$\begin{aligned} \max_{0 \leqq n \leqq [t^*/k]} \| \omega^n - u(nk) \|_{L^\infty} \leqq & \, C [\gamma(h) (\| u^0 \|_{s_0} + \| u_t^0 \|_{s_0 - 1}) \\ & + h^r (\| u^0 \|_{2s+r+2} + \| u_t^0 \|_{2s+r+1}) + k^\nu (\| u^0 \|_{2s+\nu+2} + \| u_t^0 \|_{2s+\nu+2})], \end{aligned} \tag{1.25}$$

where $s_0 = 2s + r + [N/2] - 1$.

In theorem 3.2 we prove that if r is of class C-I, $\tilde{r}$ satisfies (1.16), (1.17) and if ω^0, ω^1 are chosen as in the above announcement of theorem 3.1 then the estimate (1.25) is valid, under the condition (1.22), if (1.21) holds.

We close this section with a brief introduction to the rational functions to be used in section 4. We shall use from [3] the family of rational functions $r(\tau) \equiv r_\alpha(x; \tau)$ which satisfy

$$r_\alpha(x; \tau) = \left(\sum_{n=0}^{\alpha} \varphi_n^{(\alpha)}(x) \tau^{2n} \right) \Big/ (1 + x^2 \tau^2)^\alpha, \tag{1.26}$$

with $\alpha = \nu/2$, where $\nu \geqq 2$ is an even integer, and $x > 0$ is a real parameter. $\varphi_n^{(\alpha)}$ will be a real polynomial of degree n in x^2. In particular (1.9) will be satisfied and we show the existence of a $x^{(\alpha)}>0$, which is explicitly computable, such that for $x \geqq x^{(\alpha)}$, $r_\alpha(x; \tau)$ will be of class C–II.

It is then readily seen that for every n the computation of ω^{n+2} from ω^{n+1} and ω^n in (1.10) requires the solution of $\nu/2$ linear systems (ν is even). In [1] a family of rational functions $\tilde{r}(z) \equiv \tilde{r}_\alpha(x; z)$ is constructed, which satisfies

$$\tilde{r}_\alpha(x; z) = \left(\sum_{n=0}^{\alpha} \beta_n^{(\alpha)}(x) z^n \right) \Big/ (1 - x^2 z^2)^\alpha, \tag{1.27}$$

with $\alpha \geqq 1$ integer given by $\alpha = \nu/2$, ν even, where $\beta_n^{(\alpha)}$ is a polynomial of degree at most n in x. With the same value of x in (1.27) as in (1.26), (1.16) and (1.17) are satisfied. Also it is seen that the computation of ω^1 in (1.18), (1.19) due to this special choice of $\tilde{r}$ requires the solution of ν real systems with the same matrix used by (1.26) for the computation of ω^n, $n \geqq 2$.

We also point out that one of the main computational advantages of the schemes developed here lies in the fact that, for a given order of accuracy ν of the time stepping procedure, approximately one half the computational work is required to produce an optimal approximation to the solution, as compared with the single-step schemes of [1].

We remark that two-step schemes producing second-order accuracy in time for second-order hyperbolic equations have been proposed in [7, 8], and [6]. For high order single-step methods, *cf.* [5, 1, 9] and for multistep methods, *cf.* [8, 6].

Throughout the rest of the paper all constants appearing in the error estimates will be denoted by the generic C. Also, conditions of the type $h \leqq h_0$ (i.e., requiring h to be sufficiently small) will be implicitly assumed whenever needed.

2. CONVERGENCE IN L^2

We first find an explicit expression for ω^n for $2 \leqq n \leqq [t^*/k]$ in terms of ω^0, ω^1, *via* (1.10). Let $r(\tau)$ be a rational function of class C-II and ξ_1, ξ_2 be the roots of the quadratic equation

$$\xi^2 - 2r(\tau)\xi + 1 = 0, \qquad \tau \geqq 0. \tag{2.1}$$

Then, obviously,

$$\xi_1(\tau) = r(\tau) + i(1 - r^2(\tau))^{1/2}, \qquad \xi_2(\tau) = \overline{\xi_1(\tau)}, \quad \tau \geqq 0 \tag{2.2}$$

and

$$|\xi_j(\tau)| = 1, \qquad j = 1, 2, \quad \text{all } \tau \geqq 0. \tag{2.3}$$

It can be easily seen that the difference equation (1.10) has the solution

$$\omega^n = \xi_1^n(k L_h^{1/2})\omega^0 + \sum_{j=0}^{n-1} \xi_1^{n-1-j}(k L_h^{1/2}) \xi_2^j(k L_h^{1/2})[\omega^1 - \xi_1(k L_h^{1/2})\omega^0]. \tag{2.4}$$

Let ψ_j^h denote the (L^2-orthonormal) eigenvectors of T_h corresponding to its eigenvalues μ_j^h. For every $v \in L^2$ we then have the spectral representation

$$L_h v = \sum_j (\mu_j^h)^{-1} (v, \psi_j^h) \psi_j^h \tag{2.5}$$

and more generally, for a function g analytic in a neighborhood of the spectrum of L_h,

$$g(L_h) v = \sum_j g((\mu_j^h)^{-1}) (v, \psi_j^h) \psi_j^h. \tag{2.6}$$

We interpret e.g. (2.4) in the light of (2.6).

Now, let ρ_1, ρ_2 be the roots of the quadratic equation

$$\rho^2 - 2 \cos \tau\rho + 1 = 0, \qquad \tau \geqq 0. \tag{2.7}$$

Obviously,

$$\rho_1(\tau) = e^{i\tau}, \qquad \rho_2(\tau) = e^{-i\tau}, \qquad \text{all} \quad \tau \geqq 0, \tag{2.8}$$

i.e.:

$$|\rho_j(\tau)| = 1, \qquad j = 1, 2, \qquad \text{all} \quad \tau \geqq 0. \tag{2.9}$$

From (1.8) we conclude then that

$$\begin{aligned} u^h(nk) &= \rho_1^n(k L_h^{1/2}) u^h(0) \\ &+ \sum_{j=1}^{n-1} \rho_1^{n-1-j}(k L_h^{1/2}) \rho_2^j(k L_h^{1/2}) [u^h(k) - \rho_1(k L_h^{1/2}) u^h(0)]. \end{aligned} \tag{2.10}$$

We now let $E^n = \omega^n - u^h(nk)$, $0 \leqq n \leqq [t^*/k]$. We also let

$$f_n^{(j)}(\tau) = \xi_j^n(\tau) - \rho_j^n(\tau), \qquad j = 1, 2, \quad n = 1, 2, 3, \ldots \tag{2.11}$$

From (2.4) and (2.10) we then obtain, using $\omega^0 = u^h(0)$, the representation

$$\begin{aligned} E^n &= f_n^{(1)}(k L_h^{1/2}) u^h(0) \\ &+ \sum_{j=0}^{n-1} \xi_1^{n-1-j}(k L_h^{1/2}) \xi_2^j(k L_h^{1/2}) [(\omega^1 - u^h(k)) - f_1^{(1)}(k L_h^{1/2}) u^h(0)] \\ &+ \sum_{j=0}^{n-1} \xi_2^j(k L_h^{1/2}) f_{n-1-j}^{(1)}(k L_h^{1/2}) [u^h(k) - \rho_1(k L_h^{1/2}) u^h(0)] \\ &+ \sum_{j=0}^{n-1} \rho_1^{n-1-j}(k L_h^{1/2}) f_j^{(2)}(k L_h^{1/2}) [u^h(k) - \rho_1(k L_h^{1/2}) u^h(0)]. \end{aligned} \tag{2.12}$$

We now state the first main result of this section

THEOREM 2.1: *Let r be of class C-II, $\tilde{r}$ satisfy (1.16) and (1.17), $U^h(0)$ be given by (1.14) for $s=0$, ω^0 be given by (1.15) with $s=0$ and ω^1 be chosen by (1.18), (1.19). Then there exists a $h_0 > 0$ and a constant $C = C(t^*)$ such that for all h: $0 < h \leqq h_0$,*

$$\max_{0 \leqq n \leqq [t^*/k]} \| \omega^n - u(nk) \| \leqq C[h^r(\| u^0 \|_{r+2} + \| u_t^0 \|_{r+1}) + k^\nu(\| u^0 \|_{\nu+2} + \| u_t^0 \|_{\nu+2})]. \quad (2.13)$$

The proof of this theorem will be given in a series of lemmas:

LEMMA 2.1: *Let r be of class C-II and let $f_n^{(j)}$ be defined by (2.11). Then there exists a constant C such that for all $\tau \geqq 0$:*

$$| f_n^{(j)}(\tau) | \leqq n C \tau^l, \qquad j=1, 2, \quad 1 \leqq l \leqq \nu+1, \quad n=1, 2, \ldots \quad (2.14)$$

Also

$$| f_n^{(j)}(\tau) | \leqq 2, \qquad j=1, 2, \quad n=1, 2, \ldots \quad (2.14')$$

Proof: The proof follows from (1.9), (1.12), (2.2), (2.8) and the proof of lemma 2.3 of [3]. ■

We now recall some notation from [1]. Given $k > 0$ let J be the least integer for which $k\lambda_j^{1/2} > 1$ for $j \geqq J$. Then, given $v \in L^2$, we define

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

It is easily seen that $v^{(k)} \in C^\infty(\Omega)$ and that the following hold:

$$\| v^{(k)} \|_{s+m} \leqq k^{-m} \| v \|_s, \qquad \text{all} \quad m, s \geqq 0. \quad (2.15)$$

$$\| v - v^{(k)} \|_p \leqq k^{s-p} \| v \|_s, \qquad \text{all} \quad s \geqq 0 \quad \text{and} \quad \text{all real } p. \quad (2.16)$$

LEMMA 2.2: *Under the hypotheses of theorem 2.1, there exists a constant $C = C(t^*)$ such that for $j=1, 2$, and $1 \leqq n \leqq [t^*/k]$ we have*

$$\| f_n^{(j)}(k L_h^{1/2}) [u^h(k) - \rho_1(k L_h^{1/2}) u^h(0)] \| \leqq C k [k^\nu(\| u^0 \|_{\nu+2} + \| u_t^0 \|_{\nu+2}) + h^r(\| u^0 \|_{r+2} + \| u_t^0 \|_{r+1})]. \quad (2.17)$$

Proof: From (1.7) we have that

$$u^h(k) = \cos(k L_h^{1/2}) u^h(0) + L_h^{-1/2} \sin(k L_h^{1/2}) u_t^h(0),$$

from which, using (2.8) and (1.14) with $s=0$ we obtain

$$f_n^{(j)}(k L_h^{1/2}) [u^h(k) - \rho_1(k L_h^{1/2}) u^h(0)] \quad (2.18)$$
$$= f_n^{(j)}(k L_h^{1/2}) L_h^{-1/2} \sin(k L_h^{1/2}) u_t^0 - i f_n^{(j)}(k L_h^{1/2}) \sin(k L_h^{1/2}) T_h L u^0.$$

The first term of the right-hand side of (2.18) can be written as

$$f_n^{(j)}(k L_h^{1/2}) L_h^{-1/2} \sin(k L_h^{1/2}) u_t^0 = f_n^{(j)}(k L_h^{1/2}) L_h^{-1/2} \sin(k L_h^{1/2})(u_t^0 - u_t^{0(k)})$$
$$+ \sum_{l=0}^{\nu/2} f_n^{(j)}(k L_h^{1/2}) L_h^{-1/2} \sin(k L_h^{1/2}) T_h^l (T-T_h) L^{l+1} u_t^{0(k)}$$
$$+ f_n^{(j)}(k L_h^{1/2}) L_h^{-1/2} \sin(k L_h^{1/2}) T_h^{\nu/2+1} L^{\nu/2+1} u_t^{0(k)}. \quad (2.19)$$

We first observe that for any $\chi \in L^2$, using (2.6), (2.14') and the fact that $\sin x \leqq x$ for $x \geqq 0$, we have

$$\| f_n^{(j)}(k L_h^{1/2}) L_h^{-1/2} \sin(k L_h^{1/2}) \chi \|$$
$$= \| \sum_q f_n^{(j)}(k(\mu_q^h)^{-1/2}) (\mu_q^h)^{1/2} \sin(k(\mu_q^h)^{-1/2}) (\chi, \psi_q^h) \psi_q^h \|$$
$$\leqq k \max_q | f_n^{(j)}(k(\mu_q^h)^{-1/2}) | . \| \chi \| \leqq C k \| \chi \|. \quad (2.21)$$

Also, for $1 \leqq l \leqq \nu/2$ by (2.6) and (2.14) we have for $\chi \in L^2$:

$$\| f_n^{(j)}(k L_h^{1/2}) L_h^{-1/2} \sin(k L_h^{1/2}) T_h^l \chi \|$$
$$\leqq k \max_q | f_n^{(j)}(k(\mu_q^h)^{-1/2}) | (\mu_q^h)^l \| \chi \| \leqq C nkk^{2l} \| \chi \| \leqq C k^{2l} \| \chi \|, \quad (2.22)$$

and similarly, using (1.5) and (2.14) with $l = \nu + 1$,

$$\| f_n^{(j)}(k L_h^{1/2}) L_h^{-1/2} \sin(k L_h^{1/2}) T_h^{\nu/2+1} \chi \|$$
$$\leqq k \max_q | f_n^{(j)}(k(\mu_q^h)^{-1/2}) | (\mu_q^h)^{\nu/2+1} \| \chi \|$$
$$\leqq C nkk^{\nu+1} \max_q (\mu_q^h)^{1/2} \| \chi \| \leqq C k^{\nu+1} \| \chi \|. \quad (2.23)$$

Now by (2.21) and (2.16) we obtain

$$\| f_n^{(j)}(k L_h^{1/2}) L_h^{-1/2} \sin(k L_h^{1/2}) (u_t^0 - u_t^{0(k)}) \| \leqq C k^{\nu+1} \| u_t^0 \|_\nu. \quad (2.24)$$

Similarly, (2.21), (2.15) and (1.4) give that

$$\| f_n^{(j)}(k L_h^{1/2}) L_h^{-1/2} \sin(k L_h^{1/2}) (T-T_h) L u_t^{0(k)} \| \leqq C kh^r \| u_t^0 \|_r. \quad (2.25)$$

Also by (2.22), (2.15), and (1.4) we see that for $1 \leqq l \leqq \nu/2$:

$$\| f_n^{(j)}(k L_h^{1/2}) L_h^{-1/2} \sin(k L_h^{1/2}) T_h^l (T-T_h) L^{l+1} u_t^{0(k)} \|$$
$$\leqq C k^{2l} h^r \| u_t^{0(k)} \|_{2l+r} \leqq C kh^r \| u_t^0 \|_{r+1}. \quad (2.26)$$

Finally, by (2.23), (2.15) and (1.5) we obtain

$$\| f_n^{(j)}(k L_h^{1/2}) L_h^{-1/2} \sin(k L_h^{1/2}) T_h^{\nu/2+1} L^{\nu/2+1} u_t^{0(k)} \| \leqq C k^{\nu+1} \| u_t^0 \|_{\nu+2}. \quad (2.27)$$

Hence, by (2.19), (2.24)-(2.27) we conclude that

$$\| f_n^{(j)}(k L_h^{1/2}) L_h^{-1/2} \sin(k L_h^{1/2}) u_t^0 \| \leqq C k (k^\nu \| u_t^0 \|_{\nu+2} + h^r \| u_t^0 \|_{r+1}). \quad (2.28)$$

Now, for the second term of the right-hand-side of (2.18) we have

$$\begin{aligned} f_n^{(j)}(k L_h^{1/2}) \sin(k L_h^{1/2}) T_h L u^0 &= f_n^{(j)}(k L_h^{1/2}) \sin(k L_h^{1/2}) T_h L(u^0 - u^{0(k)}) \\ &+ \sum_{l=0}^{\nu/2-1} f_n^{(j)}(k L_h^{1/2}) \sin(k L_h^{1/2}) T_h^{l+1} (T - T_h) L^{l+2} u^{0(k)} \\ &+ f_n^{(j)}(k L_h^{1/2}) \sin(k L_h^{1/2}) T_h^{\nu/2+1} L^{\nu/2+1} u^{0(k)}. \quad (2.29) \end{aligned}$$

Using now (2.6) and (2.14) we observe that for any $\chi \in L^2$ and for $0 \leqq l \leqq \nu/2 - 1$,

$$\begin{aligned} \| f_n^{(j)}(k L_h^{1/2}) \sin(k L_h^{1/2}) T_h^{l+1} \chi \| &\leqq \max_q | f_n^{(j)}(k(\mu_q^h)^{-1/2}) \sin(k(\mu_q^h)^{-1/2}) | (\mu_q^h)^{l+1} \| \chi \| \\ &\leqq C n k^{2l+1} \max_q (\mu_q^h)^{-(l+(1/2))} k (\mu_q^h)^{-1/2} (\mu_q^h)^{l+1} \| \chi \| \\ &\leqq C k^{2l+1} \| \chi \|. \quad (2.30) \end{aligned}$$

Similarly, for $\chi \in L^2$ we see by (1.5), (2.6) and (2.14) with $l = \nu + 1$, that

$$\| f_n^{(j)}(k L_h^{1/2}) \sin(k L_h^{1/2}) T_h^{\nu/2+1} \chi \| \leqq C k^{\nu+1} \| \chi \|. \quad (2.31)$$

Hence we conclude by (2.29), (2.30) and (2.31) in analogy with previous calculations that

$$\| f_n^{(j)}(k L_h^{1/2}) \sin(k L_h^{1/2}) T_h L u^0 \| \leqq C k (k^\nu \| u^0 \|_{\nu+2} + h^r \| u^0 \|_{r+2}). \quad (2.32)$$

Finally, (2.18), (2.28) and (2.32) prove (2.17). ■

LEMMA 2.3: *Under the hypotheses of theorem* 2.1, *there exists a constant* $C = C(t^*)$ *such that*

$$\| f_1^{(1)}(k L_h^{1/2}) u^h(0) \| \leqq C k (k^\nu \| u^0 \|_{\nu+2} + h^r \| u^0 \|_{r+1}). \quad (2.33)$$

Proof: We have

$$f_1^{(1)}(k L_h^{1/2}) u^h(0) = f_1^{(1)}(k L_h^{1/2}) T_h L (u^0 - u^{0(k)})$$
$$+ \sum_{l=0}^{\nu/2-1} f_1^{(1)}(k L_h^{1/2}) T_h^{l+1} (T - T_h) L^{l+2} u^{0(k)}$$
$$+ f_1^{(1)}(k L_h^{1/2}) T_h^{\nu/2+1} L^{\nu/2+1} u^{0(k)}. \quad (2.34)$$

Using (1.4), (2.6), (2.14) with $n=1$ and (2.15) in an analogous way as in previous calculations we obtain

$$\left.\begin{aligned} &\| f_1^{(1)}(k L_h^{1/2}) T_h^{l+1} (T - T_h) L^{l+2} u^{0(k)} \| \leqq C k h^r \| u^0 \|_{r+1}, \\ &\qquad 0 \leqq l \leqq \nu/2 - 1. \end{aligned}\right\} \quad (2.35)$$

Also, by (2.6), (2.14) with $n=1$, $l=\nu+1$, (1.5) and (2.15) we obtain

$$\| f_1^{(1)}(k L_h^{1/2}) T_h^{\nu/2+1} L^{\nu/2+1} u^{0(k)} \| \leqq C k^{\nu+1} \| u^0 \|_{\nu+2}. \quad (2.36)$$

Finally by (2.6), (2.14) with $n=1$, $l=2$ and (2.16) we see that

$$\| f_1^{(1)}(k L_h^{1/2}) T_h L (u^0 - u^{0(k)}) \| \leqq C k^{\nu+1} \| u^0 \|_{\nu+1}. \quad (2.37)$$

Now, (2.34)-(2.37) give (2.33). ■

Let $\mathbf{L}^2 = L^2(\Omega) \times L^2(\Omega)$. Then we define, following [1], $((.,.))$: $\mathbf{L}^2 \to \mathbf{C}$ by

$$((X, \Psi)) = (\chi_1, \psi_1) + (T_h \chi_2, \psi_2),$$

where $X = [\chi_1, \chi_2]^T$ and $\Psi = [\psi_1, \psi_2]^T$. Note that $((.,.))$ is an inner product on $\mathscr{S}_h$. The associated seminorm (norm on $\mathscr{S}_h$) we denote by $|||X||| = ((X, X))^{1/2}$.

Recalling the definition of the operator $\mathscr{T}_h$ from the introduction we note that $\mathscr{T}_h$ restricted to $\mathscr{S}_h$ possesses a set of purely imaginary eigenvalues $\{\eta_{\pm j}\}_{j=1}^M$ given by $\eta_j = i(\mu_j^h)^{1/2}$, $\eta_{-j} = -i(\mu_j^h)^{1/2}$, $1 \leqq j \leqq M$ and a set of corresponding eigenvectors $\{\Phi_{\pm j}\}$, orthonormal with respect to $((.,.))$ given by

$$\Phi_{\pm j} = \frac{1}{\sqrt{2}} [\psi_j^h, \pm i(\mu_j^h)^{-1/2} \psi_j^h]^T, \qquad 1 \leqq j \leqq M.$$

We also set $V^{(k)} = [V_1^{(k)}, V_2^{(k)}]^T$ for $V = [V_1, V_2]^T \in \mathbf{L}^2$, and define the operator $\mathscr{T}$ by

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

We have

LEMMA 2.4: *Under the hypotheses of theorem* 2.1 *we have for some constant* $C=C(t^*)$ *that*

$$\|\omega^1-u^h(k)\| \leqq C k [k^\nu(\|u^0\|_{\nu+2}+\|u_t^0\|_\nu)+h^r(\|u^0\|_{r+1}+\|u_t^0\|_r)]. \quad (2.38)$$

Proof: Under the hypotheses of theorem 2.1, with notation introduced in section 1 we see that

$$\omega^1-u^h(k)=W_1-U_1^h(k), \quad (2.39)$$

where $W=[W_1, W_2]^T$ is given by (1.18) and $U^h(t)=[u^h(t), u_t^h(t)]^T$ satisfies for $t=0$ (1.14) with $s=0$. Hence, introducing $U^0=[u^0, u_t^0]^T$ and

$$F(z)=\tilde{r}(z)-e^{-z}, \quad (2.40)$$

we have, *cf.* [1],

$$W-U^h(k)=F(k\mathscr{L}_h)\mathscr{T}_h\mathscr{L}(U^0-U^{0(k)})$$
$$+\sum_{l=0}^{\nu-1} F(k\mathscr{L}_h)\mathscr{T}_h^{l+1}(\mathscr{T}-\mathscr{T}_h)\mathscr{L}^{l+2}U^{0(k)}+F(k\mathscr{L}_h)\mathscr{T}_h^{\nu+1}\mathscr{L}^{\nu+1}U^{0(k)}.$$

Hence, by (2.39):

$$\|\omega^1-u^h(k)\| \leqq |||W-U^h(k)|||$$
$$\leqq |||F(k\mathscr{L}_h)\mathscr{T}_h\mathscr{L}(U^0-U^{0(k)})|||+|||F(k\mathscr{L}_h)\mathscr{T}_h(\mathscr{T}-\mathscr{T}_h)\mathscr{L}^2U^{0(k)}|||$$
$$+\sum_{l=1}^{\nu-1}|||F(k\mathscr{L}_h)\mathscr{T}_h^{l+1}(\mathscr{T}-\mathscr{T}_h)\mathscr{L}^{l+2}U^{0(k)}|||$$
$$+|||F(k\mathscr{L}_h)\mathscr{T}_h^{\nu+1}\mathscr{L}^{\nu+1}U^{0(k)}|||. \quad (2.41)$$

As in [1], lemma 3.1, by (1.16), (1.17) we easily deduce that there is a constant C such that

$$|F(iy)| \leqq C|y|^l, \quad 0 \leqq l \leqq \nu+1, \quad \text{all real } y. \quad (2.42)$$

We conclude for $X \in \mathbf{L}^2$ that for $1 \leqq l \leqq \nu+1$,

$$|||F(k\mathscr{L}_h)\mathscr{T}_h^l X||| = |||\sum_q F(k\eta_q^{-1})\eta_q^l((X, \Phi_q))\Phi_q||| \leqq Ck^l|||X|||. \quad (2.43)$$

Now, by (2.43), (2.15), (2.16) and (1.5) we see that

$$|||F(k\mathscr{L}_h)\mathscr{T}_h\mathscr{L}(U^0-U^{0(k)})|||^2 \leqq Ck^2|||\mathscr{L}(U^0-U^{0(k)})|||^2$$
$$=Ck^2[\|u_t^0-u_t^{0(k)}\|^2+(T_h(Lu^0-Lu^{0(k)}), Lu^0-Lu^{0(k)})]$$
$$\leqq Ck^2(\|u_t^0-u_t^{0(k)}\|^2+\|Lu^0-Lu^{0(k)}\|^2)$$
$$\leqq [Ck^{\nu+1}(\|u^0\|_{\nu+2}+\|u_t^0\|_\nu)]^2. \quad (2.44)$$

Also, by (2.43), (2.15) and (1.4) we conclude that

$$|||F(k\mathscr{L}_h)\mathscr{T}_h(\mathscr{T}-\mathscr{T}_h)\mathscr{L}^2 U^{0(k)}||| \leqq Ck|||(\mathscr{T}-\mathscr{T}_h)\mathscr{L}^2 U^{0(k)}||| = Ck\|(T-T_h)Lu_t^{0(k)}\| \leqq Ckh^r\|u_t^0\|_r. \quad (2.45)$$

Since (1.4) and (2.15) give

$$|||(\mathscr{T}-\mathscr{T}_h)\mathscr{L}^{l+2}U^{0(k)}||| \leqq \begin{cases} \|(T-T_h)L^{l/2+1}u_t^{0(k)}\| \leqq Ch^r\|u_t^{0(k)}\|_{r+l}, & l \text{ even},\\ \|(T-T_h)L^{(l+3)/2}u^{0(k)}\| \leqq Ch^r\|u^{0(k)}\|_{r+l+1}, & l \text{ odd},\end{cases}$$

we conclude by (2.43) that

$$|||F(k\mathscr{L}_h)\mathscr{T}_h^{l+1}(\mathscr{T}-\mathscr{T}_h)\mathscr{L}^{l+2}U^{0(k)}||| \leqq Ck^{l+1}|||(\mathscr{T}-\mathscr{T}_h)\mathscr{L}^{l+2}U^{0(k)}||| \leqq Ckh^r(\|u^0\|_{r+1}+\|u_t^0\|_r). \quad (2.46)$$

Finally, since ν is even we obtain by (2.43) and (2.15):

$$|||F(k\mathscr{L}_h)\mathscr{T}_h^{\nu+1}\mathscr{L}^{\nu+1}U^{0(k)}||| \leqq Ck^{\nu+1}(\|u^0\|_{\nu+1}+\|u_t^0\|_\nu). \quad (2.47)$$

Combining now (2.41), (2.44)-(2.47) we obtain (2.38). ■

We now return to the proof of theorem 2.1. We have for $0 \leqq n \leqq [t^*/k]$,

$$\|\omega^n - u(nk)\| \leqq \|\omega^n - u^h(nk)\| + \|u^h(nk)-u(nk)\|. \quad (2.48)$$

By (2.12), using (2.3), (2.9) and (2.14′), we obtain for $0 \leqq n \leqq [t^*/k]$,

$$\|\omega^n - u^h(nk)\| \leqq n\{\|\omega^1 - u^h(k)\| + \|f_1^{(1)}(kL_h)u^h(0)\| + \max_{0\leqq m\leqq[t^*/k]}\sum_{j=1}^{2}\|f_m^{(j)}(kL_h^{1/2})[u^h(k)-\rho_1(kL_h^{1/2})u^h(0)]\|\}.$$

Hence, by (2.17), (2.33) and (2.38) we see that

$$\|\omega^n - u^h(nk)\| \leqq C[k^\nu(\|u^0\|_{\nu+2}+\|u_t^0\|_{\nu+2})+h^r(\|u^0\|_{r+2}+\|u_t^0\|_{r+1})]. \quad (2.49)$$

Now, [2], lemma 2.2, with $s=0$ implies that for $0 \leqq n \leqq [t^*/k]$:

$$\|u(nk)-u^h(nk)\| \leqq Ch^r(\|u^0\|_{r+1}+\|u_t^0\|_r). \quad (2.50)$$

Hence (2.13) follows from (2.48)-(2.50) and the proof of theorem 2.1 is now complete. ■

We now turn to the câse when $r(\tau)$ is a rational approximation of class C-I. It is now clear that the conclusions of lemma 2.1 hold for $0 \leqq \tau \leqq \varkappa$, with $\varkappa$ defined by (1.11). Under the additional hypothesis (1.21) it is clear that the condition

(1.22) implies that $k|\eta_j|^{-1} \leqq \varkappa$, all j. Retracing the steps of the proof of theorem 2.1, modifying them appropriately, we can verify the following result, the proof of which we omit:

THEOREM 2.2: *Let r be of class* C-I, *$\tilde{r}$ satisfy* (1.16), (1.17), *$U^h(0)$ be given by* (1.14) *for $s=0$, ω^0 be given by* (1.15) *with $s=0$ and ω^1 be chosen by* (1.18), (1.19). *Suppose that T_h satisfies* (1.21). *Then for h sufficiently small, provided* (1.22) *holds, the estimate* (2.13) *is valid for some constant $C=C(t^*)$.* ■

REMARK: It is clear that if instead of (1.17) we have

$$|\tilde{r}(iy)| \leqq C \quad \text{for real } y : |y| \leqq \sigma_2,$$

for some constant σ_2, then it is possible to prove (2.13) under an appropriate bound on k/h, provided (1.21) holds.

3. CONVERGENCE IN L^∞

The main result of this section is:

THEOREM 3.1: *Let r be of class* C-II, *$\tilde{r}$ satisfy* (1.16) *and* (1.17), *$U^h(0)$ be given by* (1.14), *ω^0 by* (1.15) *and ω^1 by* (1.18), (1.19) *with $s \geqq [N/2]+J_0+1$, where J_0 is defined by* (1.24). *Let $s_0 = 2s+r+[N/2]-1$ and in addition to* (1.3)-(1.5) *let T_h satisfy* (1.23) *as well. Then there exists a $h_0>0$ and a constant $C=C(t^*)$ such that for all $0<h\leqq h_0$,*

$$\max_{0\leqq n\leqq[t^*/k]} \|\omega^n - u(nk)\|_{L^\infty} \leqq C[\gamma(h)(\|u^0\|_{s_0} + \|u_t^0\|_{s_0-1}) + h^r(\|u^0\|_{2s+r+2} + \|u_t^0\|_{2s+r+1}) + k^\nu(\|u^0\|_{2s+\nu+2} + \|u_t^0\|_{2s+\nu+1})]. \quad (3.1)$$

The proof will be given in a series of lemmas. We first observe, as a consequence of the hypotheses of theorem 3.1 and of lemma 3.1 of [2], that we have the following L^∞-estimate on the eigenvectors ψ_j^h of T_h:

$$\|\psi_j^h\|_{L^\infty} \leqq C|\eta_j|^{-2K} = C(\mu_j^h)^{-K}, \quad (3.2)$$

when $K=[N/2]+1$.

LEMMA 3.1: *Under the hypotheses of theorem 3.1, there exists a constant $C=C(t^*)$ such that for $j=1$, 2 and $1\leqq n\leqq[t^*/k]$ we have*

$$\|f_n^{(j)}(kL_h^{1/2})[u^h(k)-\rho_1(kL_h^{1/2})u^h(0)]\|_{L^\infty} \leqq Ck[k^\nu(\|u^0\|_{2s+\nu+2} + \|u_t^0\|_{2s+\nu+2}) + h^r(\|u^0\|_{2s+r+2} + \|u_t^0\|_{2s+r+1})]. \quad (3.3)$$

Proof: In analogy with (2.18) we now have

$$f_n^{(j)}(kL_h^{1/2})[u^h(k)-\rho_1(kL_h^{1/2})u^h(0)]$$
$$=f_n^{(j)}(kL_h^{1/2})L_h^{-1/2}\sin(kL_h^{1/2})T_h^s L^s u_t^0$$
$$-if_n^{(j)}(kL_h^{1/2})\sin(kL_h^{1/2})T_h^{s+1}L^{s+1}u^0. \quad (3.4)$$

Now,

$$f_n^{(j)}(kL_n^{1/2})L_h^{-1/2}\sin(kL_h^{1/2})T_h^s L^s u_t^0$$
$$=f_n^{(j)}(kL_h^{1/2})L_h^{-1/2}\sin(kL_h^{1/2})T_h^s L^s(u_t^0-u_t^{0\,(k)})$$
$$+\sum_{l=0}^{\nu/2} f_n^{(j)}(kL_h^{1/2})L_h^{-1/2}\sin(kL_h^{1/2})T_h^{s+l}(T-T_h)L^{s+l+1}u_t^{0\,(k)}$$
$$+f_n^{(j)}(kL_h^{1/2})L_h^{-1/2}\sin(kL_h^{1/2})T_h^{s+\nu/2+1}L^{s+\nu/2+1}u_t^{0\,(k)}. \quad (3.5)$$

For $\chi\in L^2$ let $K=[N/2]+1$ and $1\leqq l\leqq\nu/2$. Then, using (2.6), (2.14), (3.2) and (1.24), since $s\geqq K+J_0$, we have

$$\|f_n^{(j)}(kL_h^{1/2})L_h^{-1/2}\sin(kL_h^{1/2})T_h^{s+l}\chi\|_{L^\infty}$$
$$=\|\sum_q f_n^{(j)}(k(\mu_q^h)^{-1/2})(\mu_q^h)^{1/2}\sin(k(\mu_q^h)^{-1/2})(\mu_q^h)^{s+l}(\chi,\psi_q^h)\psi_q^h\|_{L^\infty}$$
$$\leqq k(\sum_q|f_n^{(j)}(k(\mu_q^h)^{-1/2})|(\mu_q^h)^{s+l}\|\psi_q^h\|_{L^\infty})\|\chi\|$$
$$\leqq C\,knk^{2l}(\sum_q(\mu_q^h)^{s-K-J_0}(\mu_q^h)^{J_0})\|\chi\|\leqq C\,k^{2l}\|\chi\|. \quad (3.6)$$

Similarly, using (2.6), (2.14′), (3.2) and (1.24) we conclude for any $\chi\in L^2$ that

$$\|f_n^{(j)}(kL_h^{1/2})L_h^{-1/2}\sin(kL_h^{1/2})T_h^s\chi\|_{L^\infty}\leqq C\,k\|\chi\|. \quad (3.7)$$

Finally, using (2.6), (2.14) with $l=\nu+1$, (3.2), (1.24) and (1.5) we obtain for $\chi\in L^2$:

$$\|f_n^{(j)}(kL_h^{1/2})L_h^{-1/2}\sin(kL_h^{1/2})T_h^{s+\nu/2+1}\chi\|_{L^\infty}\leqq C\,k^{\nu+1}\|\chi\|. \quad (3.8)$$

Now, (3.8) and (2.15) give

$$\|f_n^{(j)}(kL_h^{1/2})L_h^{-1/2}\sin(kL_h^{1/2})T_h^{s+\nu/2+1}L^{s+\nu/2+1}u_t^{0\,(k)}\|_{L^\infty}$$
$$\leqq C\,k^{\nu+1}\|u_t^0\|_{2s+\nu+2}. \quad (3.9)$$

By (3.7), (2.16) we have

$$\|f_n^{(j)}(kL_h^{1/2})L_h^{-1/2}\sin(kL_h^{1/2})T_h^s L^s(u_t^0-u_t^{0\,(k)})\|_{L^\infty}\leqq C\,k^{\nu+1}\|u_t^0\|_{2s+\nu}. \quad (3.10)$$

Now, (3.7), (2.15) and (1.4) give

$$\| f_n^{(j)}(k L_h^{1/2}) L_h^{-1/2} \sin(k L_h^{1/2}) T_h^s (T - T_h) L^{s+1} u_t^{0\,(k)} \|_{L^\infty} \leq C k \| (T - T_h) L^{s+1} u_t^{0\,(k)} \| \leq C k h^r \| u_t^0 \|_{2s+r}. \quad (3.11)$$

In addition for $1 \leq l \leq \nu/2$, (3.6), (1.4) and (2.15) give

$$\| f_n^{(j)}(k L_h^{1/2}) L_h^{-1/2} \sin(k L_h^{1/2}) T_h^{s+l} (T - T_h) L^{s+l+1} u_t^{0\,(k)} \|_{L^\infty} \leq C k^{2l} \| (T - T_h) L^{s+l+1} u_t^{0\,(k)} \| \leq C k h^r \| u_t^0 \|_{2s+r+1}. \quad (3.12)$$

Combining now (3.5), (3.9)-(3.12) we obtain

$$\| f_n^{(j)}(k L_h^{1/2}) L_h^{-1/2} \sin(k L_h^{1/2}) T_h^s L^s u_t^0 \|_{L^\infty} \leq C k (h^r \| u_t^0 \|_{2s+r+1} + k^\nu \| u_t^0 \|_{2s+\nu+2}). \quad (3.13)$$

We now write

$$\begin{aligned} f_n^{(j)}(k L_h^{1/2}) \sin(k L_h^{1/2}) T_h^{s+1} L^{s+1} u^0 &= f_n^{(j)}(k L_h^{1/2}) \sin(k L_h^{1/2}) T_h^{s+1} L^{s+1} (u^0 - u^{0\,(k)}) \\ &+ \sum_{l=0}^{\nu/2-1} f_n^{(j)}(k L_h^{1/2}) \sin(k L_h^{1/2}) T_h^{s+l+1} (T - T_h) L^{s+l+2} u^{0\,(k)} \\ &+ f_n^{(j)}(k L_h^{1/2}) \sin(k L_h^{1/2}) T_h^{s+\nu/2+1} L^{s+\nu/2+1} u^{0\,(k)}. \quad (3.14) \end{aligned}$$

Using similar estimates as above (*cf.* also the proof of lemma 2.2), we now have

$$\| f_n^{(j)}(k L_h^{1/2}) \sin(k L_h^{1/2}) T_h^{s+1} L^{s+1} u^0 \|_{L^\infty} \leq C k (h^r \| u^0 \|_{2s+r+2} + k^\nu \| u^0 \|_{2s+\nu+2}). \quad (3.15)$$

Finally, (3.4), (3.13) and (3.15) give (3.3). ■

LEMMA 3.2: *Under the hypotheses of theorem* 3.1, *there exists a constant* $C = C(t^*)$ *such that*

$$\| f_1^{(1)}(k L_h^{1/2}) u^h(0) \|_{L^\infty} \leq C k (h^r \| u^0 \|_{2s+r+2} + k^\nu \| u^0 \|_{2s+\nu+2}). \quad (3.16)$$

Proof: Using (1.14) we obtain

$$\begin{aligned} f_1^{(1)}(k L_h^{1/2}) u^h(0) = f_1^{(1)}(k L_h^{1/2}) T_h^{s+1} L^{s+1} u^0 &= f_1^{(1)}(k L_h^{1/2}) T_h^{s+1} L^{s+1} (u^0 - u^{0\,(k)}) \\ &+ \sum_{l=0}^{\nu/2-1} f_1^{(1)}(k L_h^{1/2}) T_h^{s+l+1} (T - T_h) L^{s+l+2} u^{0\,(k)} \\ &+ f_1^{(1)}(k L_h^{1/2}) T_h^{s+\nu/2+1} L^{s+\nu/2+1} u^{0\,(k)}. \quad (3.17) \end{aligned}$$

Now, for $\chi \in L^2$, $0 \leqq l \leqq \nu/2$, $s \geqq J_0 + K$, $K = [N/2]+1$, using (2.6), (2.14), (3.2), (1.24) and (1.5) we obtain

$$\| f_1^{(1)}(k L_h^{1/2}) T_h^{s+l+1} \chi \|_{L^\infty} \leqq \left(\sum_q | f_1^{(1)}(k(\mu_q^h)^{-1/2})(\mu_q^h)^{s+l+1} \| \psi_q^h \|_{L^\infty}\right) \| \chi \|$$
$$\leqq C k^{l+1} \left(\sum_q (\mu_q^h)^{s-J_0-K+(1/2)} (\mu_q^h)^{J_0}\right) \| \chi \| \leqq C k^{2l+1} \| \chi \|. \quad (3.18)$$

By (3.18) with $l=0$, using (2.16), we have

$$\| f_1^{(1)}(k L_h^{1/2}) T_h^{s+1} L^{s+1}(u^0 - u^{0\,(k)}) \|_{L^\infty}$$
$$\leqq C k \| L^{s+1}(u^0 - u^{0\,(k)}) \| \leqq C k^{\nu+1} \| u^0 \|_{2s+\nu+2}. \quad (3.19)$$

Also, by (3.18) with $0 \leqq l \leqq \nu/2 - 1$, (2.15) and (1.4) we obtain

$$\| f_1^{(1)}(k L_h^{1/2}) T_h^{s+l+1} (T - T_h) L^{s+l+2} u^{0\,(k)} \|_{L^\infty} \leqq C k h^r \| u^0 \|_{2s+r+2}. \quad (3.20)$$

Finally, (3.18) with $l = \nu/2$ and (2.15) give

$$\| f_1^{(1)}(k L_h^{1/2}) T_h^{s+\nu/2+1} L^{s+\nu/2+1} u^{0\,(k)} \|_{L^\infty} \leqq C k^{\nu+1} \| u^0 \|_{2s+\nu+2}. \quad (3.21)$$

Combining now (3.17), (3.19)-(3.21) we obtain (3.16). ■

LEMMA 3.3: *Under the hypotheses of theorem* 3.1 *there exists a constant* $C = C(t^*)$ *such that*

$$\| \omega^1 - u^h(k) \|_{L^\infty} \leqq C k [k^\nu (\| u^0 \|_{2s+\nu+2} + \| u_t^0 \|_{2s+\nu})$$
$$+ h^r (\| u^0 \|_{2s+r+1} + \| u_t^0 \|_{2s+r})]. \quad (3.22)$$

Proof: Using (2.39), (1.18), (1.14), (2.40) and setting $U^0 = [u^0, u_t^0]^T$ we obtain

$$W - U^h(k) = F(k \mathscr{L}_h) \mathscr{T}_h^{2s+1} \mathscr{L}^{2s+1} U^0 = F(k \mathscr{L}_h) \mathscr{T}_h^{2s+1} \mathscr{L}^{2s+1} (U^0 - U^{0\,(k)})$$
$$+ \sum_{l=0}^{\nu-1} F(k \mathscr{L}_h) \mathscr{T}_h^{2s+l+1} (\mathscr{T} - \mathscr{T}_h) \mathscr{L}^{2s+l+2} U^{0\,(k)}$$
$$+ F(k \mathscr{L}_h) \mathscr{T}_h^{2s+\nu+1} \mathscr{L}^{2s+\nu+1} U^{0\,(k)}. \quad (3.23)$$

Let now $X \in \mathbf{L}^2$. For $0 \leqq l \leqq \nu$, by (2.42) and (3.2), since $s \geqq K + J_0$, $K = [N/2]+1$, we obtain

$$\| (F(k \mathscr{L}_h) \mathscr{T}_h^{2s+l+1} X)_1 \|_{L^\infty} = 2^{-1/2} \| \sum_j F(k \eta_j^{-1}) \eta_j^{2s+l+1} ((X, \Phi_j)) \psi_j^h \|_{L^\infty}$$
$$\leqq 2^{-1/2} \left(\sum_j | F(k \eta_j^{-1}) | \, | \eta_j |^{2s+l+1} \| \psi_j^h \|_{L^\infty}\right) ||| X |||$$
$$\leqq C k^{l+1} \left(\sum_j | \eta_j |^{2(s-K-J_0)} | \eta_j |^{2J_0}\right) ||| X ||| \leqq C k^{l+1} ||| X |||. \quad (3.24)$$

From (3.24) with $l=0$, (2.15), (2.16) and (1.5) we obtain

$$\begin{aligned}\| [F(k\mathscr{L}_h)\mathscr{T}_h^{2s+1}\mathscr{L}^{2s+1}(U^0-U^{0(k)})]_1\|_{L^\infty}^2 &\leqq Ck^2 |||\mathscr{L}^{2s+1}(U^0-U^{0(k)})|||^2\\ &\leqq Ck^2[\|L^s(u_t^0-u_t^{0(k)})\|^2+(T_h L^{s+1}(u^0-u^{0(k)}), L^{s+1}(u^0-u^{0(k)}))]\\ &\leqq Ck^2(k^{2\nu}\|u_t^0\|_{2s+\nu}^2+k^{2\nu}\|u^0\|_{2s+\nu+2}^2)\\ &= C[k^{\nu+1}(\|u^0\|_{2s+\nu+2}+\|u_t^0\|_{2s+\nu})]^2. \quad (3.25)\end{aligned}$$

Now from (3.24) with $0\leqq l\leqq\nu-1$ we obtain, using (1.4), (2.15) and analogous computations with the ones of lemma 2.4 that

$$\begin{aligned}\| [F(k\mathscr{L}_h)\mathscr{T}_h^{2s+l+1}(\mathscr{T}-\mathscr{T}_h)\mathscr{L}^{2s+l+2}U^{0(k)}]_1\|_{L^\infty}\\ \leqq Ck^{l+1}|||(\mathscr{T}-\mathscr{T}_h)\mathscr{L}^{2s+l+2}U^{0(k)}|||\\ \leqq Ck\left\{\begin{array}{ll} h^r\|u_t^0\|_{2s+r}, & l \text{ even},\\ h^r\|u^0\|_{2s+r+1}, & l \text{ odd}.\end{array}\right\} \quad (3.26)\end{aligned}$$

Finally, by (3.24) with $l=\nu$, (1.5) and (2.15) we see (since ν is even) that

$$\begin{aligned}\| [F(k\mathscr{L}_h)\mathscr{T}_h^{2s+\nu+1}\mathscr{L}^{2s+\nu+1}U^{0(k)}]_1\|_{L^\infty}^2 &\leqq Ck^{2(\nu+1)}|||\mathscr{L}^{2s+\nu+1}U^{0(k)}|||^2\\ &= Ck^{2(\nu+1)}[\|L^{s+\nu/2}u_t^{0(k)}\|^2+(T_h L^{s+\nu/2+1}u^{0(k)}, L^{s+\nu/2+1}u^{0(k)})]\\ &\leqq Ck^{2(\nu+1)}(\|u_t^0\|_{2s+\nu}^2+\|u^0\|_{2s+\nu+2}^2). \quad (3.27)\end{aligned}$$

Hence, since $\omega^1-u^h(k)=(W-U^h(k))_1$, (3.23)-(3.27) give (3.22). ■

We now return to the proof of theorem 3.1. For $0\leqq n\leqq[t^*/k]$, we have

$$\|\omega^n-u(nk)\|_{L^\infty}\leqq\|\omega^n-u^h(nk)\|_{L^\infty}+\|u^h(nk)-u(nk)\|_{L^\infty}. \quad (3.28)$$

Now, by (2.12), using (2.3), (2.9) and (2.14′) we obtain

$$\begin{aligned}\|\omega^n-u^h(nk)\|_{L^\infty}\leqq n(\|\omega^1-u^h(k)\|_{L^\infty}+\|f_1^{(1)}(kL_h^{1/2})u^h(0)\|_{L^\infty}\\ +\max_{0\leqq m\leqq[t^*/k]}\sum_{j=1}^{2}\|f_m^{(j)}(kL_h^{1/2})[u^h(k)-\rho_1(kL_h^{1/2})u^h(0)]\|_{L^\infty}). \quad (3.29)\end{aligned}$$

Hence, (3.3), (3.16), (3.22) and (3.29) give

$$\begin{aligned}\|\omega^n-u^h(nk)\|_{L^\infty}\leqq C[k^\nu(\|u^0\|_{2s+\nu+2}+\|u_t^0\|_{2s+\nu+2})\\ +h^r(\|u^0\|_{2s+r+2}+\|u_t^0\|_{2s+r+1})]. \quad (3.30)\end{aligned}$$

Finally, [2], theorem 2.2, gives

$$\begin{aligned}\|u(nk)-u^h(nk)\|_{L^\infty}\leqq C[\gamma(h)(\|u^0\|_{s_0}+\|u_t^0\|_{s_0-1})\\ +h^r(\|u^0\|_{2s+r+1}+\|u_t^0\|_{2s+r})]. \quad (3.31)\end{aligned}$$

Therefore, (3.29)-(3.31) prove (3.1) and the proof of theorem 3.1 is now complete. ■

We state now without proof the entirely analogous result for rational approximations of class C-I.

THEOREM 3.2: *Let r be of class* C-I *and let all other hypotheses of theorem* 3.1 *be satisfied. In addition, let* T_h *satisfy* (1.21). *Then for* h *sufficiently small, provided* (1.22) *holds, the estimate* (3.1) *is valid for some constant* $C = C(t^*)$. ■

4. EXAMPLES AND IMPLEMENTATION

In this section we give examples of high order accurate in time methods which possess certain computational advantages over other existing methods.

Let $\alpha \geqq 1$ be an integer. We define the family of real polynomials $\{\varphi_n^{(\alpha)}\}_{n \geqq 0}$ of the real variable x by

$$\varphi_n^{(\alpha)}(x) = \sum_{j=0}^{n} \frac{(-1)^j}{(2j)!} \binom{\alpha}{n-j} x^{2(n-j)}, \qquad n = 0, 1, 2, \ldots, \tag{4.1}$$

where we shall use the convention $\binom{\alpha}{j} = 0$ for $j > \alpha$.

For $x > 0$ and z complex we define the corresponding family of rational functions

$$r_\alpha(x; z) = \left(\sum_{n=0}^{\alpha} \varphi_n^{(\alpha)}(x) z^{2n} \right) \Big/ (1 + x^2 z^2)^\alpha \qquad \text{for} \quad |\operatorname{Im} z| < x^{-1}. \tag{4.2}$$

In [3] we established the following results.

LEMMA 4.1: *Let* $\alpha \geqq 1$ *be an integer and* $x > 0$. *Then there exists a constant* $C = C(\alpha, x)$ *such that*

$$|r_\alpha(x; z) - \cos z| \leqq C |z|^{2\alpha+2}, \qquad |z| < x^{-1}. \tag{4.3}$$

Furthermore, there exists a $x^{(\alpha)} > 0$ *such for all* $x \geqq x^{(\alpha)}$:

$$|r_\alpha(x; \tau)| \leqq 1, \quad \text{all } \tau \geqq 0. \tag{4.4}$$

Proof: For a proof we refer to proposition 3.1 of [3]. ■

LEMMA 4.2: *Let* $\alpha \geqq 2$ *be an even integer. Then* $\varphi_{\alpha+1}^{(\alpha)}$ *possesses at least one positive zero* $x_{\alpha+1}^{(\alpha)}$. *If we define*

$$r_a^*(z) = r_\alpha(x_{\alpha+1}^{(\alpha)}; z), \tag{4.5}$$

then there exists a constant $C=C(\alpha)$, *such that*

$$|r_\alpha^*(z)-\cos z| \leqq C|z|^{2\alpha+4} \qquad \textit{for} \quad |z|<(x_{\alpha+1}^{(\alpha)})^{-1}. \tag{4.6}$$

Furthermore, there exists a constant $\varkappa=\varkappa(\alpha)>0$ *such that*

$$|r_\alpha^*(\tau)| \leqq 1 \qquad \text{for} \quad 0 \leqq \tau \leqq \varkappa. \tag{4.7}$$

Proof: cf. proposition 3.2 of [3]. ■

In [1], the following is established.

LEMMA 4.3: *For integer* $\alpha \geqq 1$, *there exists a sequence* $\{\beta_n^{(\alpha)}\}_{n\geqq 0}$ *of real polynomials of the real variable x, of degree n such that for any* $x>0$:

$$(1-x^2 z^2)^\alpha e^{-z} = \sum_{n=0}^{\infty} \beta_n^{(\alpha)}(x) z^n, \quad \textit{all complex } z. \tag{4.8}$$

Furthermore, if we define the rational functions

$$\tilde{r}_\alpha(x;\, z) = \left(\sum_{n=0}^{\alpha} \beta_n^{(\alpha)}(x) z^n\right) \Big/ (1-x^2 z^2)^\alpha, \qquad |\operatorname{Re} z| < x^{-1} \tag{4.9}$$

then there exists a constant $C=C(\alpha, x)$ *such that*

$$|\tilde{r}_\alpha(x;\, z)-e^{-z}| \leqq C|z|^{2\alpha+1}, \qquad |z| \leqq (2x)^{-1}, \tag{4.10}$$

and

$$|\tilde{r}_\alpha(x;\, iy)| \leqq C, \quad \textit{all real } y. \tag{4.11}$$

Proof: The result (4.8) is contained in theorem 4.1 of [1]. (4.10) and (4.11) follow from (4.8) and (4.9). ■

For this work we shall use as examples of class C-II rational functions the family defined by (4.2). That $r_\alpha(\tau)=r_\alpha(x;\tau)$ is of class C-II for $\alpha \geqq 1$ and $x \geqq x^{(\alpha)}$ follows from lemma 4.1. We remark that a simple procedure for computing $x^{(\alpha)}$ is given in [3].

Our special examples of class C-I, which are not of class C-II, and which are of practical importance consist of the family $r_\alpha^*(\tau)$ defined by (4.5). That $r_\alpha^*(\tau)$, for $\alpha \geqq 2$ even, is of class C-I is the essence of lemma 4.2.

The initial approximations ω^0 and ω^1 will be generated by using a single-step procedure following [1], with the rational function $\tilde{r}_\alpha$ defined by (4.9). We note that a table of the polynomials $\beta_n^{(\alpha)}$ is provided in the appendix of [1].

For consistency with the notation of the previous sections we shall set $\nu=2\alpha$, $\alpha \geqq 1$ and r_α becomes $r_{\nu/2}$.

4.1. Class C-II schemes

Having determined the parameter $x^{(\nu/2)}$ such that (4.4) holds for $x \geqq x^{(\nu/2)}$, assuming that for $n \geqq 0$, ω^n and ω^{n+1} are known, we obtain ω^{n+2} from (1.10) as follows. Set $Z = (\omega^{n+2} + \omega^n)/2$ and (4.2) yields the computational procedure

$$[I + (x^{(\nu/2)} k)^2 L_h]^{\nu/2} Z = \left[\sum_{j=0}^{\nu/2} \varphi_j^{(\nu/2)} (x^{(\nu/2)}) k^{2j} L_h^j \right] \omega^{n+1}, \tag{4.12}$$

$$\omega^{n+2} = 2Z - \omega^n. \tag{4.13}$$

Since ν is even it is easily shown that in the case of known Galerkin methods, the determination of Z from (4.12) (and thus of ω^{n+2}) requires the solution of $\nu/2$ linear systems of equations with the same real matrix. We shall show this in the specific case of the standard Galerkin method with $\nu = 4$. The argument used can be extended by induction to the general case.

With $\nu = 4$, we find, *cf.* [3], that $x^{(2)} = (1/2 + \sqrt{5/24})^{1/2}$. Nevertheless a sharper analysis, *cf.* [3], section 4, shows that the schemes satisfy (4.4) for $x \geqq c_0 = (1/4 + \sqrt{1/24})^{1/2}$. Hence we set $x = c_0$ and $A_h = T_h + x^2 k^2 I$. Then (4.12) becomes

$$A_h^2 Z = \left[\sum_{j=0}^{2} \varphi_j^{(2)} (x) k^{2j} T_h^{2-j} \right] \omega^{n+1}. \tag{4.14}$$

Since

$$I = (xk)^{-4} (A_h^2 - T_h^2 - 2x^2 k^2 T_h),$$

setting

$$Y = Z - \varphi_2^{(2)} (x) \omega^{n+1} / x^4, \tag{4.15}$$

a staightforward substitution in (4.14) gives

$$A_h^2 Y = [\theta_0 (x) T_h^2 + \theta_1 (x) T_h] \omega^{n+1}, \tag{4.16}$$

where

$$\theta_0 (x) = \varphi_0^{(2)} (x) - \varphi_2^{(2)} (x)/x^4$$

and

$$\theta_1 (x) = k^2 [\varphi_1^{(2)} (x) - 2 \varphi_2^{(2)} (x)/x^2].$$

Thus (4.14) is equivalent to

$$A_h T_h^{-1} A_h Y = [\theta_0 (x) T_h + \theta_1 (x) I] \omega^{n+1}, \tag{4.17}$$

which we reduce to

$$A_h \zeta = [\theta_0 (x) T_h + \theta_1 (x) I] \omega^{n+1}, \tag{4.18}$$

$$A_h Y = T_h \zeta. \tag{4.19}$$

Thus, by (1.6), ζ is obtained from (4.18) as the solution of

$$(\zeta, \chi)+x^2 k^2 a(\zeta, \chi) = \theta_0(x)(\omega^{n+1}, \chi)+\theta_1(x) a(\omega^{n+1}, \chi), \qquad \forall \chi \in S_h, \quad (4.20)$$

and Y in turn, as the solution of

$$(Y, \chi)+x^2 k^2 a(Y, \chi)=(\zeta, \chi), \qquad \forall \chi \in S_h. \quad (4.21)$$

Finally, from (4.15) and (4.13),

$$\omega^{n+2} = 2\,[Y + \varphi_2^{(2)}(x)\,\omega^{n+1}/x^4] - \omega^n. \quad (4.22)$$

From (4.20)-(4.22) it follows that ω^{n+2} is obtainable from the solution of two linear systems with the same real matrix.

To generate ω^0 and ω^1 we shall use *over one step* the single-step method defined by the rational functions $\tilde{r}_\alpha$ of (4.9). To choose $\tilde{r}_\alpha$ compatible with (4.12) we set $\nu = 2\alpha$ and $x = x^{(\nu/2)}$ in (4.9). Then we define

$$W=\tilde{r}_{\nu/2}(k\mathscr{L}_h)\,U^h(0)=\tilde{r}_{\nu/2}(k\mathscr{L}_h)\,[T_h L u^0,\ P u_t^0]^T, \quad (4.23)$$

and

$$\omega^1 = W_1, \quad (4.24)$$

$$\omega^0 = u^h(0) = T_h L u^0. \quad (4.25)$$

The hypotheses of theorem 2.1 are then satisfied and with the choice (4.23)-(4.25) we obtain the optimal L^2-convergence result (2.13).

We note that from (4.23) the determination of ω^1 requires the solution of ν linear systems of equations with the same real matrix which is used at subsequent time steps obtained from (4.12). For details see [1]. Thus the entire computation may be carried out with a single matrix decomposition.

It is clear from the above that for a given accuracy $\nu \geqq 2$ of the time-stepping procedure, the above schemes provide approximations with optimal accuracy with approximately half the computational work as that required for single-step schemes of the same accuracy. In particular for the single-step schemes developed in [1] an approximation to the solution at $t=nk$, $n \geqq 2$ is obtained by solving $n\nu$ linear systems. For the present methods we obtain ω^n by solving $\nu+(n\nu/2)$ similar systems.

Our examples of class C-II schemes above also satisfy the hypotheses of theorem 3.1; if we choose

$$W=\tilde{r}_{\nu/2}(k\mathscr{L}_h)\,U^h(0)=\tilde{r}_{\nu/2}(k\mathscr{L}_h)\,[T_h^{s+1} L^{s+1} u^0,\ T_h^s L^s u_t^0]^T,$$

for $s \geqq [N/2]+J_0+1$ and $\omega^1 = W_1$, $\omega^0 = T_h^{s+1} L^{s+1} u^0$, the optimal L^∞-estimate (3.1) holds.

4.2. Class C-I schemes

We now give some interesting, from a computational standpoint, examples of class C-I schemes which are not of class C-II. These schemes will be only conditionally convergent, a condition $k/h \leqq C$ being required for convergence. But for a given amount of computational work, in terms of the number of linear systems to be solved at each time step, they are more accurate in time by two orders than the corresponding unconditionally convergent class C-II schemes.

We again set $\nu = 2\alpha$, this time for $\alpha \geqq 2$ an even integer, and choose $r^*_{\nu/2}(\tau)$ by (4.5). A root $x^{(\alpha)}_{\alpha+1}$ of $\varphi^{(\alpha)}_{\alpha+1}$ is of course computable and the constant $\varkappa = \varkappa(\alpha)$ of (4.7) is easily estimated from the details of proposition 3.2 of [3]. We now choose $\tilde{r}_{\nu/2+1}(\tau) = \tilde{r}_{\nu/2+1}(x^{(\nu/2)}_{\nu/2+1}; \tau)$ by (4.9), in which case the same real matrix is used as before.

Because of (4.6), the hypotheses of theorem 2.2 are satisfied with ν replaced by $\nu+2$. Hence we obtain the optimal L^2-convergence result (2.13) with ν replaced by $\nu+2$.

Basically the higher accuracy of two orders is obtained this way since, for the special choice of the parameter $x^{(\nu/2)}_{\nu/2+1}$, we have $\varphi^{(\nu/2)}_{\nu/2+1}(x^{(\nu/2)}_{\nu/2+1}) = 0$, giving (4.6). This however forces the scheme to be conditionally convergent.

We give the example for $\nu/2 = \alpha = 2$ which will be $O(k^6)$ in time and will require the solution of two linear systems at each time step. From (4.1) an easy computation yields that $x^{(2)}_3 = ((5+\sqrt{15})/60)^{1/2}$ is a root of $\varphi^{(2)}_3$. Hence with $r^*_2(\tau)$ given by (4.5) and $\tilde{r}_3(x^{(2)}_3; \tau)$ given by (4.9) with $x = x^{(2)}_3$, we obtain following the general procedure (4.12):

$$[T_h + (x^{(2)}_3 k)^2 I]^2 Z = \left[\sum_{j=0}^{2} \varphi^{(2)}_j (x^{(2)}_3) k^{2j} T_h^{2-j} \right] \omega^{n+1}, \tag{4.26}$$

$$\omega^{n+2} = 2Z - \omega^n, \tag{4.27}$$

which requires two linear systems to be solved at each time step and may be implemented as in (4.20)-(4.22) above. The associated bound $\varkappa$ of (4.7) is found to be 2.53724, *cf.* [3]. Hence, with $k/h \leqq C$ as in (1.22):

$$\max_{0 \leqq n \leqq [t^*/k]} \| u(nk) - \omega^n \| = O(h^r + k^6)$$

by theorem 2.2. This scheme for $\alpha = 2$ was constructed in [10] and discussed in the context of applications to systems of ordinary differential equations in [10, 3].

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