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# Highly Accurate Compact Implicit Methods and Boundary Conditions

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Compact methods are high accuracy finite-difference methods where the functions and their derivatives are considered as unknowns. Two methods are presented to eliminate the second-order derivatives in parabolic equations, while keeping the fourth-order accuracy and the tridiagonal nature of the schemes. A type of high accuracy additional boundary condition is also proposed, which is consistent with the high accuracy of the inner scheme and uses only values at interior and boundary nodes. Integration on nonregular meshes is also examined.

## INTRODUCTION

The trend toward highly accurate numerical solutions of partial differential equations has recently led to a renewed interest in Hermitian methods where derivatives are treated as unknowns, not eliminated with the help of linear combination of the basic functions. Almost at the same time, and in rather different ways, Adam [1] and Hirsh [2], developing an idea of Kreiss [3], have studied the possibility of solving pde by Hermitian compact techniques, and have shown several advantages, and also some problems arising from their effective use.

Over classical higher order methods, Hermitian approximations present the advantage of using less nodes (three instead of five) at each point of the computational grid. Moreover, the error in the discretization of the derivative is usually four to six times smaller than the error of classical highly accurate schemes of the same order. In this paper, two methods are presented to reduce the complexity and the computational cost of the compact algorithms by eliminating the higher derivatives. Additional boundary relations are derived in order to solve the set of linear equations generated by the implicit algorithms. These relations yield a third-order accuracy near the boundaries of the computational grid, which is compatible with the fourth-order accuracy at the inner points. The different methods and boundary conditions are used to solve the one-dimensional Burger's equation and a two-dimensional convective–diffusive heat equation. The advantages of compact highly accurate methods over classical schemes are shown off, mainly for moderate and high Reynolds number. The problem of integration on a nonuniform computational grid is also treated.





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## 1. Principle of Compact Methods

Let us consider the differential equation

$$u_t = L(u, u_x, u_{xx}, \ldots)$$

where $Lu$ is a differential operator of order $n$. The usual way of solving this equation by classical finite-difference methods is to approximate

$$u_x \quad \text{by} \quad \hat{u}_x = (1/2h)(u_{i+1} - u_{i-1}), \tag{1}$$

$$u_{xx} \quad \text{by} \quad \hat{u}_{xx} = (1/h^2)(u_{i+1} + u_{i-1} - 2u_i), \tag{2}$$

or by higher order approximations using more than three nodes. The principle of compact Hermitian methods is to keep $\hat{u}_x$, $\hat{u}_{xx}$ as unknowns at each point of the computational grid. Of course, the approximations $\hat{u}_x$, $\hat{u}_{xx}$ must be derived from $u$. A highly accurate way of computing these values is to solve the systems of Hermitian relations (Collatz [4])

$$\hat{u}^k_{x_{i+1}} + 4\hat{u}^k_{x_i} + \hat{u}^k_{x_{i-1}} = (3/h)(\hat{u}^k_{i+1} - \hat{u}^k_{i-1}), \tag{3}$$

$$\hat{u}^k_{xx_{i+1}} + 10\hat{u}^k_{xx_i} + \hat{u}^k_{xx_{i-1}} = (12/h^2)(\hat{u}^k_{i+1} + \hat{u}^k_{i-1} - 2\hat{u}_i{}^k), \tag{4}$$

where $k$ corresponds to a given time which can be either $n\tau$ or $(n+1)\tau$, and the $\hat{}$ is assigned to the approximated values of $u, u_x, u_{xx}, \ldots$. For example, an algorithm solving the one-dimensional convective–diffusive heat equation

$$u_t = -Vu_x + \nu u_{xx} \tag{5}$$

could be

$$\hat{u}_i^{n+1} = \hat{u}_i{}^n - \tau V\hat{u}^n_{x_i} + \tau\nu\hat{u}^n_{xx_i} \tag{6}$$

where $\hat{u}_{x_i}$ and $\hat{u}_{xx_i}$ are yielded by the systems (3) and (4), here with $k = n$. If one wishes to use an implicit scheme of the Crank–Nicholson type,

$$\hat{u}_i^{n+1} + \frac{\tau}{2} V\hat{u}^{n+1}_{x_i} - \frac{\tau}{2}\nu\hat{u}_{x_i} = u_i{}^n - \frac{\tau}{2} V\hat{u}_x{}^n + \frac{\tau}{2}\nu\hat{u}^n_{xx_i} \tag{7}$$

one has to add two sets of equations (3) and (4) with $k = n + 1$. The set of simultaneous linear equations (7), (3), and (4) must be completed by boundary relations between $\hat{u}$, $\hat{u}_x$, and $\hat{u}_{xx}$. Hirsh [2, 5] has extensively tested this method.

If the computational grid has $m$ nodes, $3m$ equations of $3m$ unknowns are to be solved. Even in this case, the Hermitian compact methods may be preferred to other highly accurate finite-difference schemes, because of their higher accuracy [6] and the tridiagonal nature of the set of linear equations [1].

## 2. Elimination of Higher Derivatives

For the sake of simplicity, only the case of second-order differential equations will be examined.

Generally, second derivatives do not appear in boundary conditions. One can thus try to eliminate the $\hat{u}_{xx_i}$'s in order to reduce the number of unknowns. This elimination is interesting only if the accuracy and the tridiagonal nature of the scheme are kept; it can be implicit or explicit.

(a) Implicit elimination: One uses relations (4); then

$$\hat{u}_{xx} \cong u_{xx} - (1/240)\, h^4 u_{xxxxxx} \tag{8}$$

if one assumes that the error is evenly distributed. Adam [1] has used such an elimination for the solution of Burger's equation

$$u_t + uu_x = \nu u_{xx}\,, \tag{9}$$

$$u\,|_\pi = 0, \tag{10}$$

$$u\,|_0 = 0. \tag{11}$$

Assuming that $\nu$ is a function $\nu(x)$, the numerical scheme is, after elimination of the linear combination $(1/12)(u_{xx_{i+1}} + 10\hat{u}_{xx_i} + \hat{u}_{xx_{i-1}})$ at times $n\tau$ and $(n+1)\,\tau$

$$\frac{1}{12}\frac{\hat{u}_{i+1}^{n+1}}{\nu_{i+1}} + \frac{10}{12}\frac{\hat{u}_i^{n+1}}{\nu_i} + \frac{1}{12}\frac{\hat{u}_{i-1}^{n+1}}{\nu_{i-1}} + \frac{\tau}{24}\left(\frac{\hat{u}_{i+1}^{n}\hat{u}_{x_{i+1}}^{n+1}}{\nu_{i+1}} + \frac{10\hat{u}_i^{n}\hat{u}_{x_i}^{n+1}}{\nu_i} + \frac{\hat{u}_{i-1}^{n}\hat{u}_{x_{i-1}}^{n+1}}{\nu_{i-1}}\right)$$

$$+ \frac{\tau}{24}\left(\frac{\hat{u}_{i+1}^{n+1}\hat{u}_{x_{i+1}}}{\nu_{i+1}} + \frac{10}{\nu_i}\hat{u}_i^{n+1}\hat{u}_{x_i}^{n} + \frac{\hat{u}_{i-1}^{n+1}\hat{u}_{x_{i-1}}^{n}}{\nu_{i-1}}\right) - \frac{\tau}{2h^2}(\hat{u}_{i+1}^{n+1} + \hat{u}_{i-1}^{n+1} - 2\hat{u}_i^{n+1})$$

$$= \frac{1}{12}\frac{\hat{u}_{i+1}^{n}}{\nu_{i+1}} + \frac{10}{12}\frac{\hat{u}_i^{n}}{\nu_i} + \frac{1}{12}\frac{\hat{u}_{i-1}^{n}}{\nu_{i-1}} + \frac{\tau}{2h^2}(\hat{u}_{i+1}^{n} + \hat{u}_{i-1}^{n} - 2\hat{u}_i^{n}) \tag{12}$$

where the last term of the left-hand side is yielded by the elimination of $(1/12)(\hat{u}_{xx_{i+1}}^{n+1} + 10\hat{u}_{xx_i}^{n+1} + \hat{u}_{xx_{i-1}}^{n+1})$ and the last term of the right-hand side by the elimination of $(1/12)(\hat{u}_{xx_{i+1}}^{n} + 10\hat{u}_{xx_i}^{n} + \hat{u}_{xx_{i-1}}^{n})$. This system of equations is closed for the interior points with Eq. (3), where $k = n$ or $n+1$.

Scheme (12) approximates Eq. (9) (divided by $\nu$) with an error

$$\frac{1}{\nu}\left(\frac{\tau^2}{12}u_{ttt} + \frac{h^4}{720}(-4uu_x + 3u_{xx})_{xxxx}\right). \tag{13}$$

The former scheme is particularly useful when the first derivative is absent from the equation to be solved; then a fourth-order accuracy scheme with three nodes and only one set of unknowns is generated, even if the diffusion coefficient $\nu$ is variable; the system of Eq. (12) can then be closed without the help of (3), saving computation time.

(b) Explicit elimination: One uses the fourth-order approximation of $u_{xx}$ :

$$\hat{u}_{xx_i} = (2/h^2)(u_{i+1} + u_{i-1} - 2u_i) - (1/2h)(u_{x_{i+1}} - u_{x_{i-1}}) \tag{14}$$

then

$$\hat{u}_{xx} \cong u_{xx} + (1/120)\, h^4 u_{xxxxxx} \tag{15}$$

if one also assumes that the error is evenly distributed.

The corresponding equations for the integration of (9) are:

$$\hat{u}_i^{n+1} + \frac{\tau}{2}\hat{u}_i{}^n\hat{u}_{x_i}^{n+1} + \frac{\tau}{2}\hat{u}_i^{n+1}\hat{u}_{x_i}^n - \frac{\tau\nu_i}{h}(\hat{u}_{i+1}^{n+1} + \hat{u}_{i-1}^{n+1} - 2\hat{u}_i^{n+1}) + \frac{\tau\nu_i}{4h}(\hat{u}_{x_{i+1}}^{n+1} - \hat{u}_{x_{i-1}}^{n+1})$$

$$= \hat{u}_i{}^n + \frac{\tau\nu_i}{h^2}(\hat{u}_{i+1}^n + \hat{u}_{i-1}^n - 2\hat{u}_i{}^n) - \frac{\tau\nu_i}{4h}(\hat{u}_{x_{i+1}}^n - \hat{u}_{x_{i-1}}^n) \tag{16}$$

and (3). The error is

$$((\tau^2/12)\, u_{ttt} - (h^4/720)(+4uu_x + 2u_{xx})_{xxx}). \tag{17}$$

A further example of this procedure is given in Section 4.

When the first derivative appears, or when the diffusion coefficient is variable, and generally, every time the "implicit elimination scheme" does not degenerate into a very simple scheme as described above, the explicit elimination should be preferred, because it is easier to handle.

Both schemes generate 2 $m$ equations with 2 $m$ unknowns ($m$ $u_i$'s and $m$ $u_{x_i}$'s). The computational effort is thus much less than that required in the previous schemes developed by Hirsh [2]. The elimination formulas are given here for a constant spatial step. On nonuniform grids, an equivalent of (4) can be found in [1] and an equivalent of (14) in the Appendix of this paper.

## 3. Additional Boundary Relations

Equations like (3) close the system at all the interior points $i$, for $i = 2,..., m-1$. Of course, they cannot be written for $i = 1$ or $i = m$. Boundary conditions for the basic function $u$ are generally written

$$r_1 u + s_1 u_x = V_1 \qquad \text{at} \quad x = x_1 \quad (i = 1), \tag{18}$$

$$r_m u + s_m u_x = V_m \qquad \text{at} \quad x = x_m \quad (i = m). \tag{19}$$

There lacks one relationship at each boundary to solve the system completely. One can derive a relationship between $\hat{u}_1$ and $\hat{u}_{x_1}$, eventually including $\hat{u}_2$, $\hat{u}_{x_2}$, $\hat{u}_3$, $\hat{u}_{x_3}$ (and the analog for $\hat{u}_m$ and $\hat{u}_{x_m}$), that preserves to some extent the high accuracy of the method. Then the tridiagonal character of the set of equations and the simplicity of the algorithm are retained.

The relationship at $i = 1$ is

$$a_2\hat{u}_{x_3} + b_2\hat{u}_{x_2} + c_2\hat{u}_{x_1} - (1/h)(m_2\hat{u}_3 + n_2\hat{u}_2 + l_2\hat{u}_1) = 0. \tag{20}$$

It can not be identical to (3) because the system of equations would then be ill-conditioned. The same argument applies at $i = m$.

Thus, fourth-order accuracy cannot be achieved without losing the tridiagonal character of the scheme, because (3) is the only three-node relationship between a function and its first derivative with an error $O(h^4)$. However a $O(h^3)$-boundary condition is consistent with a $O(h^4)$ inner scheme if the scheme is stable with regard to boundary conditions [7].

Since a condition such as (20) is a mere natural relationship between the function and its first derivative *inside* the integration domain, it cannot generate instability.

A realization of (20) could be

$$2\hat{u}_{x_1} + 4\hat{u}_{x_2} - (1/h)(-5\hat{u}_1 + 4\hat{u}_2 + \hat{u}_3) = 0, \tag{21}$$

$$4\hat{u}_{x_2} + 2\hat{u}_{x_3} - (1/h)(-\hat{u}_1 - 4\hat{u}_2 + 5\hat{u}_3) = 0, \tag{22}$$

and the analog at $i = m$

$$4\hat{u}_{x_{m-1}} + 2\hat{u}_{x_m} - (1/h)(-\hat{u}_{m-2} - 4\hat{u}_{m-1} + 5\hat{u}_m) = 0, \tag{23}$$

$$2\hat{u}_{x_{m-2}} + 4\hat{u}_{x_{m-1}} - (1/h)(-5\hat{u}_{m-2} + 4\hat{u}_{m-1} + 6\hat{u}_m) = 0. \tag{24}$$

In practice, very few, or no difference, appears in the results, whatever formulas are used. These relationships are $O(h^3)$ accurate.

Another realization of (20) is

$$u_{x_1} + u_{x_2} - (2/h)(u_2 - u_1) = 0 \tag{25}$$

and the analog at $i = m$

$$u_{x_m} + u_{x_{m-1}} - (2/h)(u_m - u_{m-1}) = 0 \tag{26}$$

which has been used by Adam [1]. This relationship is only $O(h^2)$ accurate.

## 4. Results of Numerical Experiments

Tests have been performed to check the validity of the different methods (exposed above) used to eliminate the second derivative and to yield an additional boundary condition. The test problems have been the resolution of Burger's equation in four cases, and the resolution of a two-dimensional heat equation by an ADI Hermitian procedure.

In both cases, numerical results are compared to an analytical solution. Results are given in terms of the maximum error of the Burger solution (Tables I to IV) and in terms of an averaged error for the heat equation (Table V).

TABLE I

Maximum Error of the Numerical Solution of Burger's Equation[a]

| $t$ | $\tau = 0.01\ h = \pi/20$ | $t$ | $\tau = 0.01\ h = \pi/40$ |
|---|---|---|---|
| 0.1 | −0.3884 | 0.1 | 0.0764 |
| 0.2 | −0.2192 | 0.2 | 0.0062 |
| 0.3 | −0.0597 | 0.3 | 0.0021 |
| 0.4 | −0.0149 | 0.4 | 0.0007 |
| 0.5 | −0.0040 | 0.5 | 0.0003 |
| | $\tau = 0.0025\ h = \pi/20$ | | $\tau = 0.0025\ h = \pi/40$ |
| 0.1 | −0.4754 | 0.1 | −0.0159 |
| 0.2 | −0.2257 | 0.2 | −0.0030 |
| 0.3 | −0.0605 | 0.3 | 0.0014 |
| 0.4 | −0.0149 | 0.4 | 0.0007 |
| 0.5 | −0.0042 | 0.5 | 0.0003 |

[a] $u_{max} = 20$, $\nu = 1$. Implicit elimination of the second derivative; $O(h^3)$-boundary condition.

TABLE II

Maximum Error of the Numerical Solution of Burger's Equation[a]

| $t$ | $\tau = 0.01\ h = \pi/20$ | $t$ | $\tau = 0.01\ h = \pi/40$ |
|---|---|---|---|
| 0.1 | −0.2490 | 0.1 | 0.0765 |
| 0.2 | −0.0690 | 0.2 | 0.0062 |
| 0.3 | −0.0332 | 0.3 | 0.0013 |
| 0.4 | −0.0122 | 0.4 | 0.0004 |
| 0.5 | −0.0048 | 0.5 | 0.0001 |
| | $\tau = 0.0025\ h = \pi/20$ | | $\tau = 0.0025\ h = \pi/40$ |
| 0.1 | −0.2974 | 0.1 | −0.0158 |
| 0.2 | −0.0762 | 0.2 | −0.0029 |
| 0.3 | −0.0339 | 0.3 | 0.0010 |
| 0.4 | −0.0122 | 0.4 | 0.0003 |
| 0.5 | −0.0047 | 0.5 | 0.0001 |

[a] $u_{max} = 20$, $\nu = 1$. Implicit elimination of the second derivative; $O(h^2)$-boundary condition.

TABLE III

Maximum Error of the Numerical Solution of Burger's Equation[a]

| $t$ | $\tau = 0.01\ h = \pi/20$ | $t$ | $\tau = 0.01\ h = \pi/40$ |
|---|---|---|---|
| 0.1 | 0.521 | 0.1 | 0.238 |
| 0.2 | 0.379 | 0.2 | 0.097 |
| 0.3 | 0.252 | 0.3 | 0.031 |
| 0.4 | 0.134 | 0.4 | 0.010 |
| 0.5 | 0.067 | 0.5 | 0.004 |
| | $\tau = 0.0025\ h = \pi/20$ | | $\tau = 0.0025\ h = \pi/40$ |
| 0.1 | 0.425 | 0.1 | 0.144 |
| 0.2 | 0.371 | 0.2 | 0.090 |
| 0.3 | 0.251 | 0.3 | 0.030 |
| 0.4 | 0.134 | 0.4 | 0.010 |
| 0.5 | 0.067 | 0.5 | 0.004 |

[a] $u_{\max} = 20$, $\nu = 1$. Explicit elimination of the second derivative, $O(h^3)$-boundary condition.

TABLE IV

Maximum Error of the Numerical Solution of Burger's Equation[a]

| $t$ | $\tau = 0.01\ h = \pi/20$ | $t$ | $\tau = 0.01\ h = \pi/40$ |
|---|---|---|---|
| 0.1 | 0.774 | 0.1 | 0.208 |
| 0.2 | 0.327 | 0.2 | 0.088 |
| 0.3 | 0.187 | 0.3 | 0.039 |
| 0.4 | 0.108 | 0.4 | 0.018 |
| 0.5 | 0.064 | 0.5 | 0.009 |
| | $\tau = 0.0025\ h = \pi/20$ | | $\tau = 0.0025\ h = \pi/40$ |
| 0.1 | 0.670 | 0.1 | 0.115 |
| 0.2 | 0.319 | 0.2 | 0.081 |
| 0.3 | 0.186 | 0.3 | 0.038 |
| 0.4 | 0.109 | 0.4 | 0.018 |
| 0.5 | 0.064 | 0.5 | 0.009 |

[a] $u_{\max} = 20$, $\nu = 1$. Explicit elimination of the second derivative; $O(h^3)$-boundary condition.

TABLE V

Average Error of the Numerical Solution of the Two-Dimensional Heat Equation[a]

| $t$ | $h=1/20$, $\tau=0.01$, $O(h^3)$; | $h=1/20$, $\tau=0.004$, $O(h^3)$; | $h=1/40$, $\tau=0.0025$, $O(h^3)$; | $h=1/20$, $\tau=0.004$, $O(h^2)$ |
|---|---|---|---|---|
| 0.4 | $1.27 \times 10^{-3}$ | $0.965 \times 10^{-3}$ | $1.13 \times 10^{-4}$ | $1.60 \times 10^{-3}$ |
| 0.8 | $1.26 \times 10^{-3}$ | $1.000 \times 10^{-3}$ | $1.21 \times 10^{-4}$ | $1.54 \times 10^{-3}$ |
| 1.2 | $1.00 \times 10^{-3}$ | $0.835 \times 10^{-3}$ | $1.00 \times 10^{-4}$ | $1.24 \times 10^{-3}$ |
| 1.6 | $0.80 \times 10^{-3}$ | $0.645 \times 10^{-3}$ | $0.75 \times 10^{-4}$ | $0.92 \times 10^{-3}$ |
| 2.0 | $0.59 \times 10^{-3}$ | $0.473 \times 10^{-3}$ | $0.55 \times 10^{-4}$ | $0.67 \times 10^{-3}$ |

[a] $U_x = U_y = 1$; $\nu_x = \nu_y = 0.05$.

TABLE VI

Maximum Error of the Numerical Solution of Burger's Equation[a]

| $t$ | $\epsilon_{\max}$ |
|---|---|
| 0.1 | 0.1919 |
| 0.2 | 0.0139 |
| 0.3 | 0.0105 |
| 0.4 | 0.0058 |
| 0.5 | 0.0021 |

[a] $u_{\max} = 20$, $\nu = 1$, $\tau = 0.002$. Explicit elimination of the second derivative $O(h^2)$-boundary condition. Integration on a non-uniform grid. Total number of mesh points is 21.

## 5. Burger's Equation

Let us first look at the Burger equation and compare the effect of choosing one or another additional boundary condition. For the solutions of a highly nonlinear equation ($u_{\max}(t = 0) = 20$), the $O(h^2)$-condition gives better results (Table II) than the $O(h^3)$-condition (Table I). If one leaves aside the values of the error for $t \leqslant .2$, where there is an obvious combination of time and spatial errors (the error varies strongly when $\tau$ decreases) to focus the attention on results for $t \geqslant .3$, one finds that the error decreases faster than $h^4$ (by a factor of $>2^4$). This is probably due to the fact that the error is due to the higher order terms, which is important in the region where the gradients of the solution are steep (near $x = 0$). To clarify this problem, let us examine the error on a Fourier component $A(\omega)\, e^{i\omega x}$ of the solution.

As the error introduced by (21) is

$$-\tfrac{1}{6}h^3 u_{xxxx} + (1/30)\, h^4 u_{xxxxx} \tag{27}$$

the error on the elementary solution is, near $x = 0$:

$$A(\omega)(-\tfrac{1}{6}h^3(i\omega)^4 + (1/30)\,h^4(i\omega)^5) = A(\omega)\,\omega^4h^3(-\tfrac{1}{6} + (ih/30)\,\omega). \tag{28}$$

Both components of the error are always out of phase and can never cancel each other. Moreover, for $\omega h > 5$, i.e., above the seventh harmonic, the higher order part of the error dominates, at least if $A(\omega)$ does not vanish rapidly when $\omega \to \infty$; the error introduced by (25) is

$$\tfrac{1}{6}h^2u_{xxx} - (1/12)\,h^3u_{xxxx} + (1/40)\,h^4u_{xxxxx} \tag{29}$$

or, for an elementary solution

$$A(\omega)\,\omega^3h^2(-(i/6) - (1/12)\,\omega h + (i/40)\,\omega^2h^2). \tag{30}$$

In this expression, the first and third term are in phase and of opposite signs; they nearly balance each other. For $\omega h \sim 6$, they cancel each other. As a Fourier analysis of the solution shows that the Fourier coefficients $A(\omega)$ are important up the tenth harmonic in the region near $x = 0$, relations (22) and (30) explain why the $O(h^2)$-condition gives a better result than the $O(h^3)$-condition. Further experiments (not reported here) performed on a smoother solution ($u_{\max}\,(t = 0) = 10$) have confirmed the validity of this analysis; the error behaved as predicted theoretically.

Looking at the results of the explicit elimination methods, one sees that they are less accurate than those of the implicit elimination algorithm, that the convergence is between $h^2$ and $h^3$ for the $O(h^2)$-condition, and between $h^3$ and $h^4$ for the $O(h^3)$-condition. Here again, the higher order terms are important.

## 6. Heat Equation

The two-dimensional heat equation does not exhibit such high order harmonics in its solution and the results confirm the theoretical computations.

The numerical integration scheme of the equation

$$u_t + U_1u_x + U_2u_y = \nu_1u_{xx} + \nu_2u_{yy} \tag{31}$$

is:

$$\begin{aligned}
&\hat{u}_{i,j}^{n+1/2} - \hat{u}_{i,j}^{n} + \frac{\tau}{2}\,U_1\hat{u}_{x_{i,j}}^{n+1/2} + \frac{\tau}{2}\,U_2\hat{u}_{y_{i,j}}^{n} \\
&\quad = \frac{\tau\nu_1}{h^2}\,(\hat{u}_{i+1,j}^{n+1/2} + \hat{u}_{i-1.}^{n+1/2} - 2\hat{u}_{i,jj}^{n+1/2}) - \frac{\tau\nu_1}{4h}\,(\hat{u}_{x_{i+1,j}}^{n+1/2} - \hat{u}_{x_{i-1,j}}^{n+1/2}) \\
&\qquad + \frac{\tau\nu_2}{h^2}\,(\hat{u}_{i,j+1}^{n} + \hat{u}_{i,j-1}^{n} - 2\hat{u}_{i,j}^{n}) - \frac{\tau\nu_2}{4h}\,(\hat{u}_{y_{i,j+1}}^{n} - \hat{u}_{y_{i,j-1}}^{n}),
\end{aligned} \tag{32}$$

$$\begin{aligned}
&\hat{u}_{i,j}^{n+1} - \hat{u}_{i,j}^{n+1/2} + \frac{\tau}{2}\,U_1\hat{u}_{x_{i,j}}^{n+1/2} + \frac{\tau}{2}\,U_2\hat{u}_{y_{i,j}}^{n+1} \\
&\quad = \frac{\tau\nu_1}{h^2}\,(\hat{u}_{i+i,j}^{n+1/2} + \hat{u}_{i-1,j}^{n+1/2} - 2\hat{u}_{i,j}^{n+1/2}) - \frac{\tau\nu_1}{4h}\,(\hat{u}_{x_{i+1,j}}^{n+1/2} - \hat{u}_{x_{i-1,j}}^{n+1/2}) \\
&\qquad + \frac{\tau\nu_2}{h^2}\,(\hat{u}_{i,j+1}^{n+1} + \hat{u}_{i,j-1}^{n+1} - 2\hat{u}_{i,j}^{n+1}) - \frac{\tau\nu_2}{4h}\,(\hat{u}_{x_{i,j+1}}^{n+1} - \hat{u}_{x_{i,j-1}}^{n+1}).
\end{aligned} \tag{33}$$

Here, only the explicit elimination has been used, because an implicit elimination would have required additional computations for $\hat{u}^n_{yy}$ and $\hat{u}^{n+1/2}_{xx}$ (using (4)).

The theoretical error is

$$\frac{\tau^2}{12}u_{ttt} + \frac{h^4}{51840}(624U_1u_x - 600U_2u_y + 636\nu_1u_{xx} - 600\nu_2u_{yy})_{xxxx}$$

$$+ \frac{h^4}{51840}(-600U_1u_x + 624U_2u_y - 600\nu_1u_{xx} + 636\nu_2u_{yy})_{yyyy}. \tag{34}$$

Assuming perfect symmetry in $x$ and $y$ for simplification, the error becomes, for a typical elementary solution of (31) with wave number

$$\omega = \frac{2\pi}{L}, \qquad L = mh,$$

$$\epsilon_H = \frac{2}{3}\tau^2\nu^3\left(\frac{U^2}{4\nu^2} + \omega^2\right) \tag{35}$$

$$+ \frac{h^4}{25920}\left(1224U\left(\frac{U^2}{4\nu^2} + \omega^2\right)^{5/2} + 1236\nu\left(\frac{U^2}{4\nu^2} + \omega^2\right)^3\right),$$

while for the classical Peaceman Rachford scheme,

$$\epsilon_{PR} = \frac{2}{3}\tau^2\nu^3\left(\frac{U^2}{4\nu^2} + \omega^2\right)$$

$$+ \frac{h^2}{12}\left(4U\left(\frac{U^2}{4\nu^2} + \omega^2\right)^{3/2} + \nu\left(\frac{U^2}{4\nu^2} + \omega\right)^2\right). \tag{36}$$

Introducing the Reynolds number, $R = UL/\nu$ the $\epsilon$'s become

$$\epsilon_H = \frac{1}{6}\tau^2\nu^3(R^2 + 16\pi^2) + \frac{1}{829440}\frac{h^4\nu}{L^6}(1224R(R^2 + 16\pi^2)^{5/2} + 1236(R^2 + 16\pi^2)^3), \tag{37}$$

$$\epsilon_{PR} = \frac{1}{6}\tau^2\nu^3(R^2 + 16\pi^2) + \frac{h^2\nu}{192L^4}(8R(R^2 + 16\pi^2)^{3/2} + (R^2 + 16\pi^2)^2). \tag{38}$$

For high Reynolds numbers, i.e., in this case for $R \gg 4\pi$, then

$$\epsilon_H \cong \frac{1}{6}\tau^2\nu^3R^2 + \frac{1}{337}\frac{h^4\nu}{L^6}R^6, \tag{39}$$

$$\epsilon_{PR} \cong \frac{1}{6}\tau^2\nu^3R^2 + \frac{1}{24}\frac{h^2\nu}{L^4}R^4. \tag{40}$$

If one assumes that the spatial errors must be the same for both schemes, and that a typical time frequency of the phenomenon is $f = \nu/L^2$, then:

$$(\epsilon_H)_S = \frac{1}{337}\frac{f}{m^4}R^6, \tag{41}$$

$$(\epsilon_{PR})_S = \frac{1}{24}\frac{f}{m^2}R^4, \tag{42}$$

and, for the Hermitian method,

$$m = 0.233 f^{1/4} R^{3/2} \epsilon^{-1/4} \tag{43}$$

for the PR method

$$m = 0.204 f^{1/2} R^2 \epsilon^{-1/2}. \tag{44}$$

This means that the number of nodes in each direction must increase like $R^{3/2}$ and $R^2$, respectively, and like $f^{1/4}$ and $f^{1/2}$ ($f = 1/T$), respectively; so the steeper the time gradients, or the higher the Reynolds number, or the smaller the error, the more favorable the Hermitian compact method. Even for lower $R$, like in our numerical example, ($R = 20$, $\nu = 0.05$, $L = 1$, $U = 1$), to get a 0.01 error, it takes $m = 39$ for the Hermitian method, and $m = 251$ for the PR method). The total number of nodes would have a ratio 1 to 40, with a 1 to 15 ratio in computer time (because the tridiagonal scheme needs a little more computer time, refer to [1]).

Results of the computations are shown in Table V. From the first and second columns, we can compute the time discretization error, introduce it in the third and fourth columns and compare the resulting spatial errors. For $t = 0.4$, the error with the $O(h^3)$-condition is $9.07 \times 10^{-4}$; the error with the $O(h^2)$-condition is $15.4 \times 10^{-4}$.

Halving the spatial step with the $O(h^3)$-condition gives a spatial error of $9.03 \times 10^{-5}$ and a ratio of 10, indicating a convergence like $h^{3.3}$. Similar computations can be made for other values of $t$. Equivalent values of the error are obtained with the PR method using spatial steps four times smaller.

## 7. Integration on a Nonuniform Grid

In some problems (for example, for boundary layer flows), it would be very useful to use nonuniform computational grids, i.e., a grid where the mesh can be refined or enlarged following the behavior of the solution. Most classical methods lose their accuracy on such grids; Hermitian compact methods, however, keep their good properties. Adam [1] shows that the approximation of $u_x$ with the help of a relation equivalent to (3) is $O(h^4)$, while the approximation of $u_{xx}$ with a relation equivalent to (4) is $O(h^3)$. It can easily be computed that the formula equivalent to (14), derived in the Appendix of this paper, is $O(h^3)$. Some numerical experiments have been performed using Burger's equation. A striking example is given in Table VI. The method used explicit elimination, $O(h^2)$ boundary relation, and a grid in which the mesh was refined in the region of steep gradients and enlarged in smoother regions. For the same computational effort, the error is half of the error of the best method with a uniform step (Table II).

## 5. Conclusions

From several test studies, it can be stated that Hermitian methods are promising highly accurate methods for the solution of parabolic partial differential equations. It has been shown in this paper that higher derivatives of the functions can easily be eliminated as linear combinations of the unknown functions and their first-order derivatives (treated as unknowns too), while keeping the fourth-order accuracy and the tridiagonal nature of the discrete approximation. A third-order additional boundary condition, using only the boundary and two internal points, has been proposed to close the system. Such a condition retains the tridiagonality of the solving system, is coherent with a fourth-order inner scheme, and requires no fictitious boundary point, preventing any instability originating from the boundary. Hermitian compact methods are also very accurate and easy to implement on nonuniform grids.

## Appendix

The problem is to find an approximation of $u_{xx_i}$ with the help of the values of $u_i$ and $u_{x_i}$, which should be the most accurate possible on irregular and regular meshes, using only three nodes, i.e., an approximation like

$$\hat{u}_{xx_i} = (1/h^2)(a_i u_{i+1} + b_i u_i + c_i u_{i-1}) + (1/h)(d_i u_{x_{i+1}} + e_i u_{x_i} + f_i u_{x_{i-1}}).$$

Denoting:

$$x_{i+1} - x_i = \gamma_i h,$$
$$x_i - x_{i-1} = \gamma_{i-1} h,$$

the coefficients are the solution of the system

$$\begin{bmatrix} \frac{\gamma_i^2}{2} & \frac{\gamma_{i-1}^2}{2} & \gamma_i & -\gamma_{i-1} \\ \frac{\gamma_i^3}{6} & -\frac{\gamma_{i-1}^3}{6} & \frac{\gamma_i^2}{2} & -\frac{\gamma_{i-1}^2}{2} \\ \frac{\gamma_i^4}{24} & +\frac{\gamma_{i-1}^4}{24} & \frac{\gamma_i^3}{6} & -\frac{\gamma_{i-1}^3}{6} \\ \frac{\gamma_i^5}{120} & -\frac{\gamma_{i-1}^5}{120} & \frac{\gamma_i^4}{24} & \frac{\gamma_{i-1}^4}{24} \end{bmatrix} \begin{bmatrix} a_i \\ c_i \\ d_i \\ f_i \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$b_i \quad -(a_i + c_i),$$

$$e_i = -(d_i + f_i) + \gamma_{i-1} c_i - \gamma_i a_i .$$

A simpler system arises when all the $\gamma_i$'s are equal to 1, i.e., on a regular mesh; then the system becomes

$$\begin{pmatrix} 1 & 1 & 2 & -2 \\ 1 & -1 & 3 & +3 \\ 1 & 1 & 4 & -4 \\ 1 & -1 & 5 & +5 \end{pmatrix} \begin{pmatrix} a_i \\ c_i \\ d_i \\ f_i \end{pmatrix} = \begin{pmatrix} 2 \\ 0 \\ 0 \\ 0 \end{pmatrix}.$$

and yields (14).

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