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An Operator Compact Implicit Method of Exponential Type

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A fourth-order accurate tridiagonal operator compact implicit finite-difference method for diffusion–convection equations is developed. The coefficients of the difference operator contain exponentials of the coefficients of the differential operator. In this way the method avoids spurious oscillations when the cell Reynolds number is large. Numerical results and comparisons to other methods are presented.

INTRODUCTION

The numerical simulation or modelling of physical processes involving diffusion and convection involves the approximation of spatial differential operators of the form

$$Lu = \frac{\partial}{\partial x}\left(a(x)\frac{\partial u}{\partial x}\right) + b(x)\frac{\partial u}{\partial x}. \tag{1}$$

Of extreme importance and difficulty in these physical applications is the case of convection-dominated flow, i.e., the case where the diffusion coefficient $a(x)$ is much smaller than the convection coefficient $b(x)$. Examples of this type of flow are boundary-layer flow, convective-heat transport with large Peclet numbers, and miscible-displacement processes in flow-through porous media.

The ability of numerical methods to solve problems in which Eq. (1) appears may be studied through consideration of the singular perturbation problem

$$\begin{gathered} Lu = \varepsilon\frac{\partial^2 u}{\partial x^2} + b(x)\frac{\partial u}{\partial x} = f, \qquad \text{for} \quad x \in (0, 1), \\ u(0) = \alpha_0, \qquad u(1) = \alpha_1, \end{gathered} \tag{2}$$

where f is smooth, α_0 and α_1 are given constants, and b is positive. With the above assumptions, it is well known that as $\varepsilon \to 0$, Eq. (2) has no turning points, the soution exhibits a boundary layer adjacent to $x = 0$, and obeys a maximum principle [1].

Classical finite-difference methods for Eq. (2) are constructed by developing separate difference relationships for first and second derivatives and combining these formulas to obtain an approximation to the differential operator. If central-difference

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methods are used for both first and second derivatives, then the derived scheme will have a formal cell Reynolds-number limitation. That is, with a uniform mesh length h, $f=0$, and b constant, one finds that the *cell Reynolds number*, bh/ε, must be bounded by a method-dependent constant to avoid spurious oscillations or gross inaccuracies. For small ε this requires a prohibitive number of grid points. The cell Reynolds-number problem may be avoided by replacing the central-difference approximation used for the first derivative with a noncentered- or "upwind"-difference method. The result is a method which avoids spurious oscillations. However, artificial diffusion has been added to the problem, thus smearing out any sharp fronts that exist.

The most commonly used of the above methods are a second-order method derived by using second-order central differences and having a cell Reynolds-number condition of $bh/\varepsilon < 2$, and a first-order method derived by using second-order central differences for the second derivative and a first-order upwind difference for the first derivative. Both of these methods may be classified as explicit-tridiagonal methods. That is, they have the form

$$r_j^+ u_{j+1} + r_j^c u_j + r_j^- u_{j-1} = q_j^c (Lu)_j, ..., \tag{3}$$

where u_j and $(Lu)_j$ are approximations to $u(x_j)$ and $L(u(x_j))$, respectively, and r_j^+, r_j^-, r_j^c, and q^c are coefficients which depend on the differential operator. Note that the maximum accuracy possible with any explicit-tridiagonal method is second order.

An alternative to the classical approach of separate substitution to obtain difference formulas is the class of implicit-tridiagonal methods. These methods are derived by seeking a relationship between the unknown solution and the entire differential operator on three adjacent points. The result is a method of the form

$$r_j^+ u_{j+1} + r_j^c u_j^+ r_j u_{j-1} = q_j^+ (Lu)_{j+1} + q_j^c (Lu)_j + q_j^- (Lu)_{j-1}, \tag{4}$$

with the additional coefficients q_j^+ and q_j^- nonzero and dependent on the coefficients of the differential operator. Note that the r_j^+, r_j^-, r_j^c, and q_j^+, q_j^-, q_j^c define tridiagonal-difference operators R and Q then Eq. (4) may be rewritten

$$Q(Lu)_j = Ru_j \tag{4a}$$

or

$$(Lu)_j = Q^{-1} Ru_j. \tag{4b}$$

If the method described by Eq. (4) is formally fourth-order accurate, then the method is known as an *operator compact implicit* (OCI) method. Note that formal fourth-order accuracy is the highest accuracy that can be obtained by a method of the form of Eq. (4).

The original OCI method was developed by Swartz [3] for a uniform mesh using Hermite–Birkhoff interpolation. A Taylor-series development of the method for both uniform and nonuniform mesh was given by Ciment *et al.* [4]. In [4] it was shown that for a uniform mesh the method had a formal cell Reynolds-number limitation of $bh/\varepsilon < \sqrt{12}$. In [5], Berger *et al.* showed that a class of OCI methods could be obtained by considering the OCI coefficients derived from the Taylor-series approach as asymptotic series in the mesh size h. The result is a method with nine free parameters. Using six of these parameters it is possible to obtain a formally fourth-order method with no cell Reynolds-number limitation. Moreover, the resulting tridiagonal system of equations is diagonally dominant and satisfies a maximum principle corresponding to that satisfied by Eq. (2).

All of the above methods may be classified as polynomial methods; i.e., the coefficients r_j^+, r_j^c, r_j^-, and q_j^+, q_j^c, q_j^- of the difference operator are polynomials in the mesh size h. These methods have the property that if ε is of the order h, then they reduce to $0(1)$ methods. This can be seen directly by comparing the exact solution with the finite-difference solution for the special case of Eq. (2), with $u(0)=1$, $u(1)=0, f=0$, and b constant. It can be shown that when ε is $0(h)$ the $0(1)$ behavior will occur unless r_j^-/r_j^+ becomes $\exp(-bh/\varepsilon)$ as $h \to 0$. Miller [6] has shown that uniform convergence for any positive order can be obtained only by schemes that incorporate an appropriate exponential character into their coefficients.

Finite-difference methods that incorporate this exponential character are known as methods of exponential type. An explicit-tridiagonal method of exponential type was given by Allen and Southwell in [7]. The uniform first-order accuracy of this method as applied to Eq. (2) is given in [8–10]. An implicit-tridiagonal scheme of exponential type was derived by El-Mistikawy and Werle [11]. The method of derivation involving fundamental solutions of the differential operator is a modification of the approach given in [8]. The uniform second-order convergence of this implicit scheme has recently been shown [12].

In this paper an OCI method of exponential type is developed. This is derived to be formally fourth-order accurate and in the case of ε being $0(h)$ reducing to second-order accuracy. The orders of accuracy are verified experimentally. The method is derived by introducing an integral identity for the differential operator given in Eq. (1). It is then shown that both the method of Allen, Southwell and El-Mistakawy, Werle can be derived using this identity. After deriving the exponential OCI method for Eq. (1), a numerical example comparing the polynomial schemes with the exponential schemes on a singular perturbation problem with $\varepsilon = h^P$ is given. Finally, the exponential OCI method is extended to time-dependent problems and systems of equations and its behavior is demonstarted on a problem with a moving front.

2. Derivation of the Integral Identity

Consider the diffusion–convection equation

$$Lu = \frac{\partial}{\partial x}\left(a(x)\frac{\partial u}{\partial x}\right) + b(x)\frac{\partial u}{\partial x} = f(x) \qquad \text{on} \quad [0, 1] \tag{5}$$

$$u(0) = g_1; \qquad u(1) = g_2, \tag{6}$$

where $a \geqslant a_0 > 0$ and $b \geqslant b_0 > 0$ on $[0, 1]$.

In order to derive the exponential OCI method, it is necessary to develop an integral identity for Eq. (5). Divide the interval $[0, 1]$ into a uniform mesh $x_j = jh$, $j = 0, 1, \ldots, J$ and $h = 1/J$. On the subinterval $[x_{j-1}, x_{j+1}]$ define the function P as

$$\begin{aligned} P &= \frac{\exp\left[\int_{x_j}^{x} \frac{b}{a}\, d\xi\right]}{\int_{x_j}^{x_{j+1}} \exp\left[-\int_{x_j}^{x} \frac{b}{a}\, d\xi\right] \Big/ a\, dx} \int_{x}^{x_{j+1}} \exp\left[-\int_{x_j}^{x} \frac{b}{a}\, d\xi\right] \Big/ a\, dx, \\ &\qquad\qquad x_j < x \leqslant x_{j+1} \\ &= \frac{\exp\left[\int_{x_j}^{x} \frac{b}{a}\, d\xi\right]}{\int_{x_{j-1}}^{x_j} \exp\left[-\int_{x_j}^{x} \frac{b}{a}\, d\xi\right] \Big/ a\, dx} \int_{x_{j-1}}^{x} \exp\left[-\int_{x_j}^{x} \frac{b}{a}\, d\xi\right] \Big/ a\, dx, \\ &\qquad\qquad x_{j-1} \leqslant x \leqslant x_j. \end{aligned} \tag{7}$$

The function P has the following important properties:

(1) $P(x_{j+1}) = P(x_{j-1}) = 0$,

(2) P is continuous at x_j and $P(x_j) = 1$,

(3) $\partial P/\partial x$ is discontinuous at x_j,

(4)

$$\begin{aligned} -a\frac{\partial P}{\partial x} + bP &= \left(\int_{x_j}^{x_{j+1}} \exp\left[-\int_{x_j}^{x} \frac{b}{a}\, d\xi\right] \Big/ a\, dx\right)^{-1}, \qquad x_j \leqslant x \leqslant x_{j+1} \\ &= -\left(\int_{x_{j-1}}^{x_j} \exp\left[-\int_{x_j}^{x} \frac{b}{a}\, d\xi\right] \Big/ a\, dx\right)^{-1}, \qquad x_{j-1} \leqslant x \leqslant x_j. \end{aligned} \tag{8}$$

(5) P is proportional to the discrete Green's function for the operator L.

Multiply Eq. (5) by P and integrate from x_{j-1} to x_{j+1}; i.e.,

$$\int_{x_{j-1}}^{x_{j+1}} \left[P\frac{\partial}{\partial x}\left(a\frac{\partial u}{\partial x}\right) + Pb\frac{\partial u}{\partial x}\right] dx = \int_{x_{j-1}}^{x_{j+1}} Pf\, dx. \tag{9}$$

Integrating the left-hand side of Eq. (9) by parts, first from x_{j-1} to x_j and then from x_j to x_{j+1}, Eq. (9) becomes

$$\int_{x_j}^{x_{j+1}} \left(-a\frac{\partial P}{\partial x} + bP\right)\frac{\partial u}{\partial x}\,dx + \int_{x_{j-1}}^{x_j} \left(-a\frac{\partial P}{\partial x} + bP\right)\frac{\partial u}{\partial x}\,dx + \left(aP\frac{\partial u}{\partial x}\right)\Big|_{x_j}^{x_{j+1}} + \left(aP\frac{\partial u}{\partial x}\right)\Big|_{x_{j-1}}^{x_j} = \int_{x_{j-1}}^{x_{j+1}} Pf. \tag{10}$$

Using properties (1), (2), and (4), Eq. (10) becomes

$$\frac{u_{j+1}}{\int_{x_j}^{x_{j+1}} \exp\left[-\int_{x_j}^{x} \frac{b}{a}\,d\xi\right]\Big/ a\,dx} - \left(\frac{1}{\int_{x_j}^{x_{j+1}} \exp\left[-\int_{x_j}^{x} \frac{b}{a}\,d\xi\right]\Big/ a\,dx} + \frac{1}{\int_{x_{j-1}}^{x_j} \exp\left[-\int_{x_j}^{x} \frac{b}{a}\,d\xi\right]\Big/ a\,dx}\right)u_j + \frac{u_{j-1}}{\int_{x_{j-1}}^{x_j} \exp\left[-\int_{x_j}^{x} \frac{b}{a}\,d\xi\right]\Big/ a\,dx} = \int_{x_{j-1}}^{x_{j+1}} Pf, \tag{11}$$

where $u_j = u(x_j)$.

Integrating the right-hand side of Eq. (11) by parts from x_{j-1} to x_j and then x_j to x_{j+1} the integral identity

$$\begin{aligned}
&\frac{u_{j+1}}{\int_{x_j}^{x_{j+1}} \exp\left[-\int_{x_j}^{x} \frac{b}{a}\,d\xi\right]\Big/ a\,dx} \\
&\quad - \left(\frac{1}{\int_{x_j}^{x_{j+1}} \exp\left[-\int_{x_j}^{x} \frac{b}{a}\,d\xi\right]\Big/ a\,dx} + \frac{1}{\int_{x_{j-1}}^{x_j} \exp\left[-\int_{x_j}^{x} \frac{b}{a}\,d\xi\right]\Big/ a\,dx}\right)u_j \\
&\quad + \frac{u_{j-1}}{\int_{x_{j-1}}^{x_j} \exp\left[-\int_{x_j}^{x} \frac{b}{a}\,d\xi\right]\Big/ a\,dx} = \int_{x_{j-1/2}}^{x_{j+1/2}} f\,dx \\
&\quad - \left(\int_{x_j}^{x_{j+1}} \exp\left[-\int_{x_j}^{x} \frac{b}{a}\,d\xi\right]\Big/ a\,dx\right)^{-1} \\
&\quad \times \int_{x_j}^{x_{j+1}} \left[\left(\frac{b}{a} \exp\left[\int_{x_j}^{x} \frac{b}{a}\,d\xi\right]\right.\right. \\
&\quad \times \left.\left.\int_{x}^{x_{j+1}} \exp\left[-\int_{x_j}^{x} \frac{b}{a}\,d\xi\right]\Big/ a\,dx - \frac{1}{a}\right)\int_{x_{j+1/2}}^{x} f\right] dx
\end{aligned}$$

$$- \left(\int_{x_{j-1}}^{x_j} \exp\left[-\int_{x_j}^{x} \frac{b}{a} \, d\xi \right] \Big/ a \, dx \right)^{-1}$$

$$\times \int_{x_{j-1}}^{x_j} \left[\left(\frac{b}{a} \exp\left[\int_{x_j}^{x} \frac{b}{a} \, d\xi \right] \int_{x_{j-1}}^{x} \exp\left[-\int_{x_j}^{x} \frac{b}{a} \, d\xi \right] \Big/ a \, dx + \frac{1}{a} \right) \int_{x_{j-1/2}}^{x} f \right] dx \quad (12)$$

is derived.

The integral identity (12) is known as Marchuk identity. Such an identity for $b \equiv 0$ is derived in [13].

3. Derivation of Allen–Southwell and El-Mistakawy–Werle Methods

All the finite-difference schemes to be derived using Eq. (12) are tridiagonal-difference methods. That is, they take the form

$$r_j^+ u_{j+1} + r_j^c u_j + r_j^- u_{j-1} = q_j^+ f_{j+1} + q_j^c f_j + q_j^- f_{j-1}. \quad (13)$$

These methods are explicit if $q_j^+ = q_j^- = 0$ and implicit, otherwise. The coefficients r_j^+, r_j^c, r_j^-, q_j^+, q_j^c, and q_j^- of the difference operator depend on the coefficients a and b of the differential operator and the mesh size h.

Assume in Eq. (12) that in the interval $[x_{j-1}, x_{j+1}]$, b and a are constant and they assume the value at x_j, Also, define ρ_j by

$$\rho_j = b_j h / a_j. \quad (14)$$

Under these assumptions

$$\left(\int_{x_{j-1}}^{x_j} \exp\left[-\int_{x_j}^{x} \frac{b}{a} \, d\xi \right] \Big/ a \, dx \right)^{-1} = \frac{b_j e^{-\rho_j}}{1 - e^{-\rho_j}} \quad (15a)$$

and

$$\left(\int_{x_j}^{x_{j-1}} \exp\left[-\int_{x_j}^{x} \frac{b}{a} \, d\xi \right] \Big/ a \, dx \right)^{-1} = \frac{b_j}{1 - e^{-\rho_j}}. \quad (15b)$$

Finally, approximate all the integrals on the right-hand side of Eq. (12) by the midpoint rule. The result is the explicit-tridiagonal method due to Allen and Southwell [7] defined by

$$r_j^+ = b_j/(1 - e^{-\rho_j}); \qquad r_j^- = b_j r^{-\rho_j}/(1 - e^{-\rho_j}); \qquad r_j^c = -(r_j^+ + r_j^-);$$
$$q_j^c = h \qquad \text{and} \qquad q_j^+ = q_j^- = 0. \quad (16)$$

The method described in Eq. (16) has been shown to be uniformly $0(h)$ for Eqs. (5), ([6, 8–10]). Following [5], this method is to be denoted as the explicit-fundamental solution method.

Assume now that a, b, and f are piecewise constant in $[x_{j-1}, x_{j+1}]$ with the values in $[x_{j-1}, x_j]$

$$a^- = (a_{j-1} + a_j)/2,\ b^- = (b_{j-1} + b_j)/2,\ f_{j-1/2} = (f_{j-1} + f_j)/2,$$

and the values in $[x_j, x_{j+1}]$ as

$$a^+ = (a_j + a_{j+1})/2,\ b^+ = (b_j + b_{j+1})/2,\ f_{j+1/2} = (f_j + f_{j+1})/2.$$

Also, define

$$\rho^+ = b^+ h/a^+$$

and

$$\rho^- = b^- h/a^-.$$

Under these assumptions

$$\begin{aligned} r_j^+ &= \left(\int_{x_j}^{x_{j+1}} \exp\left[-\int_{x_j}^{x} \frac{b}{a}\, d\xi\right]\Big/ a\, dx\right)^{-1} = \frac{b^+}{1 - e^{-\rho^+}}, \\ r_j^- &= \left(\int_{x_{j-1}}^{x_j} \exp\left[-\int_{x_j}^{x} \frac{b}{a}\, d\xi\right]\Big/ a\, dx\right)^{-1} = \frac{e^{-\rho^-} b^-}{1 - e^{-\rho^-}}, \end{aligned} \tag{16}$$

$$\begin{aligned} r_j^c &= -(r_j^+ + r_j^-),\ q_j = (h/2b^-)((a^-/h) - r_j^-), \\ q_j^+ &= (h/2b^+)(r_j^+ - (a^+/h)),\ q_j^c = q_j^- + q_j^+. \end{aligned} \tag{17}$$

This method, due to El-Mistakawy and Werle [11] has been shown to be uniformly $0(h^2)$ [12] for all values of b and a. Following (5), this method is to be denoted as the implicit-fundamental solution method.

4. Derivation of the Exponential OCI Method

Both the explicit- and implicit-fundamental solution methods were derived by assuming approximations for a, b, and f and then evaluating the integrals in Eq. (12). To derive the exponential OCI method, first assume that a and b are piecewise quadratic on $[x_{j-1}, x_{j+1}]$. That is, in $[x_{j-1}, x_j]$, a and b are the quadratic polynomials determined by the values a_{j-1}, $a_{j-1/2}$, a_j and b_{j-1}, $b_{j-1/2}$, b_j, respectively, and in $[x_j, x_{j+1}]$ a and b are the quadratic polynomials determined by the values a_j, $a_{j+1/2}$, a_{j+1} and b_j, $b_{j+1/2}$, b_{j+1}, respectively.

To define r_j^+, r_j^-, and r_j^c it is necessary to evaluate the terms

$$\frac{1}{r_j^+} = \int_{x_j}^{x_{j+1}} \exp\left[-\int_{x_j}^{x} \frac{b}{a}\, d\xi\right] \Big/ a\, dx \tag{18a}$$

$$\frac{1}{r_j^-} = \int_{x_{j-1}}^{x_j} \exp\left[-\int_{x_j}^{x} \frac{b}{a}\, d\xi\right] \Big/ a\, dx. \tag{18b}$$

Using integration by parts, Eq. (18) becomes

$$\begin{aligned}\frac{1}{r_j^+} = \frac{1}{b_j} - &\left(\exp\left[-\int_{x_j}^{x_{j+1}} \frac{b}{a}\, dx\right] \Big/ b_{j+1}\right) \\ &- \int_{x_j}^{x_{j+1}} \left[\exp\left[-\int_{x_j}^{x} \frac{b}{a}\, d\xi\right] \frac{1}{b^2} \frac{\partial b}{\partial x}\right] dx \end{aligned}\tag{19a}$$

$$\begin{aligned}\frac{1}{r_j^-} = \exp\left[-\int_{x_{j-1}}^{x_j} \frac{b}{a}\, dx\right] &\left(\frac{1}{b_{j-1}} - \left(\exp\left[-\int_{x_{j-1}}^{x_j} \frac{b}{a}\, dx\right] \Big/ b_j\right)\right. \\ &\left. - \int_{x_{j-1}}^{x_j} \left[\exp\left[-\int_{x_{j-1}}^{x} \frac{b}{a}\, d\xi\right] \frac{1}{b^2} \frac{\partial b}{\partial x}\right] dx\right). \end{aligned}\tag{19b}$$

The remaining integrals in Eq. (19) should be evaluated using Simpson's rule and the quadratic approximations for a and b.

The resulting formulas for r_j^-, r_j^+, and r_j^c are

$$r_j^- = \frac{\exp\left[-\int_{x_{j-1}}^{x_j} \frac{b}{a}\, d\xi\right]}{\frac{1}{b_{j-1}} - \left(\exp\left[-\int_{x_{j-1}}^{x_j} \frac{b}{a}\, d\xi\right] \Big/ b_j\right) - \int_{x_{j-1}}^{x_j} \left(\exp\left[-\int_{x_{j-1}}^{x} \frac{b}{a}\, d\xi\right] \frac{1}{b^2} \frac{\partial b}{\partial x}\right) dx}, \tag{20a}$$

$$r_j^+ = \frac{1}{\frac{1}{b_j} - \left(\exp\left[-\int_{x_j}^{x_{j+1}} \frac{b}{a}\, d\xi\right] \Big/ b_{j+1}\right) - \int_{x_j}^{x_{j+1}} \left(\exp\left[-\int_{x_j}^{x} \frac{b}{a}\, d\xi\right] \frac{1}{b^2} \frac{\partial b}{\partial x}\right) dx}, \tag{20b}$$

$$r_j^c = -(r_j^+ + r_j^-). \tag{20c}$$

In evaluating the coefficients r_j^+, r_j^c, and r_j^- integrations by parts was performed before any quadrature. This was performed so that as the function a approaches zero the OCI coefficients approach the same limit as the second-order fundamental solution method. Direct quadrature of Eq. (18) by Simpson's rule would not have this property and the method would not converge as the coefficient a approaches zero.

To evaluate q_j^-, q_j^+, and q_j^c the following terms from Eq. (12) must be computed:

$$\int_{x_{j-1/2}}^{x_{j+1/2}} f\,dx, \tag{21a}$$

$$-r_j^+ \int_{x_j}^{x_{j+1}} \left[\left(\frac{b}{a}\exp\left[\int_{x_j}^{x}\frac{b}{a}\,d\xi\right] \times \int_{x}^{x_{j+1}} \exp\left[-\int_{x_j}^{x}\frac{b}{a}\,d\xi\right]\Big/ a\,dx - \frac{1}{a}\right)\int_{x_{j+1/2}}^{x} f\right] dx, \tag{21b}$$

$$-r_j^- \int_{x_{j-1}}^{x_j} \left[\left(\frac{b}{a}\exp\left[\int_{x_j}^{x}\frac{b}{a}\,d\xi\right] \times \int_{x_{j-1}}^{x} \exp\left[-\int_{x_j}^{x}\frac{b}{a}\,d\xi\right]\Big/ a\,dx + \frac{1}{a}\right)\int_{x_{j-1/2}}^{x} f\right] dx. \tag{21c}$$

The integral in Eq. (21a) is computed using Simpson's rule and the approximation

$$f_{j-1/2} + f_{j+1/2} = \tfrac{1}{4}(f_{j-1} + 6f_j + f_{j+1}) + 0(h^4).$$

The resulting approximation is

$$\int_{x_{j-1/2}}^{x_{j+1/2}} f\,dx \approx \frac{h}{24}(f_{j-1} + 22f_j + f_{j+1}). \tag{22}$$

To evaluate the integral in Eq. (21b) first integrate by parts the term

$$\int_{x}^{x_{j+1}} \left(\exp\left[-\int_{x_j}^{x}\frac{b}{a}\,d\xi\right]\Big/ a\,dx\right).$$

Equation (21b) becomes

$$r_j^+ \int_{x_j}^{x_{j+1}} \left[\frac{b}{a}\left(\exp\left[-\int_{x}^{x_{j+1}}\frac{b}{a}\,d\xi\right]\Big/ b_{j+1}\right) + \frac{b}{a}\exp\left[\int_{x_j}^{x}\frac{b}{a}\,d\xi\right] \times \int_{x}^{x_{j+1}}\left(\exp\left[-\int_{x_j}^{x}\frac{b}{a}\,d\xi\right]\frac{1}{b^2}\frac{\partial b}{\partial x}\right)\int_{x_{j+1/2}}^{x} f\right] dx. \tag{23}$$

Now assume that f is linear in $[x_j, x_{j+1}]$; i.e.,

$$f = f_{j+1/2} + f'_{j+1/2}(x - x_{j+1/2}) \tag{24a}$$

and

$$\int_{x_{j+1/2}}^{x} f\,dx = f_{j+1/2}(x - x_{j+1/2}) + f'_{j+1/2}(x - x_{j+1/2})^2/2. \tag{24b}$$

Substituting Eq. (24b) into (23) and integrating several times by parts, Eq. (21b) becomes

$$hf_{j+1/2}\left[-\left(\frac{1}{2}+\frac{a_j}{hb_j}+\frac{1}{6}\frac{\partial}{\partial x}\left(\frac{a}{b}\right)_j\right)+r_j^+\left(\frac{1}{6}\left(\frac{1}{b_{j+1}}+\frac{4}{b_{j+1/2}}+\frac{1}{b_j}\right)\right.\right.$$
$$+\frac{2}{3}\frac{\partial}{\partial x}\left(\frac{a}{b}\right)_{j+1/2}\left(-\frac{1}{b_{j+1/2}}+\left(\exp\left[-\int_{x_{j+1/2}}^{x_{j+1}}\frac{b}{a}\,d\xi\right]\Big/b_{j+1}\right)\right.$$
$$\left.\left.\left.+\int_{x_{j+1/2}}^{x_{j+1}}\left(\exp\left[-\int_{x_{j+1/2}}^{x}\frac{b}{a}\,d\xi\right]\frac{1}{b^2}\frac{\partial b}{\partial x}\right)dx\right)\right)\right]+\frac{h^2}{24}f'_{j+1/2}. \tag{25}$$

The procedure for the evaluation of the integral in (21c) is similar. The resulting formula is

$$hf_{j-1/2}\left[-\left(\frac{1}{2}-\frac{a_j}{hb_j}+\frac{1}{6}\frac{\partial}{\partial x}\left(\frac{a}{b}\right)_j\right)+r_j^-\left(-\frac{1}{6}\left(\frac{1}{b_j}+\frac{4}{b_{j-1/2}}+\frac{1}{b_{j-1}}\right)\right.\right.$$
$$+\frac{2}{3}\frac{\partial}{\partial x}\left(\frac{a}{b}\right)_{j-1/2}\left(-\left(\exp\left[-\int_{x_{j-1}}^{x_{j-1/2}}\frac{b}{a}\right]d\xi\Big/b_{j-1}\right)+\frac{1}{b_{j+1/2}}\right.$$
$$\left.\left.\left.+\exp\left[\int_{x_{j-1}}^{x_{j-1/2}}\frac{b}{a}\,d\xi\right]\int_{x_{j-1}}^{x_{j-1/2}}\left(\exp\left[-\int_{x_{j-1}}^{x}\frac{b}{a}\,d\xi\right]\frac{1}{b^2}\frac{\partial b}{\partial x}\right)dx\right)\right)\right]$$
$$-\frac{h^2}{24}f'_{j-1/2}. \tag{26}$$

Replacing $f_{j+1/2}, f'_{j+1/2}, f_{j-1/2}$, and $f'_{j-1/2}$ by the formulas

$$f_{j+1/2}=(f_j+f_{j+1})/2, \qquad f'_{j+1/2}=(f_{j+1}-f_j)/h,$$
$$f_{j-1/2}=(f_{j-1}+f_j)/2, \qquad f'_{j-1/2}=(f_j-f_{j-1})/h,$$

and combining Eqs. (22), (25), and (26) the operator Q is defined by

$$q_j^+=h(\tfrac{1}{12}+\tilde{q}_j^+), \tag{27a}$$
$$q_j^c=h(\tfrac{10}{12}+\tilde{q}_j^++\tilde{q}_j^-), \tag{27b}$$
$$q_j^-=h(\tfrac{1}{12}+\tilde{q}_j^-), \tag{27c}$$

where

$$\tilde{q}_j^+=-\left(\frac{1}{4}+\frac{a_j}{2hb_j}+\frac{1}{12}\frac{\partial}{\partial x}\left(\frac{a}{b}\right)_j\right)+r_j^+\left(\frac{1}{12}\left(\frac{1}{b_{j+1}}+\frac{4}{b_{j+1/2}}+\frac{1}{b_j}\right)\right.$$
$$+\frac{1}{3}\frac{\partial}{\partial x}\left(\frac{a}{b}\right)_{j+1/2}\left(-\frac{1}{b_{j+1/2}}+\left(\exp\left[\int_{x_{j+1/2}}^{x_{j+1}}\frac{b}{a}\,d\xi\right]\Big/b_{j+1}\right)\right.$$
$$\left.\left.+\int_{x_{j+1/2}}^{x_{j+1}}(\exp\left[-\int_{x_{j+1/2}}^{x}\frac{b}{a}\,d\xi\right]\frac{1}{b^2}\frac{\partial b}{\partial x}dx\right)\right)$$

$$\tilde{q}_j^- = -\left(\frac{1}{4} - \frac{a_j}{2hb_j} + \frac{1}{12}\frac{\partial}{\partial x}\left(\frac{a}{b}\right)_j\right) + r_j^-\left(-\frac{1}{12}\left(\frac{1}{b_j} + \frac{4}{b_{j-1/2}} + \frac{1}{b_{j-1}}\right)\right.$$
$$+ \frac{1}{3}\frac{\partial}{\partial x}\left(\frac{a}{b}\right)_{j-1/2}\left[-\left(\exp\left[-\int_{x_{j-1}}^{x_{j-1/2}} \frac{b}{a}\, d\xi\right]\Big/ b_{j-1}\right)\right.$$
$$+ \frac{1}{b_{j-1/2}} + \exp\left[\int_{x_{j-1}}^{x_{j-1/2}} \frac{b}{a}\, d\xi\right]$$
$$\left.\left.\times \int_{x_{j-1}}^{x_{j-1/2}} \left(\exp\left[-\int_{x_{j-1}}^{x} \frac{b}{a}\, d\xi\right]\frac{1}{b^2}\frac{\partial b}{\partial x}\right) dx\right]\right)$$

and all remaining integrals are evaluated using Simpson's rule and the quadratic approximations for a and b.

Note that the exponential OCI formulas for b strictly negative are exactly the same. Care must be taken, however, in evaluating the exponentials to avoid overflows for large values of bh/a.

5. A Singular Perturbation Problem

The first numerical example to be considered is the singular perturbation problem

$$\begin{aligned} &\varepsilon \frac{\partial^2 u}{\partial x^2} + b(x)\frac{\partial u}{\partial x} = f(x, \varepsilon), \qquad x \in (0, 1), \\ &u(0) = u_e(0), \qquad u(1) = u_e(1), \end{aligned} \tag{28}$$

$$\begin{aligned} u_e(x) &= \frac{1}{b(x)} \exp\left[-\frac{1}{\varepsilon}\int_0^x b(\xi)\, d\xi\right] + \exp(-x/2), \\ b(x) &= (x+1)^3. \end{aligned} \tag{29}$$

The function $u_e(x)$ determines $f(x, \varepsilon)$. The motivation for this choice of the form of the exact solution u_e comes from the decomposition of the solution u of Eq. (28) suggested by its uniformly valid asymptotic expansion as $\varepsilon \to 0$ (see Smith [1]),

$$u(x) = A_0(x) + \frac{c}{b(x)} \exp\left[-\frac{1}{\varepsilon}\int_0^x b(\xi)\, d\xi\right] + \varepsilon R_0(x, \varepsilon), \tag{30}$$

where c is a constant, A_0 is smooth, and $R_0(x, \varepsilon)$ satisfies an equation of the same general form as Eq. (28). The first term on the right side of Eq. (29) has the form of the "most singular part" of a solution of Eq. (28), while the second term is smooth. Note that as ε becomes much smaller than the mesh size h, the first term becomes virtually zero at all grid points except $x = 0$. Thus for $\varepsilon \ll h$, $u(x)$ and, in general, its numerical approximation, are dominated by the second term on the right side of

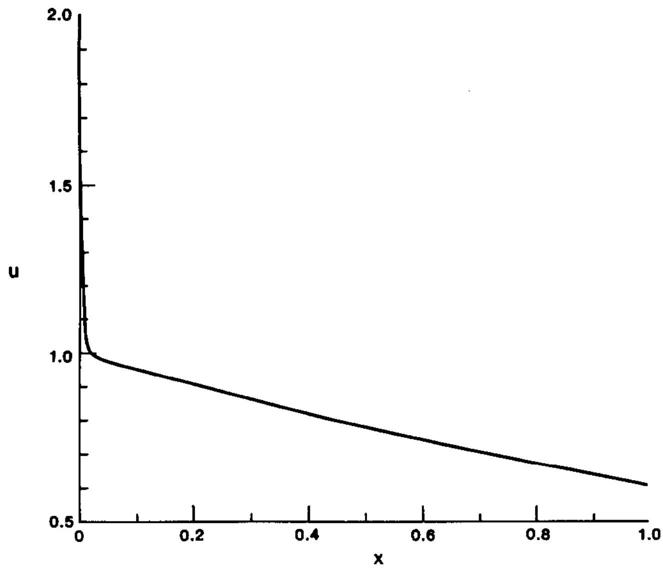

FIG. 1. Solution of singular perturbation problem. $Lu = \varepsilon u_{xx} + b(x)u_x = f(x)$, on $[0, 1]$; $u(0) = u_e(0)$, $u(1) = u_e(1)$, and $b(x) = (x+1)^3$; and $u_e(x) = (1/b(x)) \exp[-1/\varepsilon \int_0^x b(x)\,dx] + e^{-x/2}$, $\varepsilon = \frac{1}{256}$.

Eq. (29). A plot of the exact solution for $\varepsilon = \frac{1}{256}$ is given in Fig. 1. This example was also examined in detail by Berger *et al.* [5].

The methods to be compared are the standard centered second-order method, the standard OCI method [3, 4], a first-order upwind method, a second-order upwind method, the explicit- and implicit-fundamental solution methods, generalized OCI [5], and exponential OCI. The Q and R operators for the standard centered second-order method and the first- and second-order upwind methods are given in Table I. To conveniently generate a wide variation of h and ε for each method considered, Eq. (28) was solved with $\varepsilon \equiv h^P$ for various values of p. For each method and each value of p, the mesh length h was successively halved starting with $h = \frac{1}{32}$ to $h = \frac{1}{2048}$. The numerical results are summarized in Table II.

TABLE I

Q and R for Standard Polynomial Difference Methods

Method	r_j^-	r_j^c	r_j^+	q_j^-	q_j^c	q_j^+
Centered second order	$\frac{\varepsilon}{h^2} - \frac{0.5b_j}{2h}$	$\frac{-2\varepsilon}{h^2}$	$\frac{\varepsilon}{h^2} + \frac{0.5b_j}{h}$	0	1	0
Upwind first order	$\frac{\varepsilon}{h^2}$	$\frac{-2\varepsilon}{h^2} - \frac{b_j}{h}$	$\frac{\varepsilon}{h^2} + \frac{b_j}{h}$	0	1	0
Upwind second order	$\frac{\varepsilon}{h^2}$	$\frac{-2\varepsilon}{h^2} - \frac{0.5(b_j + b_{j+1})}{h}$	$\frac{\varepsilon}{h^2} + \frac{0.5(b_j + b_{j+1})}{h}$	0	0.5	0.5

TABLE II

Rate of Convergence and Maximum Error for Singular Perturbation Problem

Method	$\varepsilon = 1$	$\varepsilon = h^{0.50}$	$\varepsilon = h^{0.75}$	$\varepsilon = h$	$\varepsilon = h^{1.5}$	$\varepsilon = h^2$	$\varepsilon = h^3$
Centered	2.02	1.10	0.53	0.01			
second order	3.8E–8	1.8E–5	6.7E–4	3.5E–2			
OCI standard	4.00	2.06	1.01	0.01			
(Swartz)	[a]	7.8E–10	1.5E–6	1.5E–0			
Upwind	1.00	0.52	0.24	0.00	0.49	1.00	1.01
first order	2.0E–4	4.2E–3	2.6E–2	1.3E–1	2.2E–2	5.4E–4	4.8E–5
Upwind	1.00	0.49	0.23	0.00	0.48	1.00	2.00
second order (AKK)	2.8E–4	4.0E–3	2.6E–2	1.3E–1	2.2E–2	4.9E–4	4.8E–5
Fundamental solution explicit ($Q \equiv I$)–	1.97	1.48	1.24	1.00	0.99	1.00	1.00
first order (Allen–Southwell)	3.9E–8	6.1E–7	4.2E–6	3.1E–5	4.7E–5	4.8E–5	4.8E–5
Fundamental solution implicit (OCI)–	2.01	1.98	1.99	2.00	2.04	2.00	2.00
second order (El-Mestikawy–Werle)	2.2E–7	2.7E–7	3.5E–7	2.9E–7	2.4E–8	2.3E–8	2.3E–8
Generalized OCI	4.00	2.21	1.02	0.01	1.94	2.01	2.00
$P1 = 3$	[a]	1.1E–9	1.4E–6	1.4E–3	5.3E–6	2.0E–9	2.0E–9
Exponential OCI	4.01	2.93	2.45	2.02	2.16	2.02	2.00
	[a]	2.9E–12	9.01–11	3.85–09	2.64–08	1.88–8	1.88–8

[a] Denotes round-off error.

For each method and each p the computed rate of convergence and the maximum error for $h = \frac{1}{2048}$ are given. Note the following points in Table II:

(1) The computation for the centered second-order method and the standard OCI method could not continue for $p > 1$ because of cell Reynolds-number conditions.

(2) All the polynomial methods reduced to the predicted 0(1) accuracy for $\varepsilon = h$.

(3) The uniform first-order accuracy of explicit-fundamental solution method and the uniform second-order accuracy of implicit-fundamental solution method was demonstrated.

(4) For $\varepsilon = 1$ the fourth-order accuracy of the exponential OCI method is demonstrated. As p increases a uniform second-order accuracy appears to hold. Further proof of the fourth-order accuracy of the exponential OCI method is given in later examples.

A graphical summary of Table II is presented in Fig. 2.

The convergence results for all the methods considered for Eq. (28) do not hold if the convection term of the differential operator is in conservation form. That is, if

$$Lu = \varepsilon \frac{\partial^2 u}{\partial x^2} + \frac{\partial}{\partial x}(bu), \tag{31}$$

or more generally, if

$$Lu = \frac{\partial}{\partial x}\left(a \frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial x}(bu). \tag{32}$$

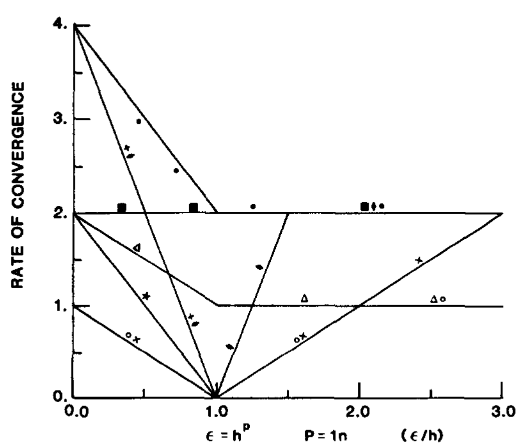

FIG. 2. Rate of convergence for singular perturbation problem. ★, CD; +, OCI Swartz; ○, UP1; ×, UP2; Δ, IFS1; ■, IFS2; ◆, generalized OCI; and ●, exponential OCI.

The results for the polynomial methods that are applicable to equations in conser- [redacted] derivative of the coefficient b. Thus, these methods would not conserve mass and are not discussed here. The exponential methods may be extended to operators of the form of Eq. (32) by introducing a new integral identity (see Appendix A for the derivation of the integral identity and the extension of the implicit-fundamental solution method and the exponential OCI method). To demonstrate the accuracy of the methods for Eq. (32) consider the problem

$$\varepsilon \frac{\partial^2 u}{\partial x^2} + \frac{\partial}{\partial x}(bu) = f, \tag{33}$$

$$\begin{aligned} u(0) &= u_e(0), \qquad u(1) = u_e(1), \\ &= \frac{1}{1-c_1}\left(\exp\left[-\frac{1}{\varepsilon}\int_0^x b(\xi)\,d\xi\right] - \frac{c_1}{b(x)}\right) + \exp(-1/2x), \\ b(x) &= (x+1)^3, \\ c_1 &= b(1)\exp\left[-\frac{1}{\varepsilon}\int_0^1 b(\xi)\,d\xi\right]. \end{aligned} \tag{34}$$

TABLE III

Results for Second-Order Fundamental Solution Method: Conservation Form

h	$\varepsilon = 1$ MER[a]	$\varepsilon = h^{0.5}$ MER	$\varepsilon = h^{0.75}$ MER	$\varepsilon = h$ MER	$\varepsilon = h^{1.5}$ MER	$\varepsilon = h^2$ MER	$\varepsilon = h^3$ MER
1/32	1.23–3	1.32–2	3.49–2	6.62–2	1.03–1	1.07–1	1.08–1
	1.88	1.32	1.00	0.84	0.94	0.95	0.96
1/64	3.46–4	5.30–3	1.75–2	3.69–2	5.36–2	5.51–2	5.53–2
	1.98	1.35	1.06	0.92	0.97	0.98	0.98
1/128	8.53–5	2.08–3	8.36–3	1.95–2	2.74–2	2.80–2	2.80–2
	2.00	1.37	1.12	0.95	0.98	0.99	0.99
1/256	2.14–5	8.05–4	3.85–3	1.01–2	1.39–2	1.41–2	1.41–2
	2.00	1.38	1.16	0.97	0.90	0.99	1.00
1/512	5.34–6	3.09–4	1.72–3	5.18–3	7.01–3	7.08–3	7.08–3
	2.00	1.40	1.19	0.98	0.99	1.00	1.00
1/1024	1.34–6	1.17–4	7.58–4	2.62–3	3.52–3	3.55–3	3.55–3
	2.00	1.42	1.20	0.99	1.00	1.00	1.00
1/2056	3.34–7	4.35–5	3.29–4	1.32–3	1.76–3	1.78–3	1.78–3

[a] Maximum error rate.

TABLE IV

Results for Exponential Operator Compact Implicit Method: Conservation Form

h	$\varepsilon = 1$ MER[a]	$\varepsilon = h^{0.5}$ MER	$\varepsilon = h^{0.75}$ MER	$\varepsilon = h$ MER	$\varepsilon = h^{1.6}$ MER	$\varepsilon = h^2$ MER	$\varepsilon = h^3$ MER
1/32	8.99–5	1.01–4	1.31–3	7.28–3	5.36–3	1.60–3	8.73–4
	5.45	2.23	1.47	0.89	1.50	1.92	2.03
1/64	2.05–6	2.15–5	4.74–4	3.93–3	1.90–3	4.21–4	2.13–4
	3.55	2.38	1.55	0.93	1.51	1.96	1.97
1/128	1.75–7	4.13–6	1.62–4	2.06–3	6.66–4	1.08–4	5.44–5
	4.02	2.40	1.60	0.96	1.52	1.98	1.99
1/250	1.08–8	7.84–7	5.34–5	1.06–3	2.33–4	2.74–5	1.37–5
	4.01	2.41	1.64	0.97	1.52	1.99	1.99
1/512	6.71–10	1.47–7	1.71–5	5.42–3	8.15–5	6.89–6	3.45–6
	4.03	2.43	1.67	0.98	1.51	2.00	2.00
1/1024	4.11–11	2.74–8	5.37–6	2.74–4	2.85–5	1.73–6	8.65–7
		2.44	1.69	0.99	1.51	2.00	2.00
1/2056	RE[b]	5.05–9	1.66–6	1.38–4	1.00–5	4.33–7	2.17–7

[a] Maximum error rate.
[b] Round-off error.

As before, Eq. (33) was solved with $\varepsilon = h^p$ for various values of p. The mesh length was successively halved starting with $h = \frac{1}{32}$ to $h = \frac{1}{2048}$. Tables III and IV give the results for the generalization of the implicit-fundamental solution method and the exponential OCI method, respectively. These results show that the uniform second-order accuracy no longer holds for the implicit-fundamental solution method; that is, the error reduces to first order for $p = 1$ and remains there. This drop to first-order accuracy also occurs for the exponential OCI method. For $p > 1$, however, there is a recovery of accuracy until second-order accuracy is achieved.

6. Extension to Time-Dependent Problems

The extension of the exponential OCI method to time-dependent problems is straightforward. Consider the problem

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(a(x,t)\frac{\partial u}{\partial x}\right) + b(x,t)\frac{\partial u}{\partial x} + f(x,t)$$

$$= Lu + f(x,t)\; x \in (0,1), \tag{35a}$$

$$u(x,0) = u_0(x), \qquad x \in (0,1), \tag{35b}$$

$$u(0,t) = g_1(t), \qquad u(1,t) = g_2(t). \tag{35c}$$

Discretize Eq. (35a) in time by some method (e.g., Crank–Nicholson) to obtain

$$(u^{n+1} - u^n)/\Delta t = [((Lu)^{n+1} + (Lu)^n)/2] + f^{n+1/2}. \tag{36}$$

Using the exponential OCI method, the spatial-differential operator L may be represented at any time t^n by

$$(Lu)_j^n = (Q^n)^{-1} R^n u_j^n, \tag{37}$$

where Q^n and R^n are defined by Eqs. (4), (20), and (27) are now time dependent because of the time dependence of a and b.

Substituting Eq. (37) into (36), and rearranging, the equation to be solved is

$$\begin{aligned}[I - (\Delta t/2)(Q^{n+1})^{-1} R^{n+1}]\, u_j^{n+1} \\ = [I + (\Delta t/2)(Q^n)^{-1} R^n]\, u_j^n + \Delta t f_j^{n+1/2} = G_j^{n+1}\end{aligned} \tag{38}$$

or

$$[Q^{n+1} - (\Delta t/2)\, R^{n+1}] u_j^{n+1} = Q^{n+1} G_j^{n+1}. \tag{39}$$

Thus, to compute each time step rquires the solution of a tridiagonal system of equations. Note that G_j^{n+1} is easily computed from the previous time level; i.e.,

$$\begin{aligned} G_j^{n+1} &= [I + (\Delta t/2)(Q^n)^{-1} R^n]\, u_j^n + \Delta t f_j^{n+1/2} = 2u_j^n \\ &\quad - [I - (\Delta t/2)(Q^n)^{-1} R^n]\, u_j^n + \Delta t f_j^{n+1/2} \\ &= 2u_j^n - G_j^n + \Delta t f_j^{n+1/2}. \end{aligned}$$

To demonstrate the effectiveness of the method on time-dependent problems, consider the example

$$\frac{\partial u}{\partial t} = \sigma \frac{\partial^2 u}{\partial x^2} + b(x, t) \frac{\partial u}{\partial x} \qquad \text{on} \quad [0, 1],$$

$$u(x, 0) = u_e(0),$$

$$u(0, t) = u_e(0, t), \qquad u(1, t) = u_e(1, t),$$

$$b(x, t) = -u_e(x, t),$$

$$u_e(x, t) = \frac{0.1e^{-A} + 0.5e^{-B} + e^{-C}}{e^{-A} + e^{-B} + e^{-C}},$$

$$A = \frac{0.05}{\sigma} (x - 0.5 + 4.95t),$$

$$B = \frac{0.25}{\sigma} (x - 0.5 + 0.75t),$$

$$C = \frac{0.5}{\sigma} (x - 0.375).$$

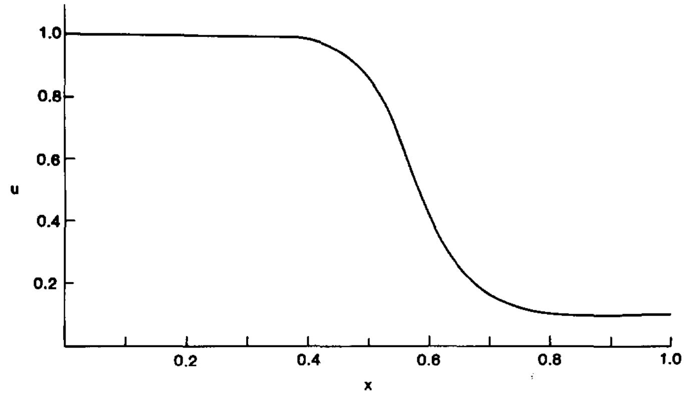

FIG. 3. Solution of wave front problem, $I = 0.4$, $\sigma = 0.01$.

This identical solution for the nonlinear Burger's equation

$$\frac{\partial u}{\partial t} = \sigma \frac{\partial^2 u}{\partial x^2} - u \frac{\partial u}{\partial x} \qquad \text{on} \quad [0, 1]$$

was studied in [14]. The exact solution $u_e(x, t)$ represents a moving wave front. The steepness of the drop at the front depends on σ; i.e., the smaller σ is the steeper the drop is. A plot of u_e for $\sigma = 0.01$, $t = 0.4$ and 1.0 may be seen in Figs. 3 and 4, respectively.

Convergence results for $\sigma = 0.1$ and $\sigma = 0.01$ are given in Tables V and VI, respectively. Table V shows that for a relatively mild drop, $\sigma = 0.1$, the fourth-order accuracy of the method is obtained. For a steep drop, however, $\sigma = 0.01$, Table VI verifies the results of the singular perturbation problem that more mesh points are needed to maintain the accuracy.

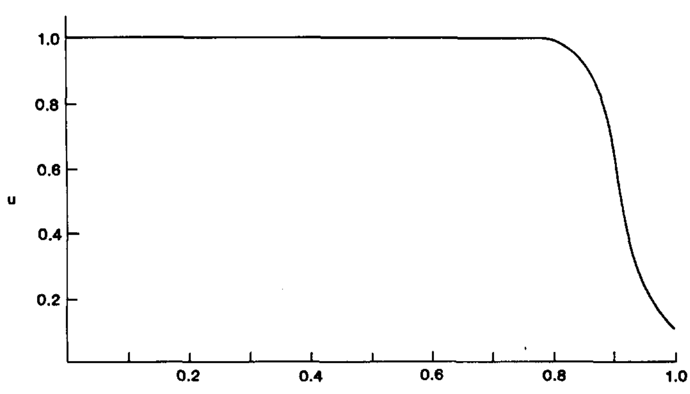

FIG. 4. Solution of wave front problem, $T = 1.0$, $\sigma = 0.01$.

TABLE V

Convergence Results for Moving Wave Front Problem ($\sigma = 0.1$)

Δx	Δt	No. of time steps	L_2-error	L_2-rate
0.1	0.05	8	3.70–05	
0.05	0.0125	32	2.325–06	3.99
0.025	0.003125	128	1.454–07	4.00
0.0125	0.00078125	512	9.089–09	4.00
0.1	0.05	20	4.332–05	
0.05	0.0125	80	2.716–06	4.00
0.025	0.004125	320	1.699–07	4.00
0.0125	0.00078125	1280	1.062–08	4.00

TABLE VI

Convergence Results for Moving Wave Front Problem ($\sigma = 0.01$)

Δx	Δt	No. of time steps	L_2-error	L_2-rate
0.1	0.05	8	1.346–02	
0.05	0.0125	32	1.942–03	2.79
0.025	0.003125	128	1.629–04	3.58
0.0125	0.00078125	512	1.0767612–05	3.92
0.1	0.05	20	1.826–02	
0.05	0.0125	80	5.380–03	1.76
0.025	0.003125	320	4.418–04	3.61
0.0125	0.00078125	1280	2.870–05	3.94

7. Extension to Systems of Equations

In [15], an OCI method for a diffusion operator in conservation form was derived. This method was extended to systems of equations by considering all the terms in the original derivation as matrices of vectors. Since there had been no necessary commutations of terms in the original derivation, the extension was straightforward. This type of extension is not possible for the exponential OCI method. The primary reason is that the exponential of a matrix does not have the same differentiation properties as the exponential of a scalar. Thus, a matrix version of the function P in Eq. (7) and the identity (12) is not possible. Therefore, the following extension of the method was conceived. Consider the system of equations

$$\frac{\partial}{\partial x}\left(a_{11}\frac{\partial u_1}{\partial x}\right)+b_{11}\frac{\partial u_1}{\partial x}+\frac{\partial}{\partial x}\left(a_{12}\frac{\partial u_2}{\partial x}\right)+b_{12}\frac{\partial u_2}{\partial x}+f_1$$

$$=h_{11}\frac{\partial u_1}{\partial t}+h_{12}\frac{\partial u_2}{\partial t}; \qquad (40a)$$

$$\frac{\partial}{\partial x}\left(a_{21}\frac{\partial u_1}{\partial x}\right)+b_{21}\frac{\partial u_1}{\partial x}+\frac{\partial}{\partial x}\left(a_{22}\frac{\partial u_2}{\partial x}\right)+b_{22}\frac{\partial u_2}{\partial x}+f_2$$

$$=h_{21}\frac{\partial u_1}{\partial t}+h_{22}\frac{\partial u_2}{\partial t}, \qquad (40b)$$

for $x \in (0, 1)$ with initial conditions

$$u_1(x,0)=u_{10}(x), \qquad u_2(x,0)=u_{20}(x),$$

and boundary conditions

$$u_1(0,t)=g_{10}(t), \qquad u_1(1,t)=g_{11}(t),$$
$$u_2(0,t)=g_{20}(t), \qquad u_2(1,t)=g_{21}(t).$$

Denoting the four spatial-differential operators in Eq. (40) by L_{11}, L_{12}, L_{21}, and L_{22} the equation may be written as

$$L_{11}u_1+L_{12}u_2+f_1=h_{11}\frac{\partial u_1}{\partial t}+h_{12}\frac{\partial u_2}{\partial t} \qquad (41a)$$

$$L_{21}u_1+L_{22}u_2+f_2=h_{21}\frac{\partial u_1}{\partial t}+h_{22}\frac{\partial u_2}{\partial t}. \qquad (41b)$$

Using a backwards in time-difference approximation and replacing the spatial-differential operators by their respective exponential OCI approximations, Eq. (41) is replaced by

$$(Q_{11}^{n+1})^{-1}R_{11}^{n+1}u_{1,j}^{n+1}+(Q_{12}^{n+1})^{-1}R_{12}^{n+1}u_{2,j}^{n+1}+f_{1,j}^{n+1}$$
$$=h_{11}^{n+1}(u_{1,j}^{n+1}-u_{1,j}^{n})/\Delta t+h_{12}^{n+1}(u_{2,j}^{n+1}-u_{2,j}^{n})/\Delta t \qquad (42a)$$

$$(Q_{21}^{n+1})^{-1}R_{21}^{n+1}u_{1,j}^{n+1}+(Q_{22}^{n+1})^{-1}R_{22}^{n+1}u_{2,j}^{n+1}+f_{2,j}^{n+1}$$
$$=h_{21}^{n+1}(u_{1,j}^{n+1}-u_{1,j}^{n})/\Delta t+h_{22}^{n+1}(u_{2,j}^{n+1}-u_{2,j}^{n})/\Delta t. \qquad (42b)$$

Rearranging Eq. (42) to obtain

$$[I(h_{11}^{n+1}/\Delta t)-(Q_{11}^{n+1})^{-1}R_{11}^{n+1}]\,u_{1,j}^{n+1}$$
$$=(h_{11}^{n+1}/\Delta t)u_{1,j}^{n}-h_{12}^{n+1}(u_{2,j}^{n+1}-u_{2,j}^{n})/\Delta t+(Q_{12}^{n+1})^{-1}R_{12}^{n+1}u_{2,j}^{n+1}+f_{1,j}^{n+1} \qquad (43a)$$

$$[I(h_{22}^{n+1}/\Delta t)-(Q_{22}^{n+1})^{-1}R_{22}^{n+1}]\,u_{2,j}^{n+1}$$
$$=h_{22}^{n+1}u_{2,j}^{n}/\Delta t-h_{21}^{n+1}(u_{1,j}^{+1}-u_{1,j}^{n}/\Delta t)+(Q_{21}^{n+1})^{-1}R_{21}^{n+1}u_{1,j}^{n+1}+f_{2,j}^{n+1}. \qquad (43b)$$

The algorithm for solving Eq. (43) for u_1^{n+1} and u_2^{n+1} follows:

(1) For every time step after the first, initialize u_2^{n+1} as

$$u_{2,j}^{n+1,0} = 2u_{2,j}^n - u_{2,j}^{n-1}$$

(on the first $u_{2,j}^{n+1,0} = u_{2,j}^n$) and set the iteration counter $i = 1$).

(2) Solve the equation

$$Q_{12}^{n+1} V_{2,j} = R_{12} u_{2,j}^{n+1,i-1}$$

and form the vector

$$G_{1,j} = (h_{11}^{n+1} u_{1,j}^n/\Delta t) - h_{12}^{n+1}[(u_{2,j}^{n+1,i-1} - u_{2,j}^n)/\Delta t] + V_{2,j} + f_{1,j}^{n+1}.$$

(3) Compute $u_1^{n+1,i}$ by solving the equation

$$[Q_{11}^{n+1}(h_{11}^{n+1}/\Delta t) - R_{11}^{n+1}]\, u_{1,j}^{n+1,i} = Q_{11}^{+1} G_{1,j}.$$

(4) Solve the equation

$$Q_{21}^{n+1} V_{1,j} = R_{21} u_{1,j}^{n+1,i}$$

and form the vector

$$G_{2,j} = (h_{22}^{n+1} u_{2,j}^n/\Delta t) - h_{21}^{n+1}[(u_{1,j}^{n+1,i} - u_{1,j}^n)/\Delta t] + V_{1,j} + f_{2,j}^{n+1}.$$

(5) Compute $u_{2,j}^{n+1,i}$ by solving the equation

$$[Q_{22}^{n+1}(h_{22}^{n+1}/\Delta t) - R_{22}^{n+1}]\, u_{2,j}^{n+1,i} = Q_{22}^{n+1} G_{2,j}.$$

(6) Check convergence by computing maximum change in $u_{1,j}^{n+1,i}$ and $u_{2,j}^{n+1,i}$ from the previous iteration. If change is less than a given tolerance, go to the next time step. If not, $i = i + 1$; go to step (2). The above algorithm is a block Gauss–Seidel method for Eq. (42).

Numerical experiments have shown that diagonal dominance is necessary for fourth-order convergence. This same condition is required by Kreiss and Nichols [16] for singularly perturbed-boundary value problems. In addition, invertibility of all the discrete operators Q_{ij}^{n+1} is required. If they are not invertible, however, alternate OCI operators for which they are invertible may be used.

The following example was chosen to verify the method

$$u_1(x, t) = (0.1e^{-A} + 0.5e^{-B} + e^{-C})/(e^{-A} + e^{-B} + e^{-C}),$$

where

$$A = (0.05/\sigma)(x - 0.5 + 4.95t),$$

$$B = (0.25/\sigma)(x - 0.5 + 0.75t),$$

$$C=(0.5/\sigma)(x-0.375);$$

$$u_2(x,t)=x^2t^2+x+t+1,$$

$$a_{11}=\sigma;\quad a_{12}=\sigma^2;\quad a_{21}=1;\quad a_{22}=1,$$

$$b_{11}=u_1;\quad b_{12}=1;\quad b_{21}=1;\quad b_{22}=1,$$

$$h_{11}=1;\quad h_{12}=0;\quad h_{21}=0;\quad h_{22}=1.$$

and f_1 and f_2 are chosen so that Eq. (40) is satisfied.

Convergence results for $\sigma=0.1$, $\sigma=0.05$, and $\sigma=0.01$ are given in Tables VII, VIII, and IX, respectively. These results confirm the expected order of convergence of the method and the increased difficulty of the problem as σ is reduced. Note that the last column in these tables indicates the number of iterations needed per time step. This number is dependent on the convergence tolerance τ. The tolerance used for a given Δx is given in Table X. The large number of iterations needed for $\sigma=0.01$, $\Delta x=0.05$, $\Delta t=0.05$ as compared to the number needed for $\sigma=0.01$, $\Delta x=0.05$, $\Delta t=0.00078125$ shows that τ should also be linked to the time-step size.

TABLE VII

Convergence Results for System of Equations ($\sigma=0.1$)

Δx	Δt	No. of time steps	L_2-error	L_2-rate	No. of iterations per time step
0.2	0.2	5	6.22–03		5
				4.31	
0.1	0.0125	80	3.13–04		2
				4.00	
0.05	0.00078125	1280	1.95–05		2
0.05	0.05	20	1.31–03		5
				4.06	
0.025	0.003125	320	7.87–05		2

TABLE VIII

Convergence Results for System of Equations ($\sigma=0.05$)

Δx	Δt	No. of time steps	L_2-error	L_2-rate	No. of iterations per time step
0.2	0.2	5	3.68–02		6
				3.91	
0.1	0.0125	80	2.44–03		2
				4.01	
0.05	0.00078125	1280	1.51–04		2
0.05	0.05	20	8.29–03		6
				3.98	
0.025	0.003125	320	5.25–04		2

TABLE IX

Convergence Results for System of Equations ($\sigma = 0.01$)

Δx	Δt	No. of time steps	L_2-error	L_2-rate	No. of iterations per time step
0.1	0.0125	16	3.25–02	3.49	4
0.05	0.00078125	256	2.89–03		
0.1	0.0125	48	1.79–01	4.57	4
0.05	0.00078125	768	7.54–03		
0.1	0.0125	80	2.25–01	3.37	4
0.05	0.00078125	1280	2.17–02		
0.05	0.05	12	1.38–01	4.47	30
0.025	0.003125	192	6.24–03		4
0.05	0.05	20	1.61–61	3.78	30
0.25	0.003125	320	1.17–02		4

TABLE X

Convergence Tolerance Used for Each Δx in Systems of Equations Example

Δx	Convergence tolerance	Δx	Convergence tolerance
0.2	1.00–03	0.05	2.50–06
0.1	5.00–05	0.025	1.25–07

8. Conclusions

(1) An integral identity was developed for diffusion–convection differential operators. This identity can be used to develop a class of exponential finite-difference methods.

(2) One method in the class is a fourth-order accurate OCI method. The OCI method is applicable to two-point boundary value problems, one-dimensional scalar-parabolic equations, and one-dimensional systems of equations.

(3) Numerical examples demonstrated the fourth-order accuracy of the method for smooth problems and a uniform second-order accuracy for singular perturbation problems.

(4) Extension of the exponential OCI method to nonlinear problems is possible by performing Newton iterations on the nonlinear differential equation and then solving the sequence of linear problems by the OCI method.

(5) Extension of the exponential OCI method to two dimension is possible [17].

(6) Application of the exponential OCI method to reservoir simulation problems is presently underway. Its effective use is dependent on a successful combination of the nonlinear algorithm and the system algorithm. Preliminary results are encouraging, however, further work is needed.

APPENDIX A

Consider the equation

$$Lu = \frac{\partial}{\partial x}\left(a\frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial x}(bu) = f \qquad \text{on} \quad (0, 1) \tag{A1}$$

$$u(0) = u_0, \qquad u(1) = u_1.$$

In this Appendix a generalization of the implicit-fundamental solution method and the exponential OCI method is derived for Eq. (A1).

Divide the interval [0, 1] into a uniform mesh $x_j = jh$, $j = 0, 1, \dots, J$ and $h = 1/J$. On the subinterval $[x_{j-1}, x_{j+1}]$ define the function P as

$$P = \frac{\int_x^{x_{j+1}} \exp\left[-\int_x^{x_{j+1}} \frac{b}{a}\,d\xi\right]\Big/ a\,dx}{\int_{x_j}^{x_{j+1}} \exp\left[-\int_x^{x_{j+1}} \frac{b}{a}\,d\xi\right]\Big/ a\,dx}, \qquad x_j \leqslant x \leqslant x_{j+1}$$

$$= \frac{\int_{x_{j-1}}^{x} \exp\left[\int_{x_j}^{x} \frac{b}{a}\,d\xi\right]\Big/ a\,dx}{\int_{x_{j-1}}^{x_j} \exp\left[\int_{x_j}^{x} \frac{b}{a}\,d\xi\right]\Big/ a\,dx}, \qquad x_{j-1} \leqslant x \leqslant x_j.$$

The function P has the following important properties:

(1) $P(x_{j+1}) = P(x_{j-1}) = 0$,

(2) P is continuous at x_j and $P(x_j) = 1$,

(3) $\partial P/\partial x$ is discontinuous at x_j and

$$\frac{\partial P}{\partial x} = \frac{-\exp\left[-\int_x^{x_{j+1}} \frac{b}{a}\,d\xi\right]\Big/ a}{\int_{x_j}^{x_{j+1}} \exp\left[-\int_x^{x_{j+1}} \frac{b}{a}\,d\xi\right]\Big/ a\,dx}, \qquad x_j \leqslant x \leqslant x_{j+1}$$

$$= \frac{\exp\left[\int_{x_j}^{x} \frac{b}{a}\,d\xi\right]\Big/ a}{\int_{x_{j-1}}^{x_j} \exp\left[\int_{x_j}^{x} \frac{b}{a}\,d\xi\right]\Big/ a\,dx}, \qquad x_{j-1} \leqslant x \leqslant x_j, \tag{A3}$$

(4) P is proportional to the discrete Green's function for the operator L.

Multiply Eq. (A1) by P and integrate from x_{j-1} to x_{j+1}; i.e.,

$$\int_{x_{j-1}}^{x_{j+1}} P\left(\frac{\partial}{\partial x}\left(a\frac{\partial u}{\partial x}\right)+\frac{\partial}{\partial x}(bu)\right)dx=\int_{x_{j-1}}^{x_{j+1}} Pf\,dx. \tag{A4}$$

Integrating the left and right side of Eq. (A4) by parts first from x_{j-1} to x_j and then from x_j to x_{j+1}, Eq. (A4) becomes

$$\begin{aligned}
&\left(\int_{x_{j-1}}^{x_{j+1}} \exp\left[-\int_x^{x_{j+1}}\frac{b}{a}\,d\xi\right]\Big/a\,dx\right)^{-1}\int_{x_j}^{x_{j+1}}\frac{\partial}{\partial x}\left(\exp\left[-\int_{x_j}^{x_{j+1}}\frac{b}{a}\,d\xi\right]u\right)dx\\
&\quad-\left(\int_{x_{j-1}}^{x_j}\left[\exp\int_{x_{j-1}}^{x_j}\frac{b}{a}\,d\xi\right]\Big/a\,dx\right)^{-1}\int_{x_{j-1}}^{x_j}\frac{\partial}{\partial x}\left(\exp\left[\int_{x_j}^{x}\frac{b}{a}\,d\xi\right]u\right)dx\\
&\quad=\int_{x_{j-1/2}}^{x_{j+1/2}} f\,dx-\int_{x_j}^{x_{j+1}}\left(\frac{\partial P}{\partial x}\int_{x_{j+1/2}}^{x} f\right)dx-\int_{x_{j-1}}^{x_j}\left(\frac{\partial P}{\partial x}\int_{x_{j-1/2}}^{x} f\right)dx
\end{aligned}$$

or

$$\begin{aligned}
&\frac{u_{j+1}}{\int_{x_j}^{x_{j+1}}\exp\left[-\int_x^{x_{j+1}}\frac{b}{a}\,d\xi\right]\Big/a\,dx}-\left(\frac{\exp\left[-\int_{x_j}^{x_{j+1}}\frac{b}{a}\,d\xi\right]}{\int_{x_j}^{x_{j+1}}\exp\left[-\int_{x_j}^{x_{j+1}}\frac{b}{a}\,d\xi\right]\Big/a\,dx}\right.\\
&\quad\left.+\left(\int_{x_{j-1}}^{x_j}\exp\left[\int_{x_j}^{x}\frac{b}{a}\,d\xi\right]\Big/a\,dx\right)^{-1}\right)u_j+\frac{\exp\left[-\int_{x_{j-1}}^{x_j}\frac{b}{a}\,d\xi\right]}{\int_{x_{j-1}}^{x_j}\exp\left[\int_{x_j}^{x}\frac{b}{a}\,d\xi\right]\Big/a\,dx}u_{j-1}\\
&\quad=\int_{x_{j-1/2}}^{x_{j+1/2}} f+\left(\int_{x_j}^{x_{j+1}}\exp\left[-\int_{x_j}^{x}\frac{b}{a}\,d\xi\right]\Big/a\,dx\right)^{-1}\\
&\quad\times\int_{x_j}^{x_{j+1}}\left(\left(\exp\left[-\int_x^{x_{j+1}}\frac{b}{a}\,d\xi\right]\Big/a\right)\int_{x_{j+1/2}}^{x} f\right)dx\\
&\quad-\left(\int_{x_{j-1}}^{x_j}\exp\left[\int_{x_j}^{x}\frac{b}{a}\,d\xi\right]\Big/a\,dx\right)^{-1}\\
&\quad\times\int_{x_{j-1}}^{x_j}\left(\left(\exp\left[\int_{x_j}^{x}\frac{b}{a}\,d\xi\right]\Big/a\right)\int_{x_{j-1/2}}^{x} f\right)dx.
\end{aligned} \tag{A5}$$

Equation (A5) is the integral identity needed to derive the methods.

To define the implicit-fundamental solution method assume that a, b, and f are piecewise constant in $[x_{j-1}, x_{j+1}]$ with their values a^-, b^-, f^- and a^+, b^+, f^+

defined in the subintervals $[x_{j-1}, x_j]$ and $[x_j, x_{j+1}]$, respectively, in the same manner as Section 3. Also, define

$$\rho^+ = b^+ h / a^+$$

and

$$\rho^- = b^- h / a^-.$$

Under these assumptions

$$r_j^+ = b^+/(1 - \exp(-\rho^+)), \qquad r_j^- = \frac{b^- \exp(-\rho^-)}{1 - \exp(-\rho^-)},$$

$$r_j^c = -(\exp(-\rho^+) r_j^+ + \exp(\rho^-) r_j^-), \qquad q_j^+ = h(0.25 + \tilde{q}_j^+),$$

$$q_j^c = h(0.5 + \tilde{q}_j^+ + \tilde{q}_j^-), \qquad q_j^- = h(0.25 + \tilde{q}_j^-),$$

where

$$\tilde{q}_j^+ = (r_j^+/b^+)(0.25 - (0.5/\rho^+) + \exp(-\rho^+)(0.25 + (0.5/\rho^+)))$$

and

$$\tilde{q}_j^- = -(\exp(\rho^-) r_j^-/b^-)(0.25 - (0.5/\rho^-) + \exp(-\rho^-)(0.25 + (0.5/\rho^-))).$$

To define the exponential OCI method assume that a and b are piecewise quadratic in $[x_{j-1}, x_{j+1}]$ with their values in $[x_{j-1}, x_j]$ determined by a_{j-1}, $a_{j-1/2}$, a_j, b_{j-1}, $b_{j-1/2}$, and b_j and their values in $[x_j, x_{j+1}]$ determined by a_j, $a_{j+1/2}$, a_{j+1}, b_j, $b_{j+1/2}$, and b_{j+1}. Proceeding as in Section 4,

$$r_j^+ = \left(\frac{1}{b_{j+1}} - \left(\exp\left[-\int_{x_j}^{x_{j+1}} \frac{b}{a}\, d\xi\right] \Big/ b_j\right) + \int_{x_j}^{x_{j+1}} \left(\exp\left[-\int_{x}^{x_{j+1}} \frac{b}{a}\, d\xi\right] \frac{1}{b^2} \frac{\partial b}{\partial x}\right) dx\right)^{-1},$$

$$r_j^- = \frac{\exp\left[-\int_{x_{j-1}}^{x_j} \frac{b}{a}\, d\xi\right]}{\frac{1}{b_j} - \left(\exp\left[-\int_{x_{j-1}}^{x_j} \frac{b}{a}\, d\xi\right] \Big/ b_{j-1}\right) + \int_{x_{j-1}}^{x_j} \left(\exp\left[-\int_{x}^{x_j} \frac{b}{a}\, d\xi\right] \frac{1}{b^2} \frac{\partial b}{\partial x}\right) dx},$$

$$r_j^c = -\left(\exp - \left[\int_{x_j}^{x_{j+1}} \frac{b}{a}\, d\xi\right] r_j^+ + \exp\left[\int_{x_{j-1}}^{x_j} \frac{b}{a}\, d\xi\right] r_j^-\right), \tag{A7}$$

$$q_j^+ = h(\tfrac{1}{12} + \tilde{q}_j^+),$$

$$q_j^c = h(\tfrac{10}{12} + \tilde{q}_j^+ + \tilde{q}_j^-), \tag{A8}$$

$$q_j^- = h(\tfrac{1}{12} + \tilde{q}_j^-),$$

where

$$\begin{aligned}\tilde{q}_j^+ = r_j^+ \Bigg[& \frac{1}{b_{j+1}} \left(\frac{1}{4} - \frac{a_{j+1}}{2hb_{j+1}} + \frac{1}{12} \frac{\partial}{\partial x} \left(\frac{a}{b} \right)_{j+1} \right) \\ & + \left(\exp\left[-\int_{x_j}^{x_{j+1}} \frac{b}{a} d\xi \right] \Big/ b_j \right) \left(\frac{1}{4} + \frac{a_j}{2hb_j} + \frac{1}{12} \frac{\partial}{\partial x} \left(\frac{a}{b} \right)_j \right) \\ & + \int_{x_j}^{x_{j+1}} \left(\exp\left[-\int_{x}^{x_{j+1}} \frac{b}{a} d\xi \right] \frac{1}{b^2} \frac{\partial b}{\partial x} \right) dx \\ & \times \left(\frac{1}{6} - \frac{a_{j+1}}{2hb_{j+1}} + \frac{1}{12} \frac{\partial b}{\partial x} \left(\frac{a}{b} \right)_{j+1} \right) \\ & + \frac{1}{3} \Bigg[\frac{\partial}{\partial x} \left(\frac{a}{b} \right)_{j+1/2} \left(\exp\left[-\int_{x_j}^{x_{j+1}} \frac{b}{a} d\xi \right] \Big/ b_{j+1/2} \right) \\ & + \int_{x_j}^{x_{j+1/2}} \left(\exp\left[-\int_{x}^{x_{j+1}} \frac{b}{a} d\xi \right] \frac{1}{b^2} \frac{\partial b}{\partial x} \right) dx \\ & \times \left(\frac{\partial}{\partial x} \left(\frac{a}{b} \right)_{j+1/2} - 1 \right) \Bigg] \Bigg] \end{aligned} \quad \text{(A9)}$$

and

$$\tilde{q}_j^- = -\tilde{q}_{j-1}^+. \quad \text{(A10)}$$

As before, the remaining integrals in Eqs. (A7)–(A10) should be evaluated using Simpson's rule and the quadratic approximations of a and b. The only exceptions, however, are the integrals of the form

$$\int_{x_j}^{x_{j+1}} \left(\exp\left[-\int_{x}^{x_{j+1}} \frac{b}{a} d\xi \right] \frac{1}{b^2} \frac{\partial b}{\partial x} \right) dx.$$

This type of integral should be evaluated using the open Newton–Cotes formula [18]

$$\int_{x_j}^{x_{j+1}} gd = \frac{h}{3} (2g_{j+1/4} - g_{j+1/2} + 2g_{j+3/4}).$$

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