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Journal of Computational and Applied Mathematics 72 (1996) 345–358

JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS

A generator of high-order embedded P-stable methods for the numerical solution of the Schrödinger equation

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Received 17 February 1995; revised 4 January 1996

Abstract

A generator of new embedded P-stable methods of order $2n+2$, where n is the number of layers used by the embedded methods, for the approximate numerical integration of the one-dimensional Schrödinger equation is developed in this paper. These new methods are called embedded methods because of a simple natural error control mechanism. Numerical results obtained for one-dimensional differential equations of the Schrödinger type show the validity of the developed theory.

Keywords: Schrödinger equation; P-stability; Error control; Phase shift problem; Resonance problem

AMS classification: 65L05

1. Introduction

Numerous numerical techniques exist in the literature for solving the Schrödinger equation [1, 4, 5, 8, 9, 11–15, 18–25, 27–29, 32–35, 37, 39–43, 46].

The one-dimensional Schrödinger equation is a boundary value problem which has the form

$$y''(x) = [l(l+1)/x^2 + V(x) - k^2]\ y(x), \tag{1}$$

with one boundary condition given by

$$y(0) = 0, \tag{2}$$

and the other boundary condition, for large values of x, determined by physical considerations. Equations of this type occur very frequently in theoretical physics (see [31]) and there is a real need to be able to solve them both efficiently and reliably by numerical methods. In (1) the function

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PII S0377-0427(96)00005-2

$W(x) = l(l+1)/x^2 + V(x)$ denotes *the effective potential*, which satisfies $W(x) \to 0$ as $x \to \infty$, k^2 is a real number denoting *the energy*, l is a given integer and V is a given function which denotes the potential.

The two-step *Numerov's method* is extremely effective as a means of solving the Schrödinger equation. This method is only of order four, but in practice it has been found to have a superior performance to certain higher-order four-step methods. The reason for this is explained in [45].

Cash and Raptis [8] have proposed the well-known Runge–Kutta type or hybrid methods. These methods are more accurate compared with Numerov's method. The reason for this is explained in [45].

Exponential fitting is another approach for developing efficient methods for the solution of (1). This approach is appropriate because for large x the solution of (1) is *periodic*. A Numerov-type exponentially fitted method has been derived in [35]. Numerical results presented there indicate that these fitted methods are much more efficient than Numerov's method for the solution of (1). Many authors have investigated the idea of exponential fitting, since Raptis and Allison. We mention the papers of Ixaru and Rizea [20], Simos [40–43], Raptis [32, 34], Raptis and Cash [37], and Cash, et al. [9].

In Section 2 we will develop the basic theory for the construction of the P-stable methods via the (m,m) Padé approximation of the exponential function. In Section 3 we will develop the P-stable m-stages methods of order $2m+2$. The computational implementation of the generator of the P-stable methods is presented in Section 4. Finally, in Section 5 an application of the new methods to the phase shift problem and to the resonance problem of the Schrödinger equation is presented.

2. The basic theory

When we applied any direct two-step integration method to the scalar test equation

$$y'' = -w^2 y, \tag{3}$$

we obtain the next difference equation

$$Q_0(H)y_{n+1} + Q_1(H)y_n + Q_0(H)y_{n-1} = 0, \quad H = \mathrm{i}wh, \tag{4}$$

where $Q_j, j = 0,1,2$ are polynomials in H, h is the integration step and y_n is the numerical approximation to $y(x_n)$ $(n = 0,1,\ldots)$. The general solution to the difference equation (4) is

$$y_n = B_1 z_1^n + B_2 z_2^n, \tag{5}$$

where B_j $(j = 1,2,\ldots,k)$ are constants which may be determined from the initial conditions and z_1 and z_2 are the zeros of the *stability polynomial*

$$P(c,H) \equiv Q_0(H)c^2 + Q_1(H)c + Q_0(H) = 0. \tag{6}$$

Definition 1 (Lambert et al. [30]). A method to solve the problem

$$y''(x) = f(x, y), \qquad y(x_0) = y_0, \qquad y'(x_0) = y_0' \tag{7}$$

is said to have a periodicity interval $(0, H_0)$ if, for all $H \in (0, H_0)$, the roots of the stability polynomial (6) satisfy

$$c_1(H) \equiv \mathrm{e}^{\mathrm{i}\theta(H)}, \; c_2(H) \equiv \mathrm{e}^{-\mathrm{i}\theta(H)}, \tag{8}$$

where θ is a real function of $H = wh$.

Definition 2 (Lambert et al. [30]). A method is said to be P-stable if its interval of periodicity is $(0, \infty)$.

We note here that for P-stable methods an important contribution is the paper of Hairer [17].

Definition 3 (Franco et al. [16]). The solution of the characteristic equation $P(c, H) = 0$ is said to be of order p, if one of the roots of $P(c, H)$ (i.e., one of the roots (8)), say c_1, satisfies

$$\mathrm{e}^H - c_1(H) = CH^{p+1} + \mathrm{O}(H^{p+2}) \quad \text{for } H \to 0 \tag{9}$$

where $C(\neq 0)$ is the error constant of $c_1(H)$.

Let us write the stability polynomial $P(c, r)$ as

$$P(c, r) \equiv [R_m(r)R_m(-r)]c^2 - [R_m^2(r) + R_m^2(-r)]c + [R_m(r)R_m(-r)] \tag{10}$$

with $r \in \mathbb{C}$ and R_m given by

$$R_m(r) \equiv 1 + \frac{mr}{2m} + \frac{m(m-1)r^2}{2m(2m-1)2!} + \frac{m(m-1)\ldots 1r^m}{2m(2m-1)(2m-2)\ldots(m+1)m!}. \tag{11}$$

The roots of (10) are given by

$$c_1(r) = c_2(r)^{-1} = R_m(r)/R_m(-r), \tag{12}$$

i.e., the roots of (10) are obtained as the (m, m) Padé approximant to $\exp(H)$ because it is valid [16]:

$$\mathrm{e}^H - c_1(H) = CH^{2m+1} + \mathrm{O}(H^{2m+2}) \quad \text{for } H \to 0. \tag{13}$$

Therefore, if we take $H = \mathrm{i}wh$, those roots are going to be conjugate complex numbers and always lie in the unity circumference, i.e., the method is going to be P-stable.

3. Construction of the generator of the high-order embedded P-stable methods

Consider the following family of two-step methods:

$$\begin{aligned} \bar{y}_{n,i} &= y_n - h^2 \left(b_{0,m+1-i}\; y''_{n+1} + b_{1,m+1-i}\; \bar{y}''_{n,i-1} + b_{0,m+1-i}\; y''_{n-1} \right), \qquad i = 1(1)m, \\ a_0 y_{n+1} + a_1 y_n + a_0 y_{n-1} &= h^2 \left(b_0 y''_{n+1} + b_1 \bar{y}''_{n,m} + b_0 y''_{n-1} \right), \end{aligned} \tag{14}$$

where $y_n'' = f(x_n, y_n), \bar{y}_{n,i-1}'' = f(x_n, \bar{y}_{n,i-1},)$, i is the number of layer, and m is the number of the family. We note that $\bar{y}_{n,0} = y_n$. We choose the parameters of the method $b_{0,m+1-i}$, $b_{1,m+1-i}$, b_0 and b_1 in order to construct P-stable methods with the maximum order.

The calculation of the values of these parameters can be obtained with the requirement of the verification of the test equation

$$y'' = \lambda^2 y, \quad \lambda = \mathrm{i}w \text{ and } w \in \mathcal{R}. \tag{15}$$

Consequently, for the above family of methods we will have

$$\bar{y}_{n,i} = y_n - H^2 \left(b_{0,m+1-i} y_{n+1} + b_{1,m+1-i} \bar{y}_{n,i-1} + b_{0,m+1-i} y_{n-1}\right), \quad i = 1(1)m, \tag{16}$$

$$a_0 y_{n+1} + a_1 y_n + a_0 y_{n-1} = H^2 \left(b_0 y_{n+1} + b_1 \bar{y}_{n,m} + b_0 y_{n-1}\right). \tag{17}$$

From the last relation we get

$$\begin{aligned} &a_0 y_{n+1} + a_1 y_n + a_0 y_{n-1} \\ &\quad = H^2 \left[b_0 y_{n+1} + b_1 \left[y_n - H^2 (b_{0,1} y_{n+1} + b_{1,1} \bar{y}_{n,m-1} + b_{0,1} y_{n-1})\right] + b_0 y_{n-1}\right] \end{aligned} \tag{18}$$

or

$$\begin{aligned} &(a_0 - b_0 H^2 + b_{0,1} b_1 H^4) y_{n+1} + (a_1 - b_1 H^2) y_n + (a_0 - b_0 H^2 + b_{0,1} b_1 H^4) y_{n-1} \\ &\quad = - b_1 b_{1,1} H^4 \bar{y}_{n,m-1} = -b_1 b_{1,1} H^4 \left[y_n - H^2 (b_{0,2} y_{n+1} + b_{1,2} \bar{y}_{n,m-2} + b_{0,2} y_{n-1})\right] \\ &\quad = - b_1 b_{1,1} H^4 y_n + b_1 b_{1,1} b_{0,2} H^6 y_{n+1} + b_1 b_{1,1} b_{1,2} H^6 \bar{y}_{n,m-2} + b_1 b_{1,1} b_{0,2} H^6 y_{n-1}. \end{aligned} \tag{19}$$

So, we have

$$\begin{aligned} &(a_0 - b_0 H^2 + b_{0,1} b_1 H^4 - b_1 b_{1,1} b_{0,2} H^6) y_{n+1} + (a_1 - b_1 H^2 + b_1 b_{1,1} H^4) y_n \\ &\qquad + (a_0 - b_0 H^2 + b_{0,1} b_1 H^4 - b_1 b_{1,1} b_{0,2} H^6) y_{n-1} \\ &\quad = - b_1 b_{1,1} b_{1,2} H^6 \bar{y}_{n,m-2} \\ &\quad = b_1 b_{1,1} b_{1,2} H^6 \left[y_n - H^2 (b_{0,3} y_{n+1} + b_{1,3} \bar{y}_{n,m-3} + b_{0,3} y_{n-1})\right] \\ &\quad = b_1 b_{1,1} b_{1,2} H^6 y_n - b_1 b_{1,1} b_{1,2} b_{0,3} H^8 y_{n+1} - b_1 b_{1,1} b_{1,2} b_{1,3} H^8 \bar{y}_{n,m-3} + b_1 b_{1,1} b_{1,2} b_{0,3} H^8 y_{n-1}. \end{aligned} \tag{20}$$

From (20) we have

$$\begin{aligned} &(a_0 - b_0 H^2 + b_{0,1} b_1 H^4 - b_1 b_{1,1} b_{0,2} H^6 + b_1 b_{11} b_{12} b_{0,3} H^8) y_{n+1} \\ &\qquad + (a_1 - b_1 H^2 + b_1 b_{1,1} H^4 - b_1 b_{1,1} b_{1,2} H^6) y_n \\ &\qquad + (a_0 - b_0 H^2 + b_{0,1} b_1 H^4 - b_1 b_{1,1} b_{0,2} H^6 + b_1 b_{1,1} b_{1,2} b_{0,3} H^8) y_{n-1} \\ &\quad = - b_1 b_{1,1} b_{1,2} b_{1,3} H^8 \bar{y}_{n,m-3}. \end{aligned} \tag{21}$$

Finally, and based on the above relations and on the fact that $\bar{y}_{n,0} = y_n$, we will have

$$Q_0(H) y_{n+1} + Q_1(H) y_n + Q_0(H) y_{n-1} = 0, \quad H = \mathrm{i}wh, \tag{22}$$

where

$$Q_0(H) \equiv a_0 - b_0H^2 + b_{0,1}b_1H^4 - b_1b_{1,1}b_{0,2}H^6 + b_1b_{11}b_{12}b_{0,3}H^8 - \cdots + \\ +(-1)^{m+1}b_1b_{1,1}b_{1,2}\ldots b_{1,m-1}b_{0,m}H^{2m+2} = a_0 - b_0H^2 + b_{0,1}b_1H^4 \\ +b_1H^6\sum_{i=1}^{m-1}(-1)^i\left(\prod_{j=1}^{i}b_{1,j}\right)b_{0,i+1}H^{2i-2}, \tag{23}$$

$$Q_1(H) \equiv a_1 - b_1H^2 + b_1b_{1,1}H^4 - b_1b_{1,1}b_{1,2}H^6 + \ldots + (-1)^{m+1}b_1b_{1,1}b_{1,2}\ldots b_{1,m}H^{2m+2} \\ = a_1 - b_1H^2 + b_1H^4\sum_{i=1}^{m-1}(-1)^{i+1}\left(\prod_{j=1}^{i}b_{1,j}\right)H^{2i-2}. \tag{24}$$

Based on the theory developed in Section 2 in order to construct P-stable methods of order $2m+2$ we require

$$Q_0(H) \equiv R_{m+1}(H)R_{m+1}(-H), \tag{25a}$$

$$Q_1(H) \equiv -[R_{m+1}^2(H) + R_{m+1}^2(-H)]. \tag{25b}$$

From (25) we will have a system of $2(m+2)$ linearly independent equations with $2(m+2)$ coefficient -parameters of the family of method (14). The order $m+1$ of the $R_k(H)$ in (25) is the required one because it is easy to see in these relations that we have only even powers of H. Based on the general form (11) it is easy to calculate the coefficient $A_{m,k}$ of H^{2k}, $k=2(1)m+1$, of the right-hand side of (25b) which is given by

$$A_{m,k} = \frac{2}{(k!)^2}\left[\prod_{j=0}^{k-1}\frac{m+1-j}{2m+2-j}\right]^2 \\ +4\left[\sum_{i=1}^{k-1}\left(\frac{1}{(2k-i)!(i!)}\prod_{j=0}^{2k-i-1}\frac{m+1-j}{2m+2-j}\prod_{j=0}^{i-1}\frac{m+1-j}{2m+2-j}\right)\right. \\ \left.+\frac{1}{(2k)!}\prod_{j=0}^{2k-1}\frac{m+1-j}{2m+2-j}\right], \quad m=3,4,\ldots, \tag{26}$$

while for the coefficient $B_{m,k}$ of H^{2k}, $k=2(1)m+1$ of the right-hand side of (25a) we have that:

$$B_{m,k} = \frac{(-1)^k}{(k!)^2}\left[\prod_{j=0}^{k-1}\frac{m+1-j}{2m+2-j}\right]^2 + \frac{2}{(2k)!}\prod_{j=0}^{2k-1}\frac{m+1-j}{2m+2-j} \\ +\sum_{i=1}^{k-1}\frac{(-1)^i+(-1)^{2k-1}}{(2k-i)!(i!)}\prod_{j=0}^{2k-i-1}\frac{m+1-j}{2m+2-j}\prod_{j=0}^{i-1}\frac{m+1-j}{2m+2-j}, \quad m=3,4,\ldots \tag{27}$$

From (23), (24) and (25) we have for the coefficient parameters a_0, a_1, b_0 and b_1 that

$$\begin{aligned} &a_0 = 1, \quad a_1 = -2, \\ &b_0 = \frac{1}{4} - \frac{m}{2(2m+1)} = \frac{1}{4(2m+1)}, \\ &b_1 = \frac{1}{2} + \frac{m}{2m+1} = \frac{4m+1}{4m+2}. \end{aligned} \tag{28}$$

For the coefficient parameters $b_{1,i}$, $i = 1(1)m$, from (25a) we obtain

$$\begin{aligned} &b_1 b_{1,1} = -A_{m,2} \text{ or } b_{1,1} = -\frac{A_{m,2}}{b_1}, \\ &-b_1 b_{1,1} b_{1,2} = -A_{m,3}, \\ &\qquad \vdots \\ &(-1)^{m+1} b_1 b_{1,1} b_{1,2} \ldots b_{1,m} = -A_{m,m+1}. \end{aligned} \tag{29}$$

So, we have

$$b_{1,k} = -\frac{A_{m,k+1}}{A_{m,k}}, \quad k = 2(1)m. \tag{30}$$

Finally, for the coefficients parameters $b_{0,i}$, $i = 1(1)m$ from (25a) we obtain

$$\begin{aligned} &b_1 b_{0,1} = -B_{m,2} \\ &-b_1 b_{1,1} b_{0,2} = -B_{m,3} \\ &\qquad \vdots \\ &(-1)^{m+1} b_1 b_{1,1} b_{1,2} \ldots b_{1,m-1} b_{0,m} = -B_{m,m+1}. \end{aligned} \tag{31}$$

From (31) and (29) we have

$$\begin{aligned} &b_{0,1} = \frac{B_{m,2}}{b_1}, \\ &b_{0,k} = \frac{B_{m,k+1}}{A_{m,k}}, \quad k = 2(1)m. \end{aligned} \tag{32}$$

4. Computational implemantation

4.1. Error estimation — Local Padé approximation error

For the integration of systems of initial-value problems, several methods have been proposed for the estimation of the local truncation error (LTE) (see, for example, [38]).

In this paper we base our local error estimation technique on an embedded pair of integration methods and on the fact that when the order of (m,m) Padé approximation of the exponential function of the P-stable method is maximal, then the approximation of the solution for the problems with oscillatory solution is better (see also [3]).

We denote the higher-order solution, i.e., the solution which we obtain using the family $m+1$ as y_{n+1}^{m+1} and the lower-order solution which we obtain using the family m as y_{n+1}^{m}; then, we have the following definition.

Definition 4. We define the Local Padé Approximation Error (LPAE) in lower-order solution y_{n+1}^{m} by the quantity

$$\text{LPAE} = | y_{n+1}^{m+1} - y_{n+1}^{m} | . \tag{33}$$

Under the assumption that h is sufficiently small, the LPAE in y_{n+1}^{m} can be neglected compared to that in y_{n+1}^{m}.

If the LPAE of acc is required and the step size of the integration used for the nth step length is h_n the estimated step size for the $(n+1)$st step, which would give a local error of acc, must be

$$h_{n+1} = h_n \left(\left| \frac{\text{acc}}{\text{LPAE}} \right| \right)^{1/q}, \tag{34}$$

where q is the order of the Padé approximation of the exponential function.

However, for ease of programming we have restricted all step changes to halving and doubling. Thus, based on the procedure developed in [36] for the local truncation error, the step control procedure which we have actually used is

$$\text{If LPAE} < \text{acc}, \quad h_{n+1} = 2h_n,$$

$$\text{If } 100\text{acc} > \text{LPAE} > \text{acc}, \quad h_{n+1} = h_n, \tag{35}$$

$$\text{If LPAE} > \text{acc}, \quad h_{n+1} = \tfrac{1}{2} h_n \text{ and repeat the step.} \tag{36}$$

We note that the LPAE estimate is in the lower-order solution y_{n+1}^{m}. However, if this error estimate is acceptable, i.e., less than acc, we adopt the widely used procedure of performing local extrapolation. Thus, although we are actually controlling an estimate of the LPAE in lower-order solution y_{n+1}^{m}, it is the higher-order solution y_{n+1}^{m+1} which we actually accept at each point.

4.2. Computational implementation

Application of method (14) to the Schrödinger equation (1) gives the following difference equation:

$$D_{n+1} y_{n+1} + D_n y_n + D_{n-1} = 0, \tag{37}$$

where

$$D_{n+1} \equiv a_0 - b_0 f_{n+1} + b_{0,1} b_1 f_{n+1} f_n + b_1 f_{n+1} f_n^2 \sum_{i=1}^{m-1} (-1)^i \left(\prod_{j=1}^{i} b_{1,j} \right) b_{0,i+1} f_n^{i-1}, \tag{38}$$

$$D_n \equiv a_1 - b_1 f_n + b_1 f_n^2 \sum_{i=1}^{m} (-1)^{i+1} \left(\prod_{j=1}^{i} b_{1,j} \right) f_n^{i-1}, \tag{39}$$

$$D_{n-1} \equiv a_0 - b_0 f_{n-1} + b_{0,1} b_1 f_{n-1} f_n + b_1 f_{n-1} f_n^2 \sum_{i=1}^{m-1} (-1)^i \left(\prod_{j=1}^{i} b_{1,j} \right) b_{0,i+1} f_n^{i-1}, \tag{40}$$

with $f_k = [l(l+1)/x_k^2 + V(x_k) - E]$, $k = n - 1(1)n + 1$.

Based on the above difference equation we have that in order to apply the developed generator of high-order P-stable methods to the one-dimensional Schrödinger equation we make the following steps:

1. We calculate $A_{m,k}$ and $B_{m,k}$, $k = 2(1)m$ from (26) and (27).
2. We calculate the values of D_{n+1}, D_n and D_{n-1} based on the Horner's scheme.
3. Now our trick to estimate the LPAE in y_{n+1}^k using the order of y_{n+1}^{k+1} is clear. At every step we start with $k = 3$, i.e., with a P-stable method of order eight, and go to m increasing k until the local error estimate be less than the bound acc $(1 \leqslant k \leqslant m)$. For reasons of round of errors of the computers, in which we have implemented our methods, m should not exceed the value 6, because for m higher the error becomes of order near to the accuracy of the computers.

5. Numerical illustrations

In this section we present some numerical results to illustrate the performance of our method. We consider the numerical integration of the one-dimensional Schrödinger equation.

The radial or one-dimensional Schrödinger equation (1) is one of the boundary-value problems, with $y(0) = 0$, and a second boundary condition for large values of x determined by physical considerations. The precise form of this second boundary condition depends crucially on the sign of E. In the case where $E = k^2 > 0$, then, in general, the potential function $V(x)$ dies away faster than the term $l(l+1)/x^2$; Eq. (1) then effectively reduces to $y''(x) + (E - l(l+1)/x^2)y(x) = 0$, for large x. The above equation has linearly independent solutions $kxj_l(kx)$ and $kxn_l(kx)$, where $j_l(kx)$ and $n_l(kx)$ are the spherical Bessel and Neumann functions, respectively. Thus, the solution of Eq. (1) has the asymptotic form

$$\begin{aligned} y(x) &\cong_{x\to\infty} Akxj_l(kx) - Bkxn_l(kx) \\ &\cong_{x\to\infty} A\left[\sin\left(kx - \tfrac{1}{2}l\pi\right) + \tan\delta_l \cos\left(kx - \tfrac{1}{2}l\pi\right)\right], \end{aligned}$$

where δ_l is the phase shift which may be calculated from the formula

$$\tan \delta_l = \frac{y(x_2)S(x_1) - y(x_1)S(x_2)}{y(x_1)C(x_2) - y(x_2)C(x_1)} \tag{41}$$

for x_1 and x_2 distinct points on the asymptotic region with $S(x) = kxj_l(kx)$ and $C(x) = -kxn_l(kx)$.

5.1. Case I: The phase shift problem—Lennard Jones potential

We illustrate the new methods derived in Section 3 by applying them to the solution of (1), where $V(x)$ is the *Lennard–Jones potential* which has been widely discussed in the literature. For this problem the potential $V(x)$ is given by

$$V(x) = m(1/x^{12} - 1/x^6) \quad \text{where } m = 500. \tag{42}$$

We solve this problem as an initial value one and, in order to be able to use a two-step method we need an extra initial condition to be specified, e.g. $y_1 (= y(h))$. It is well known that, for values of x close to the origin, the solution of (1) behaves like

$$y(x) \simeq Cx^{l+1} \quad \text{as } x \to 0. \tag{43}$$

In view of this we use $y_1 = h^{l+1}$ as our extra initial condition.

The problem we consider is the computation of the relevant phase shifts correct to 4 decimal places for energies $k = 5$ and $k = 10$. We will consider four approaches based on

(1) the well-known variable step method in [37],
(2) the variable step procedure developed in [44],
(3) the variable step procedure developed in [45],
(4) the generator of P-stable methods developed in Section 3.

The procedures (1), (2) and (3) are exactly described in [37], in [44] and in [45] and are used without modification.

The generator of P-stable methods used in (4) is developed in Section 3 and the error control procedure is described in Section 4.

In Figs. 1 and 2 we present the real time of computation of the phase shifts correct to 4 decimal places.

5.2. Case II: The resonance problem

In this section we present some numerical results to illustrate the performance of our new methods. We consider the numerical integration of the Schrödinger equation (1) in the well-known case where the potential $V(x)$ is the Woods–Saxon potential

$$W(x) = V(x) = \frac{u_0}{(1+z)} - \frac{u_0 z}{[a(1+z)^2]} \tag{44}$$

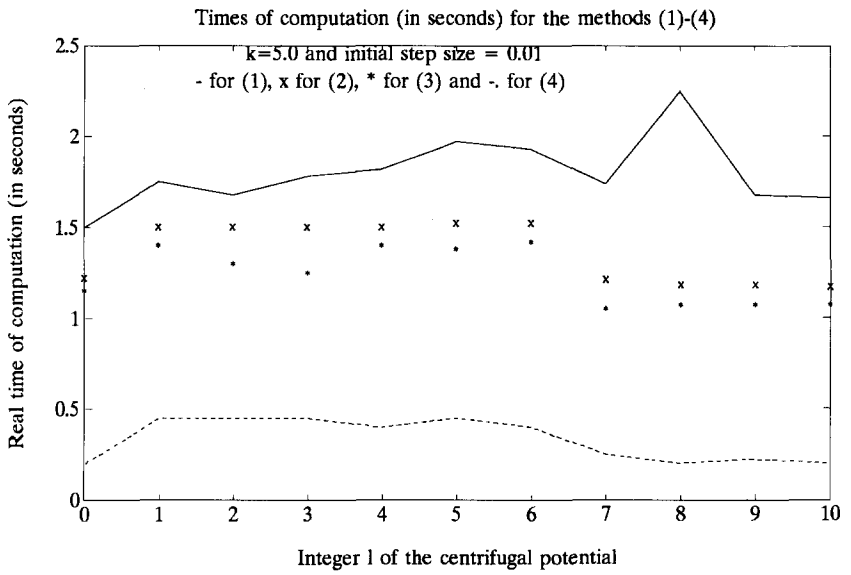

Fig. 1.

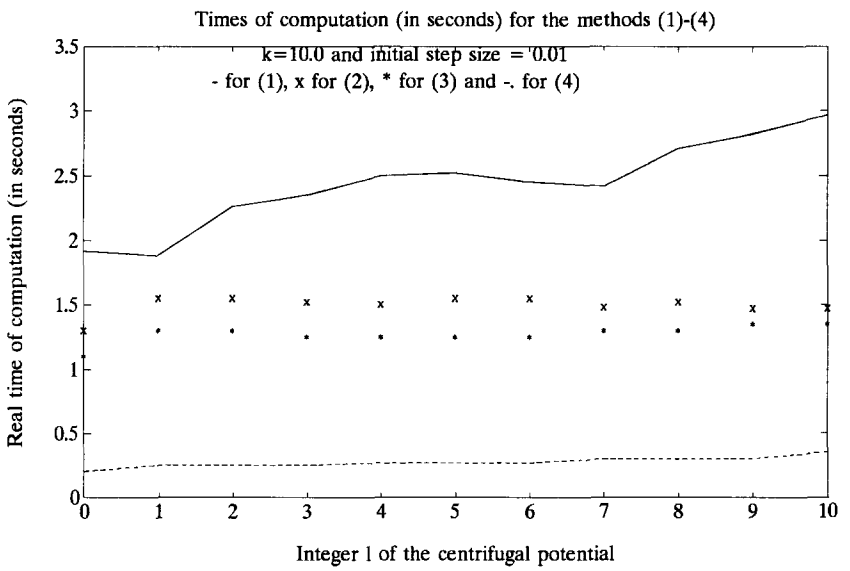

Fig. 2.

with $z=\exp[(x-X_0)/a], u_0=-50, a=0.6, X_0=7.0$ and $l=0$. In order to solve this problem numerically we need to approximate the true (infinite) interval of integration $[0,\infty)$ by a finite interval. For the purpose of our numerical illustration we take the domain of integration as $0\leqslant x\leqslant 15$. We consider (1) in a rather large domain of energies, i.e., $E=k^2\in[0,1000]$. The problem we consider is the so-called *resonance problem.*

Table 1
Deviations of the computed phase shifts from the exact one $\frac{1}{2}\pi$ in 10^{-6} units (CPU time in seconds) for the three variable-step methods. Initial step-size $h_0 = 0.001$. AbsErr=absolute error. h_{max} = the maximum step-size

	Method (1)			Method (2)			Method (3)			Method (4)		
Exact Resonances	acc	h_{max}	AbsErr (time in seconds)	acc	h_{max}	AbsErr (time in seconds)	acc	h_{max}	AbsErr (time in seconds)	acc	h_{max}	AbsErr (time in seconds)
53.588872	10^{-6}	0.128	47405 (0.050)	10^{-6}	0.128	9870 (0.040)	10^{-6}	0.128	931 (0.035)	10^{-6}	0.256	106 (0.020)
	10^{-10}	0.016	5332 (0.550)	10^{-10}	0.032	81 (0.410)	10^{-10}	0.064	35 (0.290)	10^{-10}	0.128	5 (0.120)
163.215341	10^{-6}	0.064	14159 (0.110)	10^{-6}	0.128	6123 (0.090)	10^{-6}	0.128	876 (0.035)	10^{-6}	0.512	160 (0.010)
	10^{-10}	0.016	3407 (0.490)	10^{-10}	0.032	238 (0.360)	10^{-10}	0.064	92 (0.290)	10^{-10}	0.128	3 (0.110)
341.495874	10^{-6}	0.032	10751 (0.110)	10^{-6}	0.064	5737 (0.090)	10^{-6}	0.128	832(0.035)	10^{-6}	0.256	283 (0.015)
	10^{-10}	0.008	2439 (0.610)	10^{-10}	0.016	105 (0.490)	10^{-10}	0.032	87 (0.500)	10^{-10}	0.128	3(0.155)
989.701916	10^{-6}	0.032	3351 (0.220)	10^{-6}	0.064	1458 (0.190)	10^{-6}	0.128	345(0.035)	10^{-6}	0.256	162 (0.020)
	10^{-10}	0.008	573 (0.880)	10^{-10}	0.016	130 (0.740)	10^{-10}	0.032	52 (0.580)	10^{-10}	0.128	3 (0.205)

This problem consists either of finding *the phase shift* δ_l or finding those E, for $E \in [0, 1000]$, at which δ_l equals $\frac{1}{2}\pi$. We actually solve the earlier problem.

The boundary conditions for this problem are

$$y(0) = 0,$$

$$y(x) = \cos(\sqrt{E}x) \quad \text{for large } x.$$

The domain of numerical integration is [0, 15].

In our numerical illustration we find the phase shifts δ_l by the three variable-step methods mentioned in case I.

The numerical results obtained for these methods were compared with the analytic solution $\delta_l = \frac{1}{2}\pi$. Table 1 shows the absolute errors in 10^{-6}, $h_{\max}$ and the CPU time of computation for the calculation. The empty areas indicate that the corresponding absolute errors are larger than 1.

6. Conclusions

We have constructed a generator of high-order P-stable embedded methods. The methods are embedded because of a natural error control procedure. We have proposed for this generator of P-stable methods procedures to define automatically the coefficients of the methods in order to maximize the order of the (m, m) Padé approximation of the exponential function. It can be seen from the theoretical and numerical results that the new methods is considerably more accurate than the other well-known variable-step procedure in [37], the variable step procedure developed in [44] and the variable step procedure developed in [45].

All computations were carried out on a PC i486 using double precision arithmetic (16 significant digits accuracy).

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