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A High-Accuracy Algorithm for Solving Nonlinear PDEs with High-Order Spatial Derivatives in 1 + 1 Dimensions

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We propose an algorithm to solve a system of partial differential equations of the type $\mathbf{u}_t(x, t) = \mathbf{F}(x, t, \mathbf{u}, \mathbf{u}_x, \mathbf{u}_{xx}, \mathbf{u}_{xxx}, \mathbf{u}_{xxxx})$ in 1 + 1 dimensions using the method of lines with piecewise ninth-order Hermite polynomials, where $\mathbf{u}$ and $\mathbf{F}$ are N-dimensional vectors. Nonlinear boundary conditions are easily incorporated with this method. We demonstrate the accuracy of this method through comparisons of numerically determined solutions to the analytical ones. Then, we apply this algorithm to a complicated physical system involving nonlinear and nonlocal strain forces coupled to a thermal field. © 1994 Academic Press, Inc.

1. INTRODUCTION

Many physical phenomena can be described by partial differential equations (PDEs) such as Maxwell's equations, Schrödinger's equation, and Einstein's equations. However, very few analytic solutions of these equations can be obtained if the system of PDEs involves nonlinearities. Therefore, numerical methods play a crucial role in approximately solving these equations.

The most naive algorithm for solving systems of nonlinear PDEs is to reduce the equations to a set of ordinary differential equations (ODEs) by the finite difference method, viz., to utilize finite differences to evaluate spatial derivatives approximately [1]. In order to obtain solutions of high accuracy, the discretized spatial intervals must vary with time, which makes the application of the algorithm very difficult. Even if this difficulty can be overcome, the numerical solutions in many cases will not be acceptable; a simple analysis of the intrinsic difficulties of evaluating fourth-order spatial derivatives over an interval of time is provided in Appendix A.

To overcome these difficulties, the method of lines has been developed for solving the following (1 + 1)-dimensional system [2],

$$\frac{\partial \mathbf{u}(x, t)}{\partial t} = \mathbf{F}(x, t, \mathbf{u}, \mathbf{u}_x, \mathbf{u}_{xx}) \qquad (1)$$

with the initial condition

$$\mathbf{u}(x, t = 0) = \mathbf{f}(x) \qquad (2)$$

and linear boundary conditions

$$\begin{aligned} \alpha_1 \mathbf{u} + \beta_1 \mathbf{u}_x &= \gamma_1 \quad \text{at} \quad x = x_L \\ \alpha_2 \mathbf{u} + \beta_2 \mathbf{u}_x &= \gamma_2 \quad \text{at} \quad x = x_R. \end{aligned} \qquad (3)$$

Here $\mathbf{u}$, $\mathbf{F}$, $\mathbf{f}$ are N-dimensional vectors; α_1, α_2, β_1, β_2, γ_1, and γ_2 are $N \times N$ constant matrices; x_L and x_R correspond to the left and right boundaries, respectively. However, this algorithm is inapplicable for PDE systems which contain high-order spatial derivatives or have nonlinear boundary conditions. The goal of this article is to propose a variant method of lines to solve these types of systems.

Our paper is organized as follows: First we present the details of the variant algorithm. Then, we test the algorithm by comparing our numerical solutions of systems of PDEs having a high-order spatial derivative to the analytic ones—excellent agreement is found. In Section 3, we apply the algorithm to a nonlinear, nonlocal physical system which describes a strain field coupled with a thermal field to model a first-order structural phase transition of 1 + 1 dimensions [3]. We close this article by a short conclusion.

2. ALGORITHM

The quotient difference algorithm can have severe difficulties providing accurate evaluations of the high-order spatial derivatives required to solve PDEs as time t evolves (a simple analysis is given in Appendix A). To overcome these difficulties, we introduce the variant method of lines with piecewise ninth-order Hermite polynomials to solve the system of PDEs,

$$\frac{\partial \mathbf{u}(x, t)}{\partial t} = \mathbf{F}(x, t, \mathbf{u}, \mathbf{u}_x, \mathbf{u}_{xx}, \mathbf{u}_{xxx}, \mathbf{u}_{xxxx}) \qquad (4)$$

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with the initial condition

$$\mathbf{u}(x, 0) = \mathbf{f}(x) \tag{5}$$

and the (potentially nonlinear) boundary conditions

$$\mathbf{V}_{i'}(x_L, t, \mathbf{u}, \mathbf{u}_x, \mathbf{u}_{xx}, \mathbf{u}_{xxx}) = 0 \tag{6}$$

$$\mathbf{W}_{i'}(x_R, t, \mathbf{u}, \mathbf{u}_x, \mathbf{u}_{xx}, \mathbf{u}_{xxx}) = 0 \tag{7}$$

where $\mathbf{u}$, $\mathbf{F}$, $\mathbf{f}$, $\mathbf{V}_{i'}$, and $\mathbf{W}_{i'}$ are N-dimensional vectors, and $i' = 1, 2$. We utilize piecewise ninth-order Hermite polynomials to represent $\mathbf{u}(x, t)$ in a spatial approximation; i.e., we use the polynomials $P^9_{ji}(x)$ to fit the function $\mathbf{u}(x, t)$ locally in space. In this approximation, we break up space into $M-1$ intervals whose boundaries, so-called knots, are $x = x_1 < x_2 < \cdots < x_M$ ($x_1 = x_L$ and $x_M = x_R$); the polynomials $P^9_{j1}(x)$, $P^9_{ji}(x)$ $(1 < i < M)$, and $P^9_{jM}(x)$ are nonzero only on the intervals $x_1 \leqslant x \leqslant x_2$, $x_{i-1} \leqslant x \leqslant x_{i+1}$, and $x_{M-1} \leqslant x \leqslant x_M$, respectively. The nonzero sectors of $P^9_{ji}(x)$ are ninth-order polynomials which have C_4-continuity and satisfy

$$\left.\frac{d^m}{dx^m} P^9_{ji}(x)\right|_{x=x_l} = \delta_{mj}\,\delta_{il}, \qquad 0 \leqslant j, \quad m \leqslant 4, \tag{8}$$

at the knots; the explicit forms of $P^9_{ji}(x)$ are shown in Appendix B. Thus, in our spatial approoximation

$$\mathbf{u}(x, t) = \sum_{i'=i}^{i+1} \sum_{j=0}^{4} \mathbf{C}_{i'j}(t)\, P^9_{ji'}(x) \tag{9}$$

on the interval $x_i \leqslant x \leqslant x_{i+1}$, where $i \leqslant M-1$. Because the nonzero part of $P^9_{ji}(x)$ is localized on one or two intervals, the spatial approximation of $\mathbf{u}(x, t)$ can be written as

$$\mathbf{u}(x, t) = \sum_{i=1}^{M} \sum_{j=0}^{4} \mathbf{C}_{ij}(t)\, P^9_{ji}(x) \tag{10}$$

where $\mathbf{C}_{ij}(t)$ is the approximation of jth derivative of $\mathbf{u}(x, t)$ at $x = x_i$.

If the distance between the knots is sufficiently small, the approximation will be quite good. The selection of the knots, in general, depends on the characteristic length of the physical system which one is studying, such as the width of an interface or a typical domain size. The distances between the knots can be uneven, but usually should be smaller than the characteristic length. One should always keep decreasing or increasing these distances until a converged solution is obtained.

The coefficients of the trial solution are obtained so that approximation satisfies Eq. (4) at the $5M-4$ points $\{q_m\}$ which are distributed uniformly between the knots.[1] To give an explicit form for $\{q_m\}$, we define the following numbers: $n'_i = 5 + \delta_{M/2,i}$, $n_1 = 0$, and $n_{i+1} = n_i + n'_i$, where $i = 1, ..., M-1$, and M is even number. Thus, $\{q_m\}$ are given by

$$q_{1+n_i} = x_i + (x_{i+1} - x_i)/2n'_i, \qquad q_{j+1+n_i} = q_{j+n_i} + h_i/n'_i, \tag{11}$$

where $h_i = x_{i+1} - x_i$ and $j = 1, ..., n'_i - 1$. With the defined $\{q_m\}$, we can obtain the coefficients $\mathbf{C}_{ij}$ by solving the ordinary differential equations,

$$\sum_{i=1}^{M} \sum_{j=0}^{4} \frac{d\mathbf{C}_{ij}}{dt} P^9_{ji}(q_m) = \mathbf{F}(q_m, t, \mathbf{u}(q_m, t), \mathbf{u}_x(q_m, t), ..., \mathbf{u}_{xxxx}(q_m, t)) \tag{12}$$

for $m = 1, ..., 5M-4$ and $i = 1, ..., M-1$. This is a system of $N(5M-4)$ ordinary differential equations in $5NM$ unknown coefficient funcions $\mathbf{C}_{ji}$. The number of unknown coefficients can be reduced to $N(5M-4)$ by using the $4N$ boundary conditions given in Eqs. (6) and (7) to eliminate $4N$ coefficients. As a result, we have $N(5M-4)$ unknown variables and the same number of equations, and thus the PDE system has been reduced to an ODE system with the following initial conditions:

$$\mathbf{C}_{ij}(0) = \left.\frac{\partial^j \mathbf{u}(x, 0)}{\partial x^j}\right|_{x=x_i}. \tag{13}$$

For convenience, Eq. (12) can be written in a compact form,

$$\frac{d\mathbf{C}}{dt} = \mathscr{A}^{-1}\mathbf{B}(t, y), \tag{14}$$

with the initial conditions Eq. (13), where $\mathbf{C}$ is a vector of coefficients of length $N(5M-4)$. $\mathscr{A}$ is a $N(5M-4)$ by $N(5M-4)$ sparse matrix, whose nonzero elements are $P^9_{ji}(q_m)$.

Now consider one of the simplest cases—$N = 1$ and the boundary conditions Eqs. (6) and (7) are

$$u(x, t) = u_{xx}(x, t) = 0 \qquad \text{at} \quad x = x_L \text{ and } x_R. \tag{15}$$

Equation (12) reduces to ($m = 1, ..., 5M-4$)

$$\sum_{i=1}^{M} \sum_{j=0}^{4} \frac{dC_{ij}}{dt} P^9_{ji}(q_m) = F(q_m, t, u(q_m, t), u_x(q_m, t), ..., u_{xxxx}(q_m, t)) \tag{16}$$

with $C_{10}(t) = C_{12}(t) = C_{M0}(t) = C_{M2}(t) = 0$. The sparse matrix $\mathscr{A}$ is

[1] A better way to select $\{q_m\}$ is the collocation method, viz., use Gaussian points as the $\{q_m\}$ in each subinterval. However, this method cannot easily be implemented to solve the problem discussed in Section 3, owing to the differing orders of the strain and temperature PDEs.

$$\mathscr{A} = \begin{bmatrix} P^9_{11}(q_1) & P^9_{31}(q_1) & P^9_{41}(q_1) & P^9_{02}(q_1) & \cdots & P^9_{42}(q_1) & 0 & \cdots & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ P^9_{11}(q_5) & P^9_{31}(q_5) & P^9_{41}(q_5) & P^9_{02}(q_5) & \cdots & P^9_{42}(q_5) & 0 & \cdots & 0 & \cdots \\ 0 & 0 & 0 & P^9_{02}(q_6) & \cdots & P^9_{42}(q_6) & P^9_{03}(q_6) & \cdots & P^9_{43}(q_6) & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & P^9_{02}(q_{10}) & \cdots & P^9_{42}(q_{10}) & P^9_{03}(q_{10}) & \cdots & P^9_{43}(q_{10}) & \cdots \\ 0 & 0 & 0 & 0 & 0 & 0 & P^9_{03}(q_{11}) & \cdots & P^9_{43}(q_{11}) & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & P^9_{03}(q_{15}) & \vdots & P^9_{43}(q_{15}) & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots\cdots & & & \end{bmatrix} \quad (17)$$

with a bandwidth of 10. The vector $\mathbf{C}$ is

$$\mathbf{C} = [C_{11}, C_{13}, C_{14}, C_{20}, ..., C_{24}, ..., C_{M1}, C_{M3}, C_{M4}]^{\mathrm{T}}. \quad (18)$$

and the vector $\mathbf{B}$ on the right-hand side of Eq. (14) is

$$\mathbf{B} = [F(q_1, ...), F(q_2, ...), ..., F(q_{5M-5}, ...), F(q_{5M-4}, ...)]^{\mathrm{T}}. \quad (19)$$

To test this algorithm we have numerically solved the linear equation

$$u_{tt} - u_{txx} - u_{xx} + u_{xxxx} = 0 \quad (20)$$

with the boundary condition Eq. (15) ($x_L = -L$ and $x_R = +L$) and the initial conditions

$$u(x, 0) = \sin\left(\frac{\pi}{2L}(x-L)\right),$$
$$u_t(x, 0) = -\frac{1}{2}\left(\frac{\pi}{2L}\right)^2 \sin\left(\frac{\pi}{2L}(x-L)\right) \quad (21)$$

whose analytic solution is

$$u(x, t) = \exp\left(-\frac{1}{2}\left(\frac{\pi}{2L}\right)^2 t\right) \cos\left(\frac{\pi}{4L}\sqrt{4+3\left(\frac{\pi}{2L}\right)^2}\, t\right) \times \sin\left(\frac{\pi}{2L}(x-L)\right). \quad (22)$$

The numerical solution (with $h_i = 1$ and $2L = 19$) is compared with the analytic one, Eq. (22), in Fig. 1. The discrepancies between them are so small that they cannot be distinguished in Fig. 1.

In order to quantify the discrepancies, we define the relative error as

$$E_{\mathrm{rel}}(t) = \frac{\sqrt{\int_{-L}^{L} (u(x, t) - \tilde{u}(x, t))^2\, dx}}{\int_{-L}^{L} |u(x, t)|\, dx}, \quad (23)$$

where $u(x, t)$ is Eq. (22) and $\tilde{u}(x, t)$ is the numerical solution. Up to times $t = 300$, the relative errors are list in Table I. Apparently, $E_{\mathrm{rel}}(t) < 2 \times 10^{-4}$, which is negligible and less than the error that we demand in the input of an ODE routine–a Runge–Kutta–Fehlburg integrator.

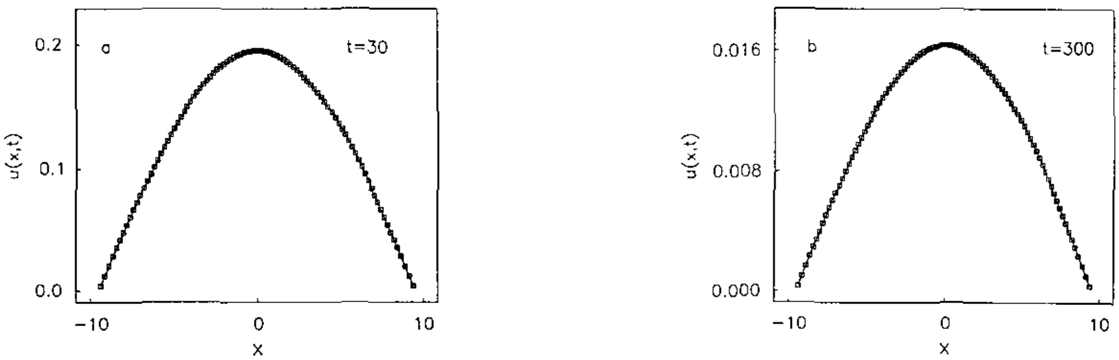

FIG. 1. The solution of Eq. (20) with the boundary condition Eq. (15) and the initial condition Eq. (21) is presented in this figure: $t = 30$ in (a), and $t = 300$ in (b). The solid line is the numerical solution, and the square symbols are the analytic solution.

TABLE I

The Relative Error, Defined in Eq. (23), at Different Times

Times	$E_{rel}(t)$
30	2.22×10^{-5}
60	8.68×10^{-6}
90	9.37×10^{-6}
120	5.29×10^{-5}
150	1.84×10^{-6}
180	1.85×10^{-4}
210	6.21×10^{-5}
240	2.57×10^{-5}
270	1.81×10^{-5}
300	5.88×10^{-6}

We have also solved Eq. (20) with a few different boundary conditions and initial conditions; the discrepancies between the numerical solutions and the analytic ones are as small as that shown in Fig. 1. In addition, we have tested this algorithm by solving other linear equations, and the results are always the same as the analytic solutions. The above example shows that our algorithm is quite reliable, although it does require that the initial conditions and the solutions have C_4-continuity. In the next section, we shall show how to apply this algorithm to a more complicated physical system.

3. A PHYSICAL EXAMPLE

In the study of interfacial dynamics at a first-order phase transition involving strain as the primary order parameter, unusual twinning dynamics is found [3]. To study the effects of the expulsion of the latent heat on the phase transition, in the heat-wave approximation, we obtain the PDE system [3, 4],

$$e_{tt} = [\delta T e - e^3 + e^5 - e_{xx} + \Gamma e_t]_{xx} \qquad (24)$$

and

$$\frac{1}{v_T^2}\frac{\partial^2 T}{\partial t^2} + \frac{1}{\alpha}\frac{\partial T}{\partial t} - \frac{\partial^2 T}{\partial x^2} = \beta\left(1 + \delta\frac{\partial}{\partial t}\right)(Tee_t). \qquad (25)$$

The boundary conditions are (again $x_L = -L$ and $x_R = +L$)

$$e_x(\pm L, t) = 0 \qquad (26)$$

$$e_t = \frac{1}{\Gamma}(e_{xx} - \delta T e + e^3 - e^5) \quad \text{at} \quad x = \pm L. \qquad (27)$$

and

$$T(\pm L, t) = T_o, \qquad (28)$$

and the initial conditions are

$$e(x, 0) = e_o \exp(-x^2/\sigma^2), \qquad e_t(x, 0) = 0. \qquad (29)$$

$$T(x, 0) = T_0, \qquad \frac{\partial T(x, 0)}{\partial t} = 0. \qquad (30)$$

Here $e(x, t)$ and $T(x, t)$ are the strain and thermal fields, respectively: $\delta T = T - T_c$, where T_c is the scaled instability temperature, which has been scaled to be unity; T_o is the initial temperature and the fixed temperature at the boundaries; e_o and σ are constants, and v_T is thermal propagation velocity; Γ, α, β, and δ are other physical constants. The derivation of the above equations will be provided elsewhere [4].

To solve Eqs. (24) and (25) with boundary conditions Eqs. (26), (27), and (28) and initial conditions Eqs. (29) and (30) using the algorithm presented in Section 2, we define

$$u^1(x, t) = e(x, t), \qquad u^2(x, t) = e_t(x, t),$$
$$u^3(x, t) = T(x, t), \qquad u^4(x, t) = \frac{\partial T(x, t)}{\partial t}. \qquad (31)$$

Thus, Eqs. (24)–(30) can be rewritten as

$$\frac{\partial \mathbf{u}}{\partial t} = \mathbf{F}(x, t, \mathbf{u}, \mathbf{u}_x, \mathbf{u}_{xx}, \mathbf{u}_{xxx}, \mathbf{u}_{xxxx}), \qquad (32)$$

where

$$\mathbf{u} = (u^1, u^2, u^3, u^4)^T, \qquad \mathbf{F} = (F^1, F^2, F^3, F^4)^T, \qquad (33)$$

and

$$F^1 = u^2,$$
$$F^2 = [(u^3 - T_c)\, u^1 - (u^1)^3 + (u^1)^5 - u^1_{xx} + \Gamma u^1_t]_{xx},$$
$$F^3 = u^4, \qquad (34)$$
$$F^4 = V_T^2\left\{u^3_{xx} - \frac{1}{\alpha}u^4 + \beta[u^3u^1u^2 + \delta(u^4u^1u^2 + u^3(u^2)^2 + u^3u^1F^2)]\right\}.$$

The boundary conditions are

$$u^1_x(\pm L, t) = 0,$$
$$u^2 = u^1_{xx} - (T_o - T_c)u^1 + (u^1)^3 - (u^1)^5 \quad \text{at} \quad x = \pm L, \qquad (35)$$
$$u^3(\pm L, t) = T_o,$$

and the initial conditions are

$$u^1(x, 0) = e_o \exp(-x^2/\sigma^2), \qquad u^2(x, 0) = 0,$$
$$u^3(x, 0) = T_o, \qquad u^4(x, 0) = 0. \qquad (36)$$

We now expand $u^1(x, t)$ and $u^2(x, t)$ in terms of piecewise ninth-order Hermite polynomials in the spatial approximation, and $u^3(x,t)$ and $u^4(x,t)$ in terms of piecewise fifth-order Hermite polynomials, respectively. To be specific, the trial solution is expanded in the series

$$\begin{aligned} u^1(x,t) &= \sum_{i=1}^{M} \sum_{j=0}^{4} C^1_{ij}(t)\, P^9_{ji}(x), \\ u^2(x,t) &= \sum_{i=1}^{M} \sum_{j=0}^{4} C^2_{ij}(t)\, P^9_{ji}(x), \\ u^3(x,t) &= \sum_{i'=1}^{M'} \sum_{j'=0}^{2} C^3_{i'j'}(t)\, P^5_{j'i'}(x), \\ u^4(x,t) &= \sum_{i'=1}^{M'} \sum_{j'=0}^{2} C^4_{i'j'}(t)\, P^5_{j'i'}(x), \end{aligned} \tag{37}$$

where we impose that $5(M-1)=3(M'-1)$, and $P^5_{ij}(x)$ are piecewise fifth-order Hermite polynomials, which are shown in Appendix B. Furthermore, for u^1 and u^2, $x_1=-L$, $x_{i+1}=x_i+h_i$, and $h_i=2L/(M-1)$; likewise, for u^3 and u^4, $x'_1=-L$, $x'_{i+1}=x'_i+h'_i$, and $h'_i=2L/(M'-1)$. For convenience, we choose $2L=w(M-1)$ and $M=4+6m'$, where m' is an arbitrary positive integer, and w is a tuning parameter which controls the distances between knots.

From the boundary conditions Eq. (35), we have

$$C^1_{11}(t)=C^1_{M1}(t)=0, \quad C^2_{11}(t)=C^2_{M1}(t)=0, \tag{38}$$

$$C^2_{10}(t)=C^1_{12}(t)-(T_o-T_c)\,C^1_{10}(t) + (C^1_{10}(t))^3-(C^1_{10}(t))^5, \tag{39}$$

$$C^2_{M0}(t)=C^1_{M2}(t)-(T_o-T_c)\,C^1_{M0}(t) + (C^1_{M0}(t))^3-(C^1_{M0}(t))^5, \tag{40}$$

$$\frac{dC^2_{10}(t)}{dt}=C^2_{12}(t)-[(T_o-T_c)+3(C^1_{10}(t))^2 - 5(C^1_{10}(t))^4]\,C^2_{10}(t), \tag{41}$$

$$\frac{dC^2_{M0}(t)}{dt}=C^2_{M2}(t)-[(T_o-T_c)+3(C^1_{M0}(t))^2 - 5(C^1_{M0}(t))^4]\,C^2_{M0}(t), \tag{42}$$

$$C^3_{10}(t)=C^3_{M'0}(t)=T_o, \quad C^4_{10}(t)=C^4_{M'0}(t)=0. \tag{43}$$

From the definition Equation (31), we also have

$$\frac{dC^1_{ij}(t)}{dt}=C^2_{ij}(t), \qquad \frac{dC^3_{i'j'}(t)}{dt}=C^4_{i'j'}(t). \tag{44}$$

Further, substituting Eq. (37) into Eq. (32) at $x=q_m$ gives us

$$\sum_{j=2}^{4}\frac{dC^2_{1j}}{dt}P^9_{j1}(q_m)+\sum_{j=0}^{4}\frac{dC^2_{2j}}{dt}P^9_{j2}(q_m) = F^2(q_m,t,\ldots)-\frac{dC^2_{10}}{dt}P^9_{01}(q_m) \tag{45}$$

for $m=1, \ldots, 5$;

$$\sum_{i=2}^{M-1}\sum_{j=0}^{4}\frac{dC^2_{ij}}{dt}P^9_{ji}(q_m)=F^2(q_m,t,\ldots) \tag{46}$$

for $m=6, \ldots, 5M-9$;

$$\sum_{j=0}^{4}\frac{dC^2_{(M-1)j}}{dt}P^9_{j(M-1)}(q_m) + \sum_{j=2}^{4}\frac{dC^2_{Mj}}{dt}P^9_{jM}(q_m)=F^2(q_m,t,\ldots) - \frac{dC^2_{M0}}{dt}P^9_{0M}(q_m) \tag{47}$$

for $m=5M-8, \ldots, 5M-4$, where dC^2_{10}/dt and dC^2_{M0}/dt are given by Eqs. (41) and (42). Similarly, $C^4_{i'j'}$ satisfies

$$\sum_{j'=1}^{2}\frac{dC^4_{1j'}}{dt}P^5_{j'1}(q_m)+\sum_{j'=0}^{2}\frac{dC^4_{2j'}}{dt}P^5_{j'2}(q_m)=F^4(q_m,t,\ldots) \tag{48}$$

for $m=1, 2, 3$;

$$\sum_{i'=2}^{M'-1}\sum_{j'=0}^{2}\frac{dC^4_{i'j'}}{dt}P^5_{j'i'}(q_m)=F^4(q_m,t,\ldots) \tag{49}$$

for $m=4, \ldots, 5M-7$;

$$\sum_{j'=1}^{2}\frac{dC^4_{(M'-1)j'}}{dt}P^5_{j'(M'-1)}(q_m) + \sum_{j'=0}^{2}\frac{dC^4_{M'j'}}{dt}P^5_{M'j'}(q_m)=F^4(q_m,t,\ldots) \tag{50}$$

for $m=5M-6, 5M-5, 5M-4$.

The above system can be written in the simple form

$$\frac{d\mathbf{C}^k}{dt}=(\mathscr{A}^k)^{-1}\,G^k(t,\mathbf{C}^1,\mathbf{C}^2,\mathbf{C}^3,\mathbf{C}^4) \quad \text{with} \quad \mathbf{C}^k(0)=\mathbf{C}^k_o. \tag{51}$$

where $k=1, 2, 3, 4$ and $\mathbf{C}^k_o$ holds the initial values of the coefficients. For $k=1$ and 2,

$$\mathbf{C}^k=[C^k_{10}, \ldots, C^k_{14}, \ldots, C^k_{M2}, C^k_{M3}, C^k_{M4}, C^k_{M1}, C^k_{M0}]^{\mathrm{T}}; \tag{52}$$

for $k=3$ and 4,

$$\mathbf{C}^k=[C^k_{10}, C^k_{11}, C^k_{12}, \ldots, C^k_{M'1}, C^k_{M'2}, C^k_{M'0}]^{\mathrm{T}}. \tag{53}$$

$\mathscr{A}^1$ and $\mathscr{A}^3$ are unit matrices; $\mathscr{A}^2$ reads as

$$\mathscr{A}^2=\begin{pmatrix} 1 & & & & \\ & 1 & & & \\ & & \mathscr{A}' & & \\ & & & 1 & \\ & & & & 1 \end{pmatrix}, \tag{54}$$

and

$$\mathscr{A}' = \begin{bmatrix} P^9_{21}(q_1) & P^9_{31}(q_1) & P^9_{41}(q_1) & P^9_{02}(q_1) & \cdots & P^9_{42}(q_1) & 0 & \cdots & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ P^9_{21}(q_5) & P^9_{31}(q_5) & P^9_{41}(q_5) & P^9_{02}(q_5) & \cdots & P^9_{42}(q_5) & 0 & \cdots & 0 & \cdots \\ 0 & 0 & 0 & P^9_{02}(q_6) & \cdots & P^9_{42}(q_6) & P^9_{03}(q_6) & \cdots & P^9_{43}(q_6) & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & P^9_{02}(q_{10}) & \cdots & P^9_{42}(q_{10}) & P^9_{03}(q_{10}) & \cdots & P^9_{43}(q_{10}) & \cdots \\ 0 & 0 & 0 & 0 & 0 & 0 & P^9_{03}(q_{11}) & \cdots & P^9_{43}(q_{11}) & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & P^9_{03}(q_{15}) & \vdots & P^9_{43}(q_{15}) & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & \cdots & \cdots \end{bmatrix} \tag{55}$$

with a bandwidth of 10. Likewise,

$$\mathscr{A}^4 = \begin{bmatrix} 1 & & & & & & & & & \\ & P^5_{11}(q_1) & P^9_{21}(q_1) & P^5_{02}(q_1) & P^5_{12}(q_1) & P^5_{22}(q_1) & 0 & 0 & 0 & \cdots \\ & P^5_{11}(q_2) & P^9_{21}(q_2) & P^5_{02}(q_2) & P^5_{12}(q_2) & P^5_{22}(q_2) & 0 & 0 & 0 & \cdots \\ & P^5_{11}(q_3) & P^9_{21}(q_3) & P^5_{02}(q_3) & P^5_{12}(q_3) & P^5_{22}(q_3) & 0 & 0 & 0 & \cdots \\ & 0 & 0 & P^5_{02}(q_4) & P^5_{12}(q_4) & P^5_{22}(q_4) & P^5_{03}(q_4) & P^5_{13}(q_4) & P^5_{23}(q_4) & \cdots \\ & 0 & 0 & P^5_{02}(q_5) & P^5_{12}(q_5) & P^5_{22}(q_5) & P^5_{03}(q_5) & P^5_{13}(q_5) & P^5_{23}(q_5) & \cdots \\ & 0 & 0 & P^5_{02}(q_6) & P^5_{12}(q_6) & P^5_{22}(q_6) & P^5_{03}(q_6) & P^5_{13}(q_6) & P^5_{23}(q_6) & \cdots \\ & 0 & 0 & 0 & 0 & 0 & P^5_{03}(q_7) & P^5_{13}(q_7) & P^5_{23}(q_7) & \cdots \\ & \vdots & \vdots & \vdots & \vdots & \vdots & P^5_{03}(q_8) & P^5_{13}(q_8) & P^5_{23}(q_8) & \cdots \\ & 0 & 0 & 0 & 0 & 0 & P^5_{03}(q_9) & P^5_{13}(q_9) & P^5_{23}(q_9) & \cdots \\ & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & \cdots & \cdots \\ & & & & & & & & & 1 \end{bmatrix} \tag{56}$$

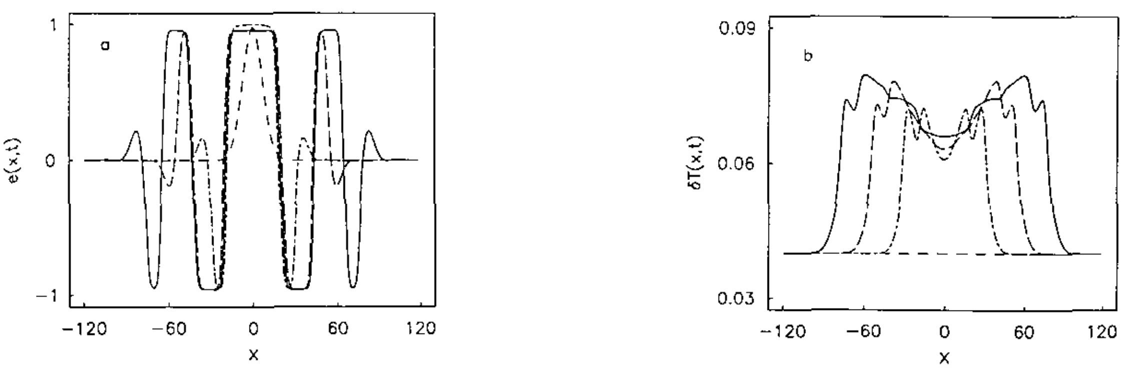

FIG. 2. The twinning solution of Eqs. (24) and (25) with the boundary conditions Eqs. (26), (27), and (28) and the initial conditions Eqs. (29) and (30) for both strain field $\varepsilon(x, t)$ (a) and thermal field $T(x, t)$ (b) at different times. The short dash, short dash–long dash, long dash, and solid lines correspond to time $t = 0$, 80, 160, and 240, respectively. The involved parameters ε_0, σ, β, δ, γ, V_T, and T_0 are $[0.5(1+\sqrt{1-4\delta T})]^{1/2}$, 10, 0.1, 1, 1, 2, and 1.04, respectively.

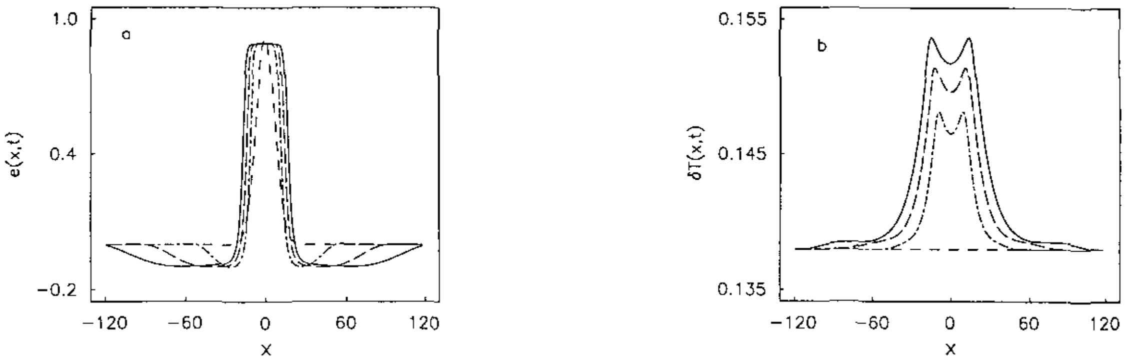

FIG. 3. The nontwinning solution of Eqs. (24) and (25) with the same boundary conditions and initial conditions as Fig. 2 for both strain field $e(x, t)$ (a) and thermal field $T(x, t)$ (b) at different times. The short dash, short dash–long dash, long dash, and solid lines correspond to time $t = 0$, 80, 160, and 240, respectively. The involved parameters are the same as Fig. 2, except that $T_0 = 1.138$.

with a bandwidth of six. The vector $\mathbf{G}^k$ follows:

$$\mathbf{G}^1 = \mathbf{C}^2, \qquad \mathbf{G}^3 = \mathbf{C}^4, \tag{57}$$

$$G_1^2 = C_{12}^2 - [(T_o - T_c) + 3(C_{10}^1)^2 - 5(C_{10}^1)^4]\, C_{10}^2, \tag{58}$$

$$G_{5M}^2 = C_{M2}^2 - [(T_o - T_c) + 3(C_{M0}^1)^2 - 5(C_{M0}^1(t))^4]\, C_{M0}^2, \tag{59}$$

$$G_2^2 = G_{5M-1}^2 = 0; \tag{60}$$

for $i = 3, ..., 7$,

$$G_i^2 = F^2(q_{i-2}) - G_1^2 P_{10}^9(q_{i-2}); \tag{61}$$

for $i = 5M - 6, ..., 5M - 2$,

$$G_i^2 = F^2(q_{i-2}) - G_{5M}^2 P_{M0}^9(q_{i-2}); \tag{62}$$

for $i = 8, ..., 5M - 7$,

$$G_i^2 = F^2(q_{i-2}). \tag{63}$$

G^4 satisfies

$$G_1^4 = G_{3M'}^4 = 0, \tag{64}$$

and for $i = 2, ..., 3M' - 1$,

$$G_i^4 = F^4(q_{i-1}). \tag{65}$$

The initial values of $\mathbf{C}_o^k$ are given by Eq. (13). Thus, we have reduced the PDEs to ODEs which can be solved by using any suitable ODE routine. Thus, so long as we know the parameters in the model, the problem becomes accessible.

Here we only briefly report some results of this model with the following involved parameters: $L = 120$, $e_0 = [0.5(1 + \sqrt{1 - 4\delta T})]^{1/2}$, $\sigma = 10$, $\beta = 0.1$, $\delta = 1$, $w = 1.5$, $V_T = 2$, and $\gamma = 1$ (the rationale for some of these choices may be found in [3, 4]). Figures 2 and 3 show the configurations of strain field and thermal field at different times for $T_o = 1.04$ and 1.138, respectively. These results indicate that for the same initial strain but differential initial temperatures, the system evolves to different states—twinning and nontwinning states [3]. The details of this model, and the underlying physics contained in similar dynamics, will be discussed elsewhere [4].

4. CONCLUSION

We have proposed a variant method of lines to solve systems of nonlinear PDEs in 1 + 1 dimensions which contain fourth-order spatial derivatives and nonlinear boundary conditions. We tested this method by solving a linear PDE system with a number of different initial conditions and linear boundary conditions. When compared with the analytical solutions, the numerical results are very accurate, and the relative errors are smaller than those that we demand in the input of an ODE routine. Therefore, we believe this method is quite reliable. Then, we used this method to investigate the physical system in which a strain field is coupled with the thermal field, both having propagating wave fronts, and the results are quite encouraging.

In general, our algorithm can be modified to solve different types of PDE systems. For instance, if a PDE system involves nth-order spatial derivatives and if its solution and initial conditions have C_n-continuity, one can construct piecewise $(2n + 1)$th-order Hermite polynomials in a similar manner to those presented in Appendix B. Thus, the spatial approximation of $\mathbf{u}(x, t)$ can be expanded in terms of piecewise $(2n + 1)$th-order Hermite polynomials, and the algorithm presented in Section 2 can be implemented for this system.

We realize that our variant method of lines has some limitations: if the solution cannot be approximately fit by piecewise ninth-order Hermite polynomials at any instant of time, the method is invalid. For instance, if the initial conditions do not have C_4-continuity, the coefficient vector $\mathbf{C}_{ij}(0)$ in Eq. (13) cannot be properly represented, and thus the solution at subsequent times cannot be obtained.

APPENDIX A

The formula of fourth derivative in the difference-quotient approximation is

$$\frac{\partial^4 u(x, t=0)}{\partial x^4} = \frac{1}{h^4}(u(x+2h, 0) - 4u(x+h, 0) + 6u(x, 0) - 4u(x-h, 0) + u(x-2h, 0)), \tag{66}$$

where we assume that $\mathbf{u}$ and $\mathbf{F}$ only have one component. Within this approximation the total absolute error, truncation plus rounding, is bounded by

$$E_{\text{abs}}(t=0) \leqslant 16\,|u(x, 0)|\,\frac{\varepsilon_o}{h^4} + \frac{1}{144}\left|\frac{\partial^6}{\partial x^6}u(x, 0)\right| h^2 \tag{67}$$

at time $t=0$, where ε_o is the relative error for $u(x, t)$ at $t=0$ and it is the machine epsilon if we start to evolve Eq. (4) from $t=0$. If we differentiate $E_{\text{abs}}(t=0)$ with respect to h and set the result equal to zero, the value of h is

$$h = 2\left|72u(x, 0)\,\varepsilon_0 \Big/ \frac{\partial^6 u(x, 0)}{\partial x^6}\right|^{1/6}, \tag{68}$$

and the minimized total absolute error at $t=0$ is

$$E_{\text{abs}}(0) \leqslant \frac{1}{4}\left|\frac{u(x, 0)}{3}\right|^{1/3}\left|\frac{\partial^6 u(x, 0)}{\partial x^6}\right|^{2/3}\varepsilon_o^{1/3}. \tag{69}$$

Assuming that $|u(x, t)| \approx |\partial^6 u(x, t)/\partial x^6|$ (e.g., $u(x, t) = f(t)\sin(x), f(t)\cos(x)$, or $f(t)\exp(x)$), we obtain the rule of thumb

$$E_{\text{rel}}(t=0) \leqslant \frac{1}{4}\left(\frac{\varepsilon_o}{3}\right)^{1/3}, \tag{70}$$

where $E_{\text{rel}}(0)$ is the relative error for $u_{xxxx}(x, t)$ at $t=0$. If we consider the inaccuracy in the calculation of $u_x(x, 0)$, $u_{xx}(x, 0)$, and $u_{xxx}(x, 0)$, the relative error of $u_t(x, t=0)$ will be order of $\varepsilon_o^{1/3}$. Therefore, when time reaches $t=1$, the relative error of $u(x, t=1)$ will be order of $\varepsilon_o^{1/3}$. Accordingly,

$$E_{\text{rel}}(t=1) \approx \frac{1}{4 \times 3^{1/3}}\,\varepsilon_o^{1/3^2}. \tag{71}$$

Using the same procedure, by induction it can be shown that

$$E_{\text{rel}}(t=n) \approx \frac{1}{4 \times 3^{1/3}}\,\varepsilon_o^{1/3^{n+1}}. \tag{72}$$

Usually, $\varepsilon_o > 10^{-18}$; therefore, $E_{\text{rel}}(t=5) > 10\%$. Besides the difficulty of changing h at different times, the relative error may be too large to obtain a reliable solution in many cases.

APPENDIX B

B.1. *Piecewise ninth-order Hermite Polynomials*

In this appendix, we first define $P^9_{4i}(x)$ and then recursively define $P^9_{3i}(x)$, $P^9_{2i}(x)$, $P^9_{1i}(x)$, and $P^9_{0i}(x)$. Let $h_i = x_{i+1} - x_i$. The polynomials $P^9_{4i}(x)$, which obey

$$\frac{d^m}{dx^m}P^9_{4i}(x_l) = \delta_{m4}\delta_{il}, \qquad 0 \leqslant m \leqslant 4, \tag{73}$$

are given by, for $i=1$,

$$P^9_{41} = \begin{cases} \dfrac{1}{4!\,h_1^5}(x-x_1)^4(x_2-x)^5, & x_1 \leqslant x < x_2, \\ 0, & x_2 \leqslant x \leqslant x_n; \end{cases} \tag{74}$$

for $i = 2, 3, ..., n-1$,

$$P^9_{4i}(x) = \begin{cases} 0, & x_1 \leqslant x < x_{i-1}, \\ \dfrac{1}{4!\,h_{i-1}^5}(x-x_{i-1})^5(x-x_i)^4, & x_{i-1} \leqslant x < x_i, \\ \dfrac{1}{4!\,h_i^5}(x_{i+1}-x)^5(x-x_i)^4, & x_i \leqslant x < x_{i+1}, \\ 0, & x_{i+1} \leqslant x \leqslant x_n; \end{cases} \tag{75}$$

for $i = n$,

$$P^9_{4n}(x) = \begin{cases} 0 & x_1 \leqslant x < x_{n-1}, \\ \dfrac{1}{4!\,h_{n-1}^5}(x-x_{n-1})^5(x-x_n)^4 & x_{n-1} \leqslant x \leqslant x_n. \end{cases} \tag{76}$$

The polynomials $P^9_{3i}(x)$ satisfying

$$\frac{d^m}{dx^m}P^9_{3i}(x_l) = \delta_{m3}\delta_{il}, \qquad 0 \leqslant m \leqslant 4, \tag{77}$$

take the following forms: for $i=1$,

$$P_{31}^9(x)=\begin{cases}\dfrac{1}{3!\,h^5}(x-x_1)^3(x_2-x)^5+\dfrac{20}{h_1}P_{41}^9(x), & \\ \qquad x_1\leqslant x<x_2, & \\ 0, \quad x_2\leqslant x\leqslant x_n; & \end{cases} \tag{78}$$

for $i=2, 3, ..., n-1$,

$$P_{3i}^9(x)=\begin{cases}0, \quad x_1\leqslant x<x_{i-1}, \\ \dfrac{1}{3!\,h_{i-1}^5}(x-x_{i-1})^5(x-x_i)^3-\dfrac{20}{h_{i-1}}P_{4i}^9(x), \\ \qquad x_{i-1}\leqslant x<x_i, \\ \dfrac{1}{3!\,h_i^5}(x_{i+1}-x)^5(x-x_i)^3+\dfrac{20}{h_i}P_{4i}^9(x), \\ \qquad x_i\leqslant x<x_{i+1}, \\ 0, \quad x_{i+1}\leqslant x\leqslant x_n; \end{cases} \tag{79}$$

for $i=n$,

$$P_{3n}^9(x)=\begin{cases}0, \quad x_1\leqslant x<x_{n-1}, \\ \dfrac{1}{3!\,h_{n-1}^5}(x-x_{n-1})^5(x-x_n)^3-\dfrac{20}{h_{n-1}}P_{4n}^9(x), \\ \qquad x_{n-1}\leqslant x\leqslant x_n. \end{cases} \tag{80}$$

The polynomials $P_{2i}^9(x)$ satisfying

$$\frac{d^m}{dx^m}P_{2i}^9(x_l)=\delta_{m2}\delta_{il}, \qquad 0\leqslant m\leqslant 4, \tag{81}$$

read as, for $i=1$,

$$P_{21}^9(x)=\begin{cases}\dfrac{1}{2!\,h_1^5}(x-x_1)^2(x_2-x)^5+\dfrac{15}{h_1}P_{31}^9(x) \\ \qquad -\dfrac{120}{h_1^2}P_{41}^9(x), \quad x_1\leqslant x<x_2, \\ 0, \quad x_2\leqslant x\leqslant x_n; \end{cases} \tag{82}$$

for $i=2, 3, ..., n-1$,

$$P_{2i}^9(x)=\begin{cases}0, & x_1\leqslant x<x_{i-1}, \\ \dfrac{1}{2!\,h_{i-1}^5}(x-x_{i-1})^5(x-x_i)^2 & \\ \qquad -\dfrac{15}{h_{i-1}}P_{3i}^9(x)-\dfrac{120}{h_{i-1}^2}P_{4i}^9(x), & x_{i-1}\leqslant x<x_i, \\ \dfrac{1}{2!\,h_i^5}(x_{i+1}-x)^5(x-x_i)^2 & \\ \qquad +\dfrac{15}{h_i}P_{3i}^9(x)-\dfrac{120}{h_i^2}P_{4i}^9(x), & x_i\leqslant x<x_{i+1} \\ 0, & x_{i+1}\leqslant x\leqslant x_n; \end{cases} \tag{83}$$

for $i=n$,

$$P_{2n}^9(x)=\begin{cases}0, \quad x_1\leqslant x<x_{n-1}, \\ \dfrac{1}{2!\,h_{n-1}^5}(x-x_{n-1})^5(x-x_n)^2 \\ \qquad -\dfrac{15}{h_{n-1}}P_{3n}^9(x)-\dfrac{120}{h_{n-1}^2}P_{4n}^9(x), \\ \qquad x_{n-1}\leqslant x\leqslant x_n. \end{cases} \tag{84}$$

The polynomials $P_{1i}^9(x)$ obeying

$$\frac{d^m}{dx^m}P_{1i}^9(x)=\delta_{m1}\delta_{il}, \qquad 0\leqslant m\leqslant 4, \tag{85}$$

are given by

$$P_{11}^9(x)=\begin{cases}\dfrac{1}{h_1^5}(x-x_1)(x_2-x)^5 \\ \qquad +\dfrac{10}{h_1}P_{21}^9(x)-\dfrac{60}{h_1^2}P_{31}^9(x)+\dfrac{240}{h_1^3}P_{41}^9(x), \\ \qquad x_1\leqslant x<x_2, \\ 0, \quad x_2\leqslant x\leqslant x_n, \end{cases} \tag{86}$$

for $i=1$;

$$P_{1i}^9(x)=\begin{cases}0, \quad x_1\leqslant x<x_{i-1}, \\ \dfrac{1}{h_{i-1}^5}(x-x_{i-1})^5(x-x_i) \\ \qquad -\dfrac{10}{h_{i-1}}P_{2i}^9(x)-\dfrac{60}{h_{i-2}^2}P_{3i}^9(x)-\dfrac{240}{h_{i-1}^3}P_{4i}^9(x), \\ \qquad x_{i-1}\leqslant x<x_i, \\ \dfrac{1}{h_i^5}(x_{i+1}-x)^5(x-x_i) \\ \qquad +\dfrac{10}{h_i}P_{2i}^9(x)-\dfrac{60}{h_i^2}P_{3i}^9(x)+\dfrac{240}{h_i^3}P_{4i}^9(x), \\ \qquad x_i\leqslant x<x_{i+1} \\ 0, \quad x_{i+1}\leqslant x\leqslant x_n; \end{cases} \tag{87}$$

for $i=2, 3, ..., n-1$;

$$P_{1n}^9(x)=\begin{cases}0, \quad x_1\leqslant x<x_{n-1}, \\ \dfrac{1}{h_{n-1}^5}(x-x_{n-1})^5(x-x_n) \\ \qquad -\dfrac{10}{h_{n-1}}P_{2n}^9(x)-\dfrac{60}{h_{n-1}^2}P_{3n}^9(x) \\ \qquad -\dfrac{240}{h_{n-1}^3}P_{4n}^9(x), \quad x_{n-1}\leqslant x\leqslant x_n, \end{cases} \tag{88}$$

for $i=n$.

The polynomials $P^9_{0i}(x)$, confined by

$$\frac{d^m}{dx^m} P^9_{0i}(x) = \delta_{m0}\delta_{il}, \qquad 0 \leqslant m \leqslant 4, \tag{89}$$

obey

$$P^9_{01}(x) = \begin{cases} \dfrac{1}{h_1^5}(x_2 - x)^5 + \dfrac{5}{h_1} P^9_{11}(x) \\ \qquad -\dfrac{20}{h_1^2} P^9_{21}(x) + \dfrac{60}{h_1^3} P^9_{31}(x) \\ \qquad -\dfrac{120}{h_1^4} P^9_{41}(x), \qquad x_1 \leqslant x < x_2, \\ 0, \qquad x_2 \leqslant x \leqslant x_n, \end{cases} \tag{90}$$

for $i = 1$;

$$P^9_{0i}(x) = \begin{cases} 0, \qquad x_1 \leqslant x < x_{i-1}, \\ \dfrac{1}{h_{i-1}^5}(x - x_{i-1})^5 - \dfrac{5}{h_{i-1}} P^9_{1i}(x) \\ \qquad -\dfrac{20}{h_{i-1}} P^9_{2i}(x) - \dfrac{60}{h_{i-2}^2} P^9_{3i}(x) - \dfrac{240}{h_{i-1}^4} P^9_{4i}(x), \\ \qquad x_{i-1} \leqslant x < x_i, \\ \dfrac{1}{h_i^5}(x_{i+1} - x)^5 + \dfrac{5}{h_i} P^9_{1i}(x) \\ \qquad -\dfrac{20}{h_i^2} P^9_{2i}(x) - \dfrac{60}{h_i^3} P^9_{3i}(x) + \dfrac{120}{h_i^4} P^9_{4i}(x), \\ \qquad x_i \leqslant x < x_{i+1} \\ 0, \qquad x_{i+1} \leqslant x \leqslant x_{n-1}; \end{cases} \tag{91}$$

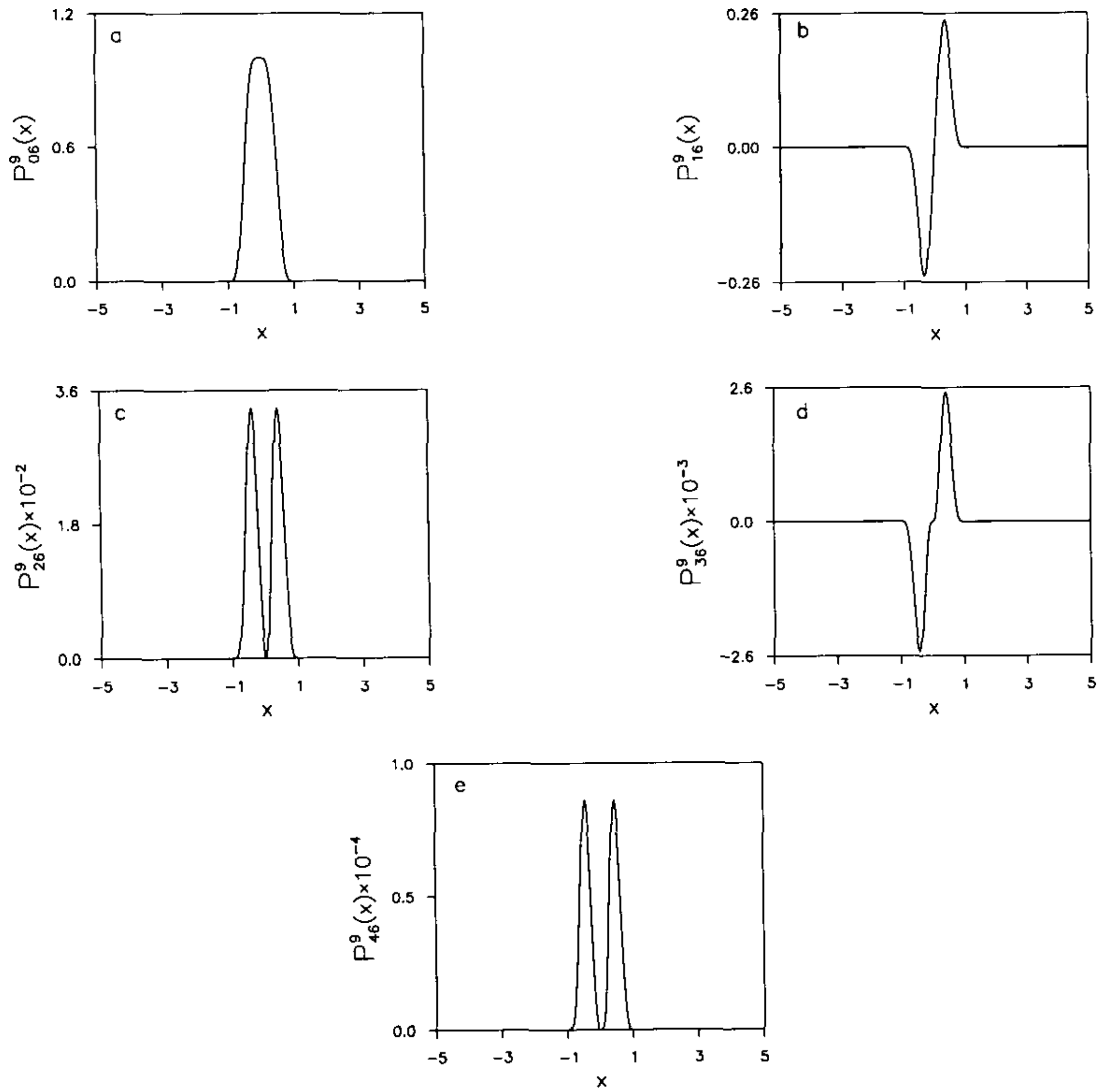

FIG. 4. $P^9_{06}(x)$ (a), $P^9_{16}(x)$ (b), $P^9_{26}(x)$ (c), $P^9_{36}(x)$ (d), and $P^9_{46}(x)$ versus x are plotted for $n = 11$ and $h_i = 1$.

for $i = 2, 3, \ldots, n-1$;

$$P^9_{0n}(x) = \begin{cases} 0, & x_1 \leqslant x < x_{n-1}, \\ \dfrac{1}{h^5_{n-1}}(x - x_{n-1})^5 - \dfrac{5}{h_{n-1}} P^9_{1n}(x) & \\ \quad - \dfrac{20}{h^2_{n-1}} P^9_{2n}(x) - \dfrac{60}{h^3_{n-1}} P^9_{3n}(x) & \\ \quad - \dfrac{120}{h^4_{n-1}} P^9_{4n}(x), & x_{n-1} \leqslant x \leqslant x_n, \end{cases} \quad (92)$$

for $i = n$.

$P^9_{06}(x)$ (a), $P^9_{16}(x)$ (b), $P^9_{26}(x)$ (c), $P^9_{36}(x)$ (d), and $P^9_{46}(x)$ verss x are plotted in Fig. 4 for $n = 11$ and $h_i = 1$.

B.2. *Piecewise Fifth-Order Hermite Polynomials*

Similar to nine-order piecewise Hermite polynomials, fifth-order piecewise Hermite polynomials can be written as follows. As in Appendix B.1, $h_i = x_{i+1} - x_i$. The polynomials $P^5_{2i}(x)$ satisfying

$$\frac{d^m}{dx^m} P^5_{2i}(x_l) = \delta_{m2}\delta_{il}, \qquad 0 \leqslant m \leqslant 2, \quad (93)$$

read as

$$P^5_{21} = \begin{cases} \dfrac{1}{2!\, h^3_1}(x - x_1)^2 (x_2 - x)^3, & x_1 \leqslant x < x_2, \\ 0, & x_2 \leqslant x \leqslant x_n; \end{cases} \quad (94)$$

for $i = 1$;

$$P^5_{2i}(x) = \begin{cases} 0, & x_1 \leqslant x < x_{i-1}, \\ \dfrac{1}{2!\, h^3_{i-1}}(x - x_{i-1})^3 (x - x_i)^2, & x_{i-1} \leqslant x < x_i, \\ \dfrac{1}{2!\, h^3_i}(x_{i+1} - x)^3 (x - x_i)^2, & x_i \leqslant x < x_{i+1}, \\ 0, & x_{i+1} \leqslant x \leqslant x_n; \end{cases} \quad (95)$$

for $i = 2, 3, \ldots, n-1$;

$$P^5_{2n}(x) = \begin{cases} 0 & x_1 \leqslant x < x_{n-1}, \\ \dfrac{1}{2!\, h^3_{n-1}}(x - x_{n-1})^3 (x - x_n)^2 & x_{n-1} \leqslant x \leqslant x_n, \end{cases} \quad (96)$$

for $i = n$.

The polynomials $P^5_{1i}(x)$ constrained by

$$\frac{d^m}{dx^m} P^5_{1i}(x_l) = \delta_{m1}\delta_{il}, \qquad 0 \leqslant m \leqslant 2, \quad (97)$$

satisfy

$$P^5_{11}(x) = \begin{cases} \dfrac{1}{h^3}(x - x_1)(x_2 - x)^3 + \dfrac{6}{h_1} P^5_{21}(x), & \\ \qquad x_1 \leqslant x < x_2, & \\ 0, \qquad x_2 \leqslant x \leqslant x_n; & \end{cases} \quad (98)$$

for $i = 1$;

$$P^5_{1i}(x) = \begin{cases} 0, \quad x_1 \leqslant x < x_{i-1}, & \\ \dfrac{1}{h^3_{i-1}}(x - x_{i-1})^3 (x - x_i) - \dfrac{6}{h_{i-1}} P^5_{21}(x), & \\ \qquad x_{i-1} \leqslant x < x_i, & \\ \dfrac{1}{h^3_i}(x_{i+1} - x)^3 (x - x_i) + \dfrac{6}{h_i} P^5_{2i}(x), & \\ \qquad x_i \leqslant x < x_{i+1}, & \\ 0, \quad x_{i+1} \leqslant x \leqslant x_n, & \end{cases} \quad (99)$$

for $i = 2, 3, \ldots, n-1$;

$$P^5_{1n}(x) = \begin{cases} 0, \quad x_1 \leqslant x < x_{n-1}, & \\ \dfrac{1}{h^3_{n-1}}(x - x_{n-1})^3 (x - x_n) - \dfrac{6}{h_{n-1}} P^5_{2n}(x), & \\ \qquad x_{n-1} \leqslant x \leqslant x_n, & \end{cases} \quad (100)$$

for $i = n$.

The polynomials $P^5_{0i}(x)$ confined by

$$\frac{d^m}{dx^m} P^5_{0i}(x_l) = \delta_{m0}\delta_{il}, \qquad 0 \leqslant m \leqslant 2, \quad (101)$$

take the form of

$$P^5_{01}(x) = \begin{cases} \dfrac{1}{h^3}(x_2 - x)^3 + \dfrac{3}{h_1} P^5_{11}(x), - \dfrac{6}{h^2_1} P^5_{21}(x), & \\ \qquad x_1 \leqslant x < x_2, & \\ 0, \qquad x_2 \leqslant x \leqslant x_n; & \end{cases} \quad (102)$$

for $i = 1$;

$$P^5_{0i}(x) = \begin{cases} 0, \quad x_1 \leqslant x < x_{i-1}, & \\ \dfrac{1}{h^3_{i-1}}(x - x_{i-1})^3 - \dfrac{3}{h_{i-1}} P^5_{1i}(x) - \dfrac{6}{h^2_{i-1}} P^5_{2i}(x), & \\ \qquad x_{i-1} \leqslant x < x_i, & \\ \dfrac{1}{h^3_i}(x_{i+1} - x)^3 + \dfrac{3}{h_i} P^5_{1i}(x) - \dfrac{6}{h^2_i} P^5_{2i}(x), & \\ \qquad x_i \leqslant x < x_{i+1}, & \\ 0, \quad x_{i+1} \leqslant x \leqslant x_n, & \end{cases} \quad (103)$$

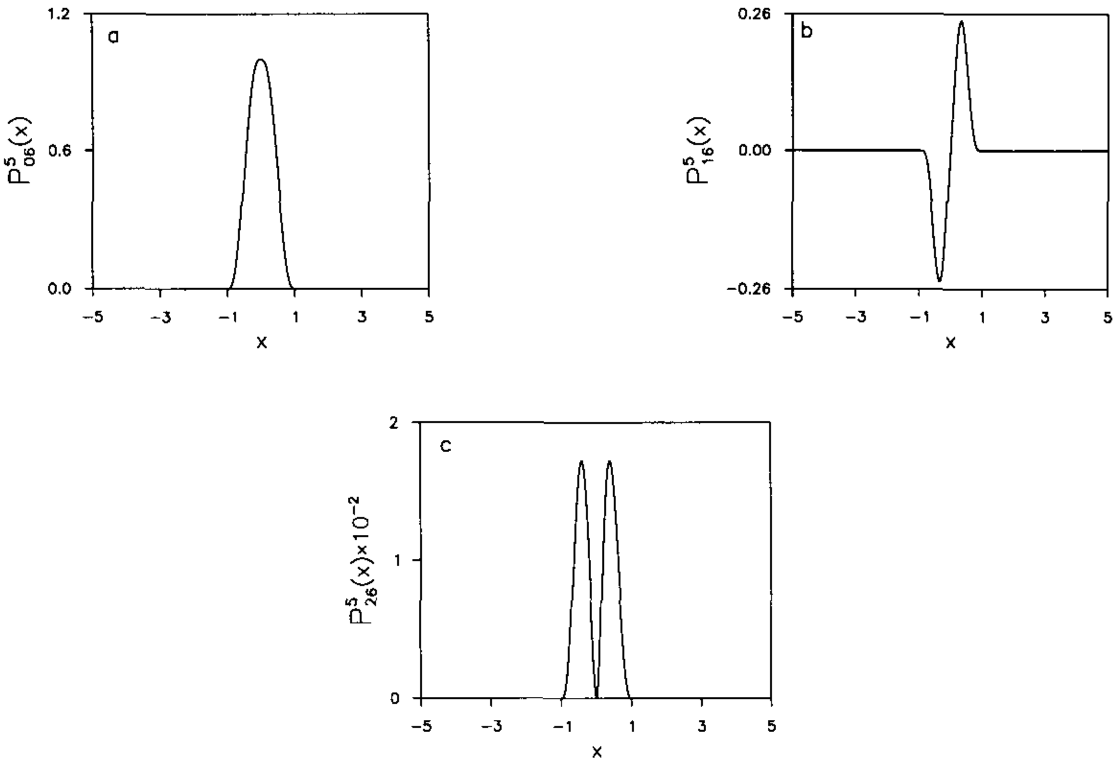

FIG. 5. $P^5_{06}(x)$ (a), $P^5_{16}(x)$ (b), and $P^5_{26}(x)$ (c) versus x are plotted for $n=11$ and $h_i=1$.

for $i=2, 3, ..., n-1$;

$$P^5_{0n}(x)=\begin{cases}0, & x_1\leqslant x<x_{n-1},\\ \dfrac{1}{h^3_{n-1}}(x-x_{n-1})^3-\dfrac{3}{h_{n-1}}P^5_{1n}(x)-\dfrac{6}{h^2_{n-1}}P^5_{2n}(x), & \\ \qquad x_{n-1}\leqslant x\leqslant x_n, & \end{cases} \tag{104}$$

for $i=n$.

$P^5_{06}(x)$ (a), $P^5_{16}(x)$ (b), and $P^5_{26}(x)$ (c) versus x are plotted in Fig. 5 for $n=11$ and $h_i=1$.

REFERENCES

1. W. H. Press, B. P. Flannery, S. A. Teukolsky, and W. T. Vetterling, *Numerical Recipes* (Cambridge Univ. Press, Cambridge, MA, 1986).
2. *User's Manual*, IMSL Math/Library, FORTRAN Subroutine for Mathematical Applications, Vol. 2, Version 1.0, (Inst. Math. Statist., Hayward, CA, 1987), p. 680.
3. G. S. Bales and R. J. Gooding, *Phys. Rev. Lett.* 67, 3412 (1991).
4. B. van Zyl and R. J. Gooding, unpublished.