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STORMER-NUMEROV APPROXIMATION FOR NUMERICAL SOLUTIONS OF ORDINARY AND PARTIAL DIFFERENTIAL EQUATIONS

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Abstract—Stormer-Numerov approximations of high accuracy were developed for solutions of nonlinear boundary value problems and nonlinear elliptic partial differential equations. The approximations can be easily adopted also for parabolic partial differential equations in one and more space dimensions and feature fourth-order accuracy. For boundary value problems only three nodes are necessary to obtain the desired fourth order accuracy. The finite difference formula for parabolic partial differential equations can be readily generalized to a nonequidistant mesh so that automatic regridding in space may be used. The Stomer-Numerov approximations are important for solution of problems where storage limitations and computer time expenditure preclude standard second order methods. Because of the fourth order approximations a low number of mesh points can be used for a majority of chemical engineering problems. The application of Stormer-Numerov approximations is illustrated on a number of examples.

INTRODUCTION

The increased use of computational techniques in studies of dissipative structures has produced a need to develop reliable and efficient algorithms to deal with a coupled set of nonlinear ordinary differential equations (boundary value problem), elliptic and parabolic differential equations. These problems feature steep space gradients so that a great number of grid points must be used to resolve the problem. Frequently we must solve the problems in two (or three) dimensions. The use of standard second order methods is precluded because of enormous number of grid points which are necessary for resolution. It has been demonstrated on simple problems several times that high order finite-difference methods may provide important improvements of codes in terms of diminishing the required number of grid points as well as the computer time for desired resolution.

The present work represents the study of Stormer-Numerov finite difference approximation to determine the feasibility of its use in chemical engineering problems. A comparison of this method with standard second order schema will be also performed.

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GENERAL APPLICATION OF STORMER-NUMEROV APPROXIMATIONS

1. Boundary value problems for ordinary differential equations

So far, several techniques have been proposed for resolution of nonlinear boundary value problems, e.g. shooting, finite-difference methods combined with the Newton-Raphson procedure, invariant imbedding, false transient method, and continuation[1]. Assessing the relative merits of different methods is not an easy task. For a number of difficult nonlinear boundary value problems finite difference methods proved to be a very reliable tool. The ultimate objective of a finite-difference scheme is generation of accurate results using a low number of grid points. Among other things, in this paper, we try to answer the following question: What is the best discretization of the given boundary value problem? What emerges from our investigation is a promising class of methods which make use of three nodes and are of fourth order accuracy.

Consider the boundary value problem

$$ay''+by'-f(x, y)=0 \tag{1a}$$

subject to linear boundary conditions

$$\alpha_0 y(0)+\beta_0 y'(0)=\gamma_0$$

$$\alpha_1 y(1)+\beta_1 y'(1)=\gamma_1 . \tag{1b}$$

Using a padé approximation, we can write [2]

$$y'_n=\left(\frac{D_0}{1+\frac{1}{6}h^2 D_+ D_-}\right) y_n \tag{2}$$

$$y''_n=\left(\frac{D_+ D_-}{1+\frac{1}{12}h^2 D_+ D_-}\right) y_n \tag{3}$$

where D_0, D_+ and D_- are operators which are defined in the following way:

$$D_0 y_n=\frac{1}{2h}(y_{n+1}-y_{n-1}) \tag{4a}$$

$$D_+ y_n=\frac{1}{h}(y_{n+1}-y_n) \tag{4b}$$

$$D_- y_n=\frac{1}{h}(y_n-y_{n-1}) . \tag{4c}$$

In practical calculations, we can set the derivatives y_n and y''_n to F_n and S_n, respectively, i.e.:

$$y'_n=F_n, \quad y''_n=S_n . \tag{5}$$

By substituting Eq. (5) into Eqs. (2) and (3) and after performing the operator operations we have:

$$\frac{1}{6}F_{n+1}+\frac{2}{3}F_n+\frac{1}{6}F_{n-1}=\frac{1}{2h}(y_{n+1}-y_{n-1}) \tag{6}$$

$$\frac{1}{12}S_{n+1}+\frac{5}{6}S_n+\frac{1}{12}S_{n-1}=\frac{1}{h^2}(y_{n+1}-2y_n+y_{n-1}) .$$

$$n=1, \cdots, N \tag{7}$$

Eq. (1) for a nodal point n reads:

$$aS_n+bF_n-f_n=0. \qquad n=0, \cdots, N+1 \tag{8}$$

Evidently Eqs. (6)-(8) represent a (3×3) block tridiagonal system of equations. This set of equations can be simplified after eliminating S_{n+1}, S_n, and S_{n-1} from Eq. (7) by using Eq. (8). The modified Eq. (7) reads:

$$-\frac{1}{12}\frac{b}{a}(F_{n+1}+10F_n+F_{n-1})+\frac{1}{12a}(f_{n+1}+10f_n$$

$$+f_{n-1})=\frac{1}{h^2}(y_{n+1}-2y_n+y_{n-1}), \; n=1, \cdots, N \tag{9}$$

Eq. (6) along with Eq. (9) forms a (2×2) block tridiagonal system. For a special type of Eq. (1), $b=0$, the calculation procedure can be further simplified. Evidently, for this case, we can rewrite Eqs. (7) and (8) in the form:

$$\frac{1}{12a}(f_{n+1}+10f_n+f_{n-1})=\frac{1}{h^2}(y_{n+1}-2y_n+y_{n-1}).$$

$$=1, \cdots, N \tag{10}$$

Eq. (10) is the classic Stormer-Numerov formula which has $0(h^4)$ accuracy [3].

The accuracy of the approximations used can be obtained by a Taylor expansion of Eqs. (6) and (7):

$$F_n-y'_n=-\frac{1}{180}h^4 y^{V} \tag{11a}$$

$$S_n-y''_n=-\frac{1}{240}h^4 y^{VI} . \tag{11b}$$

The Stormer-Numerov formula has $0(h^4)$ accuracy, but only a tridiagonal system of equations must be solved. For a case with constant coefficients, Eq. (1) can be transformed to eliminate the first derivative. Using a substitution

$$y=Y\exp\left(-\frac{b}{2a}x\right) \tag{12a}$$

Eq. (1) yields:

$$Y''=\frac{f}{a}\exp\left(\frac{b}{2a}x\right)+\left(\frac{b}{2a}\right)^2 Y=-g(x,Y) . \tag{12b}$$

This equation does not contain the first derivative and the classic Stormer-Numerov formula can be applied. Let us now discuss the different type of boundary conditions.

1-1. Boundary conditions of the first kind

These conditions result from (1b) for $\beta_0=\beta_1=0$, therefore

$$y(0)=\gamma_0/\alpha_0 \text{ and } y(1)=\gamma_1/\alpha_1 . \tag{13}$$

Eqs. (6)-(8) represent $(3N+2)$ equations for $(3N+4)$ variables $(y_n, n=1, \cdots, N; F_n, S_n, n=0, \cdots, N+1)$. The two missing equations can be easily developed by differentiation of Eq. (6):

$$\frac{1}{6}S_0+\frac{2}{3}S_1+\frac{1}{6}S_2=\frac{1}{2h}(F_2-F_0) \tag{14}$$

$$\frac{1}{6}S_{n-1}+\frac{2}{3}S_n+\frac{1}{6}S_{n+1}=\frac{1}{2h}(F_{n+1}-F_{n-1}) . \tag{15}$$

The resulting set of finite difference equations is described by a band (nine diagonal) matrix with some off-diagonal elements. Using the transformation, Eq. (12a), it is necessary to solve only N equations for N variables Y_i. It should be noticed that this procedure yields very precise values of first derivatives at the boundary, F_0 and F_{N+1}, which are necessary in chemical engineering calculations to evaluate the flux of mass or heat. In the standard $0(h^2)$ procedures, we must calculate the first derivatives from asymmetrical finite-difference formulas which may result in a very inaccurate value.

1-2. Boundary conditions of the second kind

Boundary conditions of the second kind result from (1b) for $\alpha_0=\alpha_1=0$; $\gamma_0=\gamma_1=0$. Eqs. (6)-(8) and (1b)

represent (3N+4) equations for (3N+4) variables (y_n, S_n; $n=0, \cdots, N+1$; F_n, $n=1, \ldots, N$).

1-3. Boundary conditions of the third kind

Boundary conditions (1b) can be rewritten as

$$\alpha_0 y_0 + \beta_0 F_0 = \gamma_0 \tag{16a}$$

$$\alpha_1 y_{N-1} - \beta_1 F_{N+1} = \gamma_1. \tag{16b}$$

Eqs. (6)-(8), (14), (15), (16a) and (16b) represent (3N+6) equations for (3N+6) variables y_n, F_n and S_n ($n=0, \ldots, N+1$).

Boundary conditions for Eq. (12b) were developed by Hildebrandt [3]:

$$\left(1 - h\frac{\alpha_0}{\beta_0}\right) y_0 - y_1 - \frac{h^2}{360}\left(97g_0 + 114g_1 - 39g_2 + 8g_3\right) = -h\frac{\gamma_0}{\beta_0} \tag{17a}$$

$$-y_N + \left(1 - h\frac{\alpha_1}{\beta_1}\right) y_{N-1} - \frac{h^2}{360}\left(8g_{N-2} - 39g_{N-1} + 114g_N + 97g_{N+1}\right) = h\frac{\gamma_1}{\beta_1}. \tag{17b}$$

Evidently the tridiagonal structure of the matrix is violated by the first and last rows. To restore the tridiagonal structure the first three and the last three linearized equations must be pre-solved by elimination. After the elimination procedure, the first and last rows contain only two elements, y_0, y_1, and y_N, y_{N+1}, respectively and the standard Thomas algorithm can be used.

2. Elliptic equations

There are many nonlinear elliptic equations in physics which feature very steep gradients [4] or space structurs [5,6]. Numerical resolution of such problems may represent a very difficult problem. The simplest approach consists in flooding the space by an equidistant dense grid of mesh points using some standard second order approximation. However, even on the fastest computers, the computer time may be enormous. An alternative approach may take advantage of formulas exhibiting high order of accuracy. Difference approximations to the Poisson equation on a square mesh have been extensively studied [7-9]. The 9-point difference approximation to the Poisson equation on a uniform rectangular mesh developed by Kantorovich and Krylov [8] four decades ago proved to be a very important scheme. In our considerations, we are going to deal with an elliptic nonlinear Poisson equation

$$\frac{\partial^2 y}{\partial \xi^2} + \frac{\partial^2 y}{\partial \eta^2} - g(\xi, \eta, y) = 0 \quad (\xi, \eta) \in D = (-1, 1) \times (-1, 1) \tag{18}$$

$$y(\xi, \eta) = c \quad \text{for } (\xi, \eta) \in \partial D. \tag{19}$$

Consider a uniform mesh with the spacing h. Let $y_{i,j} = y(\xi_i, \eta_j)$; $g_{i,j} = g(\xi_i, \eta_j, y_{i,j})$.

For the discretization of the elliptic equation (18) we can construct the $0(h^2)$ and $0(h^4)$ schemes:

$$0(h^2) = \diamondsuit y_{i,j} + h^2 g_{i,j} = 0 \qquad i, j = 1, \cdots, m \tag{20}$$

$$0(h^4) = \frac{1}{6}(4\diamondsuit + \square) y_{i,j} + h^2\left(g_{i,j} + \frac{1}{12}\diamondsuit g_{i,j}\right) = 0, \quad i, j = 1, \cdots, m. \tag{21}$$

Here we have introduced the symbols as follows:

$$\square y_{i,j} = y_{i+1,j+1} + y_{i-1,j-1} - y_{i+1,j-1} + y_{i-1,j-1} - 4y_{i,j} \tag{22}$$

and

$$\diamondsuit y_{i,j} = y_{i,j+1} + y_{i,j-1} + y_{i-1,j} + y_{i-1,j} - 4y_{i,j}. \tag{23}$$

The resulting set of nonlinear sparse algebraic equations can be solved by the Newton-Raphson method. The matrix generated by the 9-point formula is symmetric, block-tridiagonal matrix (each block itself is a tridiagonal matrix), and is irreducible, weakly diagonally dominant and positive difinite [9]. Symmetric block tridiagonal nature of these systems indicates that fast direct methods such as block cyclic reduction, fast Fourier transform and tensor product method [10] can be applied to the 9-point discretization.

3. Parabolic equations

A number of methods exist for numerical solution of parabolic differential equations. Among the vast variety of methods two have been extensively used in chemical engineering practice: (1) Crank-Nicolson technique [11] and (2) orthogonal collocation [12]. These methods work very well for a great deal of simple and smooth parabolic problems. The current requirements for computational fluid dynamics, reaction engineering and biomathematics codes for realistic problems resulted in the impetus for the development and implementation of higher order finite difference techniques. The most difficult problems in dealing with parabolic differential equations are those which destroy a prior error bounds (shock-like wave fronts featuring high curvature) or which are stiff. The former situation occurs for heat and mass transfer problems associated with strong exothermic reaction [13] or diffusion and autocatalytic reaction [14]. These problems can also be stiff. For numerical solution of parabolic partial differential equations, we can also apply the idea of difference formulas of hgih-order accuracy. The procedure which we are going to develop in this section is the Crank-Nicolson technique featuring tridiagonal form and fourth order accuracy.

For the sake of simplicity let us consider a simple quasilinear parabolic equation:

$$\frac{\partial y}{\partial t}=\frac{\partial^2 y}{\partial x^2}+g(x, y). \tag{24}$$

We can write this equation in the form:

$$\frac{\partial^2 y}{\partial x^2}=\frac{\partial y}{\partial t}-g(x, y)=f\left[x, y, \frac{\partial y}{\partial t}\right]. \tag{25}$$

Applying the Stormer-Numerov formula (10) to Eq. (25) we get:

$$y_{n+1}-2y_n+y_{n-1}=\frac{h^2}{12}(f_{n+1}+10f_n+f_{n-1}) \tag{26}$$

or

$$y_{n+1}-2y_n+y_{n-1}=\frac{h^2}{12}\left[\left(\frac{dy_{n+1}}{dt}+10\frac{dy_n}{dt}+\frac{dy_{n-1}}{dt}\right)-(g_{n+1}+10g_n+g_{n-1})\right]. \quad n=1, \cdots, N \tag{27}$$

Evidently, Eq. (27) is the $0(h^4)$ representation of parabolic equations (24). This equation cannot be integrated directly by explicit methods and we must presolve Eq. (27) to get the system in an explicit form. Of course, after presolving this equation the "method of lines" approach can be used [15]. However, we can integrate Eq. (27) by a trapezoidal rule:

$$\frac{1}{2}\left[(y_{n+1}^{j+1}-2y_n^{j+1}+y_{n-1}^{j+1})+(y_{n+1}^{j}-2y_n^{j}+y_{n-1}^{j})\right]$$

$$=\frac{h^2}{12k}\left[y_{n+1}^{j+1}-y_{n+1}^{j}+10y_n^{j+1}-10y_n^{j}+y_{n-1}^{j+1}-y_{n-1}^{j}\right]$$

$$-\frac{h^2}{24}\left[g_{n+1}^{j+1}+10g_n^{j+1}+g_{n-1}^{j+1}+g_{n+1}^{j}+10g_n^{j}+g_{n-1}^{j}\right].$$

$$n=1, \cdots, N \tag{28}$$

We may notice that Eq. (28) is represented by a set of algebraic equations having a tridiagonal structure. This finite-difference approximation is a Crank-Nicolson scheme having $0(h^4, k^2)$ accuracy.

For a 2D-quasilinear parabolic equation

$$\frac{\partial y}{\partial t}=\frac{\partial^2 y}{\partial \xi^2}+\frac{\partial^2 y}{\partial \eta^2}-g(y), \tag{29}$$

the Kantorovich-Krylov formula yields:

$$\frac{1}{6}(4\diamond+\square)y_{nm}+h^2\left[g_{nm}+\frac{1}{12}\diamond g_{nm}\right]=h^2\left[\left(\frac{dy}{dt}\right)_{nm}+\frac{1}{12}\diamond\left(\frac{dy}{dt}\right)_{nm}\right]. \tag{30}$$

Numerical integration of this expression by a trapezoidal formula gives rise to a Crank-Nicolson schema having $0(h^4, h^4, k^2)$ accuracy.

EXAMPLES

In this section the discretization procedures described above will be applied to physical problems. Following type of problems will be considered:

(1) Nonlinear boundary value problem for ordinary differential equations (mass transfer and autocatalytic chemical reaction).

(2) Calculation of limit points (explosion in a 2D system).

(3) Analysis of Hopf bifurcation points (onset of instability in diffusion-reaction systems).

1. Example 1

For a model reaction suggested by Nicolis and Prigogine [16],

$$A\rightarrow X$$
$$B+X\rightarrow Y+D$$
$$2X+Y\rightarrow 3X$$
$$X\rightarrow E$$

following transport equations can be written:

$$D_A\frac{d^2A}{dz^2}=A \tag{31a}$$

$$D_X\frac{d^2X}{dz^2}=(B+1)X-X^2Y-A \tag{31b}$$

$$D_Y\frac{d^2Y}{dz^2}=X^2Y-BX. \tag{31c}$$

Fixed boundary conditions are considered:

$$z=0,\ z=L;\ A=A_0,\ X=X_0,\ Y=Y_0. \tag{31d}$$

Following values of the parameters have been used for calculation:

$$D_A=0.1;\ D_X=0.0016;\ D_Y=0.008$$
$$A_0=2\ ;\ X_0=2;\ Y_0=2.3;\ B=4.6$$
$$L=0.4.$$

For this parameter values seven steady states can be calculated. The profiles of X are drawn in Fig. 1. Three steady states are symmetric, four are asymmetric. The results of calculation are reported in Table 1. The error E presented in this table is defined as:

$$E=\frac{10^4}{N}\sum_{j=1}^{N}|X_j-X_{ref}|.$$

Here N is the number of grid points and X_{ref} is the reference solution. The solution calculated for $h=0.01$ (99 internal points) has been considered as a reference solution. Fig. 2 displays the dependence log E versus

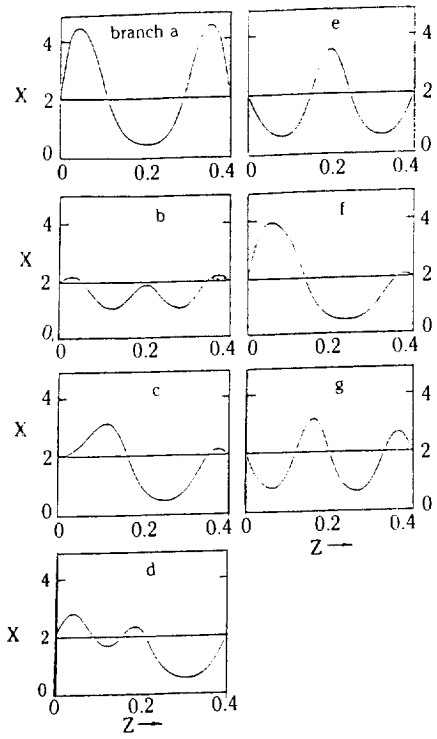

Fig. 1. Multiple solutions of nonlinear boundary value problem given by Eqs. (31a)-(31d).

log h. This figure reveals that the error is $0(h^2)$ and $0(h^4)$ for the standard difference schema and the Stormer-Numerov technique, respectively.

Based on this table we can notice that the Brandt multilevel approach [17] can fail if at the beginning of the calculation a low number of grid points is used. The table reveals that for 5 internal points only the brach a and b can be calculated and either divergence or convergence to these profiles resulted for profiles for branches c, d, e, f, and g. For N = 19 and for $0(h^2)$ schema all profiles can be located. From the table it can be inferred that 24 internal points for $0(h^4)$ scheme yield comparable accuracy with 99 points for $0(h^2)$ procedure. Since the computer time is proportional to N^2, the improvement in the economy of calculation is by at least one order of magnitude. Evidently for two dimensional problems the improvement is higher by more than two order of magnitudes.

2. Example 2

This example should illustrate the possibility of calculation of limit points for nonlinear boundary value problems and elliptic equations. For a system of nonlinear algebraic equations

$$F_i(\delta, u_1, u_2, \cdots, u_N) = 0 \quad i = 1, 2, \cdots, N, \tag{32}$$

a branching point occurs if:

Table 1. Error E versus N

N	Approx.	Branch a	Branch b	Branch c	Branch d	Branch e	Branch f	Branch g
99	$0(h^4)$	R	R	R	R	R	R	R
	$0(h^2)$	13	8	57	10	30	23	33
74	$0(h^4)$	0	0	0	0	0	0	0
	$0(h^2)$	23	14	101	17	53	41	60
49	$0(h^4)$	1	0	2	0	0	1	1
	$0(h^2)$	52	32	228	40	120	93	136
39	$0(h^4)$	3	0	4	1	2	2	3
	$0(h^2)$	83	50	355	63	189	148	214
29	$0(h^4)$	10	2	13	4	6	8	8
	$0(h^2)$	152	90	624	115	338	270	389
24	$0(h^4)$	22	4	28	8	14	16	17
	$0(h^2)$	228	131	896	172	487	396	577
19	$0(h^4)$	60	11	70	22	34	43	45
	$0(h^2)$	389	210	1387	271	766	648	944
14	$0(h^4)$	158	38	233	79	115	175	156
	$0(h^2)$	639	396	NC	551	1374	1436	1852
9	$0(h^4)$	483	204	CP	NC	624	962	717
	$0(h^2)$	826	1112	CP	NC	NC	2567	8182
5	$0(h^4)$	411	2021	CP	NC	NC	NC	NC
	$0(h^2)$	1062	2953	CP	NC	NC	NC	NC

N = number of internal mesh points
R = reference solution
O = a small number <0.5
CP = no convergence after 50 Newton iterations
NC = convergence to a solution that may not be compared with the reference

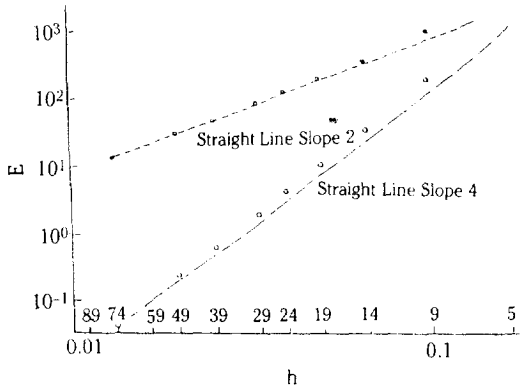

Fig. 2. Log E versus log h on the branch b.

$$F_{N+1}(\delta, u_1, u_2, \cdots, u_N) = \det G(\delta, u_1, u_2, \cdots, u_N) = 0. \quad (33)$$

Here G is the Jacobian matrix with the elements

$$g_{ij} = \frac{\partial F_i(\delta, u_1, \cdots, u_N)}{\partial u_j} \quad i, j = 1, \cdots, N. \quad (34)$$

The branching point can be determined from a simultaneous solution of Eqs. (32) and (33).

(a) Thermal explosion of solid explosives, occurring in a 2D system, is described by a nonlinear elliptic equation

$$\frac{\partial^2 \theta}{\partial x^2} + \frac{\partial^2 \theta}{\partial y^2} = -\delta \exp\theta \quad (35)$$

$$(x, y) \in D = (-1, 1) \times (-1, 1)$$

subject to boundary conditions

$$\theta = 0 \text{ for } (x, y) \in \partial D. \quad (36)$$

For $\delta < \delta^*$ a steady state solution exists while for $\delta > \delta^*$ the equation does not possess a solution. The value $\delta = \delta^*$ is referred to as the critical condition of explosion. It can be easily shown that for $\delta = \delta^*$ a limit point exists.

For discretization the Kantorovich-Krylov 9-point $0(h^4)$ formula has been used. The results of calculation are reported in Table 2.

(b) Exothermic reaction and diffusion occurring in a 1D system is described as a nonlinear boundary value problem.

Table 2. Results for critical conditions for explosion

h	δ^*	
1/2	1.6988	The correct value $\delta^* = 1.702031$
1/4	1.70188	

Table 3. Results for ignition and extinction conditions for a catalytic reaction ($\gamma = 20$, $\beta = 0.4$)

Ignition

h	δ^*	
1/2	0.13726	The correct value $\delta^* = 0.137557$
1/4	0.137540	

Extinction

h	δ^*	
1/2	0.07831	The correct value $\delta^* = 0.0779303$
1/4	0.077912	

$$\frac{d^2 Y}{dx^2} = \delta Y \exp\left(\frac{\gamma\beta(1-Y)}{1-\beta(1-Y)}\right) \quad (37)$$

$$x = \pm 1 \; ; \quad Y = 1. \quad (38)$$

This equation features, two limit points, i.e. extinction and ignition conditions exist. For the discretization the Stormer-Numerov schema has been used. The results are reported in Table 3.

3. Example 3

Transient heat conduction, diffusion and exothermic first order reaction may be described by a set of two parabolic differential equations:

$$L_w \frac{\partial y}{\partial t} = \frac{\partial^2 y}{\partial \xi^2} - \frac{\delta}{\gamma\beta} \exp\left(\frac{\theta}{1+\theta/\gamma}\right) \quad (39)$$

$$\frac{\partial \theta}{\partial t} = \frac{\partial^2 \theta}{\partial \xi^2} + \delta y \exp\left(\frac{\theta}{1+\theta/\gamma}\right) \quad (40)$$

subject to boundary conditions

$$\xi = \pm 1 \; ; \; y = 1, \quad \theta = 0. \quad (41)$$

Here y and θ represent the dimensionless concentration and temperature, respectively. From the mathematical point of view, the onset of oscillations can be characterized by so called Hopf bifurcation. The classical Hopf bifurcation occurs in a smooth automomous system of ordinary differential equations

$$\frac{du}{dt} = f(u, \delta) \quad (42)$$

when the real parameter δ has values near a critical value $\delta = \delta^{**}$ at which an isolated steady state solution u^* loses linear stability by virtue of a complex conjugated pair of eigenvalues of the Jacobian matrix $\Gamma = \{\partial f/\partial u\}_u^*$. At the Hopf bifurcation point the Jacobian matrix has a pair of pure imaginary eigenvalues.

The Stormer-Numerov scheme was used for discretization of parabolic equations (39)-(41). For calculation of the values of the Hopf bifurcation points we used a

Table 4. Hopf bifurcation points for parabolic equations ($\gamma=20$, $\beta=0.2$ $L_w=5.5$)

Mesh size	Approximation	
	$0(h^2)$	$0(h^4)$
1	1.18	1 362
1/2	1.386	1 4403
1/3	1.419	1 44363
1/4	1.430	1 44417
1/5	1.4353	1 44432
1/6	1.4380	1 444366

technique which is described elsewhere [18]. The results of calculation are reported in Table 4. From this table it can be inferred that already one internal point results in two significant digits accuracy. Two internal points for $0(h^4)$ discretization scheme yields better accuracy than 6 internal points for $0(h^2)$ scheme. Evidently, the one-point discretization makes it possible to develop analytical criteria for Hopf bifurcation [4], as a result the discretization by the Stormer-Numerov scheme can successfully compete with the "linearization" [19] and one point collocation [12].

CONCLUSIONS

The application of Stormer-Numerov high order difference approximations has proved to be a very reliable procedure for discretization of many chemical engineering problems described by elliptic or parabolic nonlinear equations. For problems where the profiles are smooth enough we can usually use a low number of points to get accurate results. For elliptic problems featuring boundary layer character it is wise to use nonequidistant mesh. The Stormer-Numerov finite-difference approximations can compete with orthogonal collocation approach both in terms of accuracy and simplicity of programming.

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