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ON THE NUMERICAL SOLUTION OF THE DIFFUSION EQUATION SUBJECT TO THE SPECIFICATION OF MASS

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Abstract

A parallel algorithm is developed for the numerical solution of the diffusion equation $u_t = u_{xx}$, $0 < x < X$, $0 < t < T$, subject to $u(x, 0) = f(x)$, $u_x(X, t) = g(t)$ and the specification of mass $\int_a^b u(x, t)\,dx = M(t)$, $0 < b < X$.

1. Introduction

It is known [2] that because certain chemicals absorb light at various frequencies, the intensity of such light on a photoelectric cell gives an electric signal which is proportional to the total amount of chemical present in the volume through which the light passes. Suppose $u(x, t)$ denotes the concentration of such a chemical which is diffusing in a straight tube with x measured in the direction of the axis of the tube. Then the electric signal produced by a light beam passing through the tube at right angles between $x = 0$ and $x = b$ is proportional to $\int_0^b u(x, t)\,dx$. This integral represents the total mass of the chemical in $0 \le x \le b$ at time t.

This paper considers the problem of obtaining numerical approximations to the concentration $u = u(x, t)$ which satisfies the partial differential equation (PDE)

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \quad 0 < x < X, t > 0, \tag{1}$$

subject to a Neumann time-dependent boundary condition on the boundary $\partial\Omega$ of the open-region Ω defined by the lines $x = 0, x = X$ given by

$$\frac{\partial u(X, t)}{\partial x} = g(t), \quad 0 \le t \le T, \tag{2}$$

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and the specification of mass

$$\int_0^b u(x,t)\,dx = M(t), \quad 0 < b < X, \tag{3}$$

with initial conditions

$$u(x,0) = f(x), \quad 0 < x < X, \tag{4}$$

where f, g and M are known functions and are assumed to be sufficiently smooth to produce a smooth classical solution of u. The existence and uniqueness properties of the solution of this problem are detailed in [1]. A number of sequential numerical procedures have been suggested in the literature for the solution of this problem; see, for instance, [2, 3].

In the present paper, the method of lines semi-discretization approach will be used to transform the model PDE into a system of first-order, linear, ordinary differential equations (ODEs), the solution of which satisfies a certain recurrence relation involving matrix exponential terms. A suitable rational approximant will be used to approximate such exponentials leading to an L_0-stable algorithm which may be parallelized through a partial-fraction splitting technique. These L_0-stable schemes, unlike A_0-stable schemes, are known to be suitable for use in integrating PDEs with time-dependent boundary conditions in which discontinuities between initial conditions and boundary conditions (such as the test problems to be considered in this paper) exist [4, 10, 11].

2. Discretization and recurrence relation

The interval $0 \leq x \leq X$ is divided into $N+1$ subintervals each of width h, so that $(N+1)h = X$ and the time variable t is discretized in steps of length ℓ. Thus at each time level $t = t_n = n\ell$ $(n = 0, 1, 2\ldots)$, the open region $\Omega = [0 < x < X] \times [t > 0]$ and its boundary $\partial\Omega$ consisting of the lines $x = 0$ and $x = X$ and the axis $t = 0$ have been superimposed by a rectangular mesh with N points within Ω and one point along each side of $\partial\Omega$.

The solution $u(x,t)$ of (1) is sought at each point $(kh, n\ell)$ in $\Omega \times [t > 0]$, where $k = 1, 2, \ldots, N$ and $n = 0, 1, 2\ldots$. The solution of an approximating numerical method will be denoted by $U(x,t)$. The space derivatives in (1) and (2) will be replaced by their second-order central-difference approximants given by

$$\frac{\partial^2 u}{\partial x^2} = h^{-2}[u(x-h),t) - 2u(x,t) + u(x+h,t)] + O(h^2) \text{ as } h \to 0 \tag{5}$$

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and

$$\frac{\partial u}{\partial x} = \frac{u(x+h,t) - u(x-h,t)}{2h} + O(h^2) \text{ as } h \to 0, \text{ respectively.} \tag{6}$$

3. Treatment of the non-local boundary condition

The integral in (3) may be approximated using a quadrature rule such as Simpson's rule to give

$$\int_0^b u(x,t)\,dx \approx \frac{h^*}{3}\left[u(0,t) + 4\sum_{i=1}^{\frac{J}{2}} u(2i-1,t) + 2\sum_{i=1}^{\frac{J}{2}-1} u(2i,t) + u(J,t)\right] + O(h^4), \tag{7}$$

in which $h^* = b/J$. Thus, the boundary conditions $u(1,t)$ and $u(0,t)$ may then be determined using (2) with (6) and (3) with (7) respectively.

Applying (1) to all the interior mesh points within Ω at time level $t_n = n\ell$, with the space derivative replaced by (5), leads to a system of N first-order, linear, ordinary differential equations of the form

$$\frac{d\mathbf{U}(t)}{dt} = A\mathbf{U}(t) + \psi(t), \quad t > 0, \mathbf{U}(0) = \mathbf{f}, \tag{8}$$

in which the matrix A is of order N and is given by

$$A = h^{-2}\begin{pmatrix} \alpha_1 & \alpha_2 & \alpha_3 & \cdots \alpha_J & & \mathbf{0} \\ 1 & -2 & 1 & & & \\ & \ddots & \ddots & \ddots & & \\ & & 1 & -2 & 1 & \\ \mathbf{0} & & & & 2 & -2 \end{pmatrix}, \tag{9}$$

where $\alpha_1 = -6$, $\alpha_2 = -1$ and $\alpha_i = \begin{cases} -4 & \text{for } i = 3(2)J-1 \\ -2 & \text{for } i = 4(2)J-2 \\ -1 & \text{for } i = J. \end{cases}$

In (8), the vector $\psi(t)$ arises from the use of the boundary conditions $u(0,t)$ and $u(1,t)$ in (5).

Solving the system of ODEs (8) subject to the initial condition $\mathbf{U}(0) = \mathbf{f}$, gives [11, p. 136],

$$\mathbf{U}(t) = \exp(tA)\mathbf{f} + \int_0^t \exp[(t-s)A]\psi(s)\,ds, \quad t \geq 0, \tag{10}$$

which satisfies the recurrence relation

$$\mathbf{U}(t+\ell) = \exp(\ell A)\mathbf{U}(t) + \int_t^{t+\ell} \exp[(t+\ell-s)A]\psi(s)\,ds, \quad t = 0, \ell, 2\ell, \ldots. \tag{11}$$

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4. The parallel algorithm

The integral in (11) may be approximated by a quadrature formula of the form

$$\int_t^{t+\ell} \exp[(t+\ell-k)A]\psi(k)\,dk \approx W_1\psi(k_1) + W_2\psi(k_2), \quad k_1 \neq k_2, \tag{12}$$

in which the weights $W_1 = W_1(\ell A)$ and $W_2 = W_2(\ell A)$. Following Lawson [7] and Swayne [9], the vector $\psi(k)$ in (12) is successively given the values $\psi(k) \equiv [1, 1, \ldots, 1]^{\mathsf{T}}$ and $\psi(k) \equiv [k, k, \ldots, k]^{\mathsf{T}}$ (with T denoting transpose) to give

$$\begin{aligned} W_1 + W_2 &= Q_1, \\ k_1 W_1 + k_2 W_2 &= Q_2, \end{aligned} \tag{13}$$

in which $Q_1 = Q_1(\ell A) = A^{-1}\exp(\ell A) - A^{-1}$ and $Q_2 = Q_2(\ell A) = A^{-1}[-(t+\ell)I + t\exp(\ell A) - A^{-1} + A^{-1}\exp(\ell A)]$, where I is the identity matrix of order N. Solving (13) for distinct abscissae k_1 and k_2 gives

$$W_1 = \frac{k_2 Q_1 - Q_2}{k_2 - k_1} \quad \text{and} \quad W_2 = \frac{k_1 Q_1 - Q_2}{k_1 - k_2}. \tag{14}$$

Substituting (13) and (14) into (12) and using $k_1 = t$ and $k_2 = t + \ell$ leads to the recurrence relation

$$\begin{aligned} \mathbf{U}(t+\ell) = {} & \exp(\ell A)\mathbf{U}(t) + (\ell A)^{-1}[\ell\exp(\ell A) + A^{-1} - A^{-1}\exp(\ell A)]\psi(t) \\ & + (\ell A)^{-1}[A^{-1}\exp(\ell A) - \ell I - A^{-1}]\psi(t+\ell); \quad t = 0, \ell, 2\ell, \ldots \end{aligned} \tag{15}$$

The development of numerical methods will be based on making appropriate approximations to the exponentials in this recurrence relation. Higher-order Padé approximants [8] are popularly employed (see, for instance, [4, 5, 11]) for such exponentials. Methods based on the use of these approximants are of high accuracy in time and, in the case of the subdiagonal Padés, have good stability properties. However, a major drawback associated with the efficient implementation of these methods is that complex arithmetic is required in the numerical computation. This is because the poles of the higher-order Padés occur in complex conjugate pairs.

In order to circumvent this drawback, a second-order rational approximant given by [4]

$$R(\ell A) \approx \left(I - e\ell A + \left(e - \frac{1}{2}\right)\ell^2 A^2\right)^{-1}[I + (1-e)\ell A], \tag{16}$$

with $e \approx 0.54$, will be used for the matrix exponentials in the recurrence relation (15). A useful feature of $R(\ell A)$ is that its denominator has real distinct poles thus

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guaranteeing the use of real arithmetic (only) in the computation. It is easy to see that the numerical method resulting from the use of (16) in (15) is second-order accurate. Assuming the eigenvalues of the matrix A are real and have negative real parts, a linearised stability analysis of the von Neumann type suggests that the numerical method arising from the use of (16) in (15) is L_0-stable. The merits of these schemes over A_0-stable methods such as the Crank-Nicholson method (arising from the use of the (1, 1) Padé approximant in (18)) and the Peaceman-Rachford method for solving problems with discontinuities between initial conditions and boundary conditions are emphasized in [6].

Using (16) in (15) gives

$$\mathbf{U}(t+\ell) = R(\ell A)\mathbf{U}(t) + \frac{\ell}{2}[S(\ell A)\psi(t) + T(\ell A)\psi(t+\ell)]; \quad t = 0, \ell, 2\ell, \ldots, \tag{17}$$

in which

$$S(\ell A) = \left[I - e\ell A + \left(e - \frac{1}{2}\right)\ell^2 A^2\right]^{-1} \tag{18}$$

and

$$T(\ell A) = \left[I - e\ell A + \left(e - \frac{1}{2}\right)\ell^2 A^2\right]^{-1}\left[I - 2\left(e - \frac{1}{2}\right)\ell A\right]. \tag{19}$$

In order to implement (17) in parallel, the functions$R(\ell A)$, $S(\ell A)$ and $T(\ell A)$ are decomposed into their partial-fraction forms given by

$$R(\ell A) = s_1(I - r_1\ell A)^{-1} + s_2(I - r_2\ell A)^{-1}, \tag{20}$$

$$S(\ell A) = s_3(I - r_1\ell A)^{-1} + s_4(I - r_2\ell A)^{-1}, \tag{21}$$

$$T(\ell A) = s_5(I - r_1\ell A)^{-1} + s_6(I - r_2\ell A)^{-1}, \tag{22}$$

with

$$s_1 = \frac{1 - e + r_1}{r_1 - r_2}, \qquad s_2 = \frac{1 - e + r_2}{r_2 - r_1}, \tag{23}$$

$$s_3 = \frac{r_1}{r_1 - r_2}, \qquad s_4 = \frac{r_2}{r_2 - r_1} \tag{24}$$

and

$$s_5 = \frac{1 - 2e + r_1}{r_1 - r_2}, \qquad s_6 = \frac{1 - 2e + r_2}{r_2 - r_1}, \tag{25}$$

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where

$$r_1 = \frac{2e-1}{e+\sqrt{(e^2-4e+2)}}, \qquad r_2 = \frac{2e-1}{e-\sqrt{(e^2-4e+2)}}. \tag{26}$$

The solution vector $\mathbf{U}(t+\ell)$ in (17) may now be obtained in parallel using two processors running concurrently as follows:

$$\begin{aligned}
\text{Processor 1}: \quad & (I - r_1\ell A)\mathbf{z}_1 = s_1\mathbf{U}(t), \\
& (I - r_1\ell A)\mathbf{z}_3 = s_3\psi(t), \\
& (I - r_1\ell A)\mathbf{z}_5 = s_5\psi(t+\ell), \\
\text{Processor 2}: \quad & (I - r_2\ell A)\mathbf{z}_2 = s_2\mathbf{U}(t), \\
& (I - r_2\ell A)\mathbf{z}_4 = s_4\psi(\mathbf{t}), \\
& (I - r_2\ell A)\mathbf{z}_6 = s_6\psi(\mathbf{t}+\ell), \\
& \text{Then } \mathbf{U}(t+\ell) = \mathbf{z}_1 + \mathbf{z}_2 + \tfrac{\ell}{2}[\mathbf{z}_3 + \mathbf{z}_4 + \mathbf{z}_5 + \mathbf{z}_6].
\end{aligned} \tag{27}$$

This algorithm is denoted by PRL. The intermediate vectors $\mathbf{z}_i (i = 1, \ldots, 6)$ need not be stored once $\mathbf{U}(t+\ell)$ is computed at each time step. The coefficient matrices $(I - r_1\ell A)$ and $(I - r_2\ell A)$ are decomposed into lower and upper (LU) triangular forms only once. These LU products are then "fed" to the two processors in order to compute the intermediate vectors $\mathbf{z}_i (i = 1, \ldots, 6)$ using forward and backward substitutions. In the case of the simple heat equation, $\psi \equiv 0$ and thus $\mathbf{z}_3 = \mathbf{z}_4 = \mathbf{z}_5 = \mathbf{z}_6 = 0$ in (27).

5. Numerical experiments

In order to test the behaviour of the L_0-stable scheme (17), four problems from the literature were considered. Comparisons were made, in terms of accuracy, with the discrete Galerkin (DG) scheme developed in [2] and the finite difference scheme DFD reported in [3].

PROBLEM 1. Following Cannon *et al.* [3], the PDE (1) subject to (2) and (3) with

$$\begin{aligned}
f(x) &= \tfrac{1}{2}x^2, \\
g(t) &= 1, \\
M(t) &= 0.75t + \tfrac{1}{6}(0.75)^3
\end{aligned} \tag{28}$$

and with theoretical solution

$$u(x,t) = \frac{1}{2}x^2 + t \tag{29}$$

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TABLE 1. Relative errors at various time lengths with $h = \ell = 0.0025$.

Time length	DG	DFD	PRL	Theoretical Solution
$t = 0.01$	$1.93E-3$	$2.40E-5$	$1.61E-6$	$4.125E-2$
$t = 0.025$	$9.93E-4$	$1.27E-4$	$8.81E-5$	$5.625E-2$
$t = 0.1$	$1.8E-3$	$4.93E-4$	$8.07E-4$	0.13125

is solved. The absolute relative errors $|(u - U)/u|$ computed at various time lengths with $h = 0.0025$ and time-step $\ell = 0.0025$ are tabulated in Table 1.

PROBLEM 2. Here

$$\begin{aligned} f(x) &= \cos(x), \\ g(t) &= -\exp(-t)\sin(1.0), \\ M(t) &= \exp(-t)\sin(0.75), \end{aligned} \tag{30}$$

with theoretical solutions

$$u(x, t) = \exp(-t)\cos(x). \tag{31}$$

TABLE 2. Relative errors at various time lengths with $h = \ell = 0.0025$.

Time length	DG	DFD	PRL	Theoretical Solution
$t = 0.01$	$8.90E-5$	$2.75E-5$	$3.73E-8$	0.9593
$t = 0.025$	$6.00E-5$	$1.05E-4$	$2.82E-6$	0.9450
$t = 0.1$	$2.81E-4$	$5.27E-4$	$6.29E-5$	0.8767

Table 2 contains the absolute relative errors at various time lengths using $h = \ell = 0.0025$.

PROBLEM 3. In this experiment,

$$\begin{aligned} f(x) &= \sin(\pi x), \\ g(t) &= -\pi \exp(-\pi^2 t), \\ M(t) &= \frac{1}{\pi}\left(\frac{1}{\sqrt{2}} + 1\right)\exp(-\pi^2 t) \end{aligned} \tag{32}$$

and the theoretical solution is

$$u(x, t) = \exp(-\pi^2 t)\sin(\pi x). \tag{33}$$

The computed results at various time lengths with $h = \ell = 0.0025$ are shown in Table 3.

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TABLE 3. Relative errors at various time lengths with $h = \ell = 0.0025$.

Time length	DG	DFD	PRL	Theoretical Solution
$t = 0.01$	$4.00E-6$	$2.44E-5$	$2.95E-6$	0.6407
$t = 0.025$	$3.00E-6$	$1.06E-4$	$2.81E-7$	0.5525
$t = 0.1$	$7.00E-6$	$8.36E-4$	$3.55E-5$	0.2635

PROBLEM 4. Following Cannon *et al.* [3], the effect of time-steps on the numerical method (27) is investigated by solving Problem 3 with three different time-steps, namely $\ell = 0.01$, $\ell = 0.05$, and $\ell = 0.025$. The relative errors at $t = 0.1$ are given in Table 4.

TABLE 4. Relative errors at $t = 0.1$ with $h = 0.0025$ using various time-steps.

Time step	DG	DFD	PRL	Theoretical Solution
$\ell = 0.01$	$1.33E-4$	$1.51E-3$	$3.99E-4$	0.2635
$\ell = 0.05$	$1.63E-2$	$1.13E-4$	$1.28E-2$	0.2635
$\ell = 0.025$	—	$8.36E-4$	$3.55E-5$	0.2635

Clearly, discontinuities between initial conditions and boundary conditions exist in all the four problems. Tables 1 to 4 confirm that the L_0-stable scheme (27) is very accurate and thus that it is suited for solving problems of this nature.

6. Conclusion

An $O(h^2 + \ell^2)$ L_0-stable parallel algorithm has been developed for the simple heat equation with non-local boundary specifications. The algorithm was found to be more accurate in comparison with two existing algorithms from the literature, and may be implemented in parallel using a machine with two processors.

References

[1] J. R. Cannon and J. van der Hoek, "The existence of and a continuous dependence result for the solution of the heat equation subject to the specification of energy", *Suppl. Bolletino Unione Mat. Ital.* **1** (1981) 253–282.

[2] J. R. Cannon, S. P. Esteva and J. van der Hoek, "A Galerkin procedure for the diffusion equation subject to the specification of mass", *SIAM J. Numer. Anal.* **24** (1987) 499–515.

[3] J. R. Cannon, Yanping Lin and Shingmin Wang, "An implicit finite difference scheme for the diffusion equation subject to mass specification", *Int. J. Engng. Sci.* **28** (7) (1990) 573–578.

[4] A. B. Gumel, "Parallel and sequential algorithms for parabolic equations with applications", (PhD Thesis, Brunel University, 1993).

[5] A. B. Gumel, E. H. Twizell and M. A. Arigu, "Parallel L_0-stable methods for multi-dimensional heat equation", *Parallel Algorithms and Applications* **11** (1997) 13–25.

[6] J. D. Lambert, *Numerical methods for ordinary differential systems: The initial-value problem* (John Wiley and Sons, Chichester, 1991).

[7] J. D. Lawson, "Some numerical methods for stiff ordinary and partial differential equations", Second Manitoba Conf. on Numerical Mathematics, Winnipeg, Canada (1972) 27–34.

[8] M. H. Padé, "Sur la répresentation approcheé d'une fonction par des fractions rationelles", *Ann. de l'Ecole Normale Supérieure* **9** (suppl) (1982).

[9] D. A. Swayne, "Time-dependent boundary and interior forcing in locally one-dimensional schemes", *SIAM J. Sci. Stat. Comput.* **8** (1987) 755–767.

[10] E. H. Twizell, *Numerical methods, with applications in the biomedical sciences* (Ellis Horwood, Chichester, and John Wiley, New York, 1988).

[11] E. H. Twizell, A. Q. M. Khaliq and D. A. Voss, "Sequential and parallel algorithms for second-order initial-value problems", WSSIA A **2** (1993) 399–412.