NASA Contractor Report 172539

ICASE REPORT NO. 85-9

ICASE

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Contract No. NAS1-17070
February 1985

INSTITUTE FOR COMPUTER APPLICATIONS IN SCIENCE AND ENGINEERING
NASA Langley Research Center, Hampton, Virginia 23665

Operated by the Universities Space Research Association

National Aeronautics and
Space Administration

Langley Research Center
Hampton, Virginia 23665

SPECTRAL METHODS IN TIME FOR PARABOLIC PROBLEMS

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Abstract

A pseudospectral explicit scheme for solving linear, periodic, parabolic problems is described. It has infinite accuracy both in time and in space. The high accuracy is achieved while the time resolution parameter M ($M = 0(\frac{1}{\Delta t})$ for time marching algorithm) and the space resolution parameter N ($N = 0(\frac{1}{\Delta x})$) have to satisfy $M = 0(N^{1+\varepsilon})$ $\varepsilon > 0$, compared to the common stability condition $M = 0(N^2)$ which has to be satisfied in any explicit finite order time algorthm.

Submitted for publication in the SIAM Journal on Numerical Analysis.

Research was supported in part by the National Aeronautics and Space Administration under NASA Contract No. NAS1-17070 while the author was in residence at the Institute for Computer Applications in Science and Engineering, NASA Langley Research Center, Hampton, VA 23665.

1. Introduction.

In recent years, it has been shown that spectral methods can provide a very useful tool for the solution of time dependent partial differential equations [3]. A standard scheme uses spectral methods to approximate the space derivatives and a finite difference approach to march the solution in time. This tactic results in an unbalanced scheme; it has infinite accuracy in space and finite accuracy in time. It is obvious that the overall accuracy is influenced strongly by the relatively poor approximation of the time derivative. Moreover, using finite order explicit scheme results in a very stringent stability condition. The time step, Δt, has to satisfy

$$\Delta t = O(\frac{1}{N^2}) \tag{1.1}$$

where N is the number of grid points in space. This severe condition is commonly overcome by resorting to implicit schemes. Varga [6], Cody, Meinardus and Varga [2] approached these problems by using Chebychev rational approximations of the evolution operator. Thus, they overcome two drawbacks - low accuracy and stringent stability condition. In fact, the implicit scheme presented in [2], [6] is unconditionally stable, and the error in time decays exponentially.

Implicit algorithms involve inverting matrices. When the space approximation is based on finite differences or finite elements (as in [2], [6]), the related matrices are banded ones (e.g. tridiagonal) which makes them relatively easy to invert. On the other hand, using spectral methods for the space discretization results in full matrices. Inverting these matrices is a time consuming procedure.

In this paper we describe an explicit scheme for the solution of parabolic problems when the space discretization is done by spectral methods. This scheme is highly efficient (its efficiency is equivalent to having a stability condition $\Delta t = O(\frac{1}{N})$) and the error in time decays exponentially. In Section 2 we present a model problem and its fully discrete solution. The new approach for approximating the evolution operator is described in Section 3. In Section 4 we carry out an error and stability analysis. Numerical experiments confirming the theoretical results are presented in Section 5.

2. The Model Problem.

Let us consider the heat equation

$$U_t - GU = 0 \qquad 0 < x < \Pi$$

$$U(x, 0) = U^0(x) \tag{2.1}$$

$$U(0, t) = U(\Pi, t) = 0$$

where G is the spatial operator

$$G = a\frac{\partial^2}{\partial x^2} . \tag{2.2}$$

Discretizing (2.1) in space using pseudospectral Fourier method results in a semidiscrete representation

$$(U_N)_t - G_N U_N = 0$$

$$U_N(x, 0) = U_N^0(x) \tag{2.3}$$

$$U_N(0, t) = U_N(\Pi, t) = 0 .$$

where

$$U_N = P_N U \quad ; \quad G_N = P_N G P_N \quad ; \quad U_N^0 = P_N U^0 \tag{2.4}$$

and where for any function $f(x)$, $P_N f(x)$ is its sine interpolant at the collocation points

$$x_j = j\Pi/N \qquad j = 0, 1, \ldots, N-1 \tag{2.5}$$

or more precisely,

$$P_N f(x) = \sum_{k=0}^{N-1} a_k \sin(kx) \tag{2.6}$$

where

$$a_k = \frac{2}{N} \sum_{j=0}^{N-1} f(x_j)\sin(kx_j) \ . \tag{2.7}$$

G_N is an operator defined on N dimensional subspace; thus it can be represented as a $N \times N$ matrix. The formal solution of (2.3) is

$$U_N(x,t) = \exp(tG_N)U_N^0(x) \tag{2.8}$$

where $\exp(tG_N)$ is the exact evolution operator. A fully discrete solution of (2.1) is achieved by approximating this evolution operator. In [5], it has been shown that any explicit time scheme can be represented as

$$V_N^M = H_M(tG_N)U_N^0 \tag{2.9}$$

where $H_M(z)$ is a polynomial of degree M which converges to e^z in the domain which includes all the eigenvalues of the operator tG_N . V_N^M is the fully discrete solution and $H_M(tG_N)$ is the numerical evolution operator.

3. The Orthogonal Polynomials Scheme.

Let E be the error that results from approximating the evolution operator. Then

$$E = [\exp(tG_N) - H_M(tG_N)]U_N^0 . \tag{3.1}$$

The eigenvectors of the matrix tG_N are $W_1,\ldots,W_N$ where $(W_k)_j = \sin(kx_j)$. Due to the orthogonality of this set of eigenvectors, tG_N is a normal matrix and there is an orthogonal matrix S_N such that

$$E = S_N D_N S_N^{-1} U_N^0 \tag{3.2}$$

where D_N is the diagonal matrix

$$(D_N)_{kk} = e^{\lambda_k t} - H_M(\lambda_k t) \tag{3.3}$$

and $\lambda_k t$ are the eigenvalues of tG_N. Since S_N is orthogonal matrix, we have $||S_N|| = ||S_N^{-1}|| = 1$. Therefore,

$$||E||_{L_2} \leq ||S_N||_{L_2} ||D_N||_{L_2} ||S_N^{-1}||_{L_2} = ||D_N||_{L_2}$$

or

$$||E||_{L_2} \leq \max_{z\in I} |e^z - H_M(z)| \tag{3.4}$$

where I is the domain which includes all the eigenvalues of tG_N. For our case

$$I = [-aN^2t, 0] . \tag{3.5}$$

A standard finite order scheme can be characterized by a polynomial $H_M(z)$ based on a Taylor expansion of e^z. Thus, it has high accuracy only for a small z. The error increases rapidly when z is increased. This property explains the poor accuracy and stringent stability condition mentioned in the introduction.

Let us take, for example, the Modified Euler scheme. The numerical evolution operator is

$$H_M(tG_N) = \left(I + \Delta t G_N + \frac{1}{2}(\Delta t G_N)^2\right)^n \tag{3.6}$$

where

$$\Delta t = t/n . \tag{3.7}$$

Thus

$$H_M(z) = \left(1 + \frac{1}{n} z + \frac{1}{2n^2} z^2\right)^n \qquad (M = 2n) \tag{3.8}$$

and

$$[H_M(z)]^{1/n} = 1 + \frac{1}{n}z + \frac{1}{2n^2} z^2 \tag{3.9}$$

(3.9) is the first three terms of Taylor expansion of $e^{z/n}$. We have

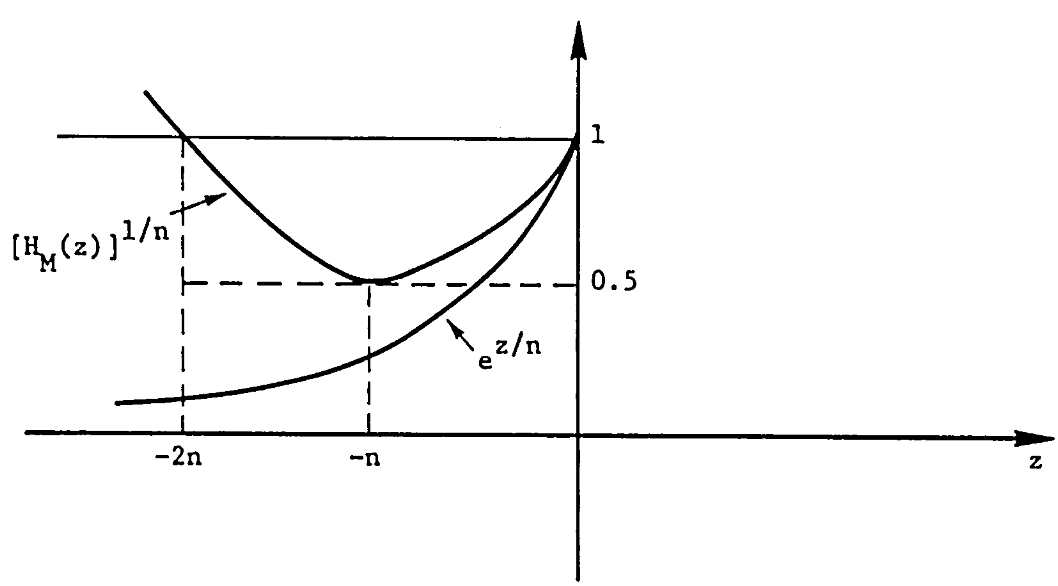

Figure 1

From Figure 1, we find that $H_M(z)$ converges to e^z when

$$-2n \leq z \leq 0 . \tag{3.10}$$

(For accuracy, a more stringent condition is necessary). Using (3.5), (3.7), and (3.10) results in the following stability condition

$$\Delta t \leq \frac{2}{a} \left(\frac{1}{N^2}\right) . \tag{3.11}$$

Expression (3.4) suggests that a uniform approximation of e^z is preferable. Such an approximation is achieved when one uses Chebychev polynomials expansion of the exponential function (see discussion in [5] for hyperbolic problems). Let

$$w = \frac{1}{R}(z + R) \qquad -1 \leq w \leq 1 \tag{3.12}$$

where

$$R = \frac{1}{2} aN^2 t . \tag{3.13}$$

It then follows

$$e^z = e^{-R} e^{Rw} = \sum_{k=0}^{\infty} b_k T_k(w) \tag{3.14}$$

where $T_k(w)$ is the Chebychev polynomial of order k and [1]

$$b_k = e^{-R} c_k \int_{-1}^{1} e^{Rw} T_k(w) (1 - w^2)^{-1/2} dw = e^{-R} c_k I_k(R) \tag{3.15}$$

and also

$$c_k = \begin{cases} 1 & k = 0 \\ 2 & k \geq 1 \end{cases} . \tag{3.16}$$

$I_k(R)$ is the modified Bessel function of order k. Thus, the M degree polynomial approximation of e^z is

$$H_M(z) = \sum_{k=0}^{M} b_k T_k(w(z)) . \tag{3.17}$$

Since (3.12) we substitute the operator F_N defined as

$$F_N = \frac{1}{R} [tG_N + RI] \tag{3.18}$$

for w. $H_M(F_N)$ is the numerical evolution operator. Thus, the fully discrete numerical solution of (2.1) is

$$V_N^M = H_M(F_N) U_N^0 = \sum_{k=0}^{M} b_k T_k(F_N) U_N^0 \tag{3.19}$$

$T_k(F_N) U_N^0$ is computed by using the recurrence relation

$$\begin{aligned} T_k(x) &= 2xT_{k-1}(x) - T_{k-2}(x) \qquad k \geq 2 \\ T_0(x) &= 1 \quad ; \quad T_1(x) = x . \end{aligned} \tag{3.20}$$

Hence

$$\begin{aligned} T_k(F_N) U_N^0 &= 2F_N T_{k-1}(F_N) U_N^0 - T_{k-2}(F_N) U_N^0 \qquad k \geq 2 \\ T_0(F_N) U_N^0 &= U_N^0 \quad : \quad T_1(F_N) U_N^0 = F_N U_N^0 . \end{aligned} \tag{3.21}$$

The algorithm defined by (3.19), (3.21) can be regarded as a three level scheme since it uses the recurrence relation. Therefore, it has the disadvantage of requiring extra memory. There are two possible ways to overcome this drawback. The first one is to convert (3.19) to a power series in F_N and using Horner scheme to compute V_N^M. The disadvantage of this approach is its sensitivity to round-off errors. The second one is based on calculating the roots of $H_M(w)$. Let us assume that the roots are

$$\Theta_1, \ldots, \Theta_M . \tag{3.22}$$

Since the b_k are real, every complex root appears with its conjugate. Rearranging (3.22) is such a way that the first $2p$ roots are p conjugate pairs, we get

$$\mu_1, \bar{\mu}_1, \ldots, \mu_p, \bar{\mu}_p, \mu_{2p+1}, \ldots, \mu_{M-p} . \tag{3.23}$$

Thus

$$H_M(w) = \alpha_0 \prod_{i=1}^{p} (1 - \alpha_i w + \beta_i w^2) \prod_{i=2p+1}^{M-p} (1 - \gamma_i w) \tag{3.24}$$

while

$$\alpha_0 = \sum_{k=0}^{M/2} b_k$$

$$\beta_i = 2R_e\mu_i / |\mu_i|^2 \quad ; \quad \beta_i = 1/|\mu_i|^2 \qquad 1 \leq i \leq p \tag{3.25}$$

$$\gamma_i = 1/\mu_i \qquad\qquad 2p+1 \leq i \leq M - p .$$

Hence we get

$$H_M(F_N) = \alpha_0 \prod_{i=1}^{p} [I - \alpha_i F_N + \beta_i F_N^2] \prod_{i=2p+1}^{M-p} [I - \gamma_i F_N] \, U_N^0 \quad (3.26)$$

Each one of the algorithms described above can be used as a one step method by calculating the solution at the final time t directly from the initial data. It can also be used as a marching scheme if one is interested in intermediate results. The size of the time step Δt depends only on the information one wants to get out of the numerical procedure. Δt enters instead of t in the expressions above, and the parameter R is determined accordingly. In any case, the refinement of the algorithm is done by increasing the degree of the polynomial and not by decreasing the size of the time step.

4. Accuracy and Stability.

Using (3.4), (3.15), and (3.17) we get

$$||E||_{L_2} \leq 2e^{-R} \left| \sum_{k=M+1}^{\infty} I_k(R) T_k(w) \right| \qquad -1 \leq w \leq 1 . \tag{4.1}$$

Since e^{Rw} is an entire function it satisfies the following theorem ([4], pp. 94-96).

Theorem. (S. N. Bernstein): Let $f(w)$ be an entire transcendental function which is real for real w. Then there exists a sequence of integers $n_1, n_2, \ldots$ with $n_\mu \to \infty$ such that the relation

$$\lim_{\mu \to \infty} \frac{E_{n_\mu}(f)}{|\alpha_{n_\mu + 1}|} = 1 \tag{4.2}$$

holds, where α_k are the coefficients in the expansion

$$f(w) = \frac{\alpha_0}{2} + \sum_{k=1}^{\infty} \alpha_k T_k(w) \tag{4.3}$$

and

$$E_n(f) = \left| f(w) - \frac{\alpha_0}{2} - \sum_{k=1}^{n} \alpha_k T_k(w) \right| . \tag{4.4}$$

There is a sequence of integers n_μ , $\mu = 1, 2, \ldots$ of the above type provided

1. $\alpha_{n_\mu + 1} \neq 0 \qquad \mu = 1, 2, \ldots \qquad (4.5)$

and

2. $$\sum_{k=n_\mu+2}^{\infty} |\alpha_k| = O(|\alpha_{n_\mu+1}|) \quad \text{as} \quad \mu \to \infty . \tag{4.6}$$

In our case we can take $n_\mu = \mu$, $\mu = 1, 2, \ldots$ and it follows that

$$||E||_{L_2} \leq 2e^{-R} I_{M+1}(R)\ (1 + O(1)) . \tag{4.7}$$

The asymptotic expansion of $I_k(R)$ is [1]

$$I_k(R) \sim \frac{e^R}{\sqrt{2\pi R}} \{1 - \frac{\mu-1}{8R} + \frac{(\mu-1)(\mu-9)}{2!(8R)^2} - \frac{(\mu-1)(\mu-9)(\mu-25)}{3!(8R)^3} + \ldots\} \tag{4.8}$$

where

$$\mu = 4k^2. \tag{4.9}$$

(4.8) can be written as

$$2e^{-R}\, I_k(R) \sim \sqrt{\frac{2}{\pi R}} \left[1 - \frac{\mu}{8R} + \frac{1}{2!} \left(\frac{\mu}{8R}\right)^2 - \ldots + O\left(\frac{1}{R}\right)\right] \tag{4.10}$$

or

$$2e^{-R}\, I_k(R) \sim \sqrt{\frac{2}{\pi R}} \quad \exp(-\mu/8R) + O\left(R^{-\frac{3}{2}}\right). \tag{4.11}$$

From (4.7), (4.9) and (4.11) we conclude that an ε time accuracy, c.e.

$$||E||_{L_2} \leq \varepsilon \quad , \tag{4.12}$$

is achieved when

$$M = O(R^{1/2}). \tag{4.13}$$

It is clear that satisfying (4.13) guarantees stability. In fact, using (3.1), (4.12) we get

$$||\exp(tG_N) - H_M(tG_N)|| \leq \varepsilon ; \tag{4.14}$$

hence

$$||H_M(tG_N)|| \leq ||\exp(tG_N)|| + \varepsilon. \tag{4.15}$$

Since $\exp(tG_N)$ is a stable operator [3], $H_M(tG_N)$ is stable as well.

R is equal to $aN^2t/2$; thus from (4.13) we can conclude the main result of this analysis: In order to achieve ε time accurate, stable solution of (2.3), M has to satisfy

$$M = O(N). \tag{4.16}$$

A similar analysis for any finite order scheme based on Taylor expansion of e^z will imply that M $[M = O(\frac{1}{\Delta t})$, see (3.7) - (3.8)] has to be proportional to N^2; thus the advantage of the orthogonal polynomials approach is obvious.

Algorithm Refinement.

From (3.13), (4.7), (4.9), and (4.11) we get

$$E \approx \frac{2}{N} \left(\frac{1}{a\pi t}\right)^{1/2} \exp\left(-(M/N)^2/at\right). \tag{4.17}$$

Expression (4.17) suggests that refinement of the algorithm while

$$M = N^{\alpha} \qquad (\alpha > 1) \tag{4.18}$$

will yield an exponential decay of the error. The accuracy thus achieved is the desired spectral accuracy.

5. Numerical Results.

Table 1 presents the stability properties of the O. P. S. (Orthogonal Polynomial Scheme) compared to modified Euler scheme which is second order in time. We have used the model problem (2.1) with $a = 1$, and initial data

$$U^0(x) = \sin(3x). \tag{5.1}$$

The solution is computed at $t = 1$.

Table 1

N	Modified Euler M	O. P. S. M
16	48	24
32	192	48
64	768	96

N - Number of grid points.
M - The degree of the evolution operator.

M indicates the minimal number of applications of the operator tG_N one has to use in order to achieve stable (meaningful) results.

The second table clarifies the spectral convergence of the O.P.S. scheme. (We included in this table the results for the Modified Euler scheme as well, for the sake of comparison.) The problem solved is

$$\begin{aligned} &U_t - U_{xx} = 0 \\ &U^0(x) = x(x - 2\pi) \end{aligned} \qquad 0 \leq x \leq 2\pi . \qquad (5.2)$$

Note that the periodic continuation of $U^0(x)$ belongs to C^0; thus the Fourier coefficients of $U^0(x)$ are decaying slowly. The solution is computed at $t = 1$.

Table 2

N	Modified Euler			O. P. S.		
	M	L_2 Error	Ratio	M	L_2 Error	Ratio
16	62	.3791-04		26	.1026-04	
			17,4			92
32	250	.2126-05		61	.1107-06	
			16.2			134
64	1000	.1339-06		140	.8263-09	

The refinement of the Modified Euler scheme is done while M satisfies

$$M = 0.97 \times (N/2)^2 .$$

For the O. P. S. algorithm, M satisfies

$$M = 2.5 \times (N/2)^{1.2} .$$

The increasing ratio between the L_2-errors of two successive refinements verifies the spectral convergence of the O. P. S. algorithm.

In Table 3 we compare the O. P. S. to the modified Euler scheme from the point of view of the amount of work needed to achieve a certain degree of accuracy. The problem solved is $U_t - U_{xx} = 0$ with $U^0(x) = \sin(3x)$. The L_2-Error is computed at the time level $t = 1$, and the space resolution is $N = 32$.

Table 3

L_2 Error	M (Modified Euler)	M (O. P. S.)
1.3 10^{-2}	200	50
1.3 10^{-4}	2000	60
1.3 10^{-6}	20000	70

6. Conclusion.

The algorithm presented in this paper achieves the goal of spectral accuracy in time and space for the simple model problem (2.1). We believe that this approach can be useful for more complicated problems. In fact the scheme described in Section 3 is applicable whenever one can represent the solution as $\exp(tG_N)U_N$ and the eigenvalues of tG_N are grouped close to the real axis.

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1. Report No. NASA CR-172539 ICASE Report No. 85-9	2. Government Accession No.	3. Recipient's Catalog No
4. Title and Subtitle: Spectral Methods in Time for Parabolic Problems		5. Report Date: February 1985
		6. Performing Organization Code
7. Author(s): Hillel Tal-Ezer		8. Performing Organization Report No.: 85-9
9. Performing Organization Name and Address: Institute for Computer Applications in Science and Engineering, Mail Stop 132C, NASA Langley Research Center, Hampton, VA 23665		10. Work Unit No.
		11. Contract or Grant No.: NAS1-17070
12. Sponsoring Agency Name and Address: National Aeronautics and Space Administration, Washington, D.C. 20546		13. Type of Report and Period Covered: Contractor Report
		14. Sponsoring Agency Code: 505-31-83-01

15. Supplementary Notes

Langley Technical Monitor: J. C. South, Jr.
Final Report

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17. Key Words (Suggested by Author(s)): spectral methods; parabolic equations	18. Distribution Statement: 64 - Numerical Analysis; Unclassified - Unlimited

19. Security Classif. (of this report): Unclassified	20. Security Classif. (of this page): Unclassified	21. No. of Pages: 20	22. Price: A02

For sale by the National Technical Information Service, Springfield, Virginia 22161

NASA-Langley, 1985