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A GOOD SPATIAL DISCRETISATION IN THE METHOD OF LIN

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ABSTRACT

In this paper, a method of lines is proposed for solving partial differential equations. A suitable spatial discretisation is introduced, then the numerical examples show that the method of lines is feasible and very effective for solving parabolic problems.

INTRODUCTION

The method of lines, MOL, is an approach to the numerical solution of quite general partial differential equations, PDE's , that involve a time variable *t* and one or more space variable x,y,... .The partial derivatives with respect to the space variables

are discretized to result in an approximating system of ODE's in the variable *t* . Two of the factors influencing the performance of the

method of lines are the choice of a spatial discretisation method and the positioning of the spatial discretization points.
The points should be chosen so that the computed solution accurately models the exact solution to the PDE . Once the spatial mesh has been chosen, it is desirable to integrate the ordinary differential equation ODE system in time. With just sufficient accuracy ,so that the temporal error does not significantly corrupt the spatial accuracy.

The purpose of this paper is to present a good spatial discretization method with diverse number of points, which introduce more accuracy when applied method of lines to solve PDE's as illustrated in section 4.This paper is structured in the following way. in section 2 new derivation of analytical form *for* approximation the spatial derivative was presented. This allows the main contribution of the paper to be given in section 3 where this approximation was used in solving PDE's by the method of lines. Finally, in section 4 discussion of the numerical experiments is presented.

DERIVATION OF ANALYTICAL APPROXIMATIONS FOR FUNCTIONS

We turn now to the production of analytical approximations *for* functions defined explicitly, that is, in closed form. Such functions may include polynomials, infinite (Taylor's) series in powers of x, rational functions, and so on . We consider the function *f(x)* defined in 0 s x S 1 ,the analytical series is given by

$$f(x) = \sum_{1=0}^{n} a_i(x)\, y_i \qquad (1)$$

In numerical practice we cannot use the infinite series, and we rely on a finite approximation of suitable accuracy.

This is obtained most obviously by truncating the series (1) at a suitable point, giving the polynomial

$$f(x) = \sum_{1=0}^{n} a_i(x) y_i \qquad (2)$$

where $0 \le x \le mh$, $m=2,4,6,\ldots\ldots\ldots$ *and we consider* $y(x) \in C^m$

If we approximate $y(x)$ by constant, linear function, second order polynomial, and so *on* , to the m order polynomial, this leads to m + I equations in $m + 1$ unknowns.

We can solve the resulting system analytically to obtain a_i as terms of x variable, and this present-an approximate to the function f(x) . If we want to approximate the first derivative of $f(x)$ we differentiate the result, and similarly to the higher derivative of $f(x)$. The resulting of our computing presents in the following tables:

i-By using three points:

$$y(x) = \sum_{i=0}^{2} a_i(x) y_i, \quad 0 \le x \le 2h, y(x) \in c^2, let\ z = \frac{x}{h}, then$$

$$a_0 = 1 - \frac{3}{2} z + \frac{1}{2} z^2$$

$$a_1 = 2z - z^2$$

$$a_2 = \frac{-1}{2} z + \frac{1}{2} z^2$$

thus, the approximate for the first derivative:

a'_0	a'_1	a'_2
-3	4	-1
-1	0	1
1	-4	3

where $a'i$, $i = 0,1,2$ factored by $\frac{1}{2ih^i}$. For the second derivative

a''_0	$a''1$	a''_2
-3	4	-1

where $a''i$, $I = 0,1;2$ factored by $\frac{1}{2ih^i}$

ii-By using five points:

$$y(x) = \sum_{i=0}^{4} a_i(x) y_i \,,\quad 0 \le x \le 4h, y(x) \in c^4 \quad then$$

$$a_0 = 1 - \frac{25}{12}z + \frac{35}{24}z^2 - \frac{5}{12}z^3 + \frac{1}{6}z^4$$

$$a_1 = 4z - \frac{13}{3}z^2 + \frac{3}{2}z^3 - \frac{1}{6}z^4$$

$$a_2 = -3z + \frac{19}{4}z^2 - 2z^3 + \frac{1}{4}z^4$$

$$a_3 = \frac{4}{3}z + \frac{7}{3}z^2 + \frac{7}{6}z^3 - \frac{1}{6}z^4$$

$$a_4 = \frac{-1}{4}z + \frac{11}{24}z^2 - \frac{1}{4}z^3 + \frac{1}{24}z^4$$

Thus we can compute the first, second, third ,and fourth derivative as follows :

the approximate for the first derivative

a'_0	a'_1	a'_2	a'_3	a'_4
-25	48	-36	16	-3
-3	-10	18	-6	1
1	-8	0	8	-1
-1	6	-18	10	3
3	-16	36	-48	25

The approximate for the second derivative

a''_0	a''_1	a''_2	a''_3	a''_4
35	- 104	114	- 56	11
11	- 20	6	4	- 1
- 1	16	- 30	16	- 1
- 1	4	6	- 20	11
11	- 56	114	- 104	35

The approximate for the third derivative

a'''_0	a'''_1	a'''_2	a'''_3	a'''_4
- 5	18	- 24	14	- 3
- 3	10	- 12	6	- 1
- 1	2	0	- 2	1
1	- 6	12	- 10	3
3	- 14	24	18	5

The approximate for the fourth derivative

a''''_0	a''''_1	a''''_2	a''''_3	a''''_4
1	- 4	6	- 4	1

iii.- By using seven points :

$$a_0 = 1 - \frac{49}{20}z + \frac{812}{360}z^2 - \frac{49}{48}z^3 + \frac{35}{144}z^4 - \frac{7}{240}z^5 + \frac{1}{720}z^6$$

$$a_1 = 6z - \frac{87}{10}z^2 + \frac{29}{6}z^3 - \frac{31}{24}z^4 - \frac{1}{6}z^5 - \frac{1}{120}z^6$$

$$a_2 = -\frac{15}{3}z - \frac{117}{8}z^2 + \frac{461}{48}z^3 - \frac{137}{48}z^4 - \frac{19}{48}z^5 - \frac{1}{48}z^6$$

$$a_3 = \frac{20}{3}z - \frac{127}{9}z^2 + \frac{31}{3}z^3 + \frac{121}{36}z^4 - \frac{1}{2}z^5 - \frac{1}{36}z^6$$

$$a_4 = -\frac{15}{4}z + \frac{33}{4}z^2 - \frac{307}{48}z^3 + \frac{107}{48}z^4 - \frac{17}{48}z^5 + \frac{1}{48}z^6$$

$$a_5 = \frac{6}{5}z - \frac{27}{10}z^2 + \frac{13}{6}z^3 - \frac{19}{24}z^4 + \frac{2}{15}z^5 - \frac{1}{120}z^6$$

$$a_6 = -\frac{1}{6}z + \frac{137}{360}z^2 - \frac{5}{16}z^3 + \frac{17}{144}z^4 - \frac{1}{48}z^5 + \frac{1}{720}z^6$$

And from this system we can compute an approximate to the first, second, third,
fourth, 5^{th} and 6^{th} derivatives as follow

a_0'	a_1'	a_2'	a_3'	a_4'	a_5'	a_6'
-1764	4320	-5400	4800	-2700	864	-120
-120	-924	1800	-1200	600	-180	24
24	-288	-420	960	-360	96	-12
-12	108	-540	0	540	-108	12
12	-96	360	-960	420	288	-24
-24	180	-600	1200	-1800	924	120
120	-864	2700	-4800	5400	-4320	1764

The approximate for the second derivative

a_0''	a_1''	a_2''	a_3''	a_4''	a_5''	a_6''
3248	-12528	21060	-20320	11880	-3888	548
548	-5880	-1020	1880	-1140	372	-52
-52	912	-1680	800	60	-48	8
8	-108	1080	-1960	1080	-108	8
8	-48	60	800	-1680	912	-52
-52	372	-1140	1880	-1020	-588	548
548	-388	11880	-20320	21060	-12528	3248

The approximate for third derivative

a_0'''	a_1'''	a_2'''	a_3'''	a_4'''	a_5'''	a_6'''
-4410	20880	-41490	44640	-27630	9360	-1350
-1350	5040	-7470	5760	-2610	720	-90
-90	-720	3150	-4320	2610	-720	90
90	-720	1170	0	-1170	720	-90
- 90	720	- 2610	4320	-3150	720	90
90	- 720	2610	- 5760	7470	- 5040	1350
1350	- 9360	27630	- 44640	41490	- 20880	4410

The approximate for the fourth derivative

$a_0^{(4)}$	$a_1^{(4)}$	$a_2^{(4)}$	$a_3^{(4)}$	$a_4^{(4)}$	$a_5^{(4)}$	$a_6^{(4)}$
4200	-22320	49320	- 58080	38520	- 13680	2040
2040	-10080	20520	-22080	13320	-4320	600
600	- 2160	2520	- 480	-1080	720	-120
- 120	1440	- 4680	6720	- 4680	1440	- 120
- 120	720	- 1080	- 480	2520	- 2160	600
600	- 4320	13320	- 22080	20520	- 10080	2040
2040	-13680	38520	-58080	49320	-22320	4200

The approximate for the 5th derivative

$a_0^{(5)}$	$a_1^{(5)}$	$a_2^{(5)}$	$a_3^{(5)}$	$a_4^{(5)}$	$a_5^{(5)}$	$a_6^{(5)}$
- 2520	14400	- 34200	43200	- 30600	11520	- 1800
- 1800	10080	- 23400	28800	- 19800	7200	- 1080
- 1080	5760	- 12600	14400	-9000	2880	- 360
- 360	1440	- 1800	0	1800	- 1440	360
360	- 2880	9000	- 14400	12600	- 5760	1080
1080	- 7200	19800	- 28800	23400	- 10080	1800
1800	- 11520	30600	- 43200	34200	- 14400	2520

The approximate for the derivative

$a_0^{(6)}$	$a_1^{(6)}$	$a_2^{(6)}$	$a_3^{(6)}$	$a_4^{(6)}$	$a_5^{(6)}$	$a_6^{(6)}$
720	-4320	10800	14400	10800	-4320	720

Where a_i' , a_i'' , a_i''' , a_i'''' , $a_i^{(5)}$, $a_i^{(6)}$, i= 1,2,3,4,5,6 factored by $\frac{1}{6!h}$

iv-By using eleven points:

We cannot use the 11-point formulas naturally in all numerical MOL applications. If we could be assured that the spatial variation of the POE will always be a polynomial, this would be logical But in general, this will not be the case .Also all of the preceding approximations for the derivative are based on polynomials. However, polynomials of increasing order have derivatives with an increasing number of roots.

For example ,the fourth-order polynomial, which is the basis of table (1), differentiates once to a third order polynomial that has three roots; at each of these three roots, the polynomial will therefore have a maximum or a minimum, suggesting that it can oscillate between three maximum and minimum values. Similarly ,a tenth- order polynomial will have nine maxima and minima, and it will in general oscillate between these nine values. in other words, as the order of the approximating polynomial increases, the possibility of unrealistic oscillation in the numerical method of lines solution of PDE also increases, and this is frequently observed. Schiesser [4] concluded that the fourth-order formulas of table (1) are good compromise between accuracy, and the minimization of oscillation. Other approximations can be used that might be better behaved (not have the oscillation of polynomials) .

In fact, essentially any approximation can be considered for the PDE spatial derivatives, and some approximations will generally be found to be better than others. Thus, the numerical method of lines is really open-ended, and can be implemented in many ways. Commonly used approximations for PDE spatial derivatives include splines, finite elements, and weighted residual methods. We could obviously devote much more discussion to the development of spatial derivatives approximations, but in order to keep the discussion to reasonable length, we shall consider a few other selected polynomial approximations that have been useful in the solution of a range of PDE problems.

Method of Lines Approximations

To illustrate MOL approximations, we consider the problem discussed by Hicks and Wei[2] :

$$\frac{\partial^2 y}{\partial x^2} = \frac{\partial y}{\partial t} \qquad (1)$$

with approximate reduction of y, x and t to dimensionless variables, eq. (1) describes diffusion or heat conduction in a slab. With proper definition of y, (1) also describes the same phenomena in a sphere, if the effects are radial only. Without loss of generality, then, discussion is limited to eq. (1) in the region $-1 \le x \le 1$. Boundary conditions are:

$$y(-1,t) = a \qquad t \ge 0$$

$$y(1,t) = b \qquad t \ge 0 \qquad (2)$$

$$y(x,0) = 0 \qquad -1 < x < 1$$

It is convenient to restate the problem as follows:

Let y = u + [(b - a) /2]x + (a + b) / 2 ; then (1) becomes:

$$\frac{\partial^2 u}{\partial x^2} = \frac{\partial u}{\partial t} \qquad (1)'$$

And (2) become:

$$u(-1,t) = 0 \qquad , t \ge 0$$

$$u(1,t) = 0 \qquad , t > 0 \qquad (2)'$$

$$u(x,0) = \frac{(b-a)}{2} \times - \frac{(a+b)}{2} \qquad , -1 < x < 1$$

by discretizing (1)′ with respect to *x* , the following system of ordinary differential equations is obtained

$$\frac{du}{dt} = \sum a_{ji} u_i \qquad (3)$$

where we often consider $\sum a_{ji}u_i$ as a finite difference approximation to $\frac{\partial^2 u}{\partial x^2}=\frac{\partial u}{\partial t}$

In dealing with, for example," 5" point central difference approximations to the second

partial derivative, Fisher[1] proposed that, at the end points, where $u_N, \frac{du_N}{dt}, \frac{d^2u_N}{dt^2}$ all equal zero. This assumption leads to the requirement that $u_{N+1}=-u_{N-1}$ and $u_{-(N+1)}=-u_{-(N-1)}$. All equally spaced central difference approximations to the second derivative are symmetric in the values of the coefficients of the u_j about the central point.

In [2] Hicks and Wei mentioned that; the use of a central difference approximation of order greater than "3" point requires explicit specification of dependent variable values outside of the interval of interest (-1,1) , and they consider the use of non central difference approximations. The well known second order finite difference

Approximation for the first derivative $\frac{du(x_i)}{dx}$ is given by the equation

$$\frac{du(x_i)}{dx}=\frac{u(x_{i+1})-u(x_{i-1})}{2\Delta x+O(\Delta x^2)} \tag{4}$$

and this equation can be applied over spatial grid at points i = 2,3,4,... , N - 1

However, a problem occurs at the end points i = 1 and i = N , equation(3) requires $u(x_{N+1})$ which is also non existent. Schiesser [4] developed an approximation for $\dfrac{du(x_i)}{dx}$ that requires the use of the points $u(x_1)$, $u(x_2)$ and $u(x_3)$

Similarly, he developed an approximation $\dfrac{du(x_N)}{dx}$ He gave "3" points formula and" 5" points formula, indicate to "9" points formula and" 11" points formula for first and second derivatives. Here we complete his work in "7" points formula and introduce the derivative up to m order.

As known any stable, convergent numerical algorithm applied to solve the system of ordinary differential equations by MOL will then also produce a stable, convergent numerical solutions of the equations, and consequently produce a stable, convergent numerical solutions of the associated partial differential equation.

Whither or not the use of higher order approximations will improve convergence depends on the improve of the higher eigenvalues. As the number of points "n" used to approximate $\dfrac{\partial^2 u}{\partial x^2}$ is increased (keeping N , the measure of number of divisions of the x interval, constant), the eigenvalues of the approximating system of ordinary differential equation must be all real and negative. Equations (3) for a "3" point centeral difference are in matrix form

$$\frac{1}{h^2}\begin{bmatrix} -2 & 1 & 0 & 0 & \dots & 0 & 0 \\ 1 & -2 & 1 & 0 & \dots & 0 & 0 \\ 0 & 1 & -2 & 0 & \dots & 0 & 0 \\ . & . & . & . & \dots & . & . \\ . & . & . & . & \dots & . & . \\ . & . & . & . & \dots & . & 1 \\ 0 & . & . & . & \dots & 1 & -2 \end{bmatrix}\begin{bmatrix} u_{N-1} \\ \\ . \\ . \\ . \\ . \\ u_{-(N-1)} \end{bmatrix} = \begin{bmatrix} \dfrac{du_{N-1}}{dt}. \\ . \\ . \\ . \\ \dfrac{du_{-(N-1)}}{dt} \end{bmatrix}$$

Or
$$\frac{1}{h^2} A_3\, u = \frac{d}{dt} u$$

where $h = \dfrac{1}{N}$ then:

$$u = \sum_{k=1}^{2N-1} c_k\, E_k \exp\left(\frac{\lambda_k t}{h^2}\right)$$

where λ_k are the eigenvalues of A_3 , E_k are eigenvectors of A_3 and C_k are the Fourier coefficients of (2)' .
The eigenvalues of A_3 are given by :

$$\lambda_k = -2 + 2\cos\frac{k\pi}{2N} \quad , \; k = 1,2,\ldots,2N-1$$

Now, as in [2] , we can show, by direct calculation (for 11 = 5,7,9,11) , that the recursion formula:

$$A_n = (-1)^{\frac{(n+1)}{2}} \left[\left(\frac{n-3}{2}\right)! \right]^2 A_3^{\frac{n-1}{2}} + (n-1)(n-2) A_{n-2} \qquad (5)$$

hold.
The significance of (5) is that each of the matrices, A_n , is a polynomial in A_3 ,and therefore ,commutes with A_3 ,which implies that A_n has the same eigenvectors as A_3 Now the eigenvalues of A_3 are all real and negative. Formula (5) can also be used to compute the eigenvalues of A_n , which are always real and negative, and which approach the eigenvalues of (1) with increasing *N,* as shown by Fisher [1] .

Hence, the formulas which introduced ,in section (2) give stable, convergent numerical solution of equation (1)' basis on the recursion formula (5) .

4. Computer Experimentation:

Simple example of the use of this method is given in schiesser [4], the testing that was carried out developing the method had been shown in tables with (3,5,7) points formulas on parabolic problems. Similarly we can apply the same method on elliptic problems. Detailed results of tests on the hyperbolic problems are given in [3]

Problem(I): Consider the special case of Heat conduction equations:

$$u_t = u_{xx} \qquad (1)$$

$$u(x,0) = \sin(\frac{\pi x}{L})$$

$$u(o,t) = u(1,t) = 0 \qquad (2)$$

where exact solution for this problem is

$$u(x,t) = e^{-(\pi^2/L^2)t}\sin(\pi x/L)$$

For $L = 1, 0 \le t \le 0.5$, $0 \le x \le 1, N = 51$, $h = \frac{1}{50}$, the output from Matlab programs is in table (I)

t	x	MOL3	MOL5	MOL7	Exact
0.1	0.1	0.1152	0.1840	0.2238	0.1152
	0.2	0.2191	0.2699	0.3030	0.2191
	0.3	0.3017	0.3395	0.3624	0.3015
	0.4	0.3545	0.3848	0.4042	0.3015
	0.5	0.3729	0.4006	0.4177	0.3727

Table(I) : MOL solution of equations (1),(2) using (3,5,7) points for spatial approximation

Problem(2):

$$u_t = u_{xx}$$

$$u(x,0) = 1 \qquad ,0 \le x \le 1$$

$$\frac{\partial u}{\partial x} = u \qquad at \qquad x = 0 \text{ for all } t$$

$$\frac{\partial u}{\partial x} = -u \qquad at \qquad x = 1 \text{ for all}$$

with $N = 51$ *and* $0 \le t \le 0.01$, **we listed the results in table II**

For L = 1 , $0 \le t \le 0.5$, $0 \le x \le 1$, $N = 51$, $h = \frac{1}{50}$,

the out put from Matlab programs is in table (II)

t	x	MOL3	MOL5	MOL7	Exact
0.0025	0.1	0.8289	1.0000	1.0003	0.9951
	0.2	0.9945	1.0004	1.0001	0.9999
	0.3	1.0000	1.0002	0.9999	1.0000
	0.4	1.0000	1.0000	1.0001	1.0000
	0.5	1.0000	1.0000	1.0000	1.0000

Table(II)

CONCLUSIONS:

From the example problems, it appears that the spatial approximation will give best result to any problem which can be solved using method of line if we used the 3point formula. These results indicate that the increasing of the points of the formula, cannot bring the MOL and exact solutions into closer agreement. Although this is logically theoretically. The previous results conformed on parabolic problems , but not necessary conformed on Hyperbolic or elliptic problems, where the

Hyperbolic problems were sensitive by the increasing of the points of formula. However, the previous tables in section 2 are too useful. tool for many kind of problems which based on approximate function or derivatives.

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الملخص العربي

في هذا البحث ، قدمنا حل المعادلات التفاضلية الجزئية بطريقة الخطوط باعتبار عدة اختيارات مناسبة لنقاض التجزئة وقد قمنا بتطبيق تلك التجزئة المكانية على أمثلة عددية من النوع المكافئ أثبتت فعالية هذا الحل