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A Research on the Numerical Solution of Partial Differential Equations Using Matrix Theory

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Abstract – The study commences with a description and classification of partial differential equations and the related matrix and eigenvalue theory. Almost in all cases the study of parabolic equations leads to initial boundary value problems and it is to this problem that the study is mainly concerned with. This paper will focus on basic (finite difference) methods to solve a (parabolic) partial differential equation. Within the text, it is included various references to distinct detailed reviews that are related to research field in this area.

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1.1 INTRODUCTION

The majority of the problems of physics and engineering fall naturally into one of three *physical* categories: *equilibrium problems, eigen value problems* and *propagation problems.* Equilibrium problems are problems of steady state in which the equilibrium configurations in a certain domain to be determined. Eigenvalue problems may be thought of as extension of equilibrium problems wherein critical values of certain parameters are to be determined in addition to the corresponding steady-state configurations. Propagation problems are initial value problems that have an unsteady state or transient nature [2]. Normally, in most cases, the dependent variable to any of these problems is expressed in terms of several independent variables. Such problems inherently give rise to the need for partial derivatives in the description of their behaviour. The study of differential equations arising from these problems constitutes the field of *Partial Differential Equations.*

Mathematically, a *partial differential equation* (henceforth abbreviated as p.d.e.) for a dependent variable u(x,y,...) is a relation of the form

$$F(x,y,\ldots,u,\frac{\partial u}{\partial x},\frac{\partial u}{\partial y},\ldots,\frac{\partial^2 u}{\partial x^2},\frac{\partial^2 u}{\partial x\partial y},\ldots)=0 \qquad (1.1.1)$$

where F is a given function of the independent variables x,y,... and the "unknown" function u and of a *finite* number of its partial derivatives.

We call u as a *solution* of (1.1.1) if after substitution of u(x,y,...) and its partial derivatives (1.1.1) is satisfied identically in x,y,... in some region ft in the space of these independent variables. The independent variables x,y,... are real (unless if stated otherwise) and u and the derivatives of u occurring in (1.1.1) are continuous functions of x,y,... in the real domain ft.

As in the theory of Ordinary Differential Equations (henceforth abbreviated as o.d.e.) a p.d.e. (1.1.1) is said to be of *order n* if the order of the highest partial derivatives involved is n. Equation (1.1.1) is said to be *linear* if F is linear in the unknown function and its derivatives and *quasi-linear* if F is linear in at least the highest order derivatives [1].

For example, the equation

$$\sqrt{x}\frac{\partial u}{\partial x}+u\frac{\partial u}{\partial y}=-u^2 , \qquad (1.1.2)$$

as a first order quasi-linear p.d.e., and the equation

$$\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}-32u=0 \qquad (1.1.3)$$

is a second order linear p.d.e. Meanwhile the equation

$$\left(\frac{\partial^2 u}{\partial x^2}\right)\left(\frac{\partial^2 u}{\partial y^2}\right)-\left(\frac{\partial^2 u}{\partial x\partial y}\right)^2=0 , \qquad (1.14)$$

is the example of a second order *non-linear.* In equation (1.1.2)—(1.1.4) above, x and y are the independent variables and u=u(x,y) is the dependent variable whose form is to be found.

A linear p.d.e. is said to be *homogeneous* if each term contains either the dependent variable or one of its derivatives. For example equation

$$\frac{\partial u}{\partial t} - k\frac{\partial^2 u}{\partial x^2} = 0 \quad \text{(Heat Equation)} \qquad (1.1.5)$$

is homogeneous, whereas

$$\frac{\partial u}{\partial t} - a\frac{\partial^2 u}{\partial x^2} = f(x,t), \qquad a>0 \qquad (1.1.6)$$

where f(x,t) is a given function, is an *inhomogeneous* or *non- homogeneous* equation.

The problem of finding the solution to the p.d.e. is very difficult as the general method of solution is not available except for certain special types of linear or quasi-linear equations. Furthermore, the *general solution* of the linear p.d.e. which contains *arbitrary functions*

is of little use, since it has to be made to satisfy other conditions called *boundary conditions[7]* which arise from the physical problem itself .

Similar to o.d.e., if $u_1, u_2, u_3, \ldots, u_n$ are n different solutions of a

linear homogeneous p.d.e, in some given domain then

$$u = c_1u_1 + c_2u_2 + \ldots + c_nu_n \qquad (1.1.7)$$

is also a solution in the same domain with $c_1, c_2, \ldots, c_n$ as arbitrary constants.

1.2 CLASSIFICATION OF PARTIAL DIFFERENTIAL EQUATIONS

As the p.d.e. arise from different categories of physical phenomenon [1,11] (e.g. steady viscous flow, resonance in electric circuits, propagation of heat), this suggests that the governing equations are also quite different in nature. Normally, they are classified in terms of their mathematical form such as elliptic, hyperbolic and parabolic equation, or in terms of the type of problems to which they apply i.e. the heat equation and the wave equation.

The most general second order linear p.d.e. in two independent variables, is given by,

$$LU \equiv A(x,y)\frac{\partial^2 u}{\partial x^2} + 2B(x,y)\frac{\partial^2 u}{\partial x \partial y} + C(x,y)\frac{\partial^2 u}{\partial y^2} + E\left(x,y,u,\frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}\right) = 0 . \qquad (1.2.1)$$

It is called *elliptic, hyperbolic* and *parabolic* according to the determinant

$$\begin{vmatrix} B & A \\ C & B \end{vmatrix} \qquad (1.2.2)$$

is negative, positive or zero. This classification depends in general on the region of the (x,y)-plane under consideration. Thus it is possible for a p.d.e. to change its classification within the different regions of the domain for which the problem is defined. The differential equation

$$y\frac{\partial^2 u}{\partial x^2} + x\frac{\partial^2 u}{\partial x \partial y} + y\frac{\partial^2 u}{\partial y^2} = F\left(x,y,u,\frac{\partial u}{\partial x},\frac{\partial u}{\partial y}\right) \qquad (1.2.3)$$

for instance, is elliptic for $|x|<2|y|$, hyperbolic for $|x|>2|y|$ and parabolic along $|x|=2|y|$, This type of equation is said to be mixed type.

For a linear p.d.e. in more than two independent variables, for systems and for non-linear p.d.e., a similar but complicated classification can be carried out. In the case of three independent variables, the terms elliptic parabolic and hyperbolic are replaced by their three dimensional analogous such as ellipsoidal, etc.

The elliptic class is related to equilibrium problems and are usually described in terms of a closed region having boundary conditions prescribed at every point on the region’s boundary. These are called the *boundary value problems[7].* The parabolic and hyperbolic problems are of propagation type and normally have a prescribed boundary condition on some part of the boundaries and an initial condition along the other part. It can also have open-ended regions into which the solution propagates. In mathematical parlance such problems are known as *initial (boundary) value problems.*

Another important aspect of the classification of the p.d.e. into hyperbolic, parabolic and elliptic is due to the characteristic equation [2].

Here we can see that at every point of the x-y plane there are two directions in which the integration of the p.d.e. reduces to the integration of an equation involving total differential only. In other words, the integration of an equation in certain directions is not complicated by the presence of partial derivatives in other directions.

Let the derivatives in equation (1.2.1) be denoted by

$$\frac{\partial u}{\partial x} = p \; ; \quad \frac{\partial u}{\partial y} = q \; ; \quad \frac{\partial^2 u}{\partial x^2} = r; \quad \frac{\partial^2 u}{\partial x \partial y} = s \text{ and } \frac{\partial^2 u}{\partial y^2} = t .$$

Let C be a curve in the x-y plane on which the values of u and its derivatives satisfy equation (1.2.1). (C is not a curve on which initial values of u,p and q are given). Therefore, the differentials of p and q in the directions tangential to C are given by

$$dp = \frac{\partial p}{\partial x}dx + \frac{\partial p}{\partial y}dy = rdx + sdy \qquad (1.2.4)$$

and

$$dq = \frac{\partial q}{\partial x}dx + \frac{\partial q}{\partial y}dy = sdx + tdy \qquad (1.2.5)$$

where the p.d.e. (1.2.1) is written as

$$Ar + 2Bs + Ct + E = 0\ . \qquad (1.2.6)$$

Elimination of r and t in (1.2.6) using (1.2.4) and (1.2.5) gives:

$$A\frac{d}{dx}(dp-sdy) + 2Bs + C\frac{d}{dy}(dq-sdx) + E = 0$$

i.e.

$$s\{A(\frac{dy}{dx})^2 - B(\frac{dy}{dx}) + C\} - \{A\frac{dp}{dx}\cdot\frac{dp}{dy} + C\frac{dq}{dx} + E\frac{dy}{dx}\} = 0. \qquad (1.2.7)$$

Now choose $\frac{dy}{dx}$, the tangent to C at a point P(x,y) to satisfy

$$A(\frac{dy}{dx})^2 - 2B(\frac{dy}{dx}) + C = 0\ . \qquad (1.2.8)$$

Therefore (1.2.7) leads to

$$A\frac{dp}{dx}\cdot\frac{dq}{dy} + C\frac{dp}{dx} + E\frac{dy}{dx} = 0 \qquad (1.2.9)$$

which gives the relationship between the total differential dp and dq with respect to x and y.

This shows that at every point P(x,y) of the solution domain there are two directions, given by the roots of equation (1.2.8), along which there is a relationship given by equation (1.2.9). The directions given by the roots of equation (1.2.8) are called the characteristic directions and the p.d.e. is said to be hyperbolic, parabolic or elliptic according to similar determinant requirement as in (1.2.2).

1.3 BOUNDARY CONDITIONS

The solution of the p.d.e. has to be made to satisfy the boundary conditions which arise from the problem formulation. There are four main types of such conditions which arise frequently in the description of physical phenomena, these are:

The First Boundary-Value Problem (the Dirichlet Problem), where the solution u has to satisfy the given values

$$u|_s = \phi \qquad (1.3.1)$$

on the boundary s. If $\phi \equiv 0$ the problem is called *Homogeneous Dirichlet* problem[7].

1. *The Second Boundary-Value Problem (the Neumann Problem),* where the solution u has to satisfy the normal derivatives

$$\frac{\partial u}{\partial \nu}\Big|_s = \psi \qquad (1.3.2)$$

on the boundary of that region.

2. *The Third Boundary-Value Problem (Mixed or Robin's Problem),*where the solution u has to satisfy a combination of u and its derivatives namely

$$[\frac{\partial u}{\partial \nu} + hu]_s = \psi \qquad (1.3.3)$$

on the boundary s.

4. The Fourth Boundary-Value Problem (Periodic Boundary Problem).

In this case we seek the solution such that it satisfies the periodicity conditions, for example,

$$u|_x = u|_{x+\ell}\ ,\ \frac{\partial u}{\partial \nu}\Big|_x = \frac{\partial u}{\partial \nu}\Big|_{x+\ell} \qquad (1.3.4)$$

where *l* is called the period.

The physical meaning of the first three boundary-value problems can be illustrated by the problem of steady-state temperature distribution.

In the Dirichlet problem, the temperature is given on the boundary of a solid. In the Neumann problem the loss or gain of heat through the boundary is given (it is proportional to $\partial u/\partial \nu$). In this problem in order to keep a steady-state distribution of temperature, the net flow of thermal energy passing through the boundary of a solid must be equal to zero, i.e.,

$$\int_s \psi\, ds = 0 \qquad (1.3.5)$$

The third-boundary problem deals with the heat exchange with the surrounding medium the temperature of which is ψ/h, where h is the coefficient of thermal conductivity divided by the specific heat.

1.4 BASIC MATRIX ALGEBRA

In the numerical solution of p.d.e.'s by the finite difference method or finite element method, the differential system is replaced by a matrix system. In this section some useful properties of a matrix are outlined. Notations 1.4.1

A square matrix of order n

a_{ij} real number which is the element in the i^{th} row and j^{th} column of the matrix A.

A^{-1} inverse of A

A^T transpose of A

$|A|$ determinant of A

I unit matrix of order n

0 null matrix •

$\rho(A)$ spectral radius of A .

$\underline{x}$ column vector with element x_i, $i=1,2,\dots,n$

$\underline{x}^T$ row vector with element x_j, $j=1,2,\dots,n$

$\bar{\underline{x}}$ complex conjugate of $\underline{x}$

$||A||$ norm of A

$||\underline{x}||$ norm of vector x

π permutation matrix which has entries of zeros and one only, with one non-zero entry in each row and column.

Definitions 1.4.1

The matrix A is said to be

i. non-singular if $|A| \neq 0$

ii. *diagonal* if its only non-zero elements lie on the diagonal

iii. *symmetric* if $A=A^T$ i.e. $a_{ij}=a_{ji}$ » $i,j=1,2,\dots,n$

orthogonal if $A^{-1}=A^T$.

null if $a_{ij}=0$ for all i and j, $i,j=1,2,\dots,n$ diagonally dominant if $|a_{ii}| \geq \sum_{\substack{j=1 \\ j\neq i}}^{n} |a_{ij}|$ for all i tridiagonal if block diagonal if $a_{ij}=0$ for $|i-j|>1$. where each

$$A = \begin{bmatrix} B_1 & & & \\ & B_2 & & 0 \\ & & \ddots & \\ 0 & & & B_s \end{bmatrix}$$

is a square matrix of order $k_1,k_2,\dots,k_s$

B_k $(k=1,2,\dots,s)$

with $k_1+k_2+\dots+k_s=n.$

upper triangular if $a_{ij}=0$ for $i>j$

lower triangular if $a_{ij}=0$ for $j>i$

sparse if many of the elements are zero.

For the matrix A whose elements a_{ij} which are not necessarily real numbers we denote A^H as the conjugate transpose of A. A is called *Hermitian* if $A^H=A$, i.e. if $\bar{a}_{j,i}=a_{i,j}$, for all i and j, i,j=l,2,...,n. The definition of a Hermitian matrix implies that the diagonal elements of the matrix are real. A real symmetric matrix is always Hermitian, but a Hermitian matrix is symmetric only if it is real.

If A is real and $\underline{x}$ is complex, then A is *positive definite* if $(\underline{x},A\underline{x})>0$ for all $\underline{x}\neq 0$. (Note that the inner product $(\underline{x},\underline{y})$ of two complex vectors is $\sum_{i=1}^{n} x_i\bar{y}_i$ where $\bar{y}_i$ is the complex conjugate of y^). A is non-negative or semi-positive definite if $(\underline{x},A\underline{x})\geq 0$ for all $\underline{x}\neq\underline{0}$ with equality for at least one $\underline{x}\neq 0$.

A is a band matrix of bandwidth $w=p+q+1$ if. $a_{ij}=0$ for $j>i+p$ or $i>j+q$.

If p=q=l, then A is tridiagonal and a pentadiagonal matrix can be obtained when p=q=2.

1.5 EIGENVALUES AND EIGENVECTORS OF A MATRIX

Definition 1.5.1

If A is a square matrix of order n and if $\underline{x}$ is a non-zero vector such that $A\underline{x}=\lambda\underline{x}$, where λ is some number, then $\underline{x}$ is said to be an *eigenvector* of A with corresponding *eigenvalue* λ *[13].*

Theorem 1.5.1

If A is a square matrix of order n, any eigenvalue λ satisfies the n[th] degree polynomial equation $|A-\lambda I|=0$; this equation is known as the characteristic equation of A.

Proof:

We seek a scalar λ and non-zero vector $\underline{x}$ such that $A\underline{x}=\lambda\underline{x}$ or $(A-\lambda I)\underline{x}=0$.

Since this is a system of n simultaneous homogeneous equations in the n unknowns, $x_1,x_2,\ldots,x_n$ (not all are zero), therefore $A-\lambda I$ must be singular, or in other words $|A-\lambda I|=0$

Theorem 1.5.2 (Gerschgorin's first theorem)

The largest of the moduli of the eigenvalues of the square matrix A cannot exceed the largest sum of the moduli of the elements along any row or any column.

Proof:

Let λ_i be an eigenvalue of A and $\underline{x}_i$ is the corresponding eigenvector with components $v_1,v_2,\ldots,v_n$. Then the equation $A\underline{x}_i=\lambda\underline{x}_i$ is in detail given by

$$\begin{aligned} a_{1,1}v_1 + a_{1,2}v_2 + \ldots + a_{1,n}v_n &= \lambda_i v_1 \\ a_{2,1}v_1 + a_{2,2}v_2 + \ldots + a_{2,n}v_n &= \lambda_i v_2 \\ \vdots \qquad \vdots \qquad & \quad \vdots \\ a_{s,1}v_1 + a_{s,2}v_2 + \ldots + a_{s,n}v_n &= \lambda_i v_s \\ \vdots \qquad \vdots \qquad & \quad \vdots \\ a_{n,1}v_n + a_{n,2}v_2 + \ldots + a_{n,n}v_n &= \lambda_i v_n \end{aligned} \qquad (1.5.1)$$

Let v_s be the largest in modulus of $v_1,v_2,\ldots,v_n$. Select the s[th] equation and divide by v_s giving

$$\lambda_i = a_{s,1}\left(\frac{v_1}{v_s}\right) + a_{s,2}\left(\frac{v_2}{v_s}\right) + \ldots + a_{s,n}\left(\frac{v_n}{v_s}\right).$$

Since $\left|\frac{v_i}{v_s}\right|\leq 1,\ i=1,2,\ldots,n,$ therefore

$$|\lambda_i| \leq |a_{s,1}| + |a_{s,2}| + \ldots + |a_{s,n}|.$$

In particular this holds for $|\lambda_i|=\max|\lambda_s|$, $s=1,2,\ldots,n$

As the eigenvalues of the transpose of A are the same as those of A, the proof is also true for columns.

Theorem 1.5.3 (Gerschgorin's circle theorem)

Let A have n eigenvalues $\lambda_i,\ i=1,2,\ldots,n.$ Then each λ_i lies in the union of the n circles,

$$|\lambda-a_{i,i}| \leq \sum_{\substack{j=1\\j\neq i}}^{n} |a_{i,j}| \qquad (1.5.2)$$

Proof:

By the previous proof

$$\lambda_i = a_{s,1}\left(\frac{v_1}{v_s}\right) + a_{s,2}\left(\frac{v_2}{v_s}\right) + \ldots + a_{s,s} + \ldots + a_{s,n}\left(\frac{v_n}{v_s}\right)$$

Therefore,

$$\begin{aligned} |\lambda_i-a_{s,s}| &= \left|a_{s,1}\left(\frac{v_1}{v_s}\right) + a_{s,2}\left(\frac{v_2}{v_s}\right) + \ldots + a_{s,s-1}\left(\frac{v_{s-1}}{v_s}\right) + a_{s,s+1}\left(\frac{v_{s+1}}{v_s}\right) + \ldots + a_{s,n}\left(\frac{v_n}{v_s}\right)\right| \\ &\leq |a_{s,1}| + |a_{s,2}| + \ldots + |a_{s,s-1}| + |a_{s,s+1}| + \ldots + |a_{s,n}| \end{aligned}$$

As λ_i is any eigenvalue, therefore,

$$|\lambda - a_{i,i}| \leq \sum_{\substack{j=1\\j\neq i}}^{n} |a_{i,j}| \qquad (1.5.3)$$

Corollary 1: If A is a square matrix of order n and

$$\nu = \max_{1\leq i\leq n} \sum_{j=1}^{n} |a_{i,j}|, \qquad (1.5.4)$$

Then $\rho(A)\leq\nu$.

1.6 CONCLUSION

In this paper, it is shown that with the increasingly high standard of technology used in society today and the accelerating use of digital computers, the numerical solution of parabolic partial differential equations remains an important subject for research for the future. The discovery of the Group Explicit method is an important landmark in methods of solving partial differential equations as in principle the method is simple, stable, accurate and flexible in the sense that it allows the calculation of more than one point at a time - a new and original idea.

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