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THE NUMERICAL SOLUTION OF ELLIPTIC PARTIAL DIFFERENTIAL EQUATIONS BY THE METHOD OF LINES*

by

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ABSTRACT. The Method of Lines is shown to be a practical and convenient technique for the numerical solution of elliptic partial differential equations. The method produces a system of coupled two-point boundary value problems which are solved using state-of-the-art software.

Section 1. The Method of Lines has long been a popular and convenient technique for the numerical solution of parabolic partial differential equations. The idea is to discretize all but one of the independent variables, which results in a system of coupled ordinary differential equations. In the parabolic case the system of initial value problems can then be solved using state-of-the-art software.

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Because of the recent availability of high quality software for two-point boundary value problems, the Method of Lines has become an attractive technique for elliptic partial differential equations as well ([4], [6]). In this paper we analyze certain aspects of this numerical method applied to Poisson's equation with Dirichlet boundary conditions on a rectangular domain. Extensions to equations with Neumann conditions are immediate.

As observed by the referee, comparisons with other numerical techniques must ultimately be made. We do not pretend that the Method of Lines competes favorably with finite elements or finite differences on most problems. However, it has been successful on certain specific elliptic equations ([4], [6]). Current work on the Method of Lines applied to Fracture Mechanics (to appear) has produced good results compared to such classical techniques as finite difference and boundary elements.

In Section 2 we outline the basic discretization schemes and in Section 3 solve the five-point scheme. Section 4 presents a matrix technique for explicitly solving the system of two-point boundary value problems. The inherent instability for this system is briefly discussed in Section 5. A specific example from [4] is presented in Section 6, which was solved using the two-point boundary value problem code SUPORT [8]. A nonlinear problem [5] having nine distinct solutions is completely solved in Section 7. Here we use the nonlinear two-point boundary value problem code PASVA3 [7], now available through the International Mathematics and Statistics Library IMSL.

<u>Section</u> 2. Following Berezin and Zhidkov [2], we consider Poisson's equation with Dirichlet boundary conditions on a rectangle:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f(x,y), \qquad (1)$$

$$u(x,c) = \gamma(x), u(x,d) = \delta(x), a \le x \le b,$$

 $u(a,y) = \alpha(y), u(b,y) = \beta(y), c \le y \le d.$

For n > 3, let h = (d-c)/(n+1) and $y_k = c+kh$, k = 0,1,2,...,n+1 (see Figure 1). The second partial derivative with respect to y is approximated by a three-point central difference scheme

$$\frac{\partial^2 u}{\partial y^2}(x,y_k) = \frac{1}{h^2}(u(x,y_{k+1}) - 2u(x,y_k) + u(x,y_{k-1})) + 0(h^2),$$

$$k = 1,2,...,n.$$
(2)

Putting $U_k(x) = u(x,y_k)$ and $f_k(x) = f(x,y_k)$, we have the $O(h^2)$ accurate system of coupled two-point boundary value problems:

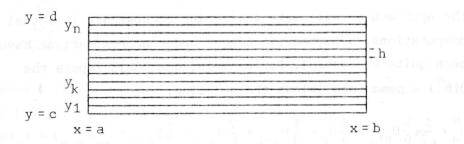


Figure 1

$$U_{k}^{"} + \frac{1}{h^{2}}(U_{k+1} - 2U_{k} + U_{k-1}) = f_{k}(x), \qquad k = 1, 2, ..., n, \qquad (3)$$

$$U_{0}(x) = \gamma(x), \quad U_{n+1}(x) = \delta(x).$$

$$U_{k}(a) = \alpha(y_{k}), \quad U_{k}(b) = \beta(y_{k}).$$

Similarly, if we approximate the second partial derivative by a five point scheme,

$$\begin{split} \frac{\partial^2 \mathbf{u}}{\partial \mathbf{y}^2} (\mathbf{x}, \mathbf{y}_k) &= \frac{1}{h^2} (\frac{-1}{12} \mathbf{u} (\mathbf{x}, \mathbf{y}_{k+2}) + \frac{4}{3} \mathbf{u} (\mathbf{x}, \mathbf{y}_{k+1}) - \frac{5}{2} \mathbf{u} (\mathbf{x}, \mathbf{y}_k) \\ &+ \frac{4}{3} \mathbf{u} (\mathbf{x}, \mathbf{y}_{k-1}) - \frac{1}{12} \mathbf{u} (\mathbf{x}, \mathbf{y}_{k-2})) + 0(h^4) \,, \end{split}$$

we arrive at the $O(h^4)$ system:

$$U_{k}'' + \frac{1}{h^{2}}(-\frac{1}{12}U_{k+2} + \frac{4}{3}U_{k+1} - \frac{5}{2}U_{k} + \frac{4}{3}U_{k-1} - \frac{1}{12}U_{k-2}) = f_{k},$$

$$k = 1, 2, \dots, n,$$

$$(4)$$

$$U_{o}(x) = \gamma(x), \quad U_{n+1}(x) = \delta(x),$$

 $U_{k}(a) = \alpha(y_{k}), \quad U_{k}(b) = \beta(y_{k}).$

Of course, there is now the need to impose further boundary conditions. One idea [3] is to require that the five-point scheme be compatible with the three-point scheme. This is the approach we will take in Section 3. However, in actual computations, nonsymmetric higher order approximations have been quite successful. For example, one could impose the $O(h^4)$ scheme (see [4]) at the n^{th} line:

$$U_{n}'' + \frac{1}{h^{2}} (\frac{5}{6} U_{n+1} - \frac{5}{4} U_{n} - \frac{1}{3} U_{n-1} + \frac{7}{6} U_{n-2} - \frac{1}{2} U_{n-3} + \frac{1}{12} U_{n-4}) = f_{n}(x).$$
(5)

Berezin [2] also derives the O(h4) system

$$\frac{5}{6} U_{k}'' + \frac{1}{12} (U_{k+1}'' + U_{k-1}'') + \frac{1}{h^{2}} (U_{k+1} - 2U_{k} + U_{k-1})$$

$$= \frac{5}{6} f_{k} + \frac{1}{12} (f_{k+1} + f_{k-1}), \quad k = 1, 2, ..., n, \quad (6)$$

$$U_{o}(x) = \gamma(x), \quad U_{n+1}(x) = \delta(x),$$

$$U_{k}(a) = \alpha(y_{k}), \quad U_{k}(b) = \beta(y_{k}).$$

Section 3. Berezin [2] and Jones [4] both solve the three-point scheme (3). Berezin further states the solution to (6). Hence, we will illustrate the techniques involved by solving the five-point scheme (4). Consider first the homogeneous system of two-point boundary value problems:

$$U_{k}^{"} + \frac{1}{h^{2}} \left(-\frac{1}{12} U_{k+2} + \frac{4}{3} U_{k+1} - \frac{5}{2} U_{k} + \frac{4}{3} U_{k-1} - \frac{1}{12} U_{k-2} \right) = 0$$

$$U_{0}(x) = 0, \quad U_{n+1}(x) = 0; \quad k = 1, 2, \dots, n.$$

This is solved by separation of variables: $U_k(x) = r(k)v(x)$. Substituting into (7) and simplifying, we obtain

$$\frac{v''(x)}{v(x)} = \frac{r(k+2) - 16r(k+1) + 30r(k) - 16r(k-1) + r(k-2)}{12r(k)h^2} = \delta^2$$
 (8)

where δ is a constant. Note that the equation corresponding to (8) for the three-point scheme (3) is

$$\frac{v''(x)}{v(x)} = \frac{r(k+1) - 2r(k) + r(k-1)}{-r(k)h^2} = \bar{\delta}^2,$$
 (9)

while that for the scheme of equation (6) is

$$\frac{\mathbf{v''}(\mathbf{x})}{\mathbf{v}(\mathbf{x})} = \frac{\mathbf{r}(\mathbf{k}+1) - 2\mathbf{r}(\mathbf{k}) + \mathbf{r}(\mathbf{k}-1)}{-(\mathbf{r}(\mathbf{k}+1) + 10\mathbf{r}(\mathbf{k}) + \mathbf{r}(\mathbf{k}-1))\mathbf{h}^2/12} = \hat{\delta}^2.$$
(10)

The boundary conditions for (7) give r(0)v(x) = 0, and r(n+1)v(x) = 0, which imply r(0) = 0 and r(n+1) = 0. If we further require that the five-point scheme be compatible with the three-point shceme, we can establish two more boundary conditions. From (9),

$$r(k+1) - (2-h^2\bar{\delta}^2)r(k) + r(k-1) = 0.$$

Since r(0) = 0, we get r(-1) = -r(1). And since r(n+1) = 0, r(n+2) = -r(n).

We see, therefore, from (8) that the problem is to solve the difference equation:

$$r(k+2)-16r(k+1)+(30-12\delta^2h^2)r(k)-16r(k-1)+r(k-2) = 0,$$
 (11)

$$k = 1,2,...,n$$
, $r(0) = r(n+1) = 0$, $r(-1) = -r(1)$; $r(n+2) = -r(n)$.

The general solution is of the form

$$r(k) = c_1 \lambda_1^k + c_2 \lambda_2^k + c_3 \lambda_3^k + c_4 \lambda_4^k$$

where $\lambda_1, \lambda_2, \lambda_3$ and λ_4 are the roots of the polynomial

$$\lambda^4 - 16\lambda^3 + (30-12\delta^2h^2)\lambda^2 - 16\lambda + 1$$

Since this a reciprocal polynomial,

$$\lambda_2 = \lambda_1^{-1}$$
 and $\lambda_4 = \lambda_3^{-1}$

Putting Z = 30 - $12\delta^2 h^2$ and $\omega_i = \lambda_i + \lambda_i^{-1}$ (i = 1,2,), an easy calculation gives

$$\omega_1 = 8 + \sqrt{66-Z}$$

$$\omega_2 = 8 - \sqrt{66-Z} . \tag{12}$$

Solving for the roots λ_i (i = 1,2,3,4), we obtain

$$\lambda_{1} = \frac{\omega_{1} + \sqrt{\omega_{1}^{2} - 4}}{2} , \qquad \lambda_{2} = \frac{\omega_{1} - \sqrt{\omega_{1}^{2} - 4}}{2}$$

$$\lambda_{3} = \frac{\omega_{3} + \sqrt{\omega_{3}^{2} - 4}}{2} , \qquad \lambda_{4} = \frac{\omega_{3} - \sqrt{\omega_{3}^{2} - 4}}{2}$$

We now apply the boundary conditions given in (11) in order to find the constants C_i (i = 1,2,3,4,):

$$\begin{split} \mathbf{r}(0) &= 0 \colon \mathbf{C}_{1} + \mathbf{C}_{2} + \mathbf{C}_{3} + \mathbf{C}_{4} &= 0 \\ \\ \mathbf{r}(\mathbf{n}+1) &= 0 \colon \mathbf{C}_{1} \lambda_{1}^{n+1} + \mathbf{C}_{2} \lambda_{2}^{n+1} + \mathbf{C}_{3} \lambda_{3}^{n+1} + \mathbf{C}_{4} \lambda_{4}^{n+1} &= 0 \\ \\ \mathbf{r}(-1) &= -\mathbf{r}(1) \colon \mathbf{C}_{1} \lambda_{1}^{-1} + \mathbf{C}_{2} \lambda_{2}^{-1} + \mathbf{C}_{3} \lambda_{3}^{-1} + \mathbf{C}_{4} \lambda_{4}^{-1} \\ \\ &= -(\mathbf{C}_{1} \lambda_{1} + \mathbf{C}_{2} \lambda_{2} + \mathbf{C}_{3} \lambda_{3} + \mathbf{C}_{4} \lambda_{4}) \\ \\ \mathbf{r}(\mathbf{n}+2) &= -\mathbf{r}(\mathbf{n}) \colon \mathbf{C}_{1} \lambda_{1}^{n+2} + \mathbf{C}_{2} \lambda_{2}^{n+2} + \mathbf{C}_{3} \lambda_{3}^{n+2} + \mathbf{C}_{4} \lambda_{4}^{n+2} \\ \\ &= -(\mathbf{C}_{1} \lambda_{1}^{n} + \mathbf{C}_{2} \lambda_{2}^{n} + \mathbf{C}_{3} \lambda_{3}^{n} + \mathbf{C}_{4} \lambda_{4}^{n}) \,. \end{split}$$

However, $\lambda_2 = \lambda_1^{-1}$ and $\lambda_4 = \lambda_3^{-1}$, and we can simplify these four equations to:

$$C_1 + C_2 + C_3 + C_4 = 0$$

These four equations can be solved for C_1, C_2, C_3, C_4 to give $C_1 = -C_2$; $C_3 = -C_4$ and

$$\lambda_1^{n+1}c_1 + \lambda_1^{-(n+1)}c_2 = 0$$

$$\lambda_3^{n+1}c_3 + \lambda_3^{-(n+1)}c_4 = 0.$$

Hence,

$$\lambda_1^{n+1} = \lambda_1^{-(n+1)}$$
 and $\lambda_3^{n+1} = \lambda_3^{-(n+1)}$.

That is,

$$\lambda_1^{2(n+1)} = 1$$
 and $\lambda_3^{2(n+1)} = 1$.

This implies that

$$\lambda_1 = \exp(\pi i s/(n+1)), \quad \lambda_3 = \exp(\pi i s/(n+1)), s = 0,1,...,n.$$

Then

$$\begin{split} \mathbf{r}(\mathbf{k}) &= c_1 \lambda_1^k + c_2 \lambda_2^k + c_3 \lambda_3^k + c_4 \lambda_4^k \\ &= c_1 (\lambda_1^k - \lambda_1^{-k}) + c_3 (\lambda_3^k - \lambda_3^{-k}) \\ &= c_1 \big[\exp(\pi \mathbf{i} \mathbf{s} \mathbf{k} / (\mathbf{n} + 1)) - \exp(\pi \mathbf{i} \mathbf{s} \mathbf{k} / (\mathbf{n} + 1)) \big] \\ &+ c_3 \big[\exp(\pi \mathbf{i} \mathbf{s} \mathbf{k} / (\mathbf{n} + 1)) - \exp(-\pi \mathbf{i} \mathbf{s} \mathbf{k} / (\mathbf{n} + 1)) \big] \end{split}$$

=
$$C_{s}\sin(\frac{\pi sk}{n+1})$$
, s = 0,1,...,n.

Of course, the value s = 0 is the trivial solution, so the solution to (11) is:

$$r(k) = \sum_{s=1}^{n} C_{s} \sin(\frac{\pi s k}{n+1})$$
, $k = 1, 2, ..., n$.

The values of δ can now be calculated from (12):

$$8 + \sqrt{66-Z} = w_1 = \lambda_1 + \lambda_1^{-1} = \exp(\pi i s/(n+1)) + \exp(-\pi i s/(n+1))$$
$$= 2\cos(\frac{\pi s}{n+1}) , \qquad s = 1, 2, ..., n.$$

Hence

$$8 + \sqrt{66 - (30 - 12\delta^{2}h^{2})} = 2\cos(\frac{\pi s}{n+1})$$

$$\sqrt{9 + 3\delta^{2}h^{2}} = \cos(\frac{\pi s}{n+1}) - 4$$

$$\delta_{s}^{2} = \frac{\cos^{2}(\frac{\pi s}{n+1}) - 8\cos(\frac{\pi s}{n+1}) + 7}{3h^{2}}, \quad s = 1, 2, ..., n.$$

To complete the solution to equation (8) we have

$$\frac{v''(x)}{v(x)} = \delta_s^2$$
 s = 1,2,...,n,

whose solution is

$$v_s(x) = A_s \exp(\delta_s x) + B_s \exp(-\delta_s x)$$

Finally, the solution to (7) is

$$U_{k}(x) = \sum_{s=1}^{n} \sin(\frac{\pi ks}{n+1}) (A_{s} \exp(\delta_{s} x) + \exp(-\delta_{s} x))$$
 (13)

$$(k = 1, 2, ..., n),$$

where

$$\delta_{s}^{2} = \frac{\cos^{2}(\frac{\pi s}{n+1}) - 8\cos(\frac{\pi s}{n+1}) + 7}{3h^{2}}$$

Problem (4) can now be resolved by variation of parameters.

Note that the solution to (3) is derived in Berezin [2]:

$$U_{k}(\mathbf{x}) = \sum_{s=1}^{n} \sin(\frac{\pi k s}{n+1}) (A_{s} \exp(\overline{\delta}_{s} \mathbf{x}) + B_{s} \exp(-\overline{\delta}_{s} \mathbf{x}))$$
(14)

where

$$\bar{\delta}_{s}^{2} = \frac{4\sin^{2}(\frac{\pi s}{2(n+1)})}{h^{2}}$$

The solution to (6) is also stated in Brezin:

$$U_{k}(\mathbf{x}) = \sum_{n=1}^{n} \sin(\frac{\pi s k}{n+1}) (A_{s} \exp(\hat{\delta}_{s} \mathbf{x}) + B_{s} \exp(-\hat{\delta}_{s} \mathbf{x}))$$
 (15)

where

$$\hat{\delta}_{s}^{2} = \frac{24 \sin^{2}(\frac{\pi s}{2(n+1)})}{h^{2}(5 + \cos(\frac{\pi s}{n+1}))}.$$

Section 4. There is a matrix technique that can also be used to solve the system of two-point boundary value problems. This will be illustrated by solving the homogeneous system corresponding to the three-point scheme (3):

$$U_{k}'' + \frac{1}{h^{2}}(U_{k+1} - 2U_{k} + U_{k-1}) = 0$$
 (16)

$$U_{o}(x) = 0$$
, $U_{n+1}(x) = 0$, $k = 1, 2, ..., n$.

In matrix form, we have: U'' = AU, where $U = (U_1, ..., U_n)^T$ and A is the n×n matrix:

$$A = \frac{1}{h^2} \begin{bmatrix} 2 & -1 & 0 & \dots & 0 \\ -1 & 2 & -1 & 0 & \dots & 0 \\ & & & & -1 \\ & & & -1 & 2 \end{bmatrix}$$

Now put $V_i = U_i'$ and $V_i' = U_i''$. We then have (16) written as a system of (2n) first order differential equations:

$$\begin{bmatrix} U_1' \\ \vdots \\ U_n \\ V_1' \\ \vdots \\ V_n' \end{bmatrix} = \begin{bmatrix} 0 & I_n \\ & & \\ A & 0 \end{bmatrix} \begin{bmatrix} U_1 \\ \vdots \\ U_n \\ V_1 \\ \vdots \\ V_n \end{bmatrix}$$

where 0 is the n×n zero matrix and I_n is the identity matrix. The eigenvalues λ of the $(2n)\times(2n)$ matrix above are easy to determine. For if $U=(U_1,\ldots,U_n)^T$ and $V=(V_1,\ldots,V_n)^T$ then

$$\begin{bmatrix} 0 & I \\ A & 0 \end{bmatrix} \begin{bmatrix} U \\ V \end{bmatrix} = \lambda \begin{bmatrix} U \\ V \end{bmatrix}$$

implies $V = \lambda U$ and $AU = \lambda V$. That is, $AU = \lambda^2 U$. The eigenvalues of A are known to be

$$\frac{2-2\cos(\frac{\pi s}{n+1})}{h^2} , s = 1,2,...,n,$$

with corresponding eigenvectors

$$E_{s} = \begin{bmatrix} \sin(\frac{s\pi}{n+1}) \\ \sin(\frac{2s\pi}{n+1}) \\ \sin(\frac{ns\pi}{n+1}) \end{bmatrix}, \quad s = 1, 2, \dots, n.$$

Hence the λ must satisfy

$$\lambda^{2} = \frac{2 - 2\cos(\frac{\pi s}{n+1})}{h^{2}} = \frac{4\sin^{2}(\frac{\pi s}{2(n+1)})}{h^{2}},$$

which implies

$$\lambda_{s} = \pm \frac{2}{h} \sin(\frac{\pi s}{2(n+1)});$$
 $s = 1, 2, ..., n.$

This leads to the same solution as (14).

Section 5. Is is apparent from the previous work that the method of lines leads to a system of unstable two-point boundary value problems. An exponential of the form $\exp(\delta x)$ occurs in each of the solutions (13), (14), (15). Let us analyze (13) in more detail. The worst case would occur if

$$\delta_{s}^{2} = \frac{\cos^{2}(\frac{\pi s}{n+1}) - 8\cos(\frac{\pi s}{n+1}) + 7}{3h^{2}}$$

were as large as possible. This happens if s = n and we would have

$$\delta_{\rm n}^2 = \frac{\cos^2(\pi) - 8\cos(\pi) + 7}{3{\rm h}^2}$$

$$\delta_n \cong 4/\sqrt{3h}$$
.

We summarize this result with those of the other two schemes (3) and (6):

Scheme

(4)
$$4/\sqrt{3}h = 2.31/h$$
,

(3) $2/h$,

(6) $\sqrt{6/h} = 2.45/h$.

Section 6. Jones [4] considers the example

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 , \qquad (17)$$

$$u(0,y) = u(1,y) = 0$$
, $u(x,b) = u(x,-b) = \sin(\pi x)$,

where b = .475. The exact solution is known to be

$$u(x,y) = \frac{\cosh(\pi y) \sin(\pi x)}{\cosh(\pi b)}$$
(18)

By symmetry considerations he is able to simplify the problem to

$$\frac{\partial^2 \mathbf{u}}{\partial \mathbf{x}^2} + \frac{\partial^2 \mathbf{u}}{\partial \mathbf{v}^2} = 0 \tag{19}$$

$$u(0,y) = u_{x}(.5,y) = 0, u(x,b) = \sin(\pi x), u(x,y) = u(x,-y).$$

He then solves the three-point method of lines scheme for (19) using the technique of section 2 together with Chebyshev polynomials for the particular solution. The solution to the three-point scheme is

$$U_{k}(x) = \frac{\cosh(k\theta)\sin(\pi x)}{\cosh((n+1)\theta)}, \qquad (20)$$

where $cosh(\theta) = 1 + \pi^2 h^2/2$.

The solution to the five-point scheme is much more complicated and of little interest. Details are available upon request.

It is important to prove that the Method of Lines solution (20) converges to the exact solution (18) as the number of lines n tends to infinity. To this end, consider

$$\cosh(\theta) = 1 + \pi^2 h^2 / 2 = 1 + \theta^2 / 2 + \theta^4 / 4! + \dots$$

So for small h, $\theta \approx \pi h = \pi b/(n+1)$. Furthermore, $y_k = kb/(n+1) = kh$, which implies that $\pi y \approx k\theta$. Hence, as $n \to \infty$,

$$U_{k}(x) = \frac{\cosh(k\theta)\sin(\pi x)}{\cosh((n+1)\theta)} \rightarrow \frac{\cosh(\pi y)\sin(\pi x)}{\cosh(\pi b)}$$

The convergence question for arbitrary elliptic partial differential questions is much more complicated. Thompson [9] proves that under suitable hypotheses convergence is assured (see Theorem 5.1, page 36).

SUPORT [8] was used successfully to solve this example with both the three and five-point schemes. The results agree with those of Jones [4]. Other codes for two-point boundary value problems could be used as well. This author has had good results with COLSYS [1] and the IMSL routines DTPTB and DVCPR. Details are available from the author upon request.

Section 7. The Method of Lines can be an effective technique for solving nonlinear equations as well. We illustrate this by solving

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + 20u - u^3 = 0$$

with boundary conditions u = 0 on the square $[0,\pi] \times [0,\pi]$. The system of boundary value problems is now non-linear:

$$U_{k}'' + \frac{1}{h^{2}}(U_{k+1} - 2U_{k} + U_{k-1}) + 20U_{k} - U_{k}^{3} = 0.$$

It can be shown theoretically that this elliptic partial differential equation has nine distinct solution [5], page 213 . We used the IMSL routine DVCPR which was originally called PASVA3 [7]. By suitably adjusting the initial profiles, all nine solutions were successfully obtained. For a theoretical analysis of partial differential equations of this type reader is referred to [5].

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