

THE ROLE OF ANALYSIS IN THE SOLUTION OF PARTIAL DIFFERENTIAL EQUATIONS

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1. INTRODUCTION

By definition, the end result of a numerical calculation is one or more numbers. From a practical point of view, such numbers are not particularly useful unless they can be related back to the 'real world'. Therefore, when discussing the numerical solution of partial differential equations (or for that matter any mathematical equations), it is not unreasonable to focus attention on problems which attempt to model some physical, biological or social phenomenon. We shall in any case do so here.

Given that our equation (or equations) do indeed fall into this category, we might ask what role mathematical analysis plays in obtaining a solution to the problem. It is sometimes argued that questions such as existence and uniqueness are superfluous. After all, the phenomenon in question actually occurs in the real world. Clearly then, the model equations should also have a solution. As for the calculation of a numerical solution, surely the basic principles and intuition available about the subject matter in hand are a sufficient guide to achieve a satisfactory answer.

Unfortunately, "life wasn't meant to be easy" and the above approach to computational problem solving can (and often does) fail (though it must be conceded that many problems have been and will continue to be solved satisfactorily in this manner). Often, some mathematical analysis of the problem and the numerical scheme for its approximate solution, is an essential ingredient in obtaining a meaningful result. Conversely, the

context and origin of the equation should not be discarded either as the approach most likely to succeed is one that takes advantage of all relevant knowledge about the problem.

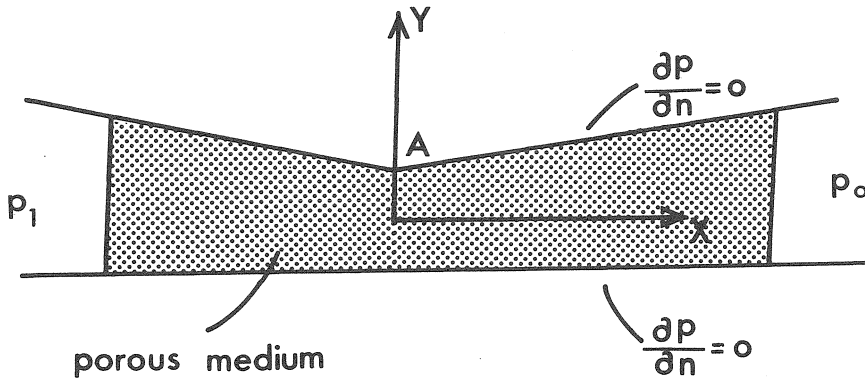
In this paper we shall try to illustrate the role of analysis when partial differential equations are used in mathematical modelling. Because of the diversity of the subject, we have adopted the approach of choosing a number of simple examples which illustrate the need for mathematical analysis at every stage from model formulation to the calculation of a numerical solution. In section 2 we demonstrate that the mathematical model chosen should reflect the particular aspect of that problem of interest and that partial differential equations whose solutions have features that are physically unrealistic may still yield relevant information about the problem in hand. The fact that well posedness of a mathematical formalism is not guaranteed even for equations that initially appear to be reasonable models for well defined physical processes is demonstrated in section 3. Then in section 4 some applications of analysis in the construction of numerical schemes is discussed. Finally, some concluding remarks are made in section 5.

2. NONPHYSICAL FEATURES OF MATHEMATICAL MODELS

All mathematical models are idealisations and contain many features that are non-physical. For example, points and lines are concepts which can never be realised in the real world. Furthermore, most mathematical models attempt to be as economical as possible and include only mechanisms which are thought to be important for the feature of the problem under investigation. For example, viscous terms are neglected in some fluid flow problems while nonlinear terms are neglected in many problems in elasticity. Thus, not only do models contain features that are purely mathematical in

concept, but they also neglect mechanisms deemed to have little effect on the required results. Of course, the mechanisms neglected should depend on the question for which an answer is sought. Thus, when examining the lift on an airfoil, it is appropriate to neglect viscous terms but if the quantity required is the drag on the airfoil, then viscous terms need to be taken into account and the relevant boundary layer equations examined (see for example Schlichting [10]).

Because the mathematical model is an idealisation of reality it is only to be expected that solutions will occasionally exhibit features that are physically unrealistic. To demonstrate this, consider the following example.



Here, we examine the flow of an incompressible fluid through a porous medium in a two dimensional duct as is shown above. Darcy's law states that the fluid velocity is proportional to the pressure gradient. Thus

$$\nabla p = -k \underline{y}, \quad \underline{y} = (u, w)^T$$

where u is the velocity in the x direction and w is the velocity in

the y direction. The equation of continuity is

$$\nabla \cdot \vec{v} = 0$$

and hence the pressure p satisfies Laplace's equation

$$\nabla \cdot \nabla p = \Delta p = 0 .$$

It turns out that this problem has a flow in which the velocity becomes infinite as we approach the re-entrant corner at the point A . Clearly this is physically unrealistic. Nevertheless, quantities such as the total flow through and the pressure distribution in the duct are meaningful and provide approximations that are often used in practice. The conclusion here is that a mathematical model which is useful in answering a particular question is not necessarily applicable for all aspects of the same physical problem.

It should also be pointed out that even when the solution becomes 'unphysical' the result may still be meaningful. Thus, in the above example, the fact that the velocity at A is infinite in the model provide the qualitative information that in reality the velocity in a neighbourhood of this point can be expected to be large. Sometimes the nature of a singularity of a solution may even provide quantitative information as is the case of the singularity in the stress at the crack tip in an elastic plate. Such 'stress intensity factors' are used to estimate crack growth (see Broeck [3]).

The above discussion has indicated that the solutions of partial differential equations may not be as well behaved as the process which they are modelling. Sometimes however it is to our advantage to have the least amount of regularity possible. To clarify this statement, consider the Neumann problem for Poisson's equation on a bounded domain Ω in \mathbb{R}^2 whose boundary we denote by Γ . Thus we have

$$\Delta u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f, \quad (x, y) \in \Omega$$

$$\frac{\partial u}{\partial n} = 0 \quad \text{on } \Gamma.$$

For a classical solution we require the existence of the second partial derivatives of u . However, the variational formulation of the problem requires only that

$$(2.1) \quad \int_{\Omega} \nabla u \cdot \nabla u \, dx \, dy < \infty.$$

For numerical schemes (such as finite element schemes) that are based on approximating the solution u , it is substantially simpler to find approximations satisfying (2.1) than it is to find approximations for which the partial derivatives exist. It is in fact often possible to use approximations that have less regularity than implied by (2.1). This is the case for nonconforming finite elements (see for example Strang and Fix [12]). However, the justification for the utilization of such elements requires substantial sophisticated analysis.

3. POSEDNESS OF PROBLEMS

A mathematical model is said to be properly posed if all of the following hold.

- (i) it has at least one solution;
- (ii) any solution it has is unique;
- (iii) its unique solution depends continuously on the data.

Of course, the above really need to be made more precise for complete rigour. For example, the meaning of continuous dependence depends on which spaces and norms are being considered. However, the above definition is sufficient for our purpose.

In the construction of a mathematical model, it is easy to obtain

equations for which a solution does not exist. Consider for example an elastic membrane which is fixed on its boundary (for simplicity take the unit disc as the domain). The physical picture we envisage here is a drum. Suppose we now prescribe a small constant displacement on a small circle contained in the unit disc (for simplicity a small concentric circle). This boundary condition corresponds to putting a coin in the centre of the drum and pressing down on it to cause a given displacement. Intuitively, we might expect that the coin can be replaced by a point. The problem then is

$$\Delta u = 0, \quad 0 < x^2 + y^2 < 1$$

$$u = 0, \quad x^2 + y^2 = 1; \quad u(0,0) = 1,$$

where u is the normalized displacement. However, it is easy to verify that this problem does not have a solution. For a finite coin (of radius ϵ say) the problem is

$$\Delta u = 0, \quad \epsilon^2 < x^2 + y^2 < 1$$

$$u = 0, \quad x^2 + y^2 = 1; \quad u = 1, \quad x^2 + y^2 = \epsilon^2.$$

This problem does have a solution and it is given by

$$u = \log(x^2 + y^2) / \log(\epsilon^2), \quad \epsilon^2 \leq x^2 + y^2 \leq 1.$$

Note however that the limit as $\epsilon \rightarrow 0$ of this solution does not exist.

As another example consider the equation

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left(D(u) \frac{\partial u}{\partial x} \right), \quad 0 < x < 1, \quad t > 0$$

with initial and boundary conditions

$$u(0, x) = 0$$

$$u(t, 0) = 1, \quad \frac{\partial u}{\partial x}(t, 1) = 0.$$

This is a standard diffusion equation if $D(u) > 0$ is smooth. Furthermore,

if $D(u)$ is given, the numerical solution of the problem can be calculated in a relatively straightforward manner and a number of packages for this task are readily available (see Barton [1]). However, suppose that $D(u)$ is unknown but $u(t,1)$ is given. Can we now calculate $D(u)$ for $0 \leq u \leq 1$? This is an example of an inverse problem (see Deuflhard and Haireiss [7] for other examples). The problem now is an order of magnitude more difficult than the standard diffusion problem. Usually, inverse problems are not well posed and special techniques must be employed to give meaningful answers. An approach to the problem outlined above may be found in Eriksson and Dahlquist [8].

As a final illustration consider the exterior Dirichlet problem

$$\Delta u = 0, \quad r = (x^2 + y^2)^{\frac{1}{2}} > 1$$

$$u = f(\theta), \quad r = 1$$

$$|u(r, \theta)| < \infty$$

where $f(\theta) = f(\theta + \pi)$, $0 \leq \theta \leq \pi$. This is a well posed problem and, because of the simple geometry involved can be solved analytically.

However, suppose we represent the solution as a distribution of sinks along the x axis between $x = -\frac{1}{2}$ and $x = \frac{1}{2}$. That is, we represent the solution as

$$u(r, \theta) = \frac{1}{4\pi} \int_{-\frac{1}{2}}^{\frac{1}{2}} \log[r^2 + x^2 - 2rx \cos \theta] g(x) dx.$$

In order that u remains bounded we require

$$\int_{-\frac{1}{2}}^{\frac{1}{2}} g(x) dx = 0$$

and to satisfy the boundary condition we need

$$\frac{1}{4\pi} \int_{-\frac{1}{2}}^{\frac{1}{2}} \log[1 + x^2 - 2x \cos \theta] g(x) dx = f(\theta), \quad 0 \leq \theta \leq 2\pi.$$

The equation we need to solve is therefore a first kind Fredholm equation

with a smooth kernel. Such equations are known to be very poorly posed and techniques such as regularization need to be employed for their numerical solution (see de Hoog [4] for a review of such techniques). In this example, mathematical manipulation has turned a well posed problem into an ill posed problem. However the above technique has found some use (in three dimensions and more complex geometry) in calculations involving cavitation bubbles (Bevir and Fielding [2]). Of course, the ill posed nature of the underlying equation must be recognised and appropriate numerical schemes used if such calculations are to be successful.

It is clear from the above example that the question of posedness of equations is an important one. Even when no solution exists for an equation there is no guarantee that the same is true for a numerical scheme designed to solve it. Indeed if we apply a five point finite difference scheme to the membrane problem, the resulting algebraic equations do have a solution that appears to be physically meaningful. On the other hand if the equation does have a solution that does not depend continuously on the data, special techniques must be employed to obtain a meaningful numerical approximation.

4. THE CONSTRUCTION AND ANALYSIS OF NUMERICAL SCHEMES

In the construction of numerical schemes, an appeal to the physics or basic processes underlying the mathematical equations is often invaluable. An example of this is the notion of conservative schemes which attempt to conserve global quantities such as mass or energy. On the other hand, a scheme derived by appealing to the underlying physical process alone may be far from optimal.

Consider for example the following discretization for the diffusion problem

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} .$$

Let us use the spatial discretization

$$x_j = j\Delta x$$

and approximate the solution on the grid by appealing to a random walk process underlying the diffusion equation. Then we obtain (Lin and Segel [9])

$$\frac{u_{j,j+1} - u_{jk}}{\Delta t} = \frac{u_{j+1,k} - 2u_{jk} + u_{j-1,k}}{(\Delta x)^2}$$

where u_{jk} is the approximation to $u(j\Delta x, k\Delta t)$. This is the explicit Euler scheme for the diffusion equation and it is well known that the stability constraint imposed by the Coarant, Friedrichs, Lewy condition (Smith [11])

$$\frac{\Delta t}{(\Delta x)^2} \leq \frac{1}{2}$$

makes this scheme very inefficient. For most applications, schemes (such as the Crank-Nickolson scheme) which are derived by examining the stability and consistency of finite difference equations, are far more efficient.

However, in some situations the analysis of a finite difference scheme can also give misleading results. Consider for example the Dirichlet problem for Poisson's equation on a square

$$\Delta u = f \quad , \quad 0 < x, y < 1$$

$$u(x, 0) = g_1(x) \quad , \quad u(x, 1) = g_2(x) \quad , \quad 0 < x < 1$$

$$u(0, y) = g_3(y) \quad , \quad u(1, y) = g_4(y) \quad , \quad 0 < y < 1 .$$

The standard finite difference scheme for this problem is

$$\begin{aligned}
& 2[(u_{i+1,j} - u_{i,j})/h_i - (u_{i,j} - u_{i-1,j})/h_{i-1}]/(h_i + h_{i-1}) \\
& \quad + 2[(u_{i,j+1} - u_{i,j})/k_j - (u_{i,j} - u_{i,j-1})/k_{j-1}]/(k_j + k_{j-1}) \\
& = f(x_i, y_j), \quad 0 < i, j < N \\
& u_{i,0} = g_1(x_i), \quad u_{i,N} = g_2(x_i), \quad 0 < i < N \\
& u_{0,j} = g_3(y_j), \quad u_{N,j} = g_4(x_j), \quad 0 < j < N
\end{aligned}$$

where

$$\begin{aligned}
x_0 = y_0 = 0, \quad x_N = y_N = 1 \\
x_i = x_{i-1} + h_{i-1}, \quad y_j = y_{j-1} + k_{j-1}, \quad 0 < i, j < N.
\end{aligned}$$

The local truncation error (that is, the remainder when the actual solution is substituted into the finite difference equation) is

$$\tau_{ij} = \frac{(h_i - h_{i-1})}{3} \frac{\partial^3 u}{\partial x^3}(x_i, y_j) + \frac{(k_j - k_{j-1})}{3} \frac{\partial^3 u}{\partial y^3}(x_i, y_j) + O(h^2 + k^2)$$

where

$$h = \max_i (h_i), \quad k = \max_j (k_j)$$

The standard analysis based on consistency and stability now yields

$$|u_{i,j} - u(x_i, y_j)| \leq C \max_{i,j} \{|h_i - h_{i-1}| + |k_j - k_{j-1}|\}$$

and thus we may expect $O(h+k)$ convergence in general. Such analysis has motivated the use of coordinate transformations to generate non-uniform grids that satisfy

$$h_i - h_{i-1} = O(1/N^2), \quad k_j - k_{j-1} = O(1/N^2)$$

(see for example de Rivas [6]). Then, we have

$$u_{ij} - u(x_i, y_j) = O(1/N^2).$$

However let us now perform some calculations with a very non-uniform grid.

Specifically let

$$h_{2i} = 2h_{2i-1} = 4/3N, \quad k_{2j} = k_{2j-1} = 4/3N$$

and

$$u(x,y) = \exp(x-y) .$$

We then obtain

N	Max. Error	Ratio
20	$.5934 \cdot 10^{-4}$	4.61
40	$.1287 \cdot 10^{-4}$	4.31
80	$.2985 \cdot 10^{-5}$	4.16
160	$.7178 \cdot 10^{-6}$	

The numerical results tabulated below indicate that the convergence is approximately second order rather than the first order convergence estimated by the analysis. For the corresponding one dimensional problem, de Hoog and Jackett [5] have shown that the convergence is indeed second order. But such an analysis has yet to be performed for the scheme above. Clearly, the necessity for coordinate transformations when solving partial differential equations requires further analysis.

Thus, while analysis plays an important role in the construction of numerical schemes, it must be realised that the estimates obtained may be gross overestimates.

5. CONCLUDING REMARKS

When a mathematical model is constructed, the solutions of the resulting equations may have features that are physically unrealistic. This does not imply that the results obtained from such a model are not meaningful but it does imply that the solution may have features that are

unintuitive. As a consequence, an approach to problem solving that is based on intuition alone may fail and clearly a balanced approach which includes mathematical analysis has a greater chance of achieving success.

Even though a differential equation has been constructed to model an observable phenomenon, it does not follow automatically that the mathematical formalism is well posed. Since ill posed problems require special treatment for their numerical solution, it is important that such problems be identified before a numerical solution is attempted.

Finally, although there are a wide variety of numerical schemes for the solution of partial differential equations, it is often possible to perform a simple analysis to eliminate those that are clearly inefficient for the problem in hand.

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