PARTIAL DIFFERENTIAL EQUATIONS IN MATHEMATICAL MODELING.

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PARTIAL DIFFERENTIAL EQUATIONS IN MATHEMATICAL MODELING**

Robert VICHNEVETSKY*

Partial differential equations have, for the past two and a half centuries, played a preponderant role in the success of mankind to develop mathematical models of the universe that surrounds us. This preponderance has persisted throughout those past few decades which we call "the computer age".

A review of theoretical milestones, fields of applications and, for the more recent past, developments of computer mathematics, hardware and software in which partial differential equations were important either as a motivating force or as a tool covers a remarkably diversified spectrum of questions in physics, applied mathematics and computer science.

Some comments about semantics may be in order: widespread use of the term <u>mathematical modeling</u> seems to be relatively recent, most often used in connection with the development of computer simulations. The <u>mathematical model</u> of some entity or system is the set of equations or statements which describe that system in a language sufficiently precise to allow <u>computer</u> codes or programs to be written, with the specific purpose of obtaining <u>particular solutions</u>. Those particular solutions of the mathematical model <u>simulate</u> the system's behavior, and are used to investigate its properties in a manner which lies somewhere in-between direct experimentation and theoretical analysis.

Partial differential equations are central to the mathematical model of a large variety of systems. One of their important characteristics though, is that exact computer solutions cannot in general be obtained: numerical solutions or "simulations" must be <u>approximations</u> obtained by the use of discrete algorithms which rely on reasonably detailed mathematical theory (or more precisely approximation theory) in their development. It comes as no surprise, therefore, that we should find out that the segment of numerical analysis which is concerned with the approximation of partial differential equations has been an area of intense activity over the past few decades, i.e. since the appearance of the electronic computer.

The removal of the necessity to solve partial differential equations analytically in order to use them, which has come with computers, has resulted in a spectacular increase in the spectrum of systems which can be modeled today. But before talking about these recent developments, it seems more than appropriate that we be reminded of the overwhelming role played by partial differential equations in the rise of mathematical physics through the past few centuries.

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**Invited paper

It is in attempting to describe the physical world that scientists of the 18th and 19th centuries were led to the first formulation of partial differential equations. The model of hyperbolic equations is the <u>wave equation</u>.

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} \tag{1}$$

which describes for instance small amplitude vibrations of a taut string. It was first expressed by Jean le Rond d'Alembert in 1747, in what may amount to the "discovery" of partial differential equations [1]. His own description of this discovery in the <u>Encyclopedie</u> reads as follows (d'Alembert refers to himself in the third person) [9]:

> *"Mr. d'Alembert is the inventor of this branch of analysis, without which one could not solve in a rigorous and general manner the problems where one deals with fluid or flexible bodies. This discovery, as important and possibly more difficult than that of integral calculus, has been less spectacular only because its author has expressed an entirely new thing by words and signs already known."*

What is worth noting is that d'Alembert, as most mathematicians of his time, was primarily concerned with finding a mathematical explanation of the physical world, and that he points to the usefulness of partial differential equations in solving new problems of physics as the main (and possibly only) reason for their interest.

This is more than a note of mere historical value: it is difficult , and sometimes futile to think of partial differential equations as abstract mathematical objects. There are many instances where an equation in itself fails to allow for a unique solution or even a solution at all to exist because of ambiguities or contradictions. It is then only by returning to the physical world whence the equation is an abstraction (sometimes imperfect), that those ambiguities and contradictions may be removed, and the intended solution be found. The concept of well posedness introduced by Hadamard at the turn of the century is an expression of this reality, and the recent work of Lax in the solution of non linear hyperbolic equations relies, in the same vein, heavily on physical notions such as entropy to generalize solutions of ideal (but incomplete) equations.

The model of parabolic equations is the <u>heat equation</u>:

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

first derived by Joseph Fourier in the early 1800's. As suggested by its name, it describes in its original derivation the important physical phenomenon of diffusion of heat in solid bodies. That this equation is an idealization can be inferred from the fact that it implies infinite speed of propagation of information.

The model of elliptic equations is Laplace's equation (sometimes called the potential equation):

$$\nabla^2 v = \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2} = 0 \qquad (3)$$

An important difference between this equation and the preceding two is that none of the independent variables (x, y and z) can be associated with Newtonian time as we perceive of it through our own cognition of the physical world. By contrast, parabolic and hyperbolic equations are generally associated with phenomena which are evolutionary in their very nature, and the variable t in (1) and (2) is indeed intended to denote a non-reversible time-like variable.

Elliptic equations appear in the description of several dimensional steady state (i.e. time-invariant) fields of different physical origin. For instance, Fourier's heat equation in three spatial dimensions and time is:

$$\frac{\partial u}{\partial t} = \sigma\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}\right) \qquad (4)$$

from which one may conclude that a steady-state temperature distribution must satisfy (3) (from $\partial u/\partial t = 0$).

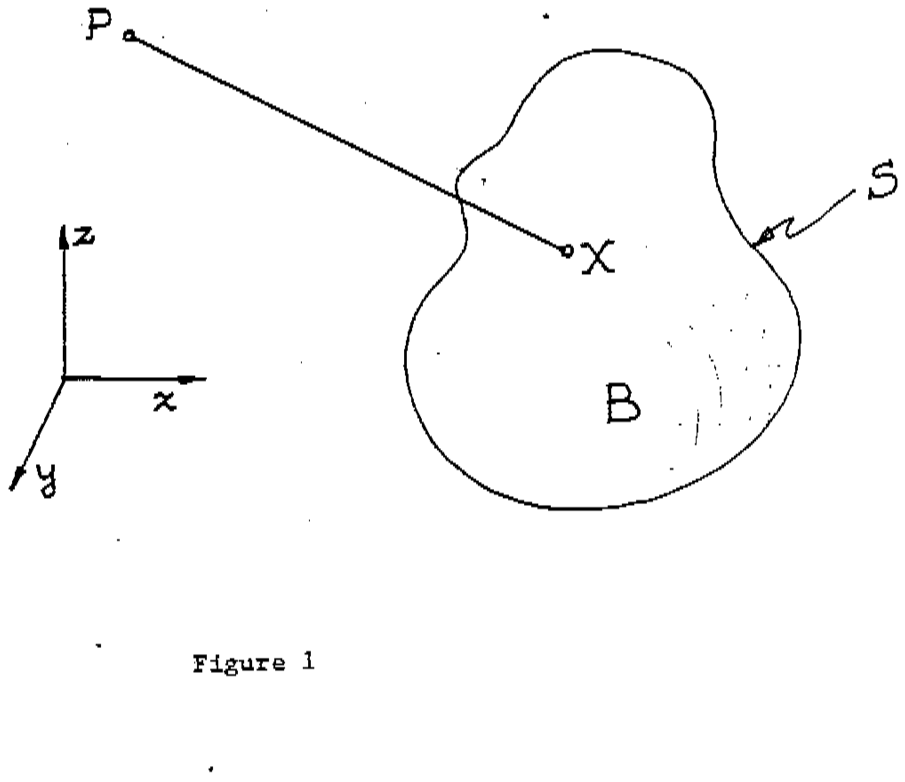

Figure 1

Elliptic equations were known well before Fourier's time. One of the ways in which they came about was in the extensions by eighteenth century mathematicians of Newton's law of gravitation to cases where masses cannot be considered as point-concentrated. In modern notations, the original formulation of the inverse square law of attraction states that the gravity vector in a point P external to a body B (figure 1) is given by the integral equation

$$\vec{g}_P = -k \iiint_B \rho(x,y,z) \cdot \frac{\overrightarrow{(P-X)}}{|P-X|^3} dxdydz \tag{5}$$

where

$$\vec{P} = \begin{vmatrix} x_p \\ y_p \\ z_p \end{vmatrix} \; ; \; \vec{X} = \begin{vmatrix} x \\ y \\ z \end{vmatrix}$$

This integral must be evaluated separately for each external point P. It was discovered, however, that $\vec{g}_P$ could be defined as minus the gradient of a <u>potential function</u>:

$$\vec{g}_P = -\nabla V \tag{6}$$

and, remarkably, that V satisfies the "potential-equation" (3). This was formalized in the last quarter of the eighteenth century by Laplace, whence the name of <u>Laplace's equation</u> given to (3). The important consequence of this is that if V can somehow be computed on the external surface S of B, then computing the gravity vector in any point exterior to B can be obtained by merely solving Laplace's equation as an exterior problem subjected to the given boundary condition on S: It was then shown that V_S may be computed by evaluation of the integral:

$$V_S = \iiint_B \frac{\rho(x,y,z)}{|P_S-X|} dxdydz \tag{7}$$

whence completing a mathematical formulation of the question.

As is often the case with names, Laplace's equation was not discovered by Laplace: it had probably been used at first by Euler in the 1750's. In 1752 he published a paper dealing with the motion of incompressible fluids, in which he defines a potential function from which velocity may be derived:

$$\text{velocity} = -\nabla V$$

and in which he showed that conservation of mass implies that V must satisfy equation (3), later to be known as Laplace's equation.

The next important step in the formulation of gravitation theory and elliptic equations came in the 19th century, when Poisson showed that for a point P located <u>inside</u> of B, the gravity potential does not satisfy (3), but obeys

$$\nabla^2 V = -4\pi\rho \tag{8}$$

to be known as Poisson's equation. This completed the transformation of the expression of the law of Newtonian gravity of distributed bodies from its original integral formulation to the analytically more convenient differential formulation. (It should be noted with interest that numerical analysts have attempted recently to approximate elliptic equations by returning to their integral equation formulation.)

By the end of the 19th century partial differential equation had been used to describe viscous fluid motion (the Navier-Stokes equations, as they are known today), hydrodynamics (e.g. the shallow wave equation), sound propagation, elasticity, electromagnetic theory (Maxwell's equations, which were to play such an important role in the theory of relativity and modern physics). They had become one of the most fundamental tools of mathematical physics.

PROBABILITY DENSITY FUNCTIONS

Up to the middle of the nineteenth century, the dependent variable of partial differential equations was meant to represent physical, measureable, deterministic quantities. An important development came with the introduction of the concept of probability density function. This occurred in the context of questions in thermodynamics such as the kinetic theory of gases and the theory of heat. The names of Maxwell, Boltzmann and Gibbs (the father of statistical mechanics) are associated with these developments. The rise of atomic physics in the first half of our century borrowed heavily on these ideas. The wave function of subatomic particles obtained as the eigenfunctions of Schrödinger's equations were interpreted by Max Born (1926) as being directly associated with the probability of presence of those particles, in a step that was to play an important role in bridging the gap between particle and wave theories of matter. More recently, statistical distributions and partial differential equations have been used to describe the evolution or randomly perturbed dynamical systems. The Fokker-Planck-Kolmogorov equation is parabolic, describing the evolution of a probability function in phase space as a diffusion process. (The "fundamental" paper of Kolmogorov was published in 1931 [2] - see also [3]). Norbert Wiener was also to play an important role in these theories.

THE IMPACT OF COMPUTERS

Mathematical models are useful only to the extent that their solution can be obtained. The appearance of electronic computers, capable of generating numerical solutions without concern for their analytic form has extended the range of applicability of models formulated as partial differential equations far beyond the few which could be solved analytically, thus opening the door to the usefulness of modeling much more complicated systems, and to a host of new applications.

Progress in those applications has been measureable by the ability of researchers to formulate new mathematical models, by the efficiency of computer algorithms to approximate them numerically, and by the size and speed of computers available for their solution.

The development of computer algorithms and methods has occupied recently schools of numerical analysts and engineers.

As for computers, one would not be far from the truth by asserting that one of the important forces behind the development of the large scientific electronic computers used today was the existence of large, complex systems described by partial differential equations whose solution had significant enough ramifications to justify multi-million dollar investments.

As new generations of larger and faster computers saw the light, more ambitious studies involving more complex mathematical models were soon to be formulated. It is, in this respect, almost amusing to look back at some of the commentaries about electronic computing that were made in the 1940's. We read for instance the following, written by Von Neumann on the occasion of one of the several Seminars on Scientific Computation that were organized by IBM (this one was in 1949 [15]):

> *"A major concern which is frequently voiced with very fast computing machines, particularly in view of the extremely high speeds which may now be hoped for, is that they will do themselves out of business rapidly".*

He then goes on expressing the opinion that this would not happen, and cites problems involving partial differential equations as the only examples of those "likely to be of the right size for fast machines", namely:

1. Problems in hydrodynamics
2. Problems involving the interaction of hydrodynamics with chemical or nuclear reaction kinetics
3. Determination of wave functions in quantum mechanics.

As in many (though not all) of his predictions, he was to be right. Successive generations of large scientific computers, up to today's machines with several million words of fast memory and speeds in the range of 10^2 MOPS (millions of operations per second) such as the Texas Instruments ASC are used to a large extent to solve partial differential equations.

No less amusing to us is another view of the 1940's, this one in the famous 1946 Burks, Goldstine and Von Neumann report on the "Logical Design of an Electronic Computing Instrument", discussing memory requirements for solving partial differential equations [5]:

> *"We consequently plan a fully automatic electronic storage facility of about 4000 numbers of 40 binary digits each..... We believe that this memory capacity exceeds the capacities required for most problems that one deals with at present by a factor of about 10 (!)."*

That even the most modest of today's users would find 4000 words of fast memory lamentably deficient demonstrates how much computers have allowed researchers to become ambitious in their expectations, not that Von Neumann *et al's* evaluation was incorrect.

NUMERICAL METHODS IN THE PRE-COMPUTER DAYS

Numerical and graphical methods for partial differential equations predate computers. What may be considered as one of the first such tools is that of Junius Massau who, in 1899 described the method of characteristics for the graphical solutions of hyperbolic equations [16]. This method has been widely used by hydraulic engineers early in this century to study transients in channels and pipes.

What is considered as one of the first descriptions of truly numerical methods was given by L. F. Richardson. In a paper presented in 1909 [21], he describes well what the state of the art was among engineers at the turn of the century:

> "*The object of this paper is to develop methods whereby the differential equations of physics may be applied more freely than hitherto in the approximate form of difference equations to problems concerning irregular bodies.*"

> "*Though very different in method, it is in purpose a continuation of a former paper by the author, on a "Freehand Graphic Way of Determining Stream Lines and Equipotentials". And all that was there said, as to the need for new methods, may be taken to apply here also. In brief, analytical methods are the foundation of the whole subject, and in practice they are the most accurate when they will work, but in the integration of partial equations, with reference to irregular-shaped boundaries, their field of application is very limited.*"

> "*Both for engineering and for many of the less exact sciences, such as biology, there is a demand for rapid methods, easy to be understood and applicable to unusual equations and irregular bodies. If they can be accurate, so much the better; but 1 per cent would suffice for many purposes. It is hoped that the methods put forward in this paper will help to supply this demand.*"

It is remarkable how much these comments remain applicable almost three quarters of a century later and, unfortunately, how many of today's numerical analysts have a much poorer perspective than Richardson had of what they aim at (or should aim at) in terms of overall accuracy.

On the more theoretical side, the now famous Courant, Friedrichs and Lewy paper of 1928 contributed a considerable amount of insight into the properties of difference approximations of partial differential equations. While the authors' objective in that paper was not computation but existence of solutions, their work became in the 1950's one of the starting points of the many studies of convergence of numerical finite difference methods used with computers.

That approximate methods for partial differential equations were of more than academic interest in precomputer days is well illustrated by the number of those whose name remains attached to basic methods in use today. Among those Rayleigh, Ritz and Galerkin hold an important place.

THE FINITE ELEMENT METHOD

Progress in the numerical or "discrete" approximation to partial differential equations had been more or less evolutionary, from a slow start in the pre-computer days, gaining momentum over the past three decades or so. The advent of the finite element method, which had been lingering since the 1940's but got its real start in the 1960's came close to a revolution or a "revival" [10].

Attempts to explain the success of this method are based on a variety of arguments. Many of them, those used mostly by the more theoretically inclined, are based on justified claims of a better accuracy over conventional finite difference techniques. (e.g. the property of "superconvergence" for second order elliptic problems.) There is however another argument which, in our opinion is at least as cogent: the numerical approximation of partial differential equations consists in two steps, viz. the formulation and the solution of discrete equation. Whereas with finite difference methods the solution step is in general the only one to be computerized, the better part of the formulation can be likewise automated within the finite element method.

A large number of operations having to do with bookkeeping and somewhat trivial "assembling operations" (rather than actual computation, in the "number crunching" sense) can be delegated to the computer in the finite element method much more conveniently so than with the older finite difference techniques. Flexible, general purpose codes can be constructed. Examples are the several structural analysis packages such as ASKA (Automatic System for Kinematic Analysis, Institute for Statics and Dynamics, Stuttgart, West Germany), STRUDL (Structural Design Language, Integrated Civil Engineering System, MIT), SAP (Structural Analysis Program, University of California, Berkeley), NASTRAN (Nasa Structural Analysis, developed for NASA by R. H. MacNeal and co-workers), and many others which are in current use today.

The age of these codes, which came when large computers with sizeable memory at reasonable cost and sophisticated graphic displays had just become available, reflects their obvious dependence on hardware.

APPLICATIONS

A true measure of the impact of partial differential equations in modeling for science and engineering is obtained by reviewing some of their applications:

CHEMICAL AND PROCESS ENGINEERING

The mathematical model of large chemical production units and subcomponents such as packed bed reactors, tubular reactors, heat exchangers and the like are replete with partial differential equations. The physical laws, correlations and mathematical equations leading to such models is well illustrated by the diversity of subjects covered in the book "Transport phenomena" by Bird, Stewart and Lightfoot which is to be found on the bookshelf of almost every chemical and process engineer. The importance of developing "simulations" has resulted in the fact that much of the early work in the development of practical numerical methods for partial differential equations was carried out by chemical and process engineers. (See e.g. Lapidus [12]).

NUCLEAR PHYSICS AND ENGINEERING

I have already mentioned the role of partial differential equations in the development of mathematical models of the atom.

Engineering aspects of nuclear power have generated over the years a remarkably large number of problems involving somewhat similar mathematics. The late 1940's and early 1950's were years in which large nuclear reactors of the fission type were being designed. Neutron diffusion in such reactors' core is described by sets of parabolic equations; heat flow is described by both parabolic equations and (in relation to transport by coolant) hyperbolic equations.

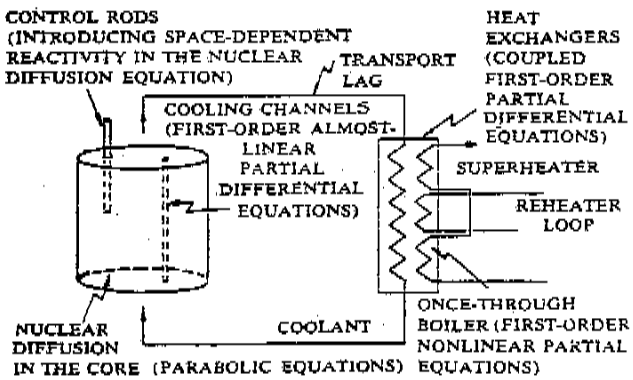

Figure 2 — Simplified schematic of the nuclear-thermal part of a gas-cooled nuclear power plant.

Fundamental mathematics in the description of the steady state and transient behavior of nuclear fission reactors was well developed by the early 1950's, as illustrated for instance by the variety and completeness of topics to be found in Glasstone and Edlund's book "Elements of Nuclear Reactor Theory", published in 1952. The first use of partial differential equations in this context is probably that found in Szilard's work of the 1930's, including several of his patents of nuclear reactors (and bombs), containing the supporting partial differential equations of neutron diffusion to prove the feasibility of those devices (see Collected Works of Szilard [24]).

Many of the actual calculations dating from the early days of nuclear power were done with the aid of computers, in which Von Neumann was to play an important role. Partial differential equations occurring in the engineering design of large fission reactors led to the use of methods of the variational and Galerkin type, implemented on large computers of which CDC's 6000 series (in the mid 1960's) is illustrative. Analog and hybrid computers also held an important place in carrying out those calculations, in particular during the late 1950's and 1960's in Europe where many nuclear-electric power plants were under construction. (see e.g. [26] and references cited.)

Research in the area of fusion reactors for power generation, which is currently funded at a rate of the order of 10^9 dollars/year depends on theory and experiment. The theory relies heavily on partial differential equations in its mathematics. Here too, computers are an important tool. Computer simulations are so large and expensive that considerable effort went into the development of efficient algorithms, such as the "fast" methods to solve Poisson's equation used in plasma simulations [15].

BIOLOGY

Mathematical biology is a relatively recent discipline, dating mostly from the earliest part of this century. This field is replete with examples of diffusion (substances in biological liquids and in capillaries), flows (blood flow and its interaction with flexible boundaries), waves (the propagation of excitation along nerves), all phenomena described by partial differential equations.

Many of the investigations in biophysics based on anlytic solutions may be found in Rashevsky (1938). Recent investigations relying heavily on computer simulations are illustrated by simulations of the nerval system, studies of oxygen concentrations in the brain, dynamics of the cochlea and extensive studies of blood flow to name a few.

MODELING OF THE ATMOSPHERE AND NUMERICAL WEATHER PREDICTION

The possibility of simulating the atmosphere for weather prediction was suggested by Richardson in the 1920's [22]. The first successful numerical "forecast" was implemented by J. G. Charney in 1948 on the ENIAC Computer. The first weather forecasting group to use computer forecasts "operationally" was established in the late 1950's in Suitland, Maryland [17].

Considerable work is being done today in that direction, involving efforts of large research centers such as the National Center for Atmospheric Research (NCAR) in Colorado and the NOAA Geophysical Fluid Dynamics Laboratory in Princeton, N. J. among others.

FLUID DYNAMICS

Partial differential equations and fluid dynamics are in many respects inseparable. Models of compressible and compressible flow have been used in almost every area of the physical and engineering sciences. Many analytical methods were developed for the solution of fluid flow equations (e.g. Jukowski's transformation well known to Aerodynamicists). As we come to recent years, much of the analytical work has been replaced by computer solutions: the name "Computational Fluid Dynamics" is often used today.

ENVIRONMENTAL SYSTEMS

Application of partial differential equations to model flows and waves in channels and rivers held an important place in the development of hydraulics through the nineteenth century. Protection of the environment which has become a topic of great concern has resulted in an increasing number of recent studies, most of them using computers, in which surface water, groundwater, ocean dynamics, atmospheric dynamics, pollution and other vital characteristics are modeled. Computer simulations based on those models are at the core of many "Environmental impact studies" on which regulating agencies tend to rely increasingly in their evaluation and decision making process.

SOME CLOSING REMARKS

As with many aspects of mathematical modeling, the occurrence of computers has allowed researchers to become overambitious in their formulation of models expressed as partial differential equations. Whereas numerical solutions may be expensive the fact that limits appeared to be only those placed by such down to earth factors as size and speed of hardware had led some to believe that those limits could be pushed back forever. However, they were soon to be reminded that mathematical models are only models, with their own incertitudes, idealizations and limitations. Whether the partial differential equations used for numerical weather prediction will ever be deterministic enough to predict the weather accurately is in question.

"Environmental impact statements" based on the numerical solution of mathematical models of air, water and earth based phenomena which are used more and more routinely as a predictive tool by protection and regulation agencies depend so much on what the modeler chooses to include in and exclude of his mathematical model that whether or not those simulations tell the exact story often becomes a debated question of opinions about what the premises should be.

The initial use of partial differential equations as mathematical models of reasonably small and controlled physical systems turned out to be among the most successful developments of applied mathematics. Its extension to larger engineering systems, linked with the availability of computers, is playing a key role in the development of our technological world. Attempts to extend this tool to environmental, life and other "softer" phenomena brings to the fore what has become one of the current issues in mathematical modeling: that of relevance, accuracy and "credibility" of the mathematical model.

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