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Ivo Babuška Fifty years of Applications of Mathematics

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FIFTY YEARS OF APPLICATIONS OF MATHEMATICS

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1. Development of applications of mathematics in the last fifty years

It has been fifty years since the journal Applications of Mathematics was founded. The name of the journal is somewhat unconventional compared with traditional titles like Applied Mathematics. What was the reason for the name? The reason was to emphasize the analysis of various physical phenomena in engineering and other fields by proper modeling and mathematics.

In the fifty year life of Applications of Mathematics a scientific revolution occurred. The development of computers changed all fields of applications and applied mathematics, and a new field, generally named computational science, appeared. Computational science concentrates on predicting physical phenomena by mathematical modeling and mathematical methodologies. Engineers, physicists, biologists, and others became, at least partly, computational scientists who can be considered some sort of applied mathematicians. In a strict sense, they are not mathematicians living in the realm of assumptions, definitions, theorems, and proofs; rather they design sophisticated arguments and methods for solving very complex problems. Their arguments are often heuristic, based on intuition and experience; but are verified by computations on benchmark problems. Their arguments, approaches, and methods are often later studied by means of rigorous mathematics, better understood and generalized. As an example, consider the finite element method. It was developed and used by engineers in the 1960's, but the basic mathematical theory was developed only in the 1970's. For the history of the finite element method and its relation to mathematics, see [1]. During the last 50 years, more than 150,000 papers on finite elements have appeared [8], not counting papers in computational fluid dynamics. Most of these papers (and books) are of an engineering nature, addressing numerous applications in various fields. Nevertheless, a significant number of mathematical papers and books have also appeared.

The computer revolution is still going on. Experts [4] predict that the exponential growth of computer power will continue for other 15–20 years. To illustrate this exponential growth over the last one-and-half decades let the 11/780 VAX computer of 1989 serve as the reference unit of computer capabilities. This unit involves one megabyte of memory, a half gigabyte of the disk storage, and one central processing unit (cpu) with the speed of 0.1 megaflops. In 1992 the IBM RS 580 had 54 times the memory of the VAX and its speed was 1000 times greater. In 1997, eight years later, the SGI Power Challenge had 1000 times the memory of VAX, six cpu units with a theoretical speed 18,000 times greater than the 1989 VAX. In November 2004, IBM's Blue Gene/L supercomputer came online with an expected peak performance of 360×10^{12} flops, over a hundred million times faster in unit capability than the 1989 VAX! Today, \$1000 can buy a computer as powerful as the biggest and most capable computer available at any cost in 1990.

An illustration of the influence of the power of computers is the use of the direct method for solving large systems of linear equations stemming from the finite element method. Today, systems with more than 2 million equations of three-dimensional elasticity are solved routinely in industry. This is possible because of the robustness of the direct solvers and computer speed making solution times acceptable.

It is interesting to compare these capabilities with expectations 60 years ago, captured in the following footnotes from the famous 1947 paper by Goldstine and von Neumann [5], Footnote 11: The difficulties of present day numerical methods in the problem of matrix inversion begin to assume very serious dimensions when n > 10. Footnote 12: We anticipate that $n \sim 100$ will become manageable.

2. Are computational results reliable?

As we have seen, the basic importance of computational science has been recognized. The field has great potential in all sciences and engineering disciplines, and its tools make various predictions possible, thus giving support to crucial decisions. However, a question arises: Will computational science, i.e. simulation and mathematics together with computers, fulfil the expectations [10]?

Today's computers are able to solve very complex problems. Nevertheless, the question is whether the computer data provide reliable predictions of the physical phenomena of interest. In this connection we refer to paper [11] that discusses the forthcoming crisis in computational science. Computational science faces three challenges today: (a) The performance challenge; (b) The programming challenge; and (c) The prediction challenge.

The performance challenge is related to the growth of computing capabilities. It is met very well [11]. The programming challenge has been reasonably well addressed and will be met soon [11]. In contrast, to address the prediction challenge still requires considerable advancement and maturity and, according to [11], it is the bottleneck that underlies the potential crisis. Because this prediction challenge is gaining recognition, the field of Verification and Validation is coming to the forefront.

3. VERIFICATION AND VALIDATION (V&V)

Every computational prediction is nothing more than a transformation of available information to desired information via a mathematical problem and input data. Input data are known completely or are known with uncertainties (that must be specified). More precisely, the computational problem is an approximation of the exact transformation mentioned above.

Verification is the process of determining whether the computational problem and the code implementation lead to the predictions with sufficient accuracy, i.e., whether the difference between the approximated and exact solution is sufficiently small. Hence verification has two aspects: the approximation aspect and the verification of the correctness of the code. The first part is the so-called solution verification. It is a multifaceted mathematical problem that includes theoretical analysis of things like the well-posedness of the problem, or a priori and a posteriori error estimations. Note that the existence of the physical problem is not equivalent to the existence of the mathematical problem. It is also often important to estimate the error due to the simplification of the original mathematical problem, which is another mathematical problem. Hence, verification is a purely mathematical problem. In recent years significant progress has been made in the theory and practice of a posteriori estimation. However, it is important to realize that possible agreement of the computational results with experimental data does not guarantee any convergence of computational results.

Validation is the process of determining whether the mathematical problem (model) reliably describes the physical phenomenon of our interest. In contrast to verification, validation is not purely a mathematical problem. It is a conglomerate of mathematics, physics, experiments, statistics and probability, experience, and also some subjective interpretation. Often the validation process is complicated by insufficient experimental data and uncertainties (which influence the formulation of the problem) that are not easy to describe. For more about V&V, including definitions, etc., see [3], [6], [7], [9], [12].

4. Where to go?

Applied mathematics is a tool for solving problems of interest in different fields of reality. Hence, as experience shows, it must be closely related to applications. By this we mean that the problems addressed must be related to the prediction of some physical phenomena of interest and also enable this prediction. Many of today's journals are application or domain specific. The Applications of Mathematics journal has its own niche: the mathematics related more or less directly to applications. This encompasses such different areas of mathematics as modeling, theory of differential equations, theoretical numerical analysis, probability, statistics, and others. Clearly, the last 50 years of developments in computational science have confirmed the correctness of the basic idea behind the foundation of this journal, namely to foster mathematics of applications. Looking briefly at the content of the journal, we see that this direction has been pursued successfully.

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