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Mathematics and Computing[1]

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1. INTRODUCTION

During its spectacular rise, the computational has joined the theoretical and experimental branches of science, and is rapidly approaching its two older sisters in importance and intellectual respectability. Its mark on high technology has been equally great; computational mathematical modeling has, in the last few years, replaced much experimentation, and computing makes it practical to extract hidden information from massive amounts of data by subtle mathematical manipulations. A science of computing is beginning to emerge, like Hercules from its cradle.

In this paper I plan to illustrate, by examples, anecdotes, and theoretical speculations, what mathematics has done for computing, and what computing has done for mathematics.

2. MATHEMATICAL METHODS IN COMPUTING

The rapid rise of computing was made possible by striking improvement in computer hardware, software, and peripherals, and by equally striking improvements in the discretization of the equations that model the physical phenomena, as well as by clever algorithms to solve the discretized equations. The last two named have been as important as the first three; John Rice estimated that the speedup in solving elliptic boundary value problems gained during the years from 1945 to 1975 due to improved numerical methods has been greater than the gain in speed

[1] This paper is dedicated to Nick Metropolis, in recognition of his contributions to mathematics, in particular to the mathematics of computations.

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of the Cray I over the IBM 650. The contributions of mathematics and mathematicians—and of honorary mathematicians like Nick Metropolis—to this process has been crucial; here is a partial list of mathematical ideas that have borne fruit.

The methods of alternating direction and fractional step initiated by Peaceman, Ratchford, Douglas, Yanenko, and Strang are used universally.

High-order difference schemes developed by Lax and Wendroff, MacCormack, and others have been particularly effective in meteorology and are of use for calculating any smooth flow.

The particle-in-cell method, developed by Harlow, has been very effective in problems where two different media are in contact and exert a force on each other, such as in high-velocity impact.

Spectral methods, pioneered by Leith and put on the map by Orszag and Gottlieb, have been made efficient by the use of the fast Fourier transform, introduced by Cooley and Tukey; they are of use in calculating space-periodic flows, both smooth and rough.

Implicit methods: a variety of ideas, introduced by Hirt, Warming, Beam, Hardned, and others have proved effective in both incompressible and compressible flow calculations, as well as in magnetofluid dynamics.

The vortex method of Chorin generates and propagates vorticity in a very original fashion. The method has been very effective in calculating effects that depend sensitively on vorticity, such as drag at high Reynolds numbers. The method has been used by Peskin to calculate flows around valves, real and artificial, in the beating heart.

The method of complex coordinates, developed by Garabedian, allows a unified treatment of subsonic and supersonic regimes in flows, and has been used successfully to design shockless transonic airfoils, compressor blades, and turbines.

The multigrid method suggested by Federenko and Bahvalov, and developed by Brandt, is an extremely rapid method for solving elliptic equations with variable coefficients.

The capacitance matrix method of Widlund exploits the fast algorithm for solving Poisson's equation in rectangles, developed by Bunemann and Hockney, to solve Poisson's equation, and related ones, in more general geometries.

The challenge of calculating flows with shocks has generated a number of mathematical ideas. One line of thought, shock capturing, started with v. Neumann and Richtmyer's notion of artificial viscosity; to this was added the notion of difference equation in conservation form with numerical flux function and Godunov's idea of threading together solutions of the Riemann initial value problem. Glimm's method is also based on solutions of Riemann problems; it employs a sequence of random parameters and has the virtue of calculating entropy production more realistically than other methods that employ an artificial viscosity. Chorin noted that this feature of the method makes it a good candidate for calculating reacting flows.

The far-reaching modification that Van Leer, Colella, and Woodward have made of Godunov's method has resulted in astonishingly accurate calculations of very complicated patterns of shocks.

The method of flux-corrected transport, developed by Boris and Book, and artificial compression, developed by Harten, are successful in resolving discontinuities, both contact and shock, that develop in flows of compressible, multimedium fluids.

Jameson has developed intricate, rapidly convergent iterative techniques for the calculation of steady transonic flow fields with shocks around complicated aerodynamic shapes.

An alternative to shock capturing is shock tracking, pioneered by Moretti, Richtmyer, and Lazarus, greatly advanced by Glimm and McBryan, and recently by Colella.

The finite element method is a significant alternative to finite differences, more able to cope with complicated geometrical configurations.

Last but not least, we mention the Monte Carlo method.

3. EXPERIMENTAL COMPUTING

In a prophetic lecture delivered in Montreal in 1945, see Ref. 10, v. Neumann concluded that "really efficient high-speed computing devices may, in the field of nonlinear partial differential equations as well as in many other fields which are now difficult or entirely denied of access, provide us with those heuristic hints which are needed in all parts of mathematics for genuine progress."

In precisely this fashion have Fermi, Pasta, and Ulam[2] discovered the remarkable, almost periodic, behavior of the vibrations of nonlinear chains, and Kruskal and Zabusky the generation and interaction of solitons. The complete integrability of the Toda Lattice became plausible through very careful numerical calculations by Joe Ford;[3] Mitchell Feigenbaum discovered his remarkable universal laws on iterations by analyzing numerical experiments. Numerical studies led Lorenz[8] to the concept of a strange attractor; the understanding of chaotic behavior of simple dynamic systems coexisting with islands of stability has been much enhanced by numerical studies. Not a bad prediction by v. Neumann, especially since the computers he spoke of in 1945 were then merely figments of his imagination.

Already Legendre and Gauss used tables of primes to guess the asymptotic distribution of prime numbers; with the advent of modern computers the quest for asymptotic laws can be and is pursued with a vengeance. So are the roots of Riemann's zeta function; recently van de Lune and te Riele have shown[12] that the zeta function has exactly 300,000,001 zeros whose imaginary parts lie between 0 and 119,590,809.282, and all of them have real part 1/2.

In Ref. 9, Mostow did a lot of computing to construct fundamental domains for certain special discrete groups; the computations do not enter the final proof but were essential in discovering what was to be proved.

In Ref. 11, Phillips and Sarnak used numerical computations to estimate the lowest eigenvalue of the Laplace–Beltrami operator; they were able to prove mathematically the phenomena discovered experimentally.

Many other examples, in geometry, in combinatorics, can be given of successful computing for gaining insight. Experimental computing has truly become a way of life in most branches of mathematics.

4. HOW MUCH CONFIDENCE CAN ONE PLACE IN A COMPUTATION?

There are many kinds of computations and many kinds of confidences.

(a) Some computations are part of the logical structure of a proof. If real numbers are used, the computations have to furnish ironclad bounds such as are provided by interval arithmetic; we give some examples:

i. Lanford[5] proves Feigenbaum's conjectures concerning iterates of a map. The conjecture states, roughly, that high-order iterates of all unimodal maps of an interval into itself, when rescaled appropriately, have very nearly the same shape. This shape is characterized by a functional equation of the form

$$Tf = f$$

Lanford proves the existence and stability of a fixed point f by first computing, by iteration, an approximate fixed point f_ε and then demonstrating the contractive character of a quasi-Newton type iteration in some neighborhood of f_ε.

ii. In Ref. 1, Curry studied the quadratic map

$$T\colon (x, y) \to (1 + y - ax^2, bx)$$

originally investigated by Henon. Among other things, he was looking for transverse homoclinic points, i.e., the transversal intersections of the stable and unstable manifolds issuing from fixed points of T. Such an intersection can be rigorously shown to take place, provided that one can generate enough approximate points on the stable and unstable manifolds, with guaranteed accuracy, a nontrivial task because of the inherent instability of iterating the mapping T.

iii. The most famous proof relying on machine computations is Haken and Appel's celebrated proof of the four-color theorem. Here all the needed calculations are discrete and can be carried out with absolute accuracy. This proof has been criticized by some for providing no insight why the result is true; this criticism is valid, but can be leveled with equal force against many other proofs which employ no computer. Others have criticized the proof because it is so difficult for a single reader to verify its correctness; true, but equally true of other, hand-carved, elaborate arguments extending over thousands of pages. There are also some who refuse on principle to accept a computer-assisted proof. This strikes me as headed in the wrong direction; after all, logicians agree that an unassailable mathematical proof is one executable by a Turing machine. There is something faintly ridiculous about holding up as the epitome of exactitude proofs carried out by imaginary computers and then balking at a proof carried out by a real one.

(b) Many, perhaps most, calculations are carried out to provide quantitative information about problems that are reasonably well-understood theoretically, such as initial and boundary value problems for ordinary and partial differential equations which have been shown to have unique solutions that depend continuously on the data. When solving such problems approximately we are looking for realistic, rather than ironclad, error estimates.

Realistic error estimates are, alas, not easy to come by for problems of real interest, so one proceeds otherwise. A sequence of descretized problems is set up, depending on one or several parameters Δ which measure the scale of discretization; the solution of the discretized problem is denoted by u_Δ. We require the scheme to be stable and to be compatible with the original problem; stability means that the u_Δ remain bounded as Δ tends to zero; compatibility means that if a sequence u_Δ converges in some topology as Δ tends to zero, its limit is a solution of the original problem; see Ref. 7.

It is easy to show that if all u_Δ are contained in a compact set, then the scheme converges. Compactness, however, does not always hold, and even where it does it is hard to prove. Stability, necessary for compactness, is not easy to prove either but al least we possess a number of heurisic criteria of practical value. Experience shows that stability and compatibility are valuable design principles for discretizing well-posed and reasonably well-understood problems.

(c) There is a large class of calculations, perhaps larger than we suspect, whose significance is only statistical. The investigations of the behavior of the iterates of volume preserving and other maps belong to this class. On chaotic regions, high-order iterates of such maps depend extremely sensitively on the starting point. For example, Curry[1] has found that when Henon's map T, described in paragraph (a), is iterated 60 times on a Cray 1, the outcome is completely different from the same calculations carried out on a CDC 7600; this is due to the difference in the manner in which the two computers round. Clearly, one cannot compute a sequence of thousands of iterates of such transformations. Nevertheless, for transformations about which theory has something to say, numerically computed strings of pseudoiterates behave very much as genuine iterates are supposed to. For instance, KAM theory asserts that for a Hamiltonian flow that differs little from a completely integrable one, most of the trajectories lie on tori of lower dimension. The classical calculations ɔf Henon and Heiles[4] bear this out; they deal with a Hamiltonian that is the sum of a quadratic and a cubic term, in four-dimensional phase space. For flows with low energy, the cubic terms are negligible; for these the pseudoiterates of the Poincaré map associated with the flow lie along smooth curves. For flows with medium energy, a portion of pseudoiterates of the Poincaré map lie along smooth curves; the rest are scattered chaotically. At high energy the pseudoiterates are completely chaotically distributed.

How to explain this behavior of pseudoiterates? Suppose for simplicity that the transformation T in question maps the n-dimensional torus into itself. A computer operating with N digit numbers maps n cubes of side length 10^{-N} into cubes of the same size. Denote this transformation by T_N. Numerical experimentations suggest that iterates of such approximations T_N behave, in a sense to be made precise, like iterates of the transformation T which they approximate. In fact, if this were not so, at least in an overwhelming number of cases, it would serve no purpose at all to carry out numerical experimentations!

A result of the above type would be like the KAM theory, with the additional complication that the perturbation that changes T into T_N changes the domain of the map from a manifold to a finite set. No such results are known; I would, however, like to call attention to Ref. 6, where it is shown that if T is volume-preserving, T_N can be chosen to be volume-preserving too; this is a result in the right direction, but far from what is wanted.

(d) An increasing number of calculations attempt to deal with unstable phenomena, such as the interface instabilities of Helmholtz and Rayleigh–Taylor, turbulent flows at high Reynolds number, turbulent multiphase flows, and turbulent combustion. Calculations of this kind typically contain algorithms that are discrete analogues of physical processes. The success of such modeling is measured by the extent to which the approximate flow patterns resemble actual flows observed in laboratories and in nature. There is nothing wrong with such a criterion; a scheme which fails in comparison with reality has to be rejected resolutely. Yet there is something unsatisfactory when a computational scheme usurps the place of a theory. The discrete calculations ought to be the shades cast by a Platonic continuum theory of unstable phenomena.

As more researchers carry out more and more numerical experiments, looking for guidance, it is inevitable that some will be misguided. A spectacular example from the past concerns the distribution of prime number. The number of primes less than x, denoted as $\pi(x)$, is, according to the Prime Number theorem, asymptotic to $x/\log x$. Already Gauss has suggested that the logarithmic integral, denoted as $li(x)$ and defined by

$$li(x) = PV \int_0^x \frac{du}{\log u}$$

is in some sense a better approximation to $\pi(x)$ than $x/\log x$. Numerical experiments suggest that this is indeed so; furthermore, for all values of x for which $\pi(x)$ has been computed, it appears that

$$\pi(x) < li(x)$$

This was generally believed to be true for all x, until Littlewood, in 1914, proved the contrary: $\pi(x) > li(x)$ for infinitely many values of x.

Littlewood's proof was indirect and gave no indications where the first violation might occur. A student of Littlewood's came up with a constructive proof that there is a number x less than 10 raised to the power 10 four times, for which $\pi(x) > li(x)$. Later research whittled this number down somewhat, but still way out of the range for which $\pi(x)$ is expected in the foreseeable future to be computed exactly.

REFERENCES

1. J. Curry, *Comm. Math. Phys.* **68**:129–140 (1969).
2. E. Fermi, J. R. Pasta, and S. M. Ulam, *Studies of Nonlinear Problems* (LASL Report LA 1940, 1955); also, *Nonlinear Wave Motions*, Lectures in Applied Mathematics, vol. 15, Alan Newell, ed. (AMS, 1974).
3. J. Ford, *Fundamental Problems in Statistical Mechanics*, vol. 3, E. D. G. Cohen, ed. (North Holland, Amsterdam, 1985).
4. M. Henon, and C. Heiles, *Astron. J.* **69**:73–79 (1964).
5. O. E. Lanford, *Bull. Amer. Math. Soc.*, **6**:427–434 (1982).
6. P. D. Lax, *Comm. Pure Appl. Math.* **XXIV**:133–135 (1971).
7. P. D. Lax and B. Wendroff, *Comm. Pure Appl. Math.* **13**:217–237 (1960).
8. E. N. Lorenz, *J. Atmos. Sci.* **26**:130–141 (1973).
9. G. D. Mostow, *Pacific J. Math.* **86**:171–276 (1980).
10. J. v. Neumann and H. H. Goldstine, On the principles of large scale computing machines," *Collected Works*, vol. V (Pergamon Press, The MacMillan Co., New York, 1963).
11. R. S. Phillips and P. Sarnak, (to appear).
12. J. van de Lune and H. J. J. Te Riele, *Math. Comp.* (to appear).