Computation – The new mathematics for sciences

N. D. Hari Dass

Institute of Mathematical Sciences, CIT Campus, Taramani, Chennai 600 113, India

COMPUTATION is actually old mathematics, in fact very old and basic, consisting of the basic operations of arithmetic, viz. addition, subtraction, multiplication and division. What is new is the tremendous speed with which these basic operations can be carried out on modern computers and supercomputers. The fastest supercomputer today, the BlueGene, can perform 70 thousand billion such operations in a second (70 Teraflops). The supercomputer KABRU, self-assembled at the Institute of Mathematical Sciences, Chennai, can perform at a Teraflop level.

Strictly speaking, the word computation can mean any logical operation even if it is very abstract. Here we are using it in the sense of an operation on a computer. Computers themselves can be of radically different types. The most familiar are the digital and analogue computers. The latter make use of the fact that certain physical quantities obey certain mathematical equations and by directly measuring the physical quantity in question, one obtains the solution for the relevant mathematical equation. In other words, one has 'computed' the solution. An illustrative example is the current in an electrical circuit made up of resistors, capacitors and the so-called inductors; the current is a solution to a differential equation whose parameters are determined by the capacitance, resistance and inductance of the circuit. By varying these, one has a whole family of differential equations whose solutions, represented by the current, can simply be measured directly or even graphically displayed on an oscilloscope.

In the case of the digital computer all mathematical manipulations are broken down to the basic operations of arithmetic, which are then carried out by specific pieces of hardware. There are other types of computers that have been thought about lately like the DNA-computer and the chaotic computer. In fact a computer has been built out of water pipes and junctions! Basically any physical phenomenon that 'simulates' the basic operations of arithmetic can be used to build the 'gates' of a computer. But the range of computations that can be done speedily is rather limited on analogue computers, at least for the moment.

Before discussing the significance of the tremendous speeds of computers that have jettisoned the computational methods to the forefront, it is worthwhile commenting on the 'reliability' of computers. After all, every form of computer mentioned before is made up of physical components that are liable to have fluctuations in their responses or even liable to breakdowns. How then can one rely on the results obtained on a computer? To drive the point home, in the case of the analogue computer, the resistance, for example, can have small fluctuations or could be affected by the heating of the elements due to the flowing current. This would certainly introduce errors in the computations. As the celebrated mathematician-physicist and the founder of modern computers, John von Neumann, put it, 'Can we build a reliable computer out of unreliable components?' This leads to the notion of fault tolerance which is achieved by either choosing components that have the desired level of reliability or even better, through very ingenious means of 'error correction'. These error-correcting techniques are in fact what allow us to have a clear phone conversation over a noisy channel. The modern supercomputers can perform hundred billion billion operations without a single error!

So what is the significance of such tremendous speeds for scientific investigations? To appreciate this it is instructive to say a few words about the alternative to numerical computations on a computer, namely, the so-called 'analytical' calculations. Here the aim is to derive formulae for various quantities of interest even though such formulae involve lot of approximations and even questionable metamorphosis of the basis framework (theory, model, etc.) itself. This is often considered more satisfactory than a numerical evaluation because of the belief that 'a single formula is worth more than a million numbers' somewhat similar to the adage that 'a picture is worth more than a thousand

But like all adages and beliefs this too hides more than what it reveals. Not all pictures are worth more than a thousand words nor all formulae worth more than a million numbers. What is of prime importance is, of course, the quality of numbers versus the quality of the formula. Besides, as Hamming has aptly said, 'the objective of computations is insight and not numbers'.

Many times, even when one has a formula for a quantity of interest, it is difficult to extract the desired information in a straightforward manner. For example, if it is known that the quantity of interest is the lowest zero of a theta function, no formula may be available for it explicitly despite one having an 'analytical result'. In such cases one can use computers for a numerical evaluation of the result.

But this is not where the real impact of the great strides made in computation manifests itself. That occurs in what

e-mail: dass@imsc.res.in

are called numerical simulations. Here one tries to actually simulate a system or some controlled approximation to it directly on powerful computers. To give an example that should be familiar to all, we can consider an accurate simulation of the motion of the planets of the solar system. While the motion of a single planet around the Sun as given by Newton's and Kepler's laws can be solved analytically in terms of simple formulae, the mere inclusion of a third body, say, Jupiter, makes an exact solution intractable and there are reasons to believe that this problem cannot be solved at all. Adding all the other planets and their moons aggravates the problem that much more. So one need not go to black holes or string theory to encounter mathematically very challenging problems.

However this problem can be simulated on a computer if we are willing to replace the continuum of time by grid of discrete points with the simulations becoming more and more reliable as the grids are made finer and finer. The grids can be made finer only at the cost of vastly increased computer resources both in terms of speed and of memory. The necessity of discretizing time arises as we can only deal with a finite, though very very large, number of quantities on a computer. The great speeds in computation allow, for example, to simulate the motion of all planets over several billion years in a very short time.

Today the repertoire of the class of problems that can be numerically simulated is really vast. It includes problems like turbulence in fluid flow (still an unsolved problem in the analytical sense), large scale weather forecast, behaviour of biomolecules, *ab initio* study of chemical reactions, black hole dynamics, problem of quark confinement (yet another outstanding problem of theoretical physics), quark-gluon plasma which was the state of matter in early universe, and many more.

While the simulation of planetary motion involves transcribing Newton's laws for the planets to discrete grids, simulation of the problem of quark confinement is made possible by exploiting some remarkable structures of quantum field theory whereby a quantum mechanical problem can be simulated to desired accuracy on a classical computer. Another important distinction between the planetary motion simulation and simulation of quantum field theories is that the former is deterministic while the latter is probabilistic. This means the simulation algorithm produces results according to some probability law and this is just what the laws of statistical mechanics are all about. For the simulations to be reliable one needs to understand subtle issues like ergodicity and ensure that the simulations are consistent with these principles.

The stochastic or probabilistic simulations heavily use techniques of statistical mechanics. Even though the list alluded to earlier includes areas that are vastly different, what is remarkable about them is the surprising similarity of computational techniques used. For example, the techniques of Monte Carlo or molecular dynamics are used for studying nonabelian gauge theories of particle physics as well as to study dynamics of polymers. In fact the most striking aspect of computations in science is the universality of computing techniques for very diverse applications. This helps scientists to overcome traditional barriers and boundaries and to realize science as one undivided path to understanding nature.

Be it elementary particle physics, hydrodynamics, biological systems or any of the many areas where computational approach has made a big impact, a formidable challenge is to understand phenomena over vastly differing scales in a mutually consistent unified manner. For example, knowing that all matter is made up of atoms, how do we understand the bulk properties of matter? Or knowing that all neutrons and protons consist of quarks how do we understand the forces that bind nuclei? Knowing that cells constitute living beings, how do we understand the texture of muscle tissues? This problem of relating phenomena at many different scales is a recurring theme in all sciences. On the analytical side, it is very difficult to make much progress on this front in a quantitatively precise way though physics is full of instances where ingenious insights have paved the way, as in Feynman's theory of superfluid helium or in the BCS theory of superconductivity, etc.

It is this multi-scale facet that can be most efficiently studied using numerical simulations. One way to do this is to distil from simulations at a particular scale, the relevant degrees of freedom at that scale and use these as the atomic constituents for simulations at a larger scale and iterate this procedure. This is not an approach that can be applied in a purely mechanical manner as it needs ingenuity in identifying the so-called relevant degrees of freedom at each scale. It is however possible to do the so-called multiscale or multigrid simulations whereby one can study phenomena at several scales simultaneously. In such a multiscale simulation, variables at many different scales are simultaneously manipulated which allows one a grand view of the problem across many scales.

I would like to illustrate the nature of this multiscale phenomenon with an example. Let us consider water and look at it at different scales. At one level we can understand it as a molecule of two hydrogen and one oxygen atoms. At this level we understand its structure to be that of a tetrahedron. But if we pack a lot of such water molecules together, they start forming long chains (polymerization is the technical description) and the behaviour of water is now governed by the string-like constitution. Depending on the temperature this assembly behaves like a liquid or like a complex solid called ice with varied crystalline structure. Inside a living cell, in the vicinity of biomolecules like DNA and proteins, the very structure and properties of water get modified which in turn has profound implications for the behaviour and functionality of the biomolecules. Thus the same entity, water, has vastly different properties at different scales. It makes more sense to view these properties as 'emergent', arising out of the nature of assembly, rather than as a property encoded in the microscopic constituents.

Another important reason why simulations are becoming indispensable is that the parameter space available to real experiments is restricted while in simulations one could probe arbitrary regions of the parameter space. To illustrate this we could go back to our example of the planetary system. There are peculiar phenomena like the moon always showing the same face to the earth which arise out of special confluence of parameters. To get a proper understanding of this would require studying what would happen when the parameters take more general values. But that is beyond the realm of actual experiments but is easily accessible to simulations. There are even more complex systems where this aspect of simulations becomes crucial.

Here are some of the major results that have been obtained through simulations that were not obtained through other mathematical techniques. I give only a very partial list here: (i) evidence that the planet Pluto's motion is chaotic and therefore unpredictable in the long run, (ii) the demonstration that the nature of the vacuum state of QCD is such that it leads to permanent quark confinement, (iii) synthesis of new materials, (iv) *ab initio* study of chemical kinetics, (v) vortices in Bose–Einstein condensates (first established in simulations and later verified through laboratory experiments) and many more.

The remarks made so far should not be misconstrued as saying that the numerical approach is a substitute for analytical work. That would indeed be preposterous. What is being emphasized is that for many the analytical approach is the only way of applying mathematics in sciences. We hold that view to be extremely myopic and counterproductive. The class of problems that are amenable to reliable analytical methods is fast shrinking while those that can be tackled with reliable numerical techniques are exploding. An efficient numerical algorithm always makes use of the most powerful insights afforded by the analytical route but the reverse happens seldom except in some happy exceptions like the four colour problem or some investigations in number theory.

To paraphrase one of my friends, just as the analytical techniques of mathematics made possible, the transition from premodern to modern science, computational methods will mark the transition from the modern to the future paradigms of science. I would go a step further and assert that physics and science in general will become more and more computational in character.

In summary the great speeds available to us on modern supercomputers has made possible many investigations unthinkable till now. The computational paradigms transcending the artificial boundaries between different disciplines should herald a new age of science. Many of the techniques and algorithms in numerical simulations are independent of the disciplines. This arises partly due to similarities in basic equations from unrelated disciplines if one transforms the variables adequately. Problems about DNA can be structurally very similar to those arising in cosmic strings; hydrodynamic flow equations in certain regimes look very much like the equations of general relativity; simulation algorithms for protein-folding are very much like well-known algorithms in statistical mechanics. Of course, there are important differences between disciplines but the commonality of the simulation methodology can bring sciences together so that they can appreciate and be tolerant of these differences more than was ever possible. The message of different paradigms and different notions of reality at different scales is also philosophically appealing as against a theory of everything for all scales which appears distinctly pre-Copernican in spirit.