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Experimenting by computer

by BRIAN HAYES

Science is generally conceived of as a dialogue between theory and experiment, but in recent years a third party has joined the conversation. The intruder is computer simulation, and it proposes nothing less than a new method of discovering truth — a way of understanding the world by reinventing it. In the 1980s this third way of doing science has penetrated most areas of research.

Often enough it is the only way that works. As researchers advance into ever-murkier corners of the natural world, they are finding details and complexities that were not imagined a few decades ago, and they are constantly confronting the limitations of their old methods and of their own unassisted brains. Let me give an example of what I mean.

Astronomers have known for some time now what a supernova is. In the 1930s astrophysicist Subrahmanyan Chandrasekhar showed that when a large star exhausts its fuel, it collapses under its own weight. In some cases, it was later realized, the collapse triggers an explosion — a supernova — that blows off much of the star's mass, leaving behind a dense neutron star or perhaps even a black hole. All this was revealed by the methods of paper-and-pencil physics. But those methods bog down in tracing the events of the crucial milliseconds in which the core of a star contracts, "bounces," and then explodes. There is so much going on in that brief span that theorists cannot cope; and laboratory experiments, of course, are unthinkable.

In the past decade or so computer simulations have begun to fill in the missing details of star death. Such simulations begin with a mathematical model of a star that describes its mass and chemical composition and internal structure. Starting up the simulation has the effect of turning on the laws of physics, so that the model star begins to cook. Nuclear reactions are ignited; convection currents begin to flow; gravitation compresses the stellar core; neutrinos and other particles stream through the layers of the atmosphere. Meanwhile the physicist waits to see what will happen. The wait is not negligible: even with a fast computer, the simulation may take several minutes for each millisecond of real time.

But the results are worth waiting for. Computer simulations have revealed, for example, that it is not always easy to blow up a star. Conversely, observations of real supernovas — particularly the one that erupted in the Large Magellanic Cloud in 1987 — have inspired computer modelers. The dialogue of science has become a noisier, threeway klatch, from which all parties emerge the wiser.

Actually, the use of computers to work out the detailed consequences of physical laws is not entirely new. In the 18th century, orreries with elaborate clockwork gears — mechanical computers, in effect — simulated the motions of the planets and their satellites; if you wanted to know the configuration of the solar system some years hence, you could just turn the crank. Some medieval astrolabes served a similar purpose. Indeed, the technology of such simulations is probably ancient: a hunk of corroded metal found in a shipwreck near the Greek island of Antikythera is thought to be the remains of a planetary computer built in the first century B.C.

But those devices were mere labor savers: they didn't solve any problems that couldn't be solved by other means. Only when mechanical computers were replaced by more powerful electronic ones, in the middle of this century, did simulation emerge as an alternative path to genuinely new knowledge.

One of the earliest and most famous instances of science by simulation happened just after World War II at the Los Alamos laboratories in New Mexico, where researchers needed to predict the fate of neutrons traveling through various materials. When a neutron struck an atom, it could be scattered or absorbed, or in some cases the atomic nucleus could undergo fission, thereby liberating more neutrons. For any given collision the probabilities of the various outcomes were known, but each neutron took part in a vast number of collisions.

Stanislaw Ulam, a mathematician by training, devised a simple solution — or at least it seems simple in retrospect. The outcome of each collision was determined by choosing a number at random; the numbers represented possible outcomes according to the known probabilities. The simulation could in principle be performed with the aid of a roulette wheel. For example, it might be decided that whenever a spin of the wheel produces an even number, the neutron is scattered, whereas an odd number corresponds to absorption; the rare fission events might take place when a zero turns up. (The actual probabilities are different from these.) After thousands of spins, the average properties of the neutrons' trajectories would begin to emerge.

Because of the element of chance in the procedure, it was dubbed the Monte Carlo method. For this problem and others Ulam and his colleagues employed not a roulette wheel but some of the earliest electronic digital computers. Today, the simulations run on the fastest machines available; and it is the wider availability of such machines that enabled computer simulation to blossom in the 1980s.

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It is hardly surprising that simulated science has been adopted most eagerly in those fields where other methods run into the most forbidding obstacles. Supernovas are simulated because the real thing is rare, remote, and inaccessible. Similarly, there are few alternatives to simulations in trying to understand the large-scale structure of the universe, to get an outsider's view. They show vast wispy filaments and cobwebs that resemble the tentative maps produced by observational astronomers, and they give at least preliminary hints about how these structures might have evolved.

Simulation can fill in not only for impractical experiments but also for inadequate theories. In the 1970s one of the hardest problems in theoretical physics was explaining the "confinement" of quarks (the component particles of protons, neutrons, and the like). Inside a proton, quarks seemed to move around without constraint, but any attempt to pull them apart in particle accelerators revealed unbreakable bonds between them. The bonds were those of the strong nuclear force, which is described by the theory called quantum chromodynamics; but theorists were at a loss to find an explanation of why quarks should be so free and yet so inseparable. Essentially the problem was that the force field between two quarks was too complicated to calculate.

A definitive solution to this problem has still not been found, but the best approximation so far is a type of computer simulation devised by Kenneth Wilson of Cornell University. In this technique the forcefield calculation is simplified by repalcing continuous space and time with a fictitious four-dimensional lattice, a kind of space-time jungle gym. The quarks can only occupy intersection points in the lattice, and the links connecting these points represent the forces acting on the quarks. Each link is variable, and so the number of possible configurations of the overall force field is enormous. But in the approach followed by workers who have elaborated on Wilson's original idea, the computer considers only a representative sample, which it selects at random by means of the Monte Carlo method. It then computes an average configuration.

What such simulations have done is to vindicate quantum chromodynamics, by showing that it does indeed predict that quarks should remain confined by the strong force in protons and neutrons. Beyond that, however, the simulations have also made a fascinating prediction. At temperatures of several million million degrees, they suggest, quarks might be liberated from the strongties that bind them and swim freely in kind of "quark soup." Many investigators now think that quark soup is what the universe was made of in the immediate aftermath of the Big Bang. It may still be around today inside the neutron stars left behind by supernovas.

These examples may give the impression that computer simulation is used only in extreme situations, when traditional theory and experiment fail. But in fact simulation has also found a place in sciences that have no such methodological barriers. Chemistry for example, is the prototypical experimental science, but during the past decade computational chemistry has become an important subdiscipline. Some computational chemists labor to calculate the structure of a molecule from the fundamental equations of quantum mechanics. Others employ less rigorous computational methods to describe large molecules, such as polymers, or to investigate complex systems of linked reactions, as in the combustion of fuels. A big advantage of the computational methods is that they allow the chemist to see directly things that would have to be inferred from the results of a conventional experiment. For example, a few years ago Enrico Clementi of IBM performed a Monte Carlo simulation of the water molecules surrounding a strand of DNA, the chainlike molecule that carries genetic information; whereas experiments had given only indirect evidence of how DNA interacts with water, the simulation revealed specific ways in which the water molecules tended to arrange themselves.

In biology, too, the computer has elbowed its way into the laboratory. Among the first biologists to turn to computer simulations were those who study population dynamics. A typical problem in that discipline is to figure out how the population of a predator species and that of a prey species fluctuate when the two are in contact. Field observations can take years, but in just a few minutes a computer can run through many generations of, say, hares and lynxes. Similar methods are now being applied to the study of epidemic disease, including the spread of AIDS through the human population.

Climate forecasting is another area in which computer simulations are touching on issues of immediate social concern. In the 1980s all of us became aware that the human race has the power, through the greenhouse effect, to change Earth's climate. The ultimate source of that realization was computer simulations, which forecast the effects on climate of increasing concentrations of carbon dioxide in the atmosphere. the science is still primitive, and the various models are distressingly different in their detailed forecasts. But most seem to agree on the central idea that Earth is going to get warmer.

Not everyone welcomes the new role of the computer in science. One cause of discomfort is cultural: a biologist who works with animals or a geologist who hammers rocks may be reluctant to acknowledge someone who twiddles computer bits as a member of the same fraternity. But there are also more substantial questions about the prudence of trusting answers that come from a machine.

The hazard that gets the most attention is what might be called the Ptolemaic fallacy. A computer model could work smoothly, reproduce experimental results in great detail even give accurate predictions of future observations, and yet still be totally wrong. A case in point is an orrery built to represent a geocentric universe, like the one the firstcentury astronomer Ptolemy envisioned, a theory that held sway until disproved by Copernicus in 1543. By fine-tuning the gear ratios and adding epicycles, we could continually refine the machine, covering up any discrepancies between the simulated universe and the real one. With enough effort we could match the model's accuracy to that of any available telescope, and so we would never detect a failure. That is just the problem.

Personally, I do not believe that such deceptive models present much of a threat to the pursuit of knowledge and the integrity of science. After all, conventional experiments can also be misleading, and theorists are certainly fallible; if institutional science has been able to cope with these weaknesses, then it should also be able to handle the occasional simulation gone astray. Indeed, a third mode of doing science — even if it is very imperfect — ought to improve overall reliability by providing an additional check on the two existing modes.

Another hazard of simulation may be more insidious. Suppose we set out to build a computer model of the biochemistry of a living cell. We might start with a few fundamental reactions, say, the cycle for extracting energy from nutrients. Then we could add some finer details, such as the "pumping" of ions across cell membranes. Next would come the enzymes that regulate the metabolic process, the genes that regulate the enzymes, and so on. Eventually our model might become so accurate that it could mimic the behavior of the real cell in full detail; such an achievement would have to be counted a success.

To be continued