Is It Real, or Is It Cray?

Computer experimentation gives researchers an entirely new tool with which to explore the world, opening up what some see as a major new branch of science

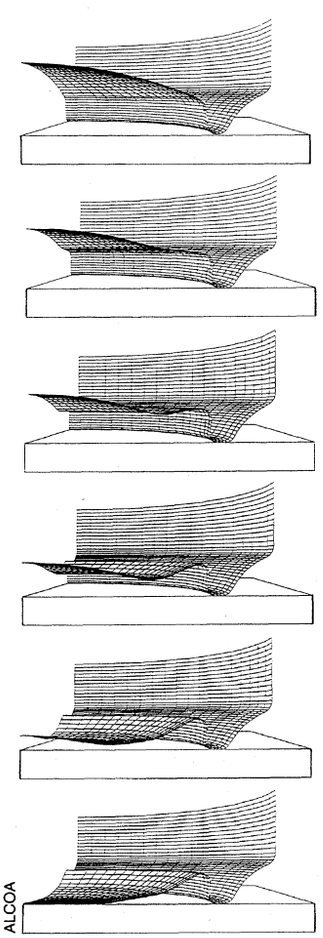
BOB DICK IS DROPPING CANS. Aluminum casings filled with beer or soda, they fall a foot or two to the floor, and Dick looks at the bottoms for damage. It is all part of a service that his employer, ALCOA, offers to can manufacturers—checking out various can designs to see which ones hold up best under abuse.

They are not real cans, however. It is not a real floor, and the beer and soda are imaginary, too. Only Dick is real. The rest of the scenario exists only as a pattern of electrical currents flashing through the circuits of a Cray Y-MP/832 supercomputer at the Pittsburgh Supercomputing Center, one of five such centers funded by the National Science Foundation.

Trained as a structural engineer, Dick is one of a new breed of experimental scientists from disciplines as diverse as biology and aerophysics who locate their laboratories inside a computer. The power of today's supercomputers lets these researchers mimic a variety of physical experiments using computer hardware and software in place of lab ware.

But not only can computer experiments substitute for many of the studies normally done in a lab, they also are allowing scientists to gather data and test hypotheses in ways that were closed to them before. And the field is still in its infancy—as computers become more powerful and as more scientists become aware of their potential, computer experiments are likely to change the way research is done. The promise of computational science has led some researchers to suggest that the field will eventually grow into a third domain of science, coequal with the traditional domains of theory and experimentation.

ALCOA is interested in computational experiments, Dick says, for two simple reasons: time and money. Andy Trageser, Dick's supervisor at ALCOA Laboratories in Pittsburgh, recalls that in the early 1980s, before the company got into computer modeling, "it would take 6 months to a year to come up with a promising design." A can manufacturer would come to ALCOA with an idea for a new shape, and the ALCOA engineers would take on the challenge of modifying this basic form so that it would best stand up to such things as drops and internal pressure. To do this, they would manufacture dozens of cans with slightly differing forms, fill them with liquid, then drop, bop, or otherwise abuse them. Today, Dick simply keys into his supercomputer the numbers that describe how he wants to modify the can—he might make the dome-like indentation on the bottom of the can a little deeper, for instance, or widen the base of the can—and then lets the Cray do the work.



ALCOA

The bottom dome of an aluminum can *pops downward after the can hits the ground. Only one-quarter of the bottom part of the can is included in the simulation.*

The simulated drop test is a marvel of number crunching. The computer knows the shape of the can, the speed at which it hits the ground, the mass and pressure of the liquid inside the can, and the physical characteristics of the aluminum. It knows the equations that describe the complicated interplay of mass, velocity, acceleration, pressure, and other relevant physical properties. To calculate the effects of the can striking the ground, it looks at the can as a collection of tiny elements, each of which acts upon and is acted upon by the other pieces around it, as well as by the ground and the liquid in the can. The computer calculates the position of each of these elements at 1 millisecond after impact, 2 milliseconds, 3 milliseconds, and so on, until the can stabilizes, usually after about 8 milliseconds.

Besides the drop test, Dick and Trageser have also used the supercomputer to check how well cans resist the internal pressure that can cause the bottom of a can to pop outwards, and to model the denting of cans as they bump into something.

The beauty of testing cans on the computer is that it is so fast and simple. With the simulated drop test, ALCOA can shoot a design back to a manufacturer in 2 weeks, sometimes in as little as 2 days. And the cost of developing a new can design with computer modeling, Trageser says, is only about $2,000, compared with about $100,000 using traditional laboratory methods.

For the same reasons that ALCOA models cans on a computer, aerodynamics researchers are increasingly swapping wind tunnel work for numerical experiments. Ron Bailey, manager of the Numerical Aerodynamic Simulation Systems Division at NASA's Ames Research Center, says that in the past engineers would go through the slow, tedious process of building different wings and testing 30 or 40 designs at a time in the wind tunnel. "With the computer we can look at many more wings in a shorter time," he says. They still end up putting four or five wings through the wind tunnel, but by using the supercomputer for an initial evaluation, "we use our wind tunnel smarter."

The convenience of computer simulations is not their only advantage over wind tunnel experiments, however. Once researchers began to play around with aerodynamic tests on computer, they found that one of the great strengths of computer experimentation is that it can tell you things you could never see in real life. The space shuttle is a good example.

"It is almost impossible to get a hot plume in a wind tunnel," says Terry Holst, chief of the applied computational fluids branch at NASA-Ames. Engineers also find it quite difficult to model the shuttle's behavior during its separation from the launch vehicle, he

says, as well as when the shuttle passes the speed of sound. In the latter instance, a shock wave bounces off the walls of the wind tunnel and interferes with the air flow around the craft. A computer-generated shuttle, on the other hand, has no walls to contend with, and a plume or a separation involves no more than writing an extra subroutine for the software.

Yet another big advantage of simulating the shuttle on a computer, Holst says, lies in the availability of the data. Measuring air pressure or wind velocity at different points along a physical model of the shuttle means sticking probes in those different places. But probes will often distort the air flow around the model, and, indeed, it is a practical impossibility to have enough probes to record data all over the shuttle. In a computer experiment, the data are there for the taking.

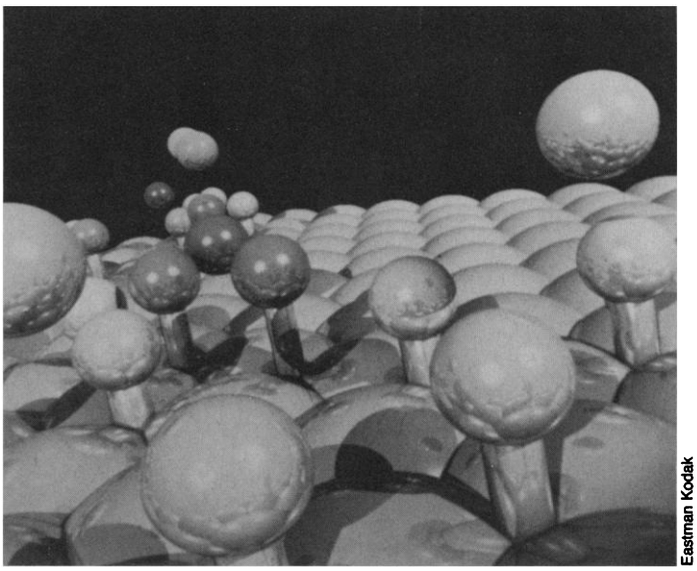
Moving from outer space to the microscopic world, another thing no researcher can ever hope to see in real life is an individual atom or molecule. Yet learning how atoms diffuse over a surface, for example, is important to understanding surface chemistry, which in turn is crucial in the study of such things as film development.

In the laboratory, since hydrogen atoms are too small to detect against a background of platinum, one can follow the diffusion in only the most general way. Working with a platinum surface already covered with hydrogen atoms, the researcher clears off a small part of the surface with a laser beam, and then lets the remaining hydrogen atoms diffuse back over the bald spot. A short time later, a second beam knocks off the hydrogen atoms that have moved into the region, and the researcher counts them. Running the experiment over and over again gives a statistical picture of how quickly the atoms diffuse over the surface. But it says nothing about how they move.

Enter Eastman Kodak's Lawrence Ray. At the University of Illinois' National Center for Supercomputing Applications, another NSF-funded project, Ray uses a supercomputer to "watch" the migration of hydrogen atoms over a platinum surface—something that no microscope can reveal. Ray's computer experiment produces videotapes of the simulated hydrogen atoms moving across the simulated platinum. "You can watch the particles bounce around on the surface," Ray says. His model, which is based on knowledge about how atoms interact and is calibrated with experimental data, agrees quite well with the laboratory results, he says. Its advantage over the laboratory is that it gives a much more detailed look at what is going on, which eventually may lead to ideas for improving procedures for such things as film developing.

Computer experiments likewise are opening a new window into biological behavior. As a result, drug researchers and molecular biologists—people normally much more comfortable with a test tube than a computer chip—have jumped at the chance to do experimental work on supercomputers.

At the Illinois supercomputing center, Riaz Abdulla, head of supercomputing applications at Eli Lilly, watches on the screen as a potential new drug interacts with an enzyme. The simulation will tell him if the drug is worth pursuing as an enzyme inhibitor—something that 5 or 10 years ago could only have been learned through tedious biochemical experiments.



Eastman Kodak

Hydrogen atoms migrate *across a platinum surface.*

Abdulla has taken several steps to reach this point. First, he modeled the structures of the enzyme and the potential inhibitor. To do this, he fed in the molecules' protein sequences and their crystalline structures, determined from x-ray crystallography, and instructed the computer to determine the molecules' structures in solution.

Although the x-ray crystal structure reveals the shape of a molecule when it is frozen into crystalline form, to understand the way in which an enzyme and inhibitor interact, one must be able to see them as "dynamic, moving entities," Abdulla says. Only a supercomputer can give this view.

Once the computer modeled the dynamic structures of the two molecules, Abdulla instructed it to bring the inhibitor up next to the active site on the enzyme and calculate the "molecular recognition" between them—how they will fit together. The computer simulations show, Abdulla says, that the standard analogy here of a lock and key is too rigid. Instead, as the two molecules approach one another, they alter each other's structure through electromagnetic forces. If the energy of interaction between the inhibitor and the active site of the enzyme is below a certain threshold, it is likely that an interaction will occur—the inhibitor will latch onto the enzyme.

The computer experiment thus provides data to Abdulla in two ways. By calculating the energy of interaction, he can tell how effective a given drug is likely to be as an inhibitor. And by watching the simulated interaction between the two molecules, he gets insight into why certain molecules work better than others as inhibitors. Eventually, he and his colleagues at Lilly hope to use this insight in the design of new drugs.

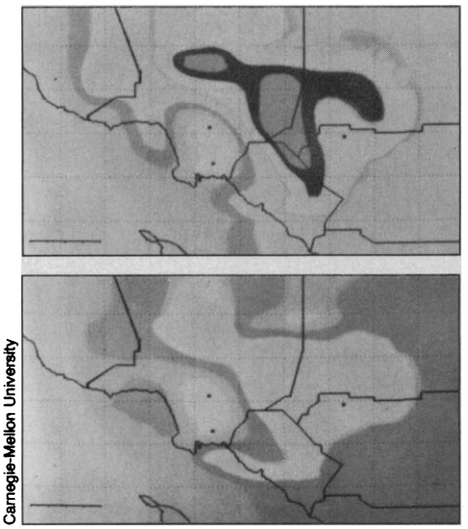
Not only can researchers use computers to see details of experiments they could never see before, they can also perform experiments they could never do before.

At NASA-Ames, for example, researchers are designing a probe to enter the Jovian atmosphere. Bailey, the manager of the aerodynamic simulation division, points out that in diving toward Jupiter, a craft will encounter conditions that cannot be mimicked in a wind tunnel on Earth. Not only does Jupiter's atmosphere have very different gases at a much higher pressure than Earth's atmosphere, but the high-speed passage of the probe will cause various chemical reactions that must also be taken into account. "Chemically, these flows can get very complex," Bailey says.

Closer to Earth, NASA is designing a National Aerospace Plane that will fly at up to 25 times the speed of sound. It is impossible to accurately represent these conditions in a wind tunnel, Bailey says, but for a supercomputer—no problem.

And researchers at the Pittsburgh Supercomputing Center performed an experiment even more difficult than putting a probe down on Jupiter: Gregory McRae, a chemical engineer, and Ted Russell, a mechanical engineer, looked at what would happen to Los Angeles smog if half the cars in the city switched over to methanol.

McRae and Russell, both at Carnegie-Mellon University, developed a computer model of the atmosphere in the Los Angeles basin, taking into account meteorology, chemistry, and the emission of air pollutants. After checking the predictions of the model against actual data, they ran a series of 200 experiments where they changed the pattern of pollution emissions in various ways. One surprising result stood out,



Carnegie-Mellon University

Ozone levels *in the Los Angeles basin drop if cars switch from gasoline (top) to methanol.*

McRae says: "Controlling hydrocarbons in the city just pushed the ozone out into the countryside." The key to the ozone level, the researchers discovered, was actually the amount of nitrogen oxide emissions. The hydrocarbons mostly affect the rate of ozone production, McRae says, so that lowering hydrocarbon emissions in the city slowed down the rate of ozone production but not the total amount produced. As a result, the city would get less ozone, but the areas downwind from the city would get more.

The two engineers ran simulations where gasoline-burning automobiles were replaced by methanol-using ones, and found they could decrease the ozone level significantly. The methanol by-products are much less reactive in their ozone-forming potential than are the gasoline by-products. As a result, changing half the cars over to methanol could cut peak ozone levels by 40%. These computer experiments played a big role in President Bush's recent decision to call for methanol-burning cars to be used in the nation's worst pollution centers, McRae and Russell say.

The best part about these simulations, McRae says, is that they are much cheaper than doing the actual experiments. Replacing all the cars in the Los Angeles area with methanol-mobiles and then seeing what happens would cost hundreds of millions of dollars. And then, "if it doesn't work, you're in a lot of trouble. If it doesn't work on the computer, you just put in a different set of numbers and try again.

Computer experimentation does have its limits, of course. The first and most obvious is that if one does not know the fundamental physical laws governing a system, one cannot use a computer to learn them. And many systems that do behave according to known physical laws may forever defy accurate simulation. "Living systems," Abdulla says, "may never be modeled on a computer because they are too complex."

Also, computer experimentation is not an end in itself; in fact, researchers say that it is most valuable when done in conjunction with physical experiments. Testing of the space shuttle was done both in wind tunnels and on computer, Holst says, because the two methods complement each other. They are prey to different types of errors, he explains—while the wind tunnel falls short in trying to mimic the features of the real world in a small, enclosed space, numerical experiments make mistakes because of the limits of the model or the limits to the computational power of the computer. A wind tunnel is vital, for example, in testing the effect of turbulence, something that no computer can yet simulate accurately.

But the power of supercomputers continues to increase, and with it the ambition of computer experimenters. Right now, Bob Dick at ALCOA has enough confidence in his simulated drop tests that he will design a can for a customer without ever having built a physical model, but no one is ready to do that with an aircraft wing, for instance. Bailey at NASA-Ames says that once computer simulations narrow a wing design down, the final work must still be done in the wind tunnel. "Basically, the wind tunnel goes into much greater detail, down to the rivet head," he says. "We don't have computers powerful enough to do that, yet." He estimates that a computer a million times faster than those now available would be necessary to get results as accurate as in the wind tunnel.

As each new generation of computers comes along, not only will researchers be able to do their old experiments with greater accuracy, but entire new lines of experimentation will open up. "We can't wait to get our hands on the next generation with several orders of magnitude more computing power," says McRae at Carnegie-Mellon. With these powerful machines, he envisions such experiments as controlling acid rain over entire regions or designing the most economically efficient strategies to curb air pollution. With enough computing power, researchers could experiment with the formation of the Milky Way galaxy, earthquakes in California, or chemical interactions between complicated organic compounds. All without getting their hands dirty. ■ ROBERT POOL

Putting the Squeeze on Hydrogen

It was hydrogen, the lightest of gases, that floated the great zeppelins across the Atlantic Ocean 60 years ago, but in the hands of Ho-Kwang "Dave" Mao and Russell Hemley, hydrogen is something else altogether.

In Mao and Hemley's lab at Carnegie Institution of Washington, hydrogen is a solid, crystalline substance with metal-like properties. As reported on page 1462 of this issue, the two researchers have squeezed hydrogen with pressures of more than 2.5 million atmospheres (2.5 megabars), and their optical measurements of hydrogen at these pressures indicate that it becomes a semimetal—a substance that conducts electricity, although to a much smaller degree than normal conductors.

Ten years ago, Mao and colleague Peter Bell at the Carnegie Institution were the first to create solid hydrogen, at about 57 kilobars. At this pressure the hydrogen is an insulator, but as the pressure increases, theory predicts it will go through a series of transformations from an insulator to a semiconductor to a semimetal and finally, somewhere between 2.5 and 4 megabars, to a metal. Checking these experimental predictions is important not only to physicists interested in bonding in solids, but also to planetary scientists. Metallic hydrogen is likely to constitute a large portion of the mantles of such gaseous planets as Jupiter and Saturn, and thus could greatly influence their electromagnetic properties. It is also possible that metallic hydrogen could be a high-temperature superconductor.

Mao, a geophysicist, and Hemley, a physical chemist, used a diamond-anvil pressure cell to put tremendous pressure on the hydrogen, and as they squeezed, they made optical measurements through the transparent diamond. At 2.5 to 3 megabars, the hydrogen becomes "virtually opaque," Hemley said. This implies that some of the electrons bound to the individual hydrogen molecules are moving into new energy levels to become conduction electrons, creating a semimetal. At some point, all of the electrons should come loose from the nuclei and the material should become fully metallic, but Hemley does not believe they have reached that point.

Unfortunately, the researchers may have trouble seeing the metallic hydrogen if they do achieve it. Above 2 megabars, the diamonds begin to glow bright red, making it hard to do optical measurements. So far, they have managed to overcome the interference, but it may get worse with increasing pressure. ■ ROBERT POOL