A computer in the test tube — Simulating a liquid

The movement of molecules in a liquid can be copied by a computer. In a calculation which lasts many hours, a split second in the life of a liquid can be investigated.

When Mike Klein begins an experiment on liquid ammonia he doesn't put on a white lab coat — he doesn't even handle a test tube — he simply enters some numbers into a computer and sits back to wait.

For the past ten years the only experiments Dr. Klein has performed have been on a computer. Klein, a chemist at NRC's Division of Chemistry, likes to think of the computer as the "Third World" of science. "Up to now, we've had two basic approaches in science," he says, "experiment and theory. But now it's possible to add a third mode of attack on chemical problems — the process of computer simulation."

Computer simulations have become an important aid in engineering, systems planning and decision-making situations. Astronauts train on computer-simulated space trips; new traffic intersections are designed on a computer-simulated model of city traffic flow; student doctors increasingly perform their first diagnoses on computer simulated patients. With their ability to handle millions of decisions in a short interval of time, computers can simulate many of the more complex situations of modern living. For research chemists, physicists and biologists, computer simulations have also entered the laboratory, mimicing the behavior of solids, liquids, chemical reactions and even simple biological systems.

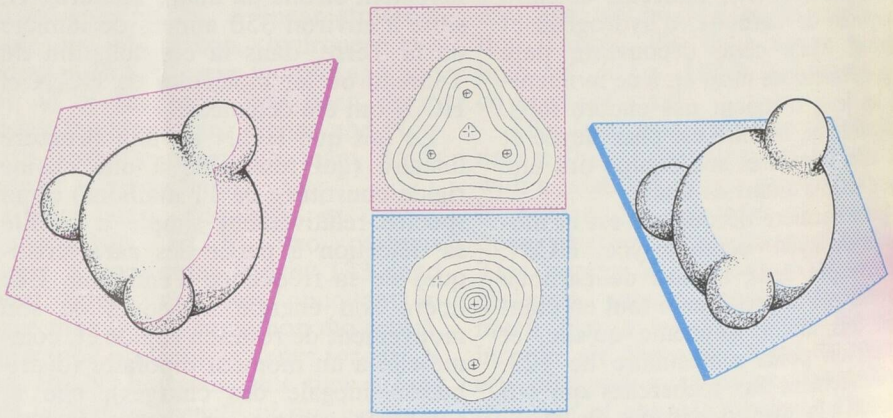
But why attempt to reproduce the behavior of a liquid on a computer? Dr. Klein explains: "The sort of systems I'm interested in are not only very important but they're very complicated. In fact, there really isn't a good theory to explain them fully. If you're investigating a relatively simple system then it's possible to construct a theory and check it out by making a few predictions and then trying to verify them by experiment. But, suppose the system is very complicated and the theory just isn't comprehensive enough to account for the wealth of behavior of the real situation. How, then, do we develop the theory? The answer is to simulate the system on a computer — or at least an important part of the system's behavior. It then becomes possible to carry out a detailed comparison between the theoretical predictions and the computer-generated system in a controlled fashion. In addition, the computer model is interesting in itself because of what it tells us about the system which could not have been found in any other way."

How does Dr. Klein go about simulating liquids on a computer? Take liquid ammonia as an example. "First, we begin by telling the computer something about an individual molecule of ammonia," he explains, "its characteristics, the way it can move, the way it will interact and behave if it hits another molecule. The next step is to work out the movement not of one molecule but several hundred as they interact and collide with one another."

Even for a modern computer, this becomes an enormously difficult task requiring hours of computer time. For a real liquid the simulation seems crude, given that a cup of liquid contains over a million, million, million, million, molecules, rather than a few hundred! But, with the aid of an ingenious mathematical trick called "periodic boundary conditions", it is possible to overcome some of the limitations of using a small number of "molecules" in the computer simulation. (The technique works in a way analagous to that of placing an object between two parallel mirrors. A seeming infinity of images can be seen in each mirror, and appear to recede into the far distance. In a similar way, periodic boundary conditions continually reflect the motions of molecules in the simulation.)

After a run time lasting several hours, not overly long for this kind of work, Mike Klein examines the readout. The computer allows him to follow the motion of several hundred "molecules" through thousands of collisions, recording the buildup and breakdown of so-called "oriented" structures within the "liquid". In terms of what happens in a real liquid, however, this simulation is stretched out in time. How much time would have elapsed in a real system for these events to take place? "About a thousand millionth of a second," Dr. Klein says. "Although this may seem an incredibly short time, on the molecular level it is long enough for us to get an idea of the structure of the liquid and understand some of its behavior. However, some important changes simply take too long to simulate on a computer. For example, we are only now beginning to study how a liquid freezes. Even if computers become much faster and computer time becomes cheaper I think it will be some while before we can follow such changes in molecular systems. What is needed is a new idea — a better way of simulating molecular motions and interactions." □

David Peat



John Bianchi

The wave function for a molecule, calculated by a computer, gives a picture of the molecule as it appears to its neighbors. These cross sections, which have the appearance of contour maps, display the density of electrons in various segments of the molecule. The cross sections are useful to scientists in visualizing how molecules fit together.

La fonction d'onde d'une molécule, calculée par un ordinateur, montre comment celle-ci apparaît à ses voisines. Grâce à ces coupes transversales ressemblant à des courbes de niveau, on peut voir les variations de densité électronique dans les différentes régions moléculaires. Elles permetttent également aux scientifiques de visualiser la disposition spatiale des molécules.