Supercomputing the liquid state of carbon

The liquid state of carbon exists under such extreme conditions that its nature has long remained an enigma. Signs of melting on graphite and diamond surfaces blasted by intense laser pulses have spurred interest in this elusive liquid, but researchers have found it difficult to produce and contain liquid carbon long enough for study. Now, sophisticated computer calculations provide a glimpse of the liquid's key characteristics at pressures close to atmospheric pressure.

"It forms quite an interesting liquid," says physicist Richard M. Martin of the University of Illinois at Urbana-Champaign. According to a computer model developed by Martin and colleague Giulia Galli and described in the Aug. 28 Physical Review Letters, carbon can exist in a liquid state at temperatures greater than 4,500 kelvins, even at relatively low pressures. Under those conditions, liquid carbon has the electrical conductivity of a metal. At the same time, each carbon atom, although free to move around, remains closely associated with two, three or four neighbors.

Such theoretical results provide information useful to researchers presently studying the formation of diamond films, which could be used in electronic devices. The findings also supply hints of what could happen to carbon that lies deep within the giant planets Uranus and Neptune or is scattered as dust across interstellar space.

Using a method developed by Roberto Car and Michele Parrinello of the International School for Advanced Studies in Trieste, Italy, Martin and Galli essentially start with Schrödinger's equation, which describes the relationships between the energies and positions of atoms and electrons. Their simulations, done on a supercomputer, represent the most exact calculations yet of a carbon system. "We think we can make the case that these calculations are accurate enough that they're real predictions of what should happen," Martin says.

"The only bad thing about [using this method] is that it takes so much computer time," says Jerry Tersoff of the IBM Thomas J. Watson Research Center in Yorktown Heights, N.Y. "If it weren't for that, I think everybody would be using it by now."

In their computer model, Martin and Galli track the behavior of a set of 54 carbon atoms, along with 216 of their electrons. These atoms, representing a microscopic sample of the material, start in a particular arrangement, such as the tetrahedral diamond lattice in which each carbon atom bonds with four others. "We give the atoms some random displacements so they're not in a nice structure anymore, which is equivalent to putting in a lot of energy," Martin says. "We find the properties of the liquid by following the atoms and their motions for a sufficiently long time."

Martin and Galli's computer simulations show that at a sufficiently high temperature, the carbon atoms break out of a rigid structure but remain close to one another. The atoms continually switch partners, making and breaking bonds but always keeping two, three or four neighbors at hand. "They never get away from one another completely," Martin says. "They're always shuffling between neighbors." Because it takes a large amount of thermal energy to form and reform the bonds between neighboring atoms, such interactions explain why diamond and graphite are so hard to melt.

Despite intensive study for nearly a century, many of carbon's properties remain poorly understood. "Carbon has so many possibilities for what it can do that we can't claim to have investigated all the possibilities," Martin says. Martin and Galli are now studying how the properties of liquid carbon depend on pressure and temperature, especially at the high pressures encountered deep inside planets. *– I. Peterson*

Bashing concrete for nuclear safety

Sandia

In less than a tenth of a second, experimenters reduced a 21-ton aircraft to a twisted mass as they rocketed it off an approach sled at 480 miles per hour into a 500-ton concrete target. The huge slab, floating on a powerful cushion of air, was moved nearly 5 feet by the surplus F-4 Phantom jet. A battery of sensors and high-speed cameras monitored the spectacular crash, which took place at Sandia National Laboratories in Albuquerque, N.M., on April 19, 1988. Researchers released details of the test for the first time at a conference last month on reactor technology in Anaheim, Calif.

The test marked the denouement of a $3.2 million, Japanese-sponsored project designed to measure how a structure, such as a nuclear reactor's containment building, responds during the eye-blink interval over which a crash progresses. "We'd previously done some fairly accurate computer analysis, but the computer models were untried on the real thing," notes Walter A. von Riesemann of Sandia's Containment Technology Division. The test data indicate computer models now used to estimate impact effects are close to the mark.

A billion digits of pi

When it comes to computing the decimal digits of pi (the ratio of a circle's circumference to its diameter), records are made to be broken. With an infinite number of digits to pursue, enthusiasts keep trying to extend the number of digits known, though they have no hope of ever reaching the end.

Now, just a few months after calculating 480 million digits (SN: 6/17/89, p.372), mathematicians Gregory V. and David V. Chudnovsky of Columbia University in New York City have broken the billion-digit barrier, using their innovative techniques to compute and verify 1,011,196,691 digits in the decimal expansion of pi.

The Chudnovskys ran their programs on an IBM-3090 computer, using two different operating systems. Printed out in a line, the digits they computed would stretch nearly halfway across the United States. The first computer calculation of pi in 1949 reached only 2,037 digits.

The Chudnovskys intend to give up their pursuit of pi, at least for now. "If somebody comes along and wants to use our algorithm, that's fine," David Chudnovsky says. "But we are out of the game."

Still in the game is computer scientist Yasumasa Kanada of the University of Tokyo, who previously held records for computing the digits of pi (SN: 4/2/88, p.215). In July, Kanada used a modified version of his pi-computing program on a Hitachi supercomputer to reach 536,870,000 digits. To speed up his program further, Kanada is investigating ways of hastening the multiplication of numbers up to a billion digits long. "I hope to continue, but it all depends on the availability of new machines," Kanada told Science News. In his effort to break the present record, he's hoping to get time on any one of several new supercomputers now being developed in Japan. *– I. Peterson*