six agencies led by the National Science Foundation (NSF), the Department of Energy (DOE), and the Department of Defense (DOD) (see table on previous page) to support research in three categories. The largest chunk—$228 million—is slated for research on new computer and software architectures to help people interact with computers and make sense of vast stores of information housed in complex databases, such as those involved in predicting weather. Another $123 million would go to develop advanced computers needed to propel research in other areas of science, including earthquake prediction, materials simulations, and modeling the evolution of the universe. Some $15 million is being set aside for research on the ethical implications of the information revolution, including data privacy issues. About 60% of funds will go to university research, says DOE research chief Ernest Moniz; the rest will go for peer-reviewed projects in industry and the national labs.

Scientists hoping to exploit massive new sources of computing power are welcoming IT^2. "Anything that would move forward the forefront of computing would help genome efforts," says J. Craig Venter, president of Celera, a Rockville, Maryland–based company hoping to sequence most of the human genome in the next 2 years. Venter points out that more powerful supercomputers are needed to handle data-intensive tasks, such as analyzing the human genome sequence. "We're talking about completely new ways of computing," adds Jane Alexander, acting deputy director of the Defense Advanced Research Projects Agency of DOD.

Although White House officials are touting the funds as "new money" that won't require cuts in other science programs, they have yet to explain how they will pay for the increases under increasingly tight budget caps. They are also fuzzy on which agency will direct the program. The presidential task force had recommended designating NSF as coordinator of IT research spending, but some agencies chafed at that idea. Gore announced that NSF's head of computing will lead a White House working group coordinating the initiative and that a second panel will report to the Administration's National Science and Technology Council. But each partner agency is expected to retain control over its own budget.

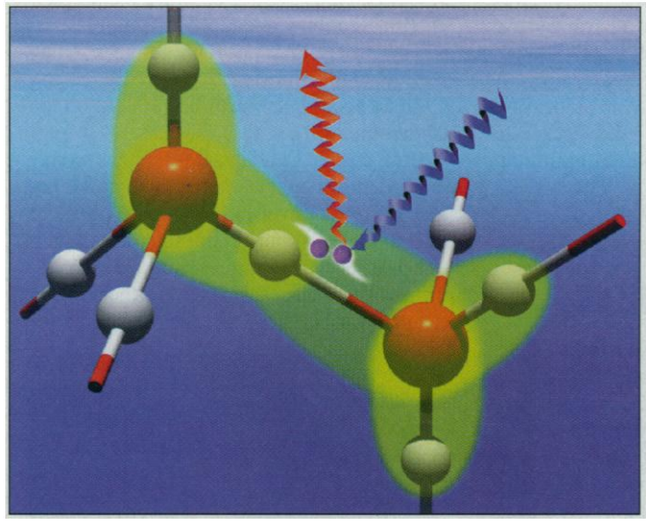
It's also unclear whether Congress will climb aboard the IT train—or whether it will prefer to construct its own version. "There's a good chance" that IT^2 will gain bipartisan support, says Representative Vernon Ehlers (R–MI). "But we need to learn about the details first and find out how they plan to pay for it."

–ROBERT F. SERVICE AND DAVID MALAKOFF

CONDENSED MATTER PHYSICS

Getting to the Bottom of Water

With the help of one of the world's most powerful x-ray sources, a team of researchers from the United States, Canada, and France has answered a simple question about a commonplace substance: What holds water together? In 1935, the Nobel Prize–winning chemist Linus Pauling suggested that the standard picture of electrostatic attractions—so-called hydrogen bonds—joining water molecules in water and ice may not be complete. He proposed that the influence of the strong "covalent" bonds within each water molecule leaks into the hydrogen bonds and lends a hand in binding one molecule to the next. More recently, quantum theory confirmed Pauling's view, and now researchers have probed the bonds in ice with intense x-rays and found that he was right.



Pulling together. Covalent bonds (darker yellow clouds) in water spread their influence into intermolecular hydrogen bonds (lighter yellow clouds).

The result, reported in the 18 January issue of *Physical Review Letters*, will allow researchers to refine their models of water and ice assuming that the bonds between molecules are part covalent and part electrostatic, says team member Phil Platzman of Lucent Technologies' Bell Labs in Murray Hill, New Jersey. "It is a nice piece of physics, and their experiment suggests that the theory must be very good," says David Clary of University College London.

The conventional picture of water molecules holds that the two types of bond are entirely separate. In a covalent bond, two atoms each donate one electron to a shared pair that no longer belongs to either atom alone, but occupies a single orbital common to both. In a water molecule, however, the sharing is not 50–50. The oxygen hogs the electron pair, leaving the positively charged nuclei of the hydrogen atoms exposed. Hence water molecules are "polar," and the positive hydrogen atoms of one molecule are attracted to the negative electron cloud around the oxygen atom of another, forming weak hydrogen bonds that, in theory, involve electrostatic attraction only and no electron sharing.

But this tidy classical picture of the hydrogen bond does not square with the quantum mechanical depiction of covalent bonds. Pauling and others since have predicted that the electrons in the covalent bonds should spread out into the hydrogen bonds. Last year, researchers from Bell Labs, Canada's Steacle Institute for Molecular Sciences in Ottawa, and the European Synchrotron Radiation Facility (ESRF) in Grenoble, France, set out to see if they could settle the matter. Their strategy relied on Compton scattering: bombarding the bonds with photons and analyzing how much energy their electrons absorbed. The chance of hitting the bonding electrons is small, but with the powerful flux of x-rays from ESRF, a new third-generation synchrotron source, the researchers hoped to get a detectable number of hits. "This experiment could not have been done 5 years ago," says team member Eric Isaacs of Bell Labs.

The researchers directed an intense, needle-sharp beam of x-ray photons with a precisely defined energy onto a tiny sample of specially prepared ice. A detector placed close to the beamline counted photons deflected backward and measured their energy. The energy distribution indicated how much energy the photons lost to electrons in the sample. The team counted photons for 23 hours, then reoriented the ice crystal and repeated the operation.

One orientation was chosen so that the hydrogen bonds, held fixed by the crystal structure of the ice, were parallel to the incoming beam; the other put the hydrogen bonds at an angle to the beam. If the bond had been purely electrostatic, there would be no difference in the energy profiles. If, however, the hydrogen bonds are partly covalent, there would be shared electrons in the bond which would behave as quantum-mechanical waves and when one energy

CREDITS: ISAACS *ET AL.*, *PHYSICAL REVIEW LETTERS* 82 (3) (18 JANUARY 1999)

distribution is subtracted from the other, an interference pattern would result. When the team subtracted the distributions, they obtained ripples which matched predictions of models of how covalent bonding electrons might intrude into the hydrogen bonds. "We see that this is really the model that explains the data. ... The classical electrostatic picture is not enough," says team member Abhay Shukla of ESRF.

Electrons spread out in this way because of a purely quantum-mechanical effect known as delocalization, says Shukla. Electrons seek the lowest possible energy state, and for the covalent bonding pairs in water, the lowest energy state apparently extends into the hydrogen bonds. Scientists studying water and other materials with hydrogen bonds will now have to take into account the complex nature of their bonds, and a commonplace material is looking increasingly strange.

–ALEXANDER HELLEMANS

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NCI Asked to Increase Focus on Minorities

Cancer researchers are likely to be asked to pay more attention to minorities and the "medically underserved" in the wake of an analysis released last week by the Institute of Medicine (IOM). The report, ordered by Congress more than 2 years ago, contends that the National Cancer Institute (NCI) is not spending as much as it claims on studies of minorities and urges it to do more. The IOM panel also proposes a significant change in the way NCI gathers incidence and mortality data: It rejects standard racial categories and recommends that data be collected in ethnic or cultural categories. NCI leaders agreed in principle but said they face many practical barriers in trying to change the way data are collected.

Bottom line. Senator Specter asked how much NCI spends on research involving minorities and the "medically underserved."

The IOM panel offered its advice more in support than in anger, noting that NCI already is headed in the right direction. "During the time that the committee was developing recommendations, we could see that they [NCI officials] were also thinking along the same lines," says M. Alfred Haynes, former president and dean of Drew Postgraduate Medical School in Los Angeles, who chaired the 16-member IOM panel.

The 272-page report, titled "The Unequal Burden of Cancer," will almost surely increase pressure on the National Institutes of Health (NIH) and NCI during this year's round of appropriations hearings to direct more research toward minorities and the medically underserved. Among the disparities the report notes: Cancer incidence is 15% higher among African-American men than among white, non-Hispanic men; all minority groups have higher rates of stomach cancer than white Americans have; and the 5-year survival rate of Native Americans from all types of cancer is only about two-thirds that of whites.

The report suggests that poverty and lifestyle are at the root of these differences, and it frequently praises NCI's "excellent" leadership and its "impressive array" of minority-oriented research efforts. But the IOM panel and NCI are not in agreement about everything. NCI says it spent $124.4 million in fiscal year 1997 on research relevant to minorities and the medically underserved. The panel, rejecting NCI's definition of relevant research, says the figure is only $24.2 million. Senator Arlen Specter (R–PA) homed in on these numbers in his very first question at a hearing of his Senate Appropriations Subcommittee on Labor, Health and Human Services, and Education on 21 January, the day after the report's release. "This is a very fundamental question as to resource allocation," Specter said. "I want to get to the bottom of it."

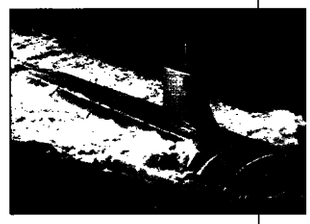
The dispute, however, may be largely a matter of accounting. NCI includes in its $124.4 million the cost of enrolling minorities in clinical trials and outcomes studies. The IOM panel contends that NCI should count only research projects that address "a priori research questions uniquely affecting minority and medically underserved groups."

NCI director Richard Klausner argues that "to segregate research this way would isolate the data we obtain, limit our ability to compare with the full population, and restrict our discovery of trends within subgroups that may only be discerned across

CREDITS: (TOP) U.S. NAVY; (BOTTOM) RICK KOZAK

ScienceScope

Dive! Dive! Scientists at the Armed Forces Institute of Pathology (AFIP) in Washington, D.C., regularly take on macabre and unusual assignments, including the grisly task of analyzing the remains of bomb blast victims. Now, thanks to controversial U.S. Navy plans to battle test one of its new Seawolf submarines (right) off the coast of Florida by detonating five nearby underwater mines, AFIP researchers may be examining corpses of another kind: whales, dolphins, and sea turtles.



Some conservationists fear that the Navy blasts—scheduled for sometime after 2000—could kill or injure the legally protected sea creatures. So, as part of a test permit, the National Marine Fisheries Service (NMFS) has required the Navy to fund, for a year after the blasts, AFIP studies of animals that strand on nearby beaches. The AFIP researchers—who have in the past conducted other studies on marine mammals—will be looking for evidence of explosion-induced "barotrauma," such as shattered ear bones. The free exams are a "wonderful" windfall to marine researchers, says Blair Mase, who coordinates regional stranding studies for NMFS in Miami.

Court Date A dozen scientists at the Georgetown University Medical Center in Washington, D.C., have followed through on their threat to sue the institution, claiming the university's directors ran roughshod over opposition to a new salary policy (*Science*, 22 January, p. 487). The complaint, filed 15 January, charges that the new policy—which ties salaries more tightly to a researcher's ability to win grants—"abrogated the core principles of tenure at the University and overturned 200 years of tradition in the treatment of Georgetown faculty." Several campus grievance committees have found in favor of the protesters over the last year. But university officials say they played by the book in overriding the rulings and implementing the new policy last July. A D.C. Superior Court judge could hear opening gambits as early as April.

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