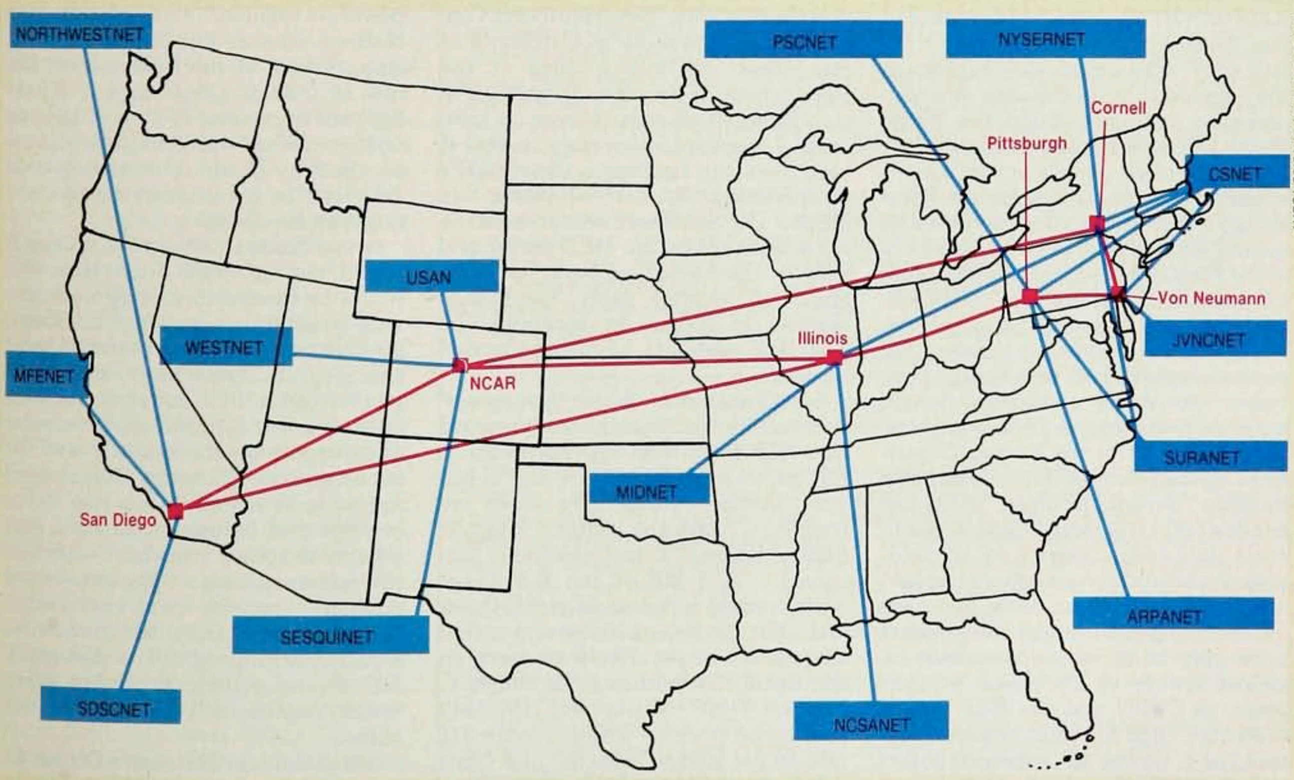
NSF supercomputer centers plan for next leap into research

Though they've been running only two years, the National Science Foundation's five supercomputer centers are a success story. In fact, while NSF still considers them an experiment, the centers have already made a difference in academic science and engineering. Since the centers were first set up in 1985, about 6000 researchers working on some 2600 different projects at 200 universities and other organizations have consumed 30 000 CPU hours on the supercomputers supported by NSF.

"Supercomputers can be characterized as scientific instruments that allow you to explore territories inaccessible to the usual experimental instruments," says Kenneth G. Wilson, director of Cornell University's Center for Theory and Simulation in Science and Engineering. "For example, an astronomer with a telescope can observe the universe over perhaps 50 years—the length of his scientific career. But an astrophysicist with a supercomputer can 'see' for a billion years. Computer simulation is therefore a theoretician's experiment."

In the past year, all five NSF centers have won high marks from reviewers. Accordingly, when their funding status came up before the National Science Board, NSF's policy oversight body, they were approved for support for the rest of their full five-year agreement. The last center to be established, the Pittsburgh Center for Advanced Computing, which is jointly operated by Carnegie Mellon University and the University of Pittsburgh, got the go-ahead from the Science Board on 20 August after only one year's operation. Now that it's attained the blessing of the Science Board, Pittsburgh proposes to sell its existing Cray X-MP/48, which is already used at 90% capacity, to buy a Cray Y-MP in fiscal 1989—though whether it does this depends on the center's ability to raise the money to buy the new machine. Although the Y-MP is still in R&D at Cray Research Inc in Minneapolis and unlikely to be available until late 1988, it should enable its users to do calculations with



ELLIOT PLOTKIN / PHYSICS TODAY

Map of supercomputing networks connected to the five NSF centers and the National Center for Atmospheric Research resembles an airline routing chart. NSFNET links the main nodes as the backbone of the entire system. For researchers on agency grants, NSF pays for time on the Defense Department's ARPANET and the Energy Department's MFENET, as well for the use of such networks as NYSERNET (New York State Educational and Research Network), SURANET (Southeastern Universities Research Association Network), NCSANET (the network of Illinois's National Center for Supercomputing Applications) and USAN (University Satellite Network).

three times the capacity and speed of the X-MP/48.

NSF and the university centers know that advances in supercomputers make last year's machines seem as stale as last week's croissants. Though they are still fledglings in the world of supercomputers, some centers have augmented their supercomputers and, like Pittsburgh, plan to upgrade their equipment in the next year or two. The original intention, says John W. D. Connolly, director of NSF's Office of Advanced Scientific Computers, was not to create a group of "FLOP shops" whose main purpose would be to keep up with the latest peak power (as measured in FLOPs, or floating-point operations per second) attained by computer manufacturers.

"We no longer speak of supercomputers in terms of maximum gigaflops but of average power for scientific applications," says Connolly. "We talk about the ability to deliver useful research results. That's much more meaningful."

White House push. NSF's interest in computers was slow in coming. Its decision to create supercomputer centers was driven in 1983 by the agency's director at the time, Edward A. Knapp, along with President Reagan's science adviser then, George A. Keyworth II. Friends and colleagues at Los Alamos National Laboratory before they were called to Washington, they agreed to push the idea of supercomputer centers through the White House Office of Management and Budget even though officials in that agency opposed the concept. The arguments of Knapp and Keyworth were endorsed by several studies conducted by members of the Science Board and the NSF staff. US computer makers and university scientists also supported their efforts.

Until then, government orders for supercomputers had principally been meant to foster weapons design, weather prediction and space exploration. In the 1970s the Energy Department opened state-of-the-art computer facilities "outside the fence" at the Los Alamos and Livermore weapons labs to some university researchers in fields such as plasma physics and atmospheric science. In addition, some scientists collaborating with foreign researchers were able to access supercomputers, almost always of US make, at such places as CERN and the Max Planck institutes. But for most academic researchers, access to supercomputers was unavailable—an elusive and expensive Holy Grail that held hope for solving complex problems of science and technology.

Enter now the NSF program, with high expectations: to enlarge the number of researchers who would be able to solve many previously intractable problems by using computers, to train a generation of students and scientists to use the latest machines, and to stimulate innovative computer design and development at both universities and industry. The discussion at the Science Board meeting on 20 August suggested that the NSF program not only is realistic but has already achieved impressive results in disciplines as diverse as astrophysics, econometrics and materials science.

Congressional support. The beginning was remarkable. NSF made its first moves cautiously in late 1983 when it bought the equivalent of some 5000 hours of supercomputer time at Boeing Computer Services, the University of Minnesota and Purdue University for distribution to academics during the gestation period before it could create its own centers. The agency requested \$20 million in its 1985 budget to set up the first center. Congress's reaction was unexpected. It was so enthusiastic about NSF's concept that it approved funds, with the agency's agreement, to start four centers in fiscal 1985.

NSF's first solicitation evoked 22 proposals from academic institutions and groups to set up centers. The first to start running, in November 1985, was the San Diego Supercomputer Center at the University of California at San Diego. It was a clone of the Department of Energy's Magnetic Fusion Energy Computer Center at Lawrence Livermore Laboratory in that it used the same machine, a Cray X-MP/48 operated at GA Technologies in San Diego. The San Diego center used the same software as the MFE center and shared the same network, MFENET. Some 15 months later San Diego marked its success by becoming the first NSF center to be fully saturated by users.

San Diego, which is run by a consortium of 25 institutions, has proposed that NSF finance an upgrade of its X-MP/48 to a Y-MP. While the X-MP was "at the cutting edge when we bought it," says the center's director, Sidney Karin, "it has now been surpassed." A Y-MP at the San Diego center would increase capacity threefold. The hitch in this scenario is that the agency is not likely to have an additional \$29 million in its budget to buy the Y-MP. Worse yet, NSF isn't sure it can come up with the extra \$12 million per year to lease the new Cray.

San Diego does not intend to trade its X-MP for the more powerful Y-MP. Having two machines with staggered upgrade paths, Karin observes, will provide for smoother transitions and economies of scale, thereby enabling the center to take advantage of the full useful life of each machine. "The need for upgrades is not an issue for some far-off year," he states. "If we are going to stay ahead in research, we must act soon."

IBM donation. Last July, Cornell University's Center for Theory and Simulation in Science and Engineering replaced its IBM 3090-400 mainframe, which had been installed only a year before, with the company's recently introduced 3090-600E, equipped with six vector processors rather than the four of its predecessor. The new machine, says Cornell's Wilson, provides 60% more capacity and twice the memory of the previous supercomputer. Like the earlier machine, the new model was donated to the center by IBM. Wilson has asked NSF to fund another 3090-600E and additional array processors produced by Floating Point Systems of Beaverton, Oregon—hardware that would overwhelm the center's present quarters, but would fit neatly into its proposed new building (see box).

The other two NSF centers are also eager to replace or supplement their machines. NSF is committed, according to C. Gordon Bell, director of the foundation's computing division, to "maintain the centers at the peak power available." Accordingly, the National Center for Supercomputing Applications at the University of Illinois in Urbana–Champaign is exploring both upgrading its Cray X-MP and adding a second supercomputer—possibly the Cray II, which has already been delivered to government defense and intelligence agencies.

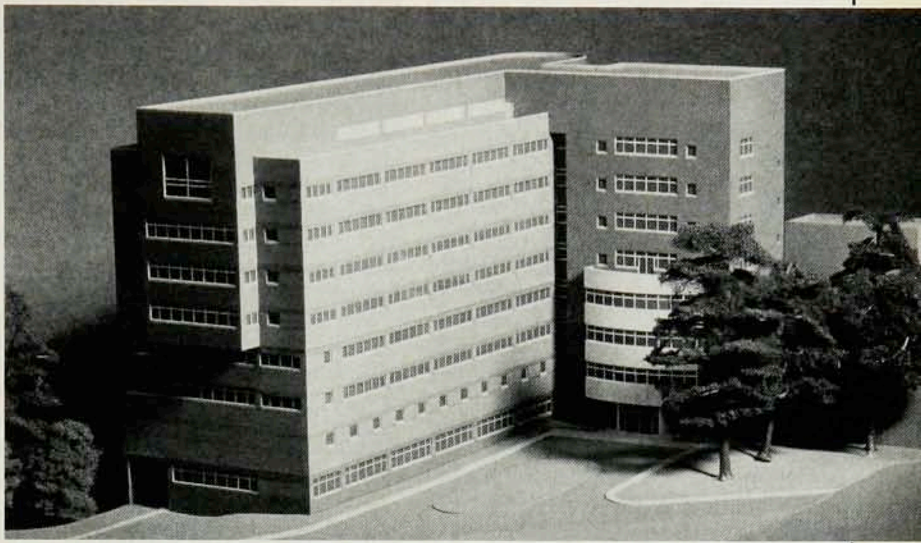
Private funding. Money for a Cray II would not all come from NSF, but would be funded in part by an industrial program, says Larry L. Smarr, director of the Illinois center. Under this program, firms may contribute as much as \$3 million in return for 3000 hours on the Illinois supercomputer and support by the center's staff for three years. Eastman Kodak and Amoco have signed on this year as the center's first industrial partners, says Smarr, and other firms have expressed interest in joining. "My goal is ten partners over the next two years," boasts Smarr. Only the first three would be accommodated on the Cray X-MP/48, he claims; the other seven would require still another big machine.

The John von Neumann Center for Scientific Computing, which is operated jointly for 12 large universities and the Institute for Advanced Study in Princeton, is to replace its two Cyber 205 supercomputers with a four-processor ETA-10 this November. As the flagship research center for ETA, a division of Control Data Inc, this center is slated to get the second ETA-10 delivered. The first, a two-processor ETA-10, went to Florida State University earlier this year. The von Neumann center expects to receive an eight-processor model next summer if all goes according to schedule at ETA. For the 1990 fiscal year, NSF is considering an even faster ETA supercomputer with even more vector processors and more powerful semiconductors.

So far, von Neumann has been the most troubled of NSF's centers. A peer review earlier this year criticized it for lacking both internal organization and commitment from its academic partners, a group including such prestigious universities as Harvard, MIT, Columbia, Princeton, New York University and Rutgers. Von Neumann's problems appeared insurmountable: It has had four presidents in two years—counting one interim and one acting head. Its board still cannot agree on whether to create a center for scientific research or simply to offer supercomputing capability. Its Cyber 205s are "half a generation older than the machines available at three of the other centers" and "not as interesting," according to Richard G. Leahy, associate dean of research of the faculty of arts and sciences at Harvard and chairman of the consortium's board. Some members of the consortium doubt that the ETA-10 will be as exciting and productive a machine as consortium members had hoped when they ordered it two years ago. Delivery of the supercomputer is now six months behind schedule and tests have indicated it is not as fast as promised.

Deep scars. NSF warned von Neumann's officials that it will cut off funds for the center unless the consortium members provide some support of their own—a condition in the NSF contract that not all the universities have honored. Despite these problems, the center's future now seems brighter than a year ago, when reports by review committees were so negative that NSF put the center on notice and changed the review cycle drastically from once a year to once a month. The foundation also cut the center's request for fiscal 1987 from $11.5 million to $8.5 million. Some financial juggling and a new agreement to lease rather than buy the ETA-10 made the cuts less than fatal, but deep scars remain. Though the board has approved hiring more staff and buying additional graphics workstations and supercomputer accessories, empty offices and vacant rooms in a new building in Princeton, New Jersey, are silent testimony that the von Neumann center

Cornell's supercomputer building at the brink



Of NSF's five supercomputing centers, only Cornell's lacks a building to house all its facilities and staff under one roof. At Cornell the IBM 3090-600E and the accompanying Floating Point Systems array processors are located in the main computer building, while the faculty and staff are jammed ears to elbows in a jumble of prefabs across the campus, as well as in the Olin Hall of Chemical Engineering. So there were cheers at Cornell's Center for Theory and Simulation in Science and Engineering when New York State's Urban Development Corporation agreed to put up $5 million in grant money and another $5 million as a loan to help fund a $29 million new home for the machine and its people in a sprawling engineering complex. In addition, an anonymous donor offered $10 million more, which would enable Cornell to double the height of the proposed building, thereby producing additional space for the planned expansion of the college of engineering.

The trouble is that the proposed building site stretches about 15 feet into the oak, maple and other hardwood trees that grace the northern rim of Cascadilla Gorge, an idyllic spot that critics contend the university promised never to build on. Environmentalists argue that 45 trees at the brink of the gorge would have to be cut down to make way for the structure. Urban planners complain that the proposed building (see the model in the photo above) is nothing special anyway, resembling thousands of nondescript contemporary structures in suburban communities and industrial parks. As such, they gripe, it is esthetically unexciting.

If built, the new building would be the third tallest structure on campus after Bradfield Hall and the McGraw Bell Tower. Varying between 140 feet (at one side) and 160 feet (at the western end of the gorge), it would rise to the height of Barton Hall, the Schoellkopf Field press box and a planned tower on the engineering quadrangle. Its design is somewhat higher than the typical eight-story building because its floors will require extra space to accommodate computer cables.

For its part, the university administration claims the proposed building is absolutely necessary to relieve the overcrowded and outmoded facilities now occupied by the theory center and engineering college. Between 1938 and 1962, when three-quarters of the engineering campus was built, Cornell never anticipated the large, sophisticated and expensive equipment, instruments and systems that are now required for education and research, the administration claims.

"We have talented young researchers who must work in hallways," says John F. Burness, Cornell's vice president for university relations. "Unless the severe space problems facing the college are solved, Cornell will lose its ability to attract and hold the world-class faculty that is the key to success. The theory center has attracted national attention to Cornell and to Ithaca. Yet for all its prominence, the center is an absurdity, in that many of its staff members are housed in temporary quarters. The theory center continues to compete for limited Federal research funding. It is vital that we show the NSF that we are making substantial progress toward providing new facilities. To the extent that the theory center thrives, research and education at Cornell will prosper. We will strengthen our nation's competitive position in vital industries and our community will benefit from clean new industry."

On 25 August the Ithaca Planning and Development Board voted unanimously to ask state officials to cancel plans to back the controversial building. It is not certain if the Urban Development Corporation will consider the city's ruling important enough to rescind the earlier decision. The UDC is expected to decide in November which way to go. In the meantime, to help the UDC make its decision, the university has hired an independent firm in Rochester, New York, to produce an environmental impact statement describing the likely consequences of the building on the gorge.

—IRWIN GOODWIN

still isn't operating at anywhere near full capacity.

Most board members prefer to talk about the accomplishments of the past year rather than the turmoil of the year before. Credit for much of the progress, say board members, goes to Joseph F. Traub, who took over the presidency last November. A canny negotiator, Traub worked out a deal with Control Data under which the second Cyber 205 is essentially free—the center is responsible only for site preparation and electric power. He also wangled new financial arrangements for the ETA-10 that take into account the slow progress in developing software for the machine.

But Traub never got to do the job for which he was hired. Instead of making von Neumann a top supercomputing center, he quit unexpectedly, for personal reasons, he declares, to return to his post as chairman of the computer science department at Columbia University. He prefers life on a vibrant university campus, he says. Although only a few miles from the main campus of Princeton University, one of the consortium members, the von Neumann center lacks the continuous stimulation of scientific and cultural activities. The other four NSF centers are on bustling college campuses. To make up for this lack, Traub says, the consortium must create an "invisible college" that will provide the infrastructure to attract and retain top scientific and computer experts. One way to do that, he suggests, would be to offer programs in such fields as molecular modeling to attract leading people. Some board members disagree with Traub's ideas and approach.

When the Science Board met on 20 August, members were told that Doyle D. Knight, a von Neumann trustee and professor of mechanical and aerospace engineering at Rutgers, had agreed to become president of the center.

Research changes. The computerization of scientific research is one of the most dominant changes in university research work. Erich Bloch, NSF's current director and himself a former computer engineer who managed IBM's 360 program, is convinced that supercomputers will change the course of some research forever. "Predicting the future is always risky," he asserts, "but I already see that computational research is practical and productive in such fields as physics, biochemistry, aeronautical engineering and atmospheric science."

For example, Michael G. Rossmann, a Purdue biologist, has used NSF supercomputer time on Purdue's machine to simulate the structure and behavior of human rhinovirus 14 in his study of common cold viruses. Rossman claims he was able to do in one month on a Cyber 205 what might have taken ten years of laboratory work. Another example involves computational simulation of interactions among vehicle emissions, meteorology and chemistry in the Los Angeles basin. Gregory J. McRae and his colleagues at Carnegie Mellon solved more than a half-million coupled, nonlinear partial differential equations on the Pittsburgh center's X-MP/48 to determine that conventional emission control technologies are likely to be extremely expensive and not particularly effective in altering ozone and NO_x concentrations in such cities as Los Angeles, Houston and New York. McRae's group suggested using methanol in cars and trucks instead. Various agencies in California and the US Environmental Protection Agency are working together to advance the introduction of vehicles that would use methanol as well as gasoline to reduce air pollution in the Los Angeles area.

Electronic networks. NSF funding of investigators using supercomputers has increased with the expansion of electronic networks to greater numbers of universities and private companies. For instance, CSNET, which is run by Bolt, Beranek & Newman in Cambridge, Massachusetts, connects Apple Computer Corp, Bell Communications Research, Emory University, Hewlett-Packard Labs, IBM Research and Rice University, among others, with more than a dozen additional networks. The networks are linked to the NSF centers and the National Center for Atmospheric Research (see map, page 61).

The foundation is taking steps with additional research implications. One innovation involves a system called EXPRES (Experimental Program of Remote Submission), which will enable researchers to transmit grant proposals to the agency by electronic mail. Another relates more directly to computer research. On 27 August NSF announced five-year projects at five universities to establish and enhance various experiments in computer or information science and engineering research. In this program the University of Washington will get $827 000 to advance understanding of memory multiprocessors and to design a networked multiprocessor with workstations. Princeton University will use its initial NSF grant of $549 000 plus university funds to set up an experimental computer science program in programming languages, graphics, very large-scale integration algorithms and algorithm animations. Purdue University will get $867 000 the first year to devise mathematical software and tools to stimulate geometric modeling. Georgia Institute of Technology will receive $708 000 for its Clouds Project, which is designed to develop a distributed object-based computer system. Rice University is to get $844 000 to create a parallel software laboratory called PARASOL, which is intended to support studies of the fundamental nature of parallel computing and applications to problems of importance in software engineering and scientific computing.

—IRWIN GOODWIN

Ride report: Charting the nation's future course in space

What happened to the nation that went first to the Moon and clearly dominated the exploration of the Solar System for more than two decades? A thoughtful answer to that question came on 12 August in a 63-page report by Sally K. Ride, the first US woman in space, who holds a PhD in astrophysics. Her report, based on a study conducted over 11 months with the help of a half-dozen unnamed members of NASA's new Office of Exploration, was commissioned by the agency's administrator, James C. Fletcher. Bearing the straightforward title *Leadership and America's Future in Space*, it is the most comprehensive recent effort within NASA to chart long-range directions for the nation's space program. Along with setting the course, the Ride report, as it is referred to at NASA, carries a disquieting message: The US space program lacks leadership, direction and, possibly most troubling, capability.

The report is certain to stoke the fires already burning in Congress on the space program. While it is addressed to NASA's management, the report serves notice that revitalizing America's space enterprise will require the commitment and support of the White House and Congress. Neither, says the report, has provided any coherent policy for a sensible and systematic program to explore space since the Apollo project began more than a quarter of a century ago. Worse still, NASA's program has been drifting aimlessly while the Administration and Congress debated whether to build a fourth orbiter to replace Challenger,