CUTTING-EDGE RESEARCH

Austin emerges as top supercomputer center

As more powerful machines help solve problems from global warming to human disease, University of Texas experts and Central Texas tech wizards claim a bigger piece of the action.

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When Earth scientists ponder the consequences of global warming, some look south to the West Antarctic Ice Sheet.

Parts of the ice sheet — which is 2½ miles thick and about the size of Mexico — have started moving more rapidly toward the sea. Its most active glacier is dumping about 4 cubic miles more ice each year than was the case 12 years ago.

Some scientists say that eventually, most or all of the ice sheet is likely to slide into the ocean, raising the world's sea level as much as 30 feet.

When? No one is entirely sure. But University of Texas scientist Don Blankenship plans to provide a better picture with the help of Ranger, the world's largest computer devoted to general research, which began operating in February at UT's J.J. Pickle Research Campus.

"Without Ranger, these results aren't possible," Blankenship said.

For many 21st-century scientists, cutting-edge research is increasingly reliant on new, more powerful computers to tackle really big problems. And several of those big new computers are being built through a federal initiative that will cost hundreds of millions of dollars.

"High-performance computing is having a greater impact in all areas of science, from climate modeling to environmental modeling to biological modeling to national security," said Jack Dongarra, a supercomputer expert at the University of Tennessee.

Coupled with immensely complex software, the machines enable scientists to make more detailed models of the natural world, sorting through mountains of research data to find new patterns and thus new knowledge on topics as varied as nanotechnology, the origins of the universe and the roots of common illnesses.

"This is the most exciting time in history to be a computational scientist because of these new instruments that are coming into the fold," said Omar Ghattas, an Earth scientist and computational science expert at UT's Institute for Computational and Engineering Sciences.

Until recently, Austin was a relative backwater in the field. The arrival of Ranger, prompted by UT's determination to keep pace with top research universities, is but one sign of a major turnaround.

Another is just across the street from Ranger in North Austin. In a dowdy, 1960s-era structure known as Building 45, hundreds of IBM Corp.'s top chip and computer engineers are helping design a machine labeled Blue Waters, which will introduce fundamental changes in how supercomputers work and will perform at about 30 times Ranger's level when it's built in three years.

These separate, high-profile projects, along with advances by chipmaker Advanced Micro Devices Inc., Dell Inc. and others, reflect the city's emergence in the past decade as a key center for innovative data-crunching technology that could help solve some of the biggest challenges facing mankind.

Though scientific supercomputers have been around for more than three decades, today's machines, fueled by dramatic leaps in performance of microprocessor chips, are vastly more powerful. Ranger, for example, packs about five times more punch than the top science research computers that came before it. The machine has a peak performance of about 504 trillion operations per second, which means it is about 30,000 times more powerful than a typical modern desktop computer.

Unlike the "big iron" supercomputers of past decades, which linked vast circuitry in a single large highly customized box, many modern supercomputers are collections of hundreds or thousands of smaller computers, or "nodes," each of which resembles a high-performance server computer that might go into a corporate data center or "server farm." The nodes are linked by super-fast communications switches that enable the different nodes to work together and share results.

Researchers with extremely complex problems flock to the new machines to tap their number-crunching power. Ghattas says Ranger will enable him to run earthquake projections that deliver twice as much "resolution" as he could previously get with less powerful machines.

Ranger's giant brain is now helping with about 150 research projects involving more than 800 scientists, a number that will top 1,000 by the end of this year. They are investigating everything from the internal control mechanisms in human cells to a more detailed picture of star formation in the first billion years after the Big Bang.

While some subjects, such as the early cosmos, might yield few practical benefits in the short term, Ranger could pay dividends in treatment of disease, in discovery of new drugs, in better understanding of climate change and violent weather and in development of nanomaterials — including substances that exhibit unique properties when manipulated on a microscopic scale.

"The computer is a kind of microscope," said Klaus Schulten, a University of Illinois biophysicist whose team uses Ranger. "The data that we work with are very complicated. We need the computer to look through the data. Without it, we are totally blind."

Schulten's 40-person team is out to discover essential processes that enable human cells to repair themselves. The team's computer models and findings have been used by thousands of other researchers to further their own research. The work is expected to be a foundation for potential new treatments of diseases, including Alzheimer's.

Ranger might well have been built at some other school were it not for Jay Boisseau, who runs the Texas

Advanced Computing Center on the north side Pickle campus. UT hired the brash, energetic Boisseau in 2001 after it was told it could not meet its goal of being a top-ranking research university without a top-ranking computing center.

"Jay has put Austin on the map," said Larry Smarr, a computer researcher at the University of California at San Diego's highly regarded computing center, where Boisseau worked before coming to UT.

Boisseau's new team won a stiff competition for a $59 million National Science Foundation grant to build Ranger and run it and provide support for researchers for four years.

The computer — consisting of nearly 4,000 smaller computers plus other equipment in about 6,000 square feet of floor space, roughly the size of three average homes — was built by Sun Microsystems. The smaller units use advanced, designed-in-Austin processors made by Advanced Micro Devices, which also works closely with supercomputer maker Cray Inc.

For Boisseau, the 2006 grant was as sweet as the Longhorns' Rose Bowl win to secure the national football championship earlier that year.

"We are instrumental in making sure the best science in the world gets done here," he said.

That science will be done by corporations as well as by academics. UT's computing center currently has fewer than 10 commercial clients; the goal is 20. A key condition is that their projects benefit the university as well as the company.

A few scientists grumble privately that supercomputing has become a tail that wags the dog: The availability of research funds tied to the big computers unduly influences decisions about which projects to pursue. Supercomputer advocates counter that they are an enormously productive investment because they do work in so many different fields, and the work they do can't be done any other way.

Like a No. 1 football ranking, the biggest-hardware title can't be held forever. A supercomputer nicknamed "Kraken" will be built this year at Oak Ridge National Laboratory in Tennessee under another National Science Foundation grant, and awards for two more machines are in the works. They all are expected to deliver performance that is slightly higher than Ranger's.

Those, in turn, will be left far behind by Blue Waters. Though IBM-Austin has a significant piece of that $208 million, federally funded project, the computer will be owned and operated by the University of Illinois' National Center for Supercomputing Applications.

The machine will depend on IBM's next-generation Power7 processor, which is still in development in Austin. Like Sun, IBM is attempting to expand supercomputer sales beyond the handful of federal contracts by selling to companies that need high-end machines, including those involved in petroleum exploration, aerospace engineering and Internet commerce.

Blue Waters is "a moon-shot kind of effort," said Ravi Arimilli, a key player in the project and one of a handful of technical workers in Austin who has been designated an IBM Fellow, the company's highest technical honor.

IBM and Sun are among a group of companies actively developing high-performance computers from high-volume commercial processor chips.

For its part, Dell has pursued sales of large technical computers for nearly a decade and says it has 24 systems among the 500 top-performing supercomputers. The company recently announced the installation of a major research computer at Purdue University.

At the start of this decade, federal money for supercomputers was intended primarily for nuclear weapons research. Scientists such as Ghattas noted that U.S. computers for academic science were falling behind.

The performance of Japan's Earth Simulator, completed in 2002 for an estimated $350 million, put all American computers in the shade, which in turn raised concerns in Congress.

"The notion that we were no longer No. 1 ... did prompt the examination of whether we were doing enough," said Daniel Atkins, director of the National Science Foundation's Office of Cyber Infrastructure.

By 2005, the foundation had new financial support from Congress and announced it would spend nearly half a billion dollars on open-science supercomputers. Scientists who want to use these machines must get permission from a foundation panel.

The results of the new federal money include Ranger, Kraken and Blue Waters, which are bargains in comparison with the Japanese model, in part because of the relentless advance of technology. Today's consumer desktops deliver more performance than the most powerful machines did 25 years ago. Ranger, built six years later than Earth Simulator with cheaper, more advanced chip technology, is several times faster, Boisseau estimates.

Now the challenge is harnessing that power.

Software for standard computers proceeds in sequence, step-by-step. But a supercomputer uses a complex kind of software called massively parallel programming, which distributes parts of a computing job among the hundreds or thousands of smaller "node" units in a supercomputer. Many scientists lack the software skills needed for that kind of programming.

For any open-science computing center, a major part of the mission is helping researchers get their software application ready to run on a big machine. Collaboration among researchers also helps bridge the gap. For example, Ghattas, who is using Ranger for his own Earth science research, is also assisting Blankenship's team on developing a model the West Antarctic Ice Sheet.

"There are many researchers — in geosciences, mathematical and physical sciences, polar programs and engineering — all these researchers are itching to get on this thing," Ghattas said. "We have gotten this machine, and now we've got to deliver."

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