UWYO

THE MAGAZINE FOR ALUMNI AND FRIENDS OF THE UNIVERSITY OF WYOMING

Summer 2010

THE NEED FOR SPEED

SUPERCOMPUTING COMES TO WYOMING

Homecoming Honors S. H. Knight

Homecoming's hoopla this year centers around an unusual theme for an unusual man. "Two Million B.C." is a salute to the man who knows as much about that year as anyone alive.

SAMUEL H. KNIGHT, retiring head of the Geology department, is the man of the hour. This year's Homecoming holds a double significance for him.

Fifty years ago S. H. Knight stood in line for his sheepskin at UW's commencement and 40 years ago he started the Homecoming tradition.

In his exclusive career at his alma mater, Knight has earned a demi-god status as one of the University's most outstanding professors.

APPROPRIATELY enough, he attended University prep and took his first geology course from his football coach. In 1929 he received his doctorate from Columbia University, but resisted the lure of the Ivy League circuit to return home.

"As an instructor," he says, "I could receive as much stimulus from teaching Wyoming youth as Massachusetts youth. Besides, I didn't think I could be completely happy away from the mountains."

So Knight returned to the city of his birth and took over the position held by his father 15 years earlier.

AFTER a busy career which included organizing Homecoming and marking off Corbett Field for old-time gridiron battles, Knight has no intentions of fading away with the typical old professors.

Looking ahead, Knight says, "Retiring isn't going to change my way of life seriously." The shock of turning in his chalk will be somewhat lessened by his light teaching schedule this year.

MEANWHILE, on the lawn of the Geology building, he continues to construct his life-sized model of a Tyrannosaurus Rex.

When completed the representative of the "Two Million B.C." era will stand 20 feet high and 45 feet long. It's the only one in the country to be constructed of fabricated steel with a hammered copper coating.

Knight will switch to an updated mode of transportation when he mounts his horse to head the Homecoming parade.

He will be a guest of honor at a dinner in his honor given by UW Pres. G. D. Humphrey. He and his fellow 50-year grads will have special seats at the game and will be feted at the All-Alumni luncheon after the game.

Images courtesy of the UW Annuals and the Emmett D. Chisum Special Collections

FEATURES

UWyo Summer 2010 volume 12 number 1

UW veteran Troy Phillips as Pistol Pete in Iraq.
photo courtesy of Troy Phillips

Travel 40 miles east of Laramie on I-80 and you will come across the birth of the future.

The need for speed

Breaking ground with great expectations

by Dave Shelles

Editor's Note: For more than a decade, the University of Wyoming has been working to build a Center for Excellence in Computational Science. While the NCAR-Wyoming Supercomputing Center will help UW reach its goal, it's not the only resource available to UW's growing roster of computational scientists.

It's as if Liqiang "Eric" Wang has been planning for a supercomputer his whole career.

Really, that's what every computer scientist wants—a massive, fast computer to run and improve code.

Wang and the rest of the University of Wyoming community will have the chance to work with one of the fastest computers in the world, as UW and the National Center for Atmospheric Research broke ground on the NCAR-Wyoming Supercomputing Center (NWSC) near Cheyenne, Wyoming on June 15.

Wang sits in his office in Engineering Hall with a smile on his face. He says he's excited about the advent of supercomputing at UW and sees two main benefits.

The first, he says, is to his own research. Wang designs tools for supercomputing that help create more dependable computer systems, and the NWSC can improve the performance of his systems by making them run faster. Faster computing means he can produce more data.

Second, his faculty collaborations will benefit. Wang is one of eight scientists at UW who is part of the Interdisciplinary Computational Sciences program, a growing multidisciplinary area that focuses on solving scientific problems through computing. Wang says the NWSC will help improve the performance of applications in other areas; for example, geology.

Shaochang Wo (UWyo, Spring 2008) sits in his office in the geology building, patiently watching a graphic replay of a simulated moving oil bank in a reservoir. A three-dimensional reservoir model shows him where the remaining oil may exist, which is a simple explanation for his work with the Enhanced Oil Recovery Institute (EORI). On another computer screen, a rolling report shows a simulation job is working slowly but steadily, drawing computing power from a cluster of 15 nodes, each node powered by two central processing units.

The NCAR supercomputer will exceed that power exponentially. For Wo, that means his simulations of oil production will take far less time and enable him to report more data more accurately.

Robert Mayes, director of the Science and Math Teaching Center at UW, looks over the concept rendering of the NWSC facility at the June 15th groundbreaking ceremony.

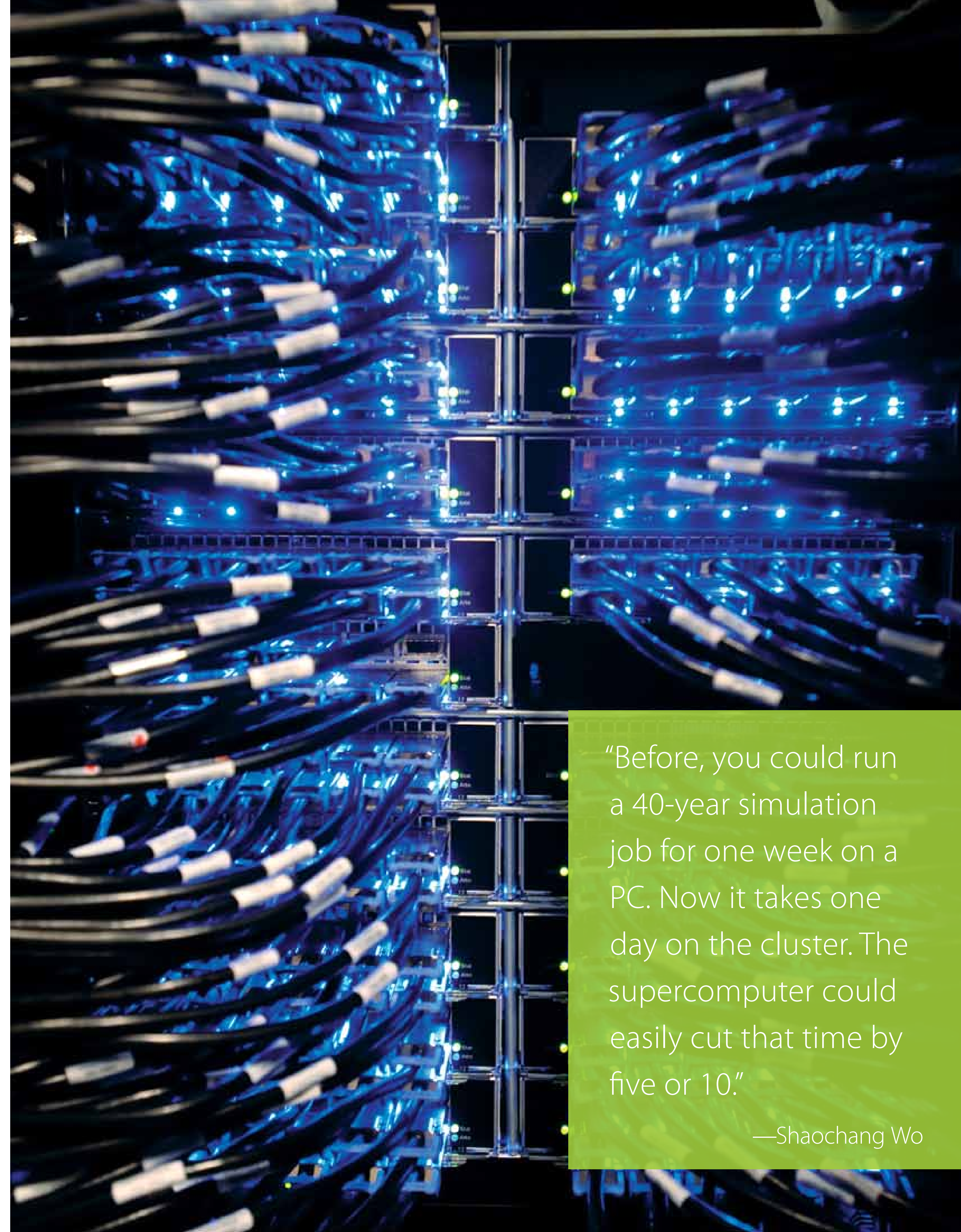
"For now we usually limit the size of a model under one or two million grids, even while running on the cluster, because of the limitation of computer memory space. Data transfer and storage is also an issue. If you want to do really detailed reservoir modeling and simulation with tens of millions of grids, for now it's almost impossible," Wo says.

"Think about this: The average Wyoming oil field has been in production for more than 40 years. If you want to know currently how the remaining oil distributes in a reservoir, you have to simulate the whole reservoir production history—it's called history matching, in which the simulated results must match the observed measurements, historical production and pressure records for example. Usually we want to have a quick turnaround time during the history matching process, like a half-hour or so, to test various scenarios. Even for this small cluster we already speed up our turnaround and it's five to six times faster. Before, you could run a 40-year simulation job for one week on a PC. Now it takes one day on the cluster. The supercomputer could easily cut that time by five or 10."

Wo also has some multidisciplinary plans, thanks to his background in mathematics. He earned his doctorate in mathematics from UW in 1997. Wo joined EORI in 2004 as a senior research scientist. With the supercomputer, he says solving the problems of advanced oil recovery gets somewhat easier.

"For me, it was definitely a really exciting moment," he says of learning UW would get the supercomputer. "The lack of computing power has been a bottleneck for us to conduct high-resolution reservoir simulation. No matter how powerful a computer is, there are always bigger and more complicated problems to challenge its capabilities."

Where Wo migrated from mathematics to oil recovery, professor Dan Stanescu started out in engineering, earning



"Before, you could run a 40-year simulation job for one week on a PC. Now it takes one day on the cluster. The supercomputer could easily cut that time by five or 10."

—Shaochang Wo

Part of the energy that's expected to power the NWSC will come from wind power. Project planners say this supercomputing center will be among the most efficient in computing speed per energy used.

his bachelor's and master's degrees in that discipline before earning his doctorate in mathematics.

Stanescu worked in aeroacoustics, the study of how to reduce the amount of noise from airplanes. At Florida State University, he worked on what at the time was the most powerful supercomputer in any university in the world, figuring out how sound waves transferred from high in the sky to the ground.

"With this computer, we have a good chance to nail down very clearly the noise signature on the ground of an aircraft with a commercial turbofan," he says. "Those are your jetliners today. We can probably model what will be the noise that someone on the ground hears from this airplane and see how we can optimize in the sense of reducing the footprint on the ground. That's really what I see from my perspective."

Stanescu points out that the majority of research done with the computer will involve climate data and predicting weather. After all, climate change is one of the most pressing issues facing our planet today, and NCAR is at the forefront of developing the computational tools for weather and climate prediction. Stanescu describes a grid over the entire planet, and the intersecting lines create the data points. The supercomputer essentially creates those lines and takes the data from an increasing number of points.

"If you put more grid points, make your grid denser, your computation is going to become more reliable," he says. It's not going to veer off so fast from the data you get from the meteorological stations, because a lot of this depends on what happens in the details in the grid.

"We can be much more reliable. It's not my research, but this is a very important research area."

The sciences of computer science, mathematics and geology dominate discussion of what to do with the supercomputing center. Associate professor Alex Buerkle, an evolutionary geneticist in the department of botany, points out that the National Science Foundation's largest grant was awarded to the University of Arizona to develop computational solutions to the biggest challenges in plant science. That illustrates the importance of computational science in biology, Buerkle says.

"The biggest computer problems today aren't restricted to math or engineering, but are also in biology," he says. "The Human Genome Project is a computational project. You get words that you need to put together into sentences that you need to put into paragraphs that you put into the whole genome. The problem of ordering all that is a computational problem."

Buerkle has worked with Stanescu and engineering professor Dimitri Mavriplis on computational science projects and teaches a course in computational biology; last offered in fall 2009, he will teach it again in the spring.

"Obviously I do computational science, and I do a lot of computing. But there is a lot yet to be determined about how UW faculty and student researchers will use this resource," Buerkle says. "We are trying to build programs and facilities for research computing at UW and this is one component of the research computing landscape."

Dimitri Mavriplis might be the luckiest one of the bunch.

The professor of mechanical engineering will spend the 2010–11 school year at ground zero of the project, working with applied mathematics and statistics groups at NCAR on developing new algorithms and parallel computing, a technique where many calculations are carried out simultaneously.

"We will be collaborating on developing and testing new algorithms and parallel computing techniques designed to scale to large numbers of cores on machines such as the NCAR supercomputer," Mavriplis says. "By being in residence at NCAR, I also expect to keep well informed on the developments of the new facility and the hardware configuration of the machine and to be able to serve as a liaison back to the UW research community on these matters."

Like Stanescu, Mavriplis has experience with supercomputers, having worked with nationally funded installations at NASA and with the U.S. Departments of Defense and Energy. He knows firsthand what a supercomputer can do for research.

"The availability of the NCAR machine to UW researchers provides a unique advantage for engaging researchers in the important aspects of developing leading edge simulation capabilities," Mavriplis says. "In the absence of supercomputer facilities, researchers naturally gravitate toward developing applications which can be run on commodity hardware, which is typically available at the department level and thus do not engage in the important aspects, which are needed to enable large scale simulations on leading-edge hardware."

While it's easy to get excited about the research aspect of supercomputing, Stanescu says the primary mission is to educate students. He cites the opportunities for educating the next generation of computational scientists that arise from having access to the supercomputer. The multidisciplinary approach benefits both from multiple departments working together, and from enthusiastic students willing to learn.

"You have to know a lot of stuff. You have to know a lot of mathematics and a lot of computer science," Stanescu says. "It's a very narrow niche in computer science, and it's not taught in most places. I'm talking about this item called 'how to use this big computer.' It's called parallel programming.

"We need to teach our students parallel programming, and a major incentive to learn that would be to have access to a big computer, at least a little bit of it. Try it out, check it out, see how it works. Of course, by the time they use that computer, they have to have their programs tested and running. So we provide some of those capabilities here. It might do well for them to have in the back of their minds the idea that there is a good possibility to work on that supercomputer at a later time.

"I think it's a very important step, a big opportunity that we have. I hope that this is going to get the kids more active in this direction," Stanescu says.

In the fall, Wang will teach a class called Introduction to High-Performance Computing. Two years away from the first experiments on the new supercomputer, Wang says he's excited about the future of this class, a core course in the interdisciplinary computational science minor.

"This class introduces students to how to do programming on a supercomputer," Wang says. "Right now we run our programs on a local cluster, not a real supercomputer. When we have the NCAR supercomputer, we can teach students how to run code on that machine. That's a very good opportunity for students. Maybe now we can have a trend of more graduate and undergraduate students interested in this kind of research." ❖

GLOSSARY OF TERMS

Bit: Short for binary digit, the basic unit of information in computing and telecommunications; it is the amount of information that can be stored by a digital device or other physical system.

Byte: A unit of digital information in computing and telecommunications. It is an ordered collection of bits, in which each bit denotes the binary value of 1 or 0.

Computer science: The study of the theoretical foundations of information and computation, and of practical techniques for their implementation and application in computer systems.

CPU: The central processing unit of a computer where computations are carried out.

Interdisciplinary Computational Science: A relatively new but rapidly growing multidisciplinary area that focuses on the solution of real-world scientific problems through the development and use of computer algorithms, methods and hardware for analysis.

NWSC: The NCAR Wyoming Supercomputing Center

Parallel computing: A form of computation in which many calculations are carried out simultaneously, operating on the principle that large problems can often be divided into smaller ones, which are then solved concurrently ("in parallel").

PUE Index: The Power Usage Effectiveness (PUE) Index reflects how much of the facility's power consumption is used for actual computing, as opposed to support functions like cooling. PUE is defined as the ratio of the total power consumed by a supercomputing center to the power consumed by the information technology equipment of the facility.

Supercomputer: A large, very fast mainframe used especially for scientific calculations. Supercomputers are used for highly calculation-intensive tasks such as problems involving quantum physics, weather forecasting, climate research, molecular modeling (computing the structures and properties of chemical compounds, biological macromolecules, polymers, and crystals), physical simulations (such as simulation of airplanes in wind tunnels, simulation of the detonation of nuclear weapons, and research into nuclear fusion).

Terabyte: A multiple measured by the International System of Units of the unit byte for digital information storage and is equal to 10^{12} (1 trillion short scale) bytes. The unit symbol for the terabyte is TB.

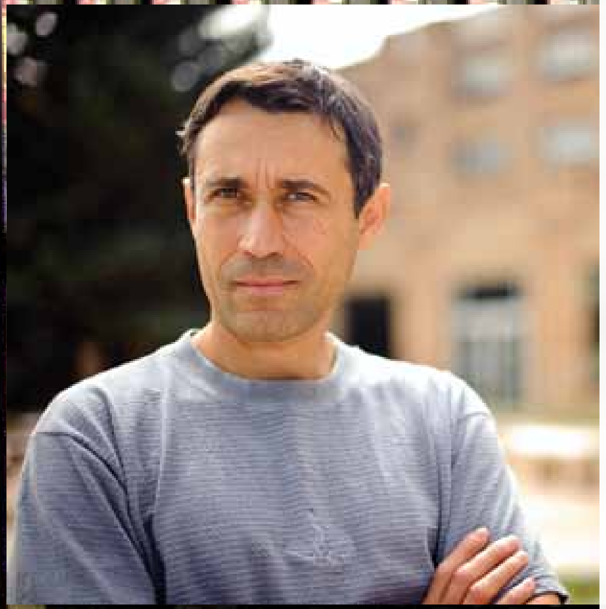
ON THE WEB

The National Center for Atmospheric Research
http://ncar.ucar.edu

Interdisciplinary Computational Science at UW
www.uwyo.edu/ICS/

The NCAR-Wyoming Supercomputing Center
http://cisl.ucar.edu/nwsc/

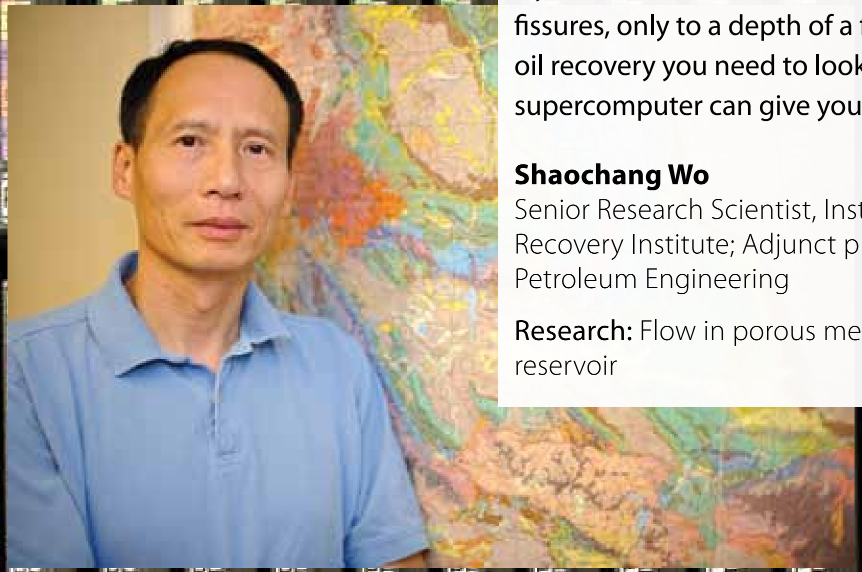
What impact does the supercomputer hold?



"It will put us in a very good position in terms of computational science, which is a major focus area for the university. If we have this capability here, we are going to be much, much more likely to attract researchers in this field. From my perspective, I also hope that we're going to attract a lot of students, in particular graduate students. Undergraduates would be good, as long as they go on after that. I think it's going to have a major impact. I'm optimistic. Maybe this will give them somewhere to come."

Dan Stanescu
Professor of mathematics

Research: Computational aeroacoustics, or the study of how sound waves from airplanes behave on the ground; also computational fluid dynamics, numerical solution of stochastic differential equations



"The most important part, for the supercomputer, is we can do high-resolution reservoir simulations. Right now, looking through seven layers of rock is difficult. You can see lots of geological features called fissures, only to a depth of a few feet. Once you get into enhanced oil recovery you need to look at where the remaining oil is. The supercomputer can give you much more information."

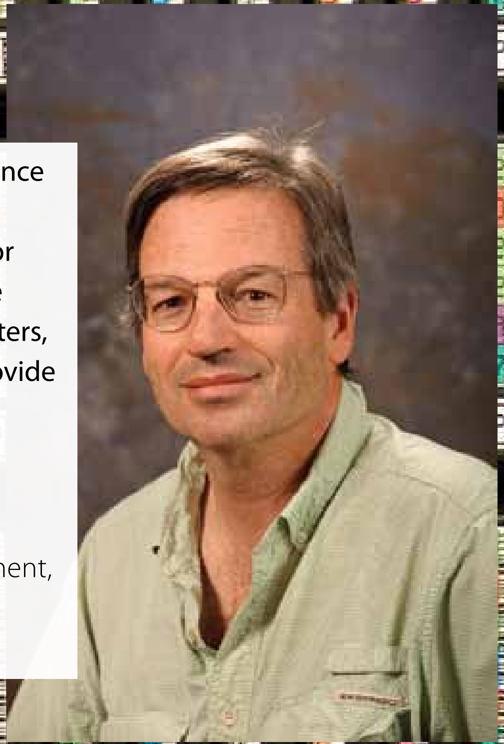
Shaochang Wo
Senior Research Scientist, Institute for Energy Research/Enhanced Oil Recovery Institute; Adjunct professor, Department of Chemical and Petroleum Engineering

Research: Flow in porous media, or seeing how fluids behave inside a reservoir

"Since we are focused on the development of high-performance algorithms and simulation capabilities, the availability of leading-edge hardware is not only desirable but necessary for us to contribute significantly in our field of research. We have traditionally had access to government-funded supercomputers, but the proximity and availability of the NCAR facility will provide us with a considerable advantage in this respect."

Dimitri Mavriplis
Professor of mechanical engineering

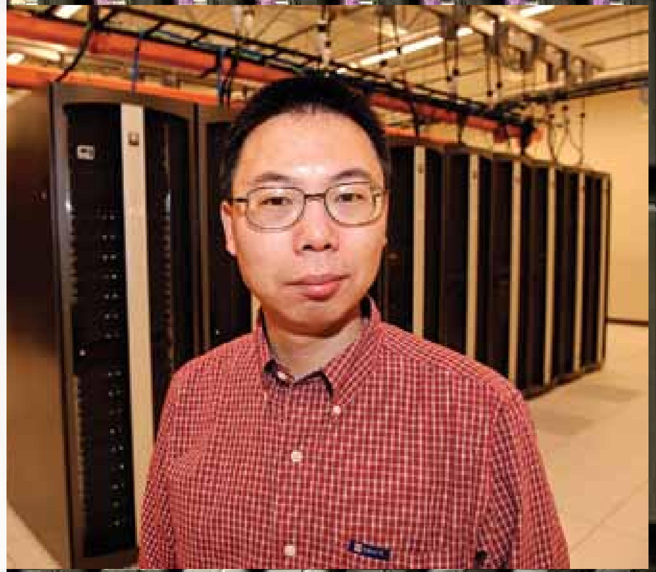
Research: Computational fluid dynamics, algorithm development, parallel computing techniques, wind energy simulations, aerospace applications

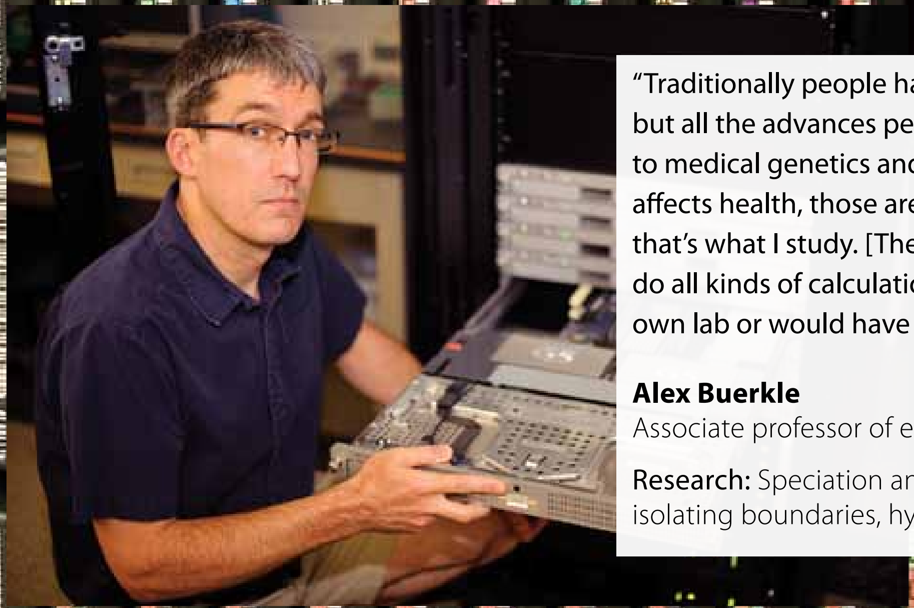


"I try to design tools to help design parallel programs, so the first benefit of the supercomputer is to provide a platform for me to conduct my research. I also work with other faculty, and we're trying to develop a code. As other faculty have said, the supercomputer will improve the performance. Based on the architecture, based on the network, based on the CPU, we would like to customize our code. To customize means we can adjust our code for this machine and make our code faster on that machine. That's our plan for when the new supercomputer is done."

Liqiang Wang
Assistant professor of computer science

Research: Design and analysis of parallel computing systems. He also is interested in integrating parallel computing with scientific workflows





"Traditionally people have thought about those problems, but all the advances people hope to make with respect to medical genetics and understanding how the genome affects health, those are huge computer problems and that's what I study. [The supercomputer] could allow us to do all kinds of calculations here that either now I do in my own lab or would have to go to national centers elsewhere."

Alex Buerkle
Associate professor of evolutionary genetics

Research: Speciation and the genetic architecture of isolating boundaries, hybridization, genetics of adaptation

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Welcome

to UWYO, the magazine that showcases the people who make the University of Wyoming great.

Our blend of features, news, and photography highlights members of the university community, its alumni, and friends who make the university a leader in research, teaching, service, and outreach.

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