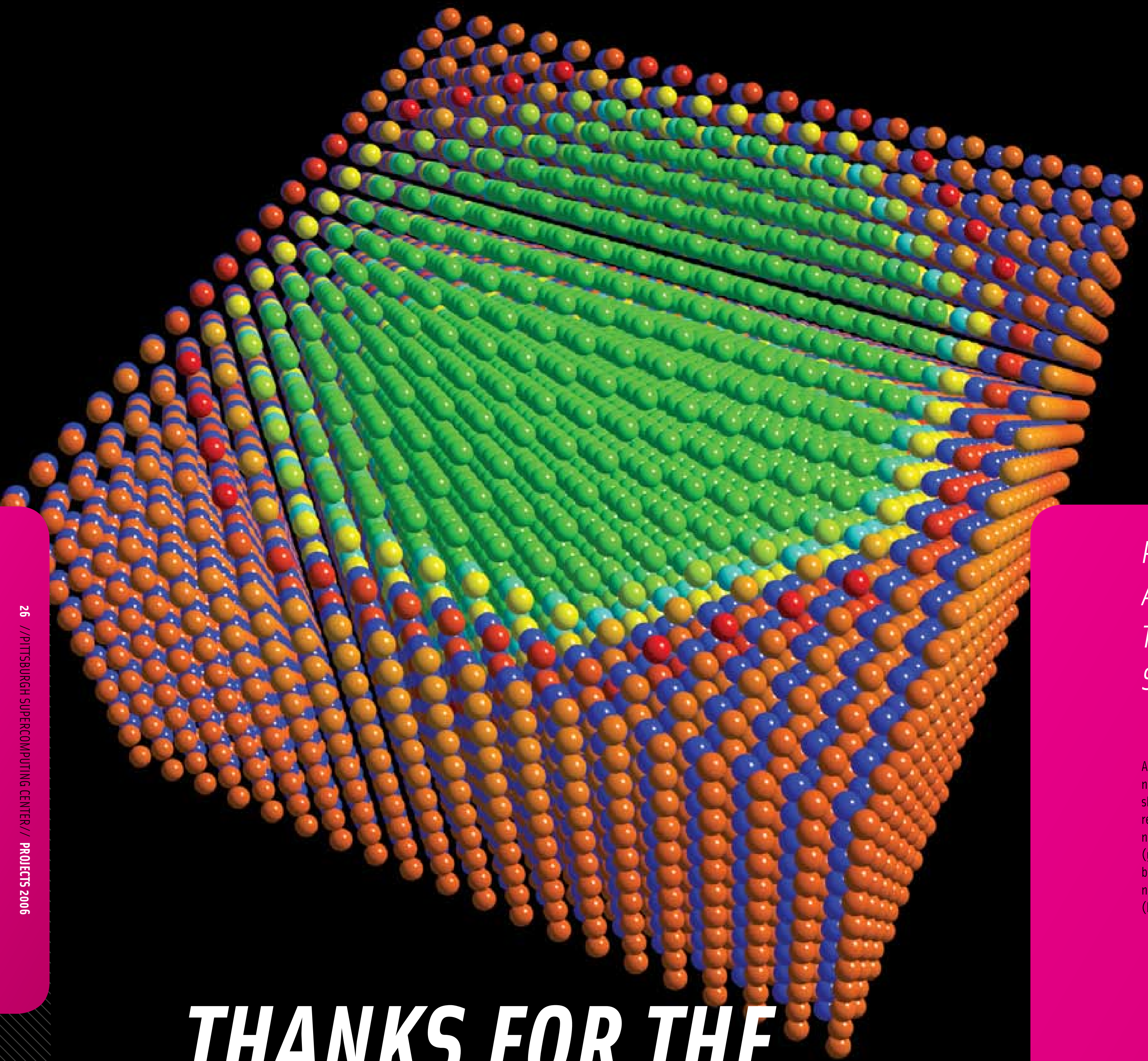
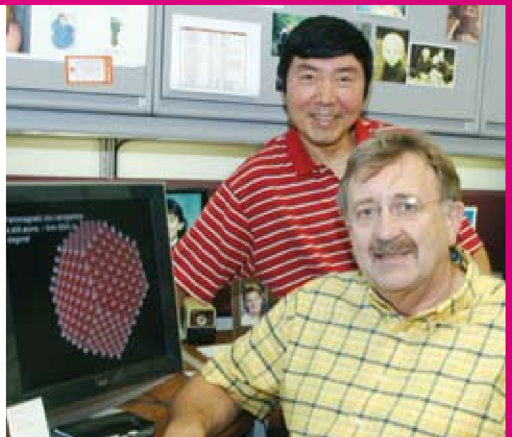


THANKS FOR THE MEMORY

POWERFUL QUANTUM METHODS AND THE CRAY XT3 OPEN A DOOR TO NEXT-GENERATION MAGNETIC STORAGE

A slice from the 2005 simulation, an iron nanoparticle embedded in an iron-aluminide matrix, shows charge distribution on the atoms (blue to red, positive to negative). In the nanoparticle itself, neutral iron (green) is bounded by iron atoms (yellow & light blue) that lose electrons. Other boundary iron atoms gain electrons to become more negative (red). In the matrix, aluminum atoms (blue) lose electrons to iron atoms (orange).



Malcolm Stocks (right), Oak Ridge National Laboratory, and **Yang Wang**, Pittsburgh Supercomputing Center

Computational scientists and other computer users in the future may hum this tune of gratitude, though perhaps few will appreciate how today's supercomputing helped to realize those even more capable hard drives of the future, as well as better iPods, DVDs, and who knows what?

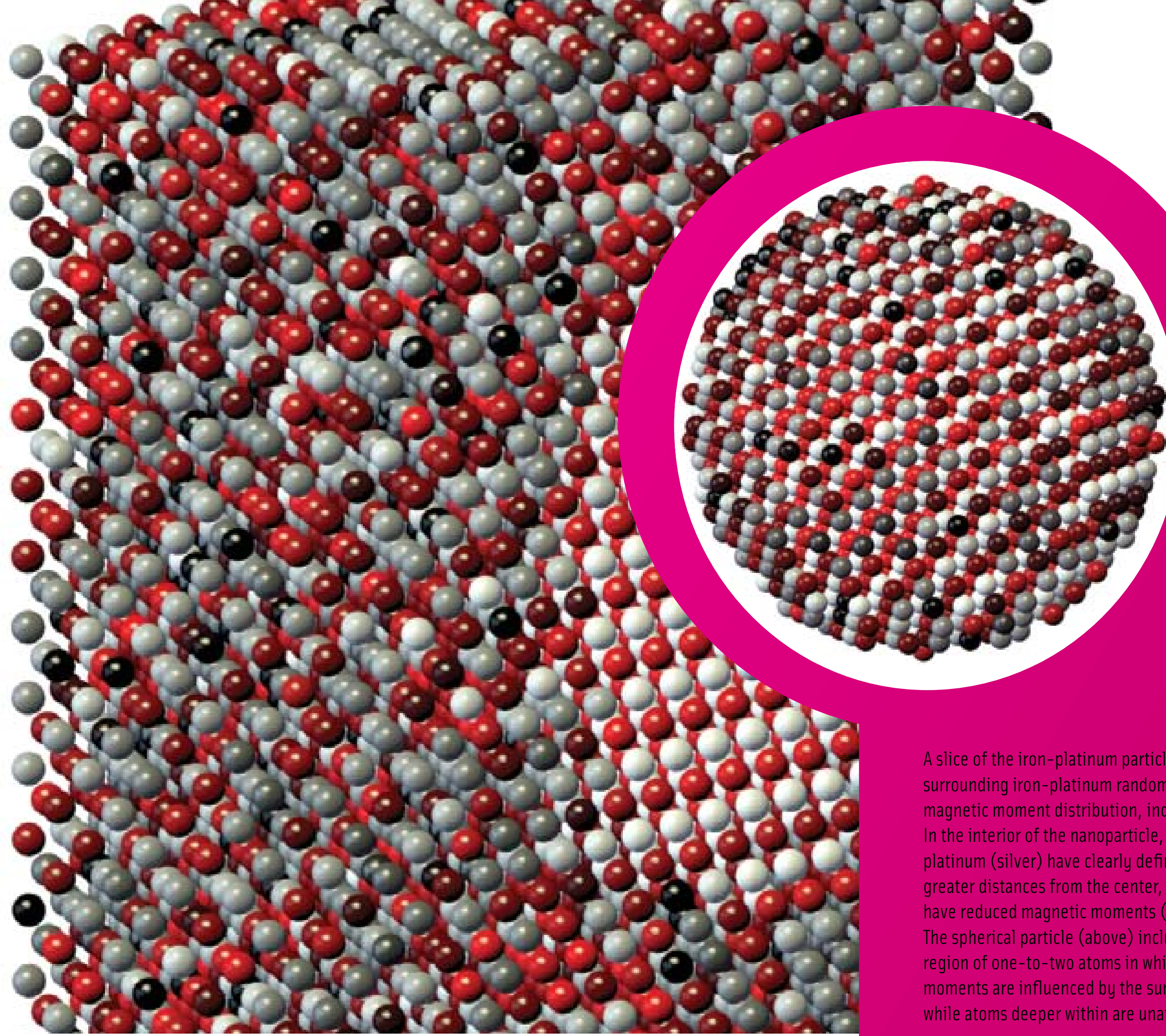
Technology has made steady advances in the ability to write and store vast quantities of information in smaller, more manageable forms, but current technologies are approaching their limit. How much smaller can you make grains of magnetized material before they start to act like the mind of an overstressed, aging human who steps out of the shower and can't remember if he's washed his hair?

Not much, which is why researchers are seeking a way to magnetize a single nanoparticle reliably, so that such a particle — rather than "grains" used in current magnetic-storage media — can record one bit of digital data. The door to this breakthrough is understanding what happens at the quantum level for each atom in a nanoparticle. Laboratory methods, for all their usefulness, can't provide this information. Over the past year, however, Malcolm Stocks, Yang Wang and their colleagues — using PSC's Cray XT3 — have shown that computational simulations can do the job.

"Experimenters can tell us a lot about the magnetic and electrical properties of a nanoparticle as a whole," says PSC physicist Wang, "but simulations are the only way we have to determine the magnetic moments and electrical charges of individual atoms and therefore to understand the underlying mechanisms that drive the particle's electro-magnetic behavior."

Quantum-level simulations of even the smallest nanoparticles present huge challenges. "Consider that even a five nanometer-sized cube of iron contains on the order of 12,000 atoms," says Oak Ridge National Labs physicist Stocks, who leads a team — including Wang, Aurelian Rusanu, Don Nicholson and Markus Eisenbach of Oak Ridge — who have carried out large-scale nanoparticle simulations with powerful software they developed and the XT3.

Along with proving the feasibility of their approach, they have with their most recent simulation — a 14,400 atom iron-platinum nanoparticle — revealed unexpected electro-magnetic features. They found that a boundary region of nanoparticle atoms isolates the particle interior from quantum disturbances — a finding that opens a new window for design and development of nanostructured magnetic materials.



A slice of the iron-platinum particle (left) with surrounding iron-platinum random alloy shows magnetic moment distribution, indicated by color. In the interior of the nanoparticle, iron (red) and platinum (silver) have clearly defined moments. At greater distances from the center, the alloy atoms have reduced magnetic moments (darker color). The spherical particle (above) includes a boundary region of one-to-two atoms in which magnetic moments are influenced by the surrounding alloy, while atoms deeper within are unaffected.

THE SUPERPARAMAGNETIC LIMIT

Steady increases in data-storage density — which have doubled annually for decades — and the similar trend in faster processors have driven us into the information age. Today's magnetic storage can record data at 100 gigabits per square inch, and the next milestone is a terabit, a trillion bits per square inch. Roughly, that's all the x-ray data in a large hospital, or about 5,000 trees worth of printed paper, on one square-inch of magnetic material.

The dominant storage media are films of magnetic particles, composed of complex alloys of various metals, on fast-spinning hard disks. Whether the information is a rap tune on an iPod or a cryptogram on a CIA server, it's written to the disk by magnetizing minute patches of these particles, one patch for each bit of information. The smaller and fewer the particles that can be given a uniform magnetic field to represent binary "1" or "0," the greater the density.

The roadblock that looms — called the superparamagnetic limit — is that as the grains become smaller, heat effects (called thermal fluctuations) disturb the magnetic moments, resulting in noise, false sensor response, and long-term data loss. Storing information reliably — 10 years is a typical industry standard — requires stable magnetization at room temperature, but at grain sizes much smaller than current technologies, thermal fluctuations, even at room temperature, tend to scramble the data.

Proposed new designs, such as a patterned magnetic nanoparticle media in which each bit is stored in a single nanoparticle, require better understanding of quantum-mechanical behaviors. "There are big pieces of the underlying physics," says Stocks, "that we don't understand."

"We want to be able to predict for each nanoparticle," says Wang, "how much energy it takes to flip the magnetic moment from up to down. And because thermal fluctuations can flip the moment, we need to know the smallest size a particle can be and resist the fluctuation, and we want to understand the interactions between nanoparticles — how close they can be one to another — because we don't want to flip one particle and affect another one."

RESULT: A DETAILED PICTURE OF A REALISTIC
NANOPARTICLE'S ELECTRONIC AND MAGNETIC STRUCTURE

AN ELECTROMAGNETIC SCREENING REGION

To get some of these answers, the Oak Ridge-PSC team turned to LSMS (the locally self-consistent multiple scattering method), powerful software they developed to simulate the quantum properties of solid-state materials. When implemented at PSC in 1998 (on the Cray T3E), LSMS broke the teraflop barrier. It was the first research software (as opposed to benchmark codes) to sustain performance over a teraflop (a trillion computations a second), an achievement that won the 1998 Gordon Bell Prize for high-performance computing.

On the XT3, running on 2,048 processors, LSMS zooms at over eight teraflops, more than 80 percent of the XT3's theoretical peak. "A powerful innovation of LSMS is its linear scaling," says Stocks. "As the number of atoms increases, computing time increases by only the same multiple." Without the innovations of LSMS, a realistically sized particle of tens-of-thousands of atoms would be too large to simulate. With a conventional approach, the amount of computing increases by the number of atoms cubed N^3 — so that as the particle size changes, for instance, from 1,000 to 10,000 atoms, the computing would take 1,000 times as long, rather than, as with LSMS, only ten times.

"Quantum-mechanical calculations are very time-consuming," says Stocks, "even on big computers. What we've done with LSMS is develop methods that allow you to do calculations for a sufficient number of atoms so the nanoparticle that the theory people talk about gets very close to the size that the experimentalists can make and measure."

In 2005, Stocks, Wang and colleagues used LSMS to carry out one of the first projects on PSC's then newly installed XT3. They calculated the electronic and magnetic structure of an iron nanoparticle embedded in an iron-aluminide matrix, a total of 16,000 atoms. This was the first quantum-based calculation of a physical system several nanometers in scale, and it successfully laid the groundwork for their next simulation.

The 2005 calculations were limited by an assumption that the magnetic moments for each atom of the nanoparticle were aligned in the same direction. "In reality," says Yang, "because of surrounding materials, that won't be the case." This year, taking the next step, they simulated an iron-platinum nanoparticle — at three different sizes, 2.5, 3.86 and 5.0 nanometers — in a matrix of surrounding alloy, totaling in each case 14,400 atoms, without any a priori assumptions about alignment of the magnetic moments. They focused on iron-platinum, says Wang, because industry leaders are interested in its potential as a storage medium. The computations occupied 1,200 XT3 processors — 12 atoms assigned to each processor — running for more than 50 hours.

"Iron-platinum," says Stocks, "is an important material because of its high magnetic anisotropy compared to most metals. This means it takes more energy for the magnetic moment to flip. As particle size gets smaller, this is more and more important."

The result of the LSMS simulations is a detailed picture of a realistic nanoparticle's electronic and magnetic structure. Atoms in the particle interior settle into an organized pattern of essentially the same amount of net charge and magnetic moment as bulk crystalline iron-platinum. Iron atoms gain electrons from the platinum atoms to become negatively charged, and conversely the platinum atoms become positively charged.

The most interesting finding is a boundary region, just a few atoms in thickness, that isolates the nanoparticle from disruptive quantum effects from the surrounding alloy. In this region, about four angstroms, net charge and magnetic moment fluctuate from influence of the alloy. The four-angstrom width of this region was constant for all three simulations, suggesting that it is independent of particle size. "The perturbed surface of the particle," says Stocks, "is like a fishbowl, separating the interior from outside effects. This is a piece of knowledge we didn't have before, and it will prove useful."

This success points to more challenging tasks ahead. Nanotechnology — such as new discoveries in nanostructured "spintronic" devices, which may be able to harness the electron's spin as well as its charge — represent problems well beyond even the latest LSMS simulation. Meeting those challenges will require characterizing electronic and magnetic structures on scales approaching millions of atoms, rather tens-of-thousands, and the computational cost will rise by a factor of hundreds.

Eventually, simulations such as these will aid in developing the more powerful computers needed for the next round of simulations. "Without the magnetic storage advances to date," says Stocks, "we wouldn't be able to do these calculations, which will help develop the next level of materials for the disk drives we'll need for the next level of calculations."

"Ultimately," says Wang, "the success of direct quantum mechanical simulation of nanostructured electronic devices relies on the advent of petaflop computing technology." (GH)

MORE INFORMATION:

http://www.psc.edu/science/2006/nano.html