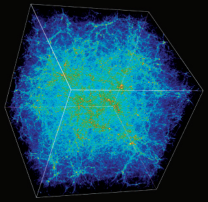
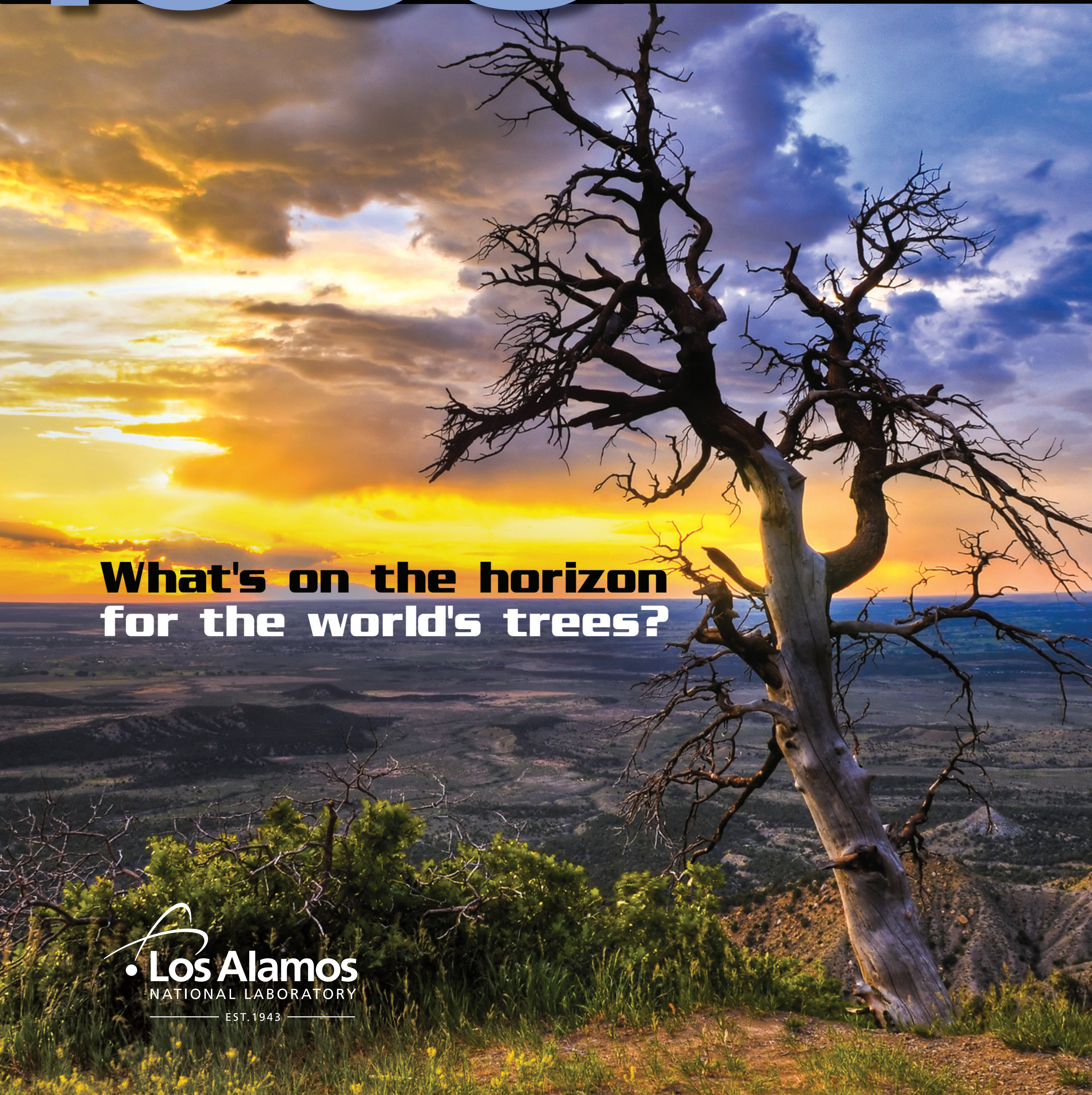


LOS ALAMOS SCIENCE AND TECHNOLOGY MAGAZINE

OCTOBER 2012

# 1663

- Plutonium's Magic Frequency
- Universe in a Box
- HOPE and Curiosity
- Sounding the Structural Alarm



## What's on the horizon for the world's trees?

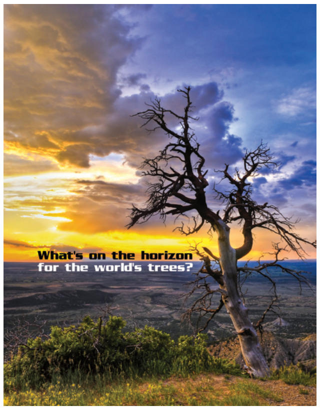
Los Alamos
NATIONAL LABORATORY
EST. 1943

# 1663

LOS ALAMOS SCIENCE AND TECHNOLOGY MAGAZINE

**About Our Name:** During World War II, all that the outside world knew of Los Alamos and its top-secret laboratory was the mailing address—P. O. Box 1663, Santa Fe, New Mexico. That box number, still part of our address, symbolizes our historic role in the nation's service.

**About the LDRD Logo:** Laboratory Directed Research and Development (LDRD) is a competitive, internal program by which Los Alamos National Laboratory is authorized by Congress to invest in research and development that is both highly innovative and vital to our national interests. Whenever *1663* reports on research that received support from LDRD, this logo appears at the end of the article.



**About the Cover:** As global temperatures rise and droughts become more severe, trees become more susceptible to an early death. Trees around the world are now dying at mortality rates far greater than they were just 40 years ago—even in rain forests and other non-arid ecosystems. And because trees take in carbon dioxide from the atmosphere while they're alive (and release much of it when they die), an acceleration in their deaths may lead to a corresponding acceleration in climate change. In order to determine how rapidly these changes will proceed—and what, if anything, can be done to slow them down—a Los Alamos research team is working to understand the detailed mechanisms behind tree mortality.

## Los Alamos Firsts

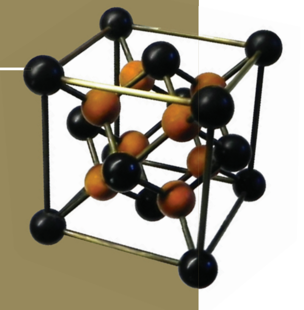
Between 1943 and 1945, a covert Los Alamos workforce accomplished the remarkable when they developed not one but two types of atomic bombs. Seven years later, the Laboratory achieved the unimaginable when it demonstrated the feasibility of an even more powerful weapon, the thermonuclear bomb.

Atomic bombs are fission devices: their explosive energy comes from splitting heavy nuclei apart. The energy of a thermonuclear bomb, also known as a hydrogen bomb, derives from both nuclear fission and nuclear fusion, the latter being when two light nuclei merge into one. For fusion to happen, the fuel must be extremely hot and dense, conditions that suggested a two-stage bomb design: the energy released by a fission-based "primary" explosive unit—i.e., an atomic bomb—is used to compress and ignite a fusion-based "secondary" explosive unit, which produces most of the thermonuclear bomb's yield.

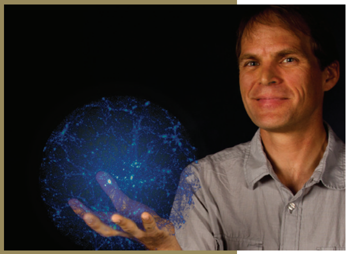
A device (left), never meant to be a deliverable weapon, was built to demonstrate proof-of-principle. The two nuclear components were encased within the massive steel cylinder (nicknamed "the sausage") that stood 20 feet tall and was more than 6 feet in diameter, with 10- to 12-inch-thick walls. The primary, one of the largest atomic bombs ever fielded by the U.S., sat above the secondary, which was a huge container of liquid deuterium (the fusion fuel) surrounded by a thick metal tamper. The entire device weighed in at 62 tons.

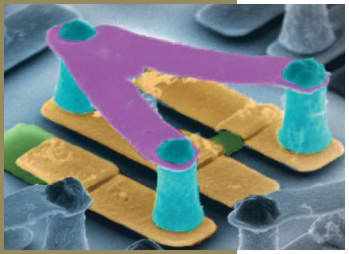
On October 31, 1952, in a test code-named Ivy Mike, the sausage exploded with the energy equivalent of 10.4 million tons of TNT. It remains one of the largest man-made explosions ever.

# IN THIS ISSUE

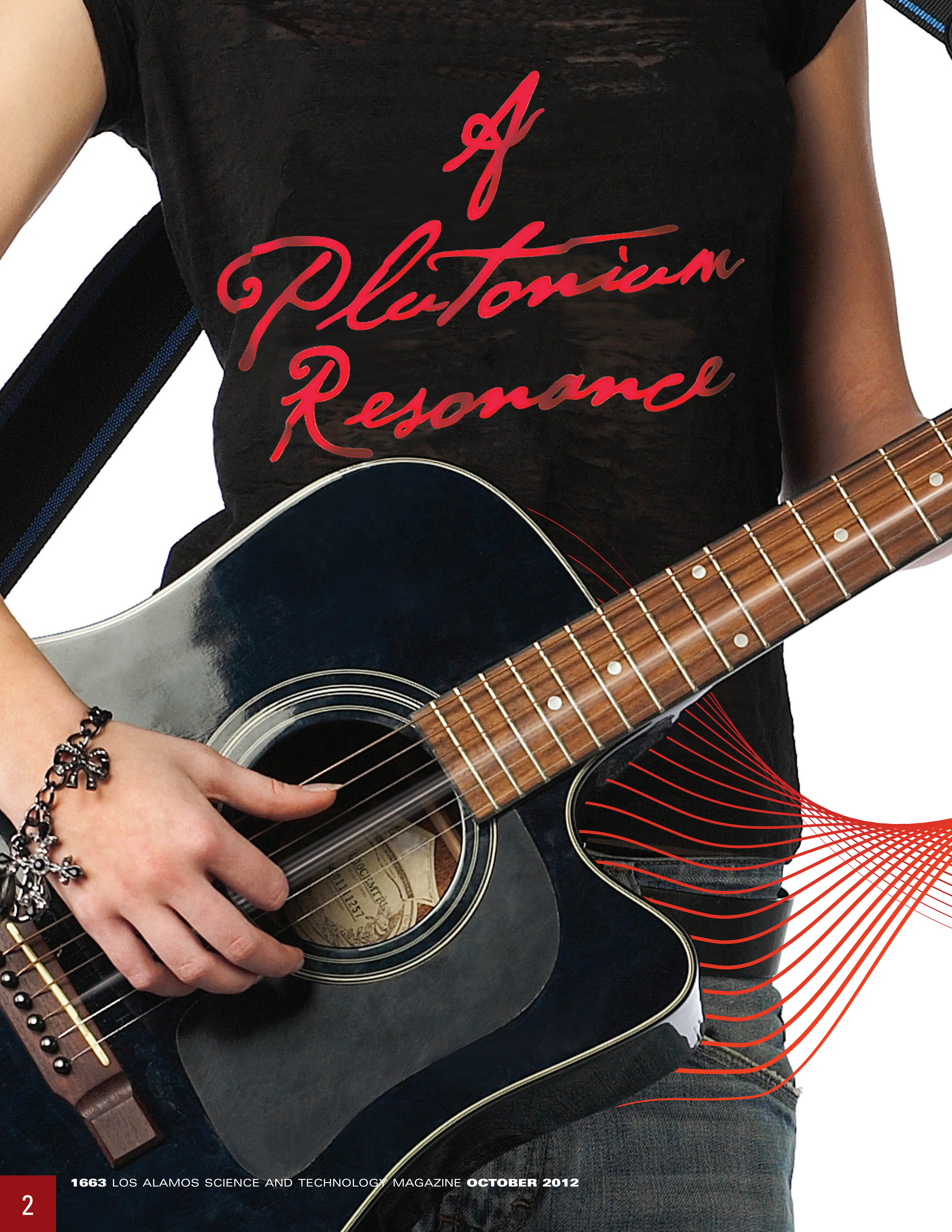


## FEATURES





## SPOTLIGHTS



# A Plutonium Resonance

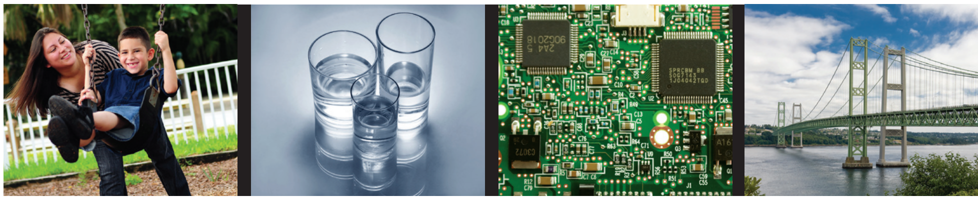
# After fifty years, plutonium-239 finally reveals one of its most important secrets.

When University of Tokyo physics professor Hiroshi Yasuoka, a visiting scholar of the Glenn T. Seaborg Institute at Los Alamos National Laboratory, teamed this summer with Los Alamos post-doctoral researcher Georgios Koutroulakis, it was one of those rare acts of providence. Using their skills and wiles, the two succeeded in measuring the nuclear magnetic resonance (NMR) frequency of the plutonium isotope Pu-239, something that scientists had been unable to pull off for the past 50 years.

“It was important to achieve scientifically,” said Yasuoka, a pioneer in NMR techniques. “But it was also a personal goal. I was very determined to make the measurement.”

Getting the result required fabricating a one-of-a-kind sample and cooling it down to near absolute zero. But with the NMR frequency in hand, scientists are positioned to gain a much better understanding of plutonium and possibly learn how to master the roguish element. And it couldn’t have come at a better time.

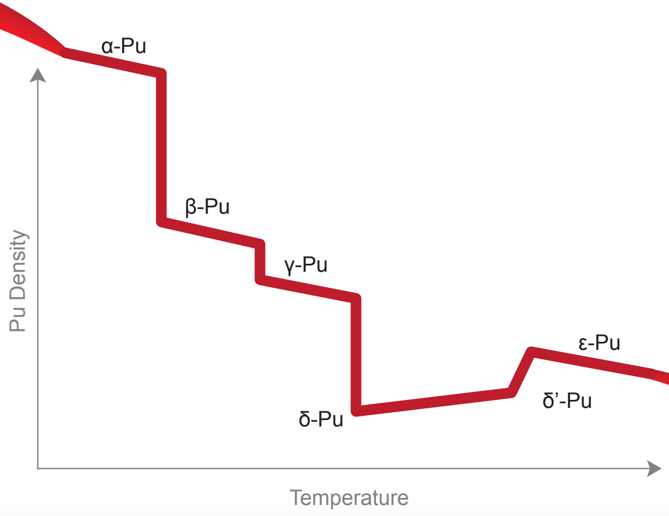
A child’s swing, glasses of water, electric circuits, even buildings and bridges—all exhibit resonance behavior: They oscillate more readily at their so-called resonance frequencies, and when fed energy at a particular resonance frequency, that particular oscillation becomes stronger. An acoustic guitar is another example. A plucked string sets the body of the guitar vibrating. Acoustic resonances then amplify not just the string’s tone, but certain overtones, so the raw sound of the string is made richer by the instrument. The plutonium-239 nucleus also exhibits a resonance—a magnetic resonance—and will readily absorb radio waves at its resonance frequency. The resonance frequency depends on the magnetic fields produced by nearby atoms and electrons, so researchers can learn how a plutonium atom behaves *in situ* by observing how its nuclear resonance frequency shifts as conditions vary.



## *A Complicated Metal*

The silvery metal plutonium has eight outermost (valence) electrons that are available to form bonds (carbon has only four). Each electron is likely to be found within a defined volume of space (an orbital) with a definite energy and angular momentum. In isolated atoms or in molecules, the orbitals are localized about the nucleus, and a bond can sometimes form between two atoms if an orbital from one overlaps an orbital from the other. The situation is a little more complicated in a solid containing lots of atoms, because overlapping valence orbitals from all the atoms merge into bands. The electrons in these bands are mobile, able to hop from atom to atom. It's the attraction between these mobile electrons and the lattice of ion cores that holds the solid together.

Much of plutonium's complexity can be traced to its three "barely's": First, many of its valence electrons extend from the nucleus just barely enough to participate in forming bands. Second, there's barely any difference in energy between different sets of orbitals, even though there are significant differences in the bonding properties of the different sets. And third, in plutonium metal and its alloys, many valence electrons are barely mobile; they can switch between being mobile or localized to a particular atom under slightly different conditions. As a result, plutonium's ability to form bands becomes extraordinarily sensitive to changes in pressure, temperature, humidity, etc., and the element has arguably the most complex metallurgy of any element in the periodic table.



For example, the pure metal is very reactive. Its corrosion rates can vary by thirteen orders of magnitude ($10^{13}$) depending on whether the material is in dry air or in a hydrogen-rich environment. Heat the metal in air to 500˚C and it bursts into flames.

The graph above shows the density versus temperature relationship for pure plutonium metal. At room temperature, plutonium is one of the densest solids, weighing more than two-and-a-half times an equal volume of iron. Like most metals, it expands as it heats up, so its density smoothly decreases. When the material reaches 120˚C, there's a sudden large change in density, because the atoms in the metal shift their positions slightly and settle into a more comfortable crystal structure. By the time it reaches 315˚C, plutonium will have assumed three different crystal structures and expanded well beyond its original size.

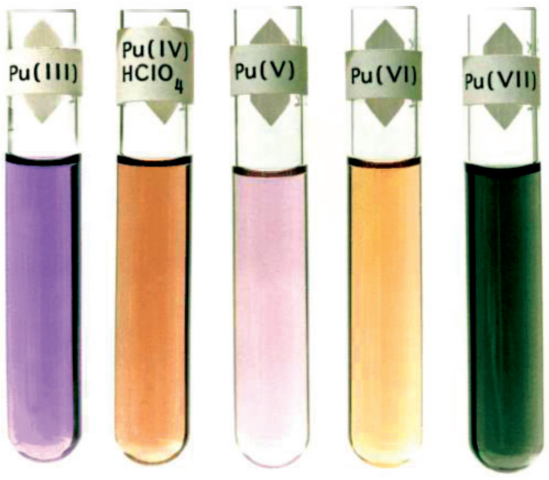
### A Most Intriguing Element

Number ninety-four in the periodic table, plutonium didn't exist in the late 19th and early 20th centuries when chemists were busy filling in the table. Although present in the primordial gas cloud that gave rise to our solar system, all versions of plutonium's nucleus (all isotopes) are unstable, and the element had all but vanished from Earth long before human beings ever appeared. (With a half-life of 80 million years, only Pu-244 lives long enough that the faintest hint of its primordial abundance remains in the Earth's crust.)

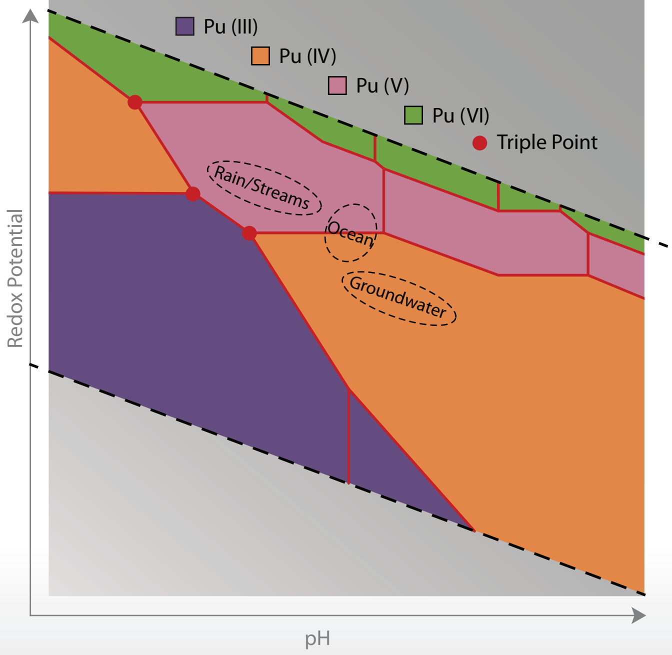
Glenn Seaborg and a team of scientists resurrected the isotope Pu-238 in the winter of 1941 by bombarding uranium with heavy hydrogen (deuterium), then a few months later used similar means to re-introduce Pu-239 to the planet. By 1944, Manhattan Project scientists were producing Pu-239 in bulk in the giant B nuclear reactor housed at the secret Hanford production site in Richland, Washington. The first the general public heard of the element and its remarkable comeback was after a plutonium sphere smaller than a cantaloupe destroyed the Japanese city of Nagasaki on August 9, 1945.

Since then, plutonium has become extraordinarily important to the security and energy needs of the world's most powerful nations. It is as essential to the U.S. nuclear arsenal as gunpowder is to a bullet. The element is also a key nuclear fuel—roughly a third of the energy produced by a standard light-water nuclear reactor comes from plutonium. The isotope Pu-238 is used as a power and heat source to keep space probes and, for example, the Mars rover Curiosity alive and well.

But there are health risks associated with plutonium. These risks can be minimized if the element remains outside the body because most of its common isotopes decay by alpha-particle emission. (Pu-241 emits a low-energy electron and turns into Am-241, which then decays by alpha emission.) The heavy alpha particles can't penetrate the body's outer layers of dead skin, and there are no harmful



Raise the temperature just a bit more, and the metal changes to a fourth crystal structure and, bizarrely, begins to shrink with increasing temperature. At 480˚C, it again changes structure and, being ornery, returns to expanding with increasing temperature. The metal melts at a relatively low 640˚C (even copper melts at over 1000˚C), and it turns out that liquid plutonium is even denser than the solid from whence it came. The result is that as it melts, a metal six times denser than granite will begin to float in its own liquid.



Plutonium chemistry is also extraordinarily complex. In solution, plutonium will readily lose between three and seven of its outer electrons, and the resulting cation can assume one of five formal oxidation states, Pu(III)–Pu(VII). Its properties in solution depend on the oxidation state. For example, the test tubes above show that each oxidation state has a characteristic color in solution. Additionally, as shown in the plot above, plutonium likes to be in several oxidation states at once (red lines and dots), depending on water conditions. As a result, it can undergo several chemical pathways simultaneously.

gamma rays associated with those decays. The alpha decay of plutonium-244, however, is an exception: It produces a daughter nucleus that emits a harmful gamma ray. If present, this isotope is a serious health risk.

The risk is much greater if plutonium gets into the body. When swallowed, a small percentage of the material will be absorbed by the body (the rest will pass through). The absorbed fraction often ends up in bone tissue, where its radiation increases the risk of bone cancer. If inhaled, plutonium particles of the right size will remain in the lungs and increase the risk of lung cancer, or they can enter the blood from the lungs and get transported to other parts of the body. (People who were alive during the 1950s and 60s inhaled plutonium that entered the environment as a result of atmospheric nuclear tests. On average, North Americans retained a negligible amount, receiving a committed effective dose of radiation of less than 1/1000 of the background dose.)

Because of the health concerns, as well as safety and security issues, plutonium is carefully regulated and kept tightly under wraps at all times. Thus, relatively few people have ever seen this material of national importance, and fewer still have ever placed their hands inside the rubber gloves of a glovebox and handled it. Consequently, researchers know far less about plutonium than they do about almost any other heavily utilized element. The irony is that if a human being were as integral to national defense and security as plutonium is, the country would want to know everything about him, from the company he keeps to how he ties his shoes.

The need to know everything about plutonium is more pressing today than it has ever been. Consider that the nuclear weapons in our stockpile have long exceeded their design lifetime, and, as outlined in the Obama administration's *Nuclear Posture Review Report*, a range of life extension programs are being considered to ensure the weapons remain safe, secure, and effective. Refurbishing warheads is a favored option, wherein new parts and components will replace old ones. But the plutonium core of the old weapon—the pit—will simply be transferred to a refurbished weapon, despite it being older in some cases than the personnel doing the refurbishing.

What's worrisome is that the certification of a weapon's performance is based, in part, on computer simulations of how the pit performs. Due to radioactive decay, the level of impurities in the plutonium increases over time, and that has the potential to alter the material's physical properties and its behavior. Plutonium is also extraordinarily sensitive to environmental changes, such as temperature, pressure, and humidity. As intriguing as that may be from a materials perspective, it means that the range of possible behaviors increases as plutonium ages, and since scientists don't know everything they'd like to about the element, their ability to simulate that behavioral range becomes an issue. As a consequence, scientists become increasingly uncertain about plutonium's behavior as it ages.

Plutonium is prized for its energy-packed nucleus, but its chemical and solid-state behavior is determined by its electrons. Enough is known about these electrons to have an appreciable understanding of plutonium's behavior in many circumstances, although the in-depth understanding that would enable true control over the element is currently lacking. But the tool that scientists would use to help gain that understanding is NMR, the workhorse of materials science, except that NMR had never been successful with plutonium—that is, not until Yasuoka and Koutroulakis measured the Pu-239 resonance frequency.

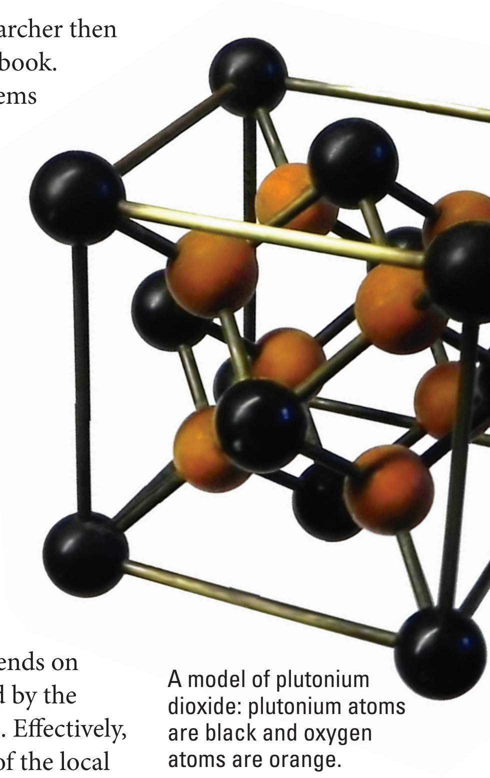
## Basic NMR

As a tool, NMR is used to gain insight into the structure of a particular nucleus or into the configuration of atoms and electrons surrounding that type of nucleus in a material.

Conceptually, the technique is straightforward. A sample containing a specific nuclear isotope is subjected to a strong magnetic field, and a radio frequency (RF) wave is directed perpendicular to the magnetic field direction. The RF wave is swept through a range of frequencies or, alternatively, the strength of the magnetic field is varied. When the frequency of the RF wave corresponds to the Pu-239 resonance frequency, the isotope absorbs energy from the RF wave. Various techniques can be employed to detect when that occurs. The researcher then jots down the frequency in a notebook.

The broad utility of NMR stems from the resonance condition, which depends on the strength of the applied magnetic field and two other parameters. The first is the so-called gyromagnetic ratio, $\gamma_n$. This quantity is related to the isotope's magnetic moment—the moment being the source of a magnetic field—which in turn depends on the detailed arrangement of protons and neutrons in a nucleus. Thus $\gamma_n$ is very much the calling card of a specific isotope.

The second parameter, $K$, is called the chemical shift. It depends on the internal magnetic field created by the electrons surrounding the isotope. Effectively, it is a one-value characterization of the local environment.

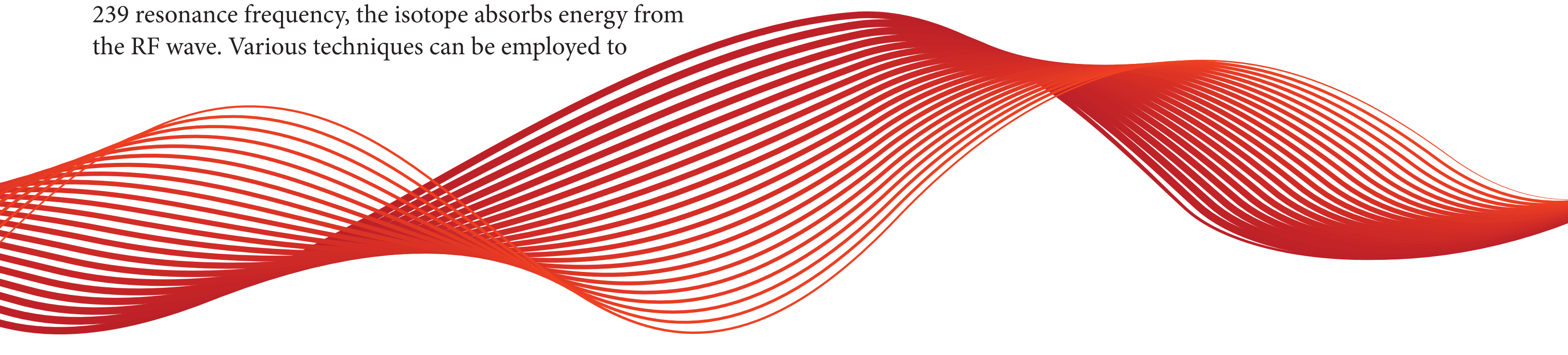


A model of plutonium dioxide: plutonium atoms are black and oxygen atoms are orange.

If the environment is known, then $K$ is known and the resonance frequency becomes a measure of $\gamma_n$. Theorists then have a number that needs to be explained in terms of the nuclear structure of the isotope. On the other hand, if $\gamma_n$ is known, the resonance frequency measures $K$, and the isotope becomes a very effective probe of local structure.

Only certain nuclei are amenable to NMR, namely those that have a non-zero "spin." The spin is a central feature of the quantum realm, an angular momentum that is intrinsic to every elementary particle. Electrons, protons, and neutrons have one-half unit of spin, whereas photons have one unit. Collective bodies, such as nuclei, have a spin that depends on the specific arrangement of protons and neutrons. If that sounds suspiciously like $\gamma_n$, it's because the two are related: $\gamma_n$ is the ratio of the nuclear magnetic moment to the nuclear spin.

There are 30 nuclei with spin ½, but Pu-239 was the only one not observed by NMR. In part that was due to the difficulty of experimenting with plutonium. But largely it's because people didn't know where to look, and even if they did, the signal didn't last long enough for them to observe it.



## High Hurdles

There are no accurate accounts of the Pu-239 magnetic moment, hence there is no reliable value of $\gamma_n$. Various experiments have tried to determine the nuclear moment indirectly, but the estimates varied so much that the possible parameter space for NMR resonance was daunting. More troublesome was the extremely strong interaction between electrons and nuclear spins in Pu-239. The unpaired electrons, as moving electric charges, give rise to a large internal magnetic field of about 100 teslas at the nucleus. This adds to the external field and shifts the resonance frequency by several orders of magnitude. Since $\gamma_n$ was unknown, where it shifted to was also unknown.

Also, the large internal magnetic field fluctuates as the electrons move around, and that lets the nuclear spins relax and assume random positions. That weakened and broadened the resonance signal—which was only present for a few millionths of a second—making it disappear into the noise.

Yasuoka and Koutroulakis had the clever idea of performing the experiment on plutonium dioxide ($PuO_2$). The plutonium ion in that case is $Pu^{4+}$, and in their lowest energy state, the electrons pair up to form a non-magnetic spin-0 state. The value of $K$ becomes close to zero, a major uncertainty as to where to find the NMR resonance disappears, and the resonance becomes sufficiently strong, sharp, and long-lived to be observed.

Unfortunately, if the electrons are given a small amount of energy, they can rearrange and form a magnetic state, and $K$ would again assume some large, unknown value. The scientists, therefore, did their experiments at a temperature of 4 kelvins, close to absolute zero, essentially freezing the electrons in their lowest energy state. They also called for a little help from the Laboratory's Kurt Veirs, who provided a high purity $PuO_2$ powder sample, with a Pu-239 isotopic abundance of about 94 percent. The result is that many nuclei could contribute to the signal and each would have the same resonance.

The experiments were performed in the laboratory of Los Alamos scientists Joe Thompson and Eric Bauer. They investigate plutonium superconductivity, which, not surprisingly, shows anomalous behavior. Their lab was well equipped to look at plutonium at low temperature.

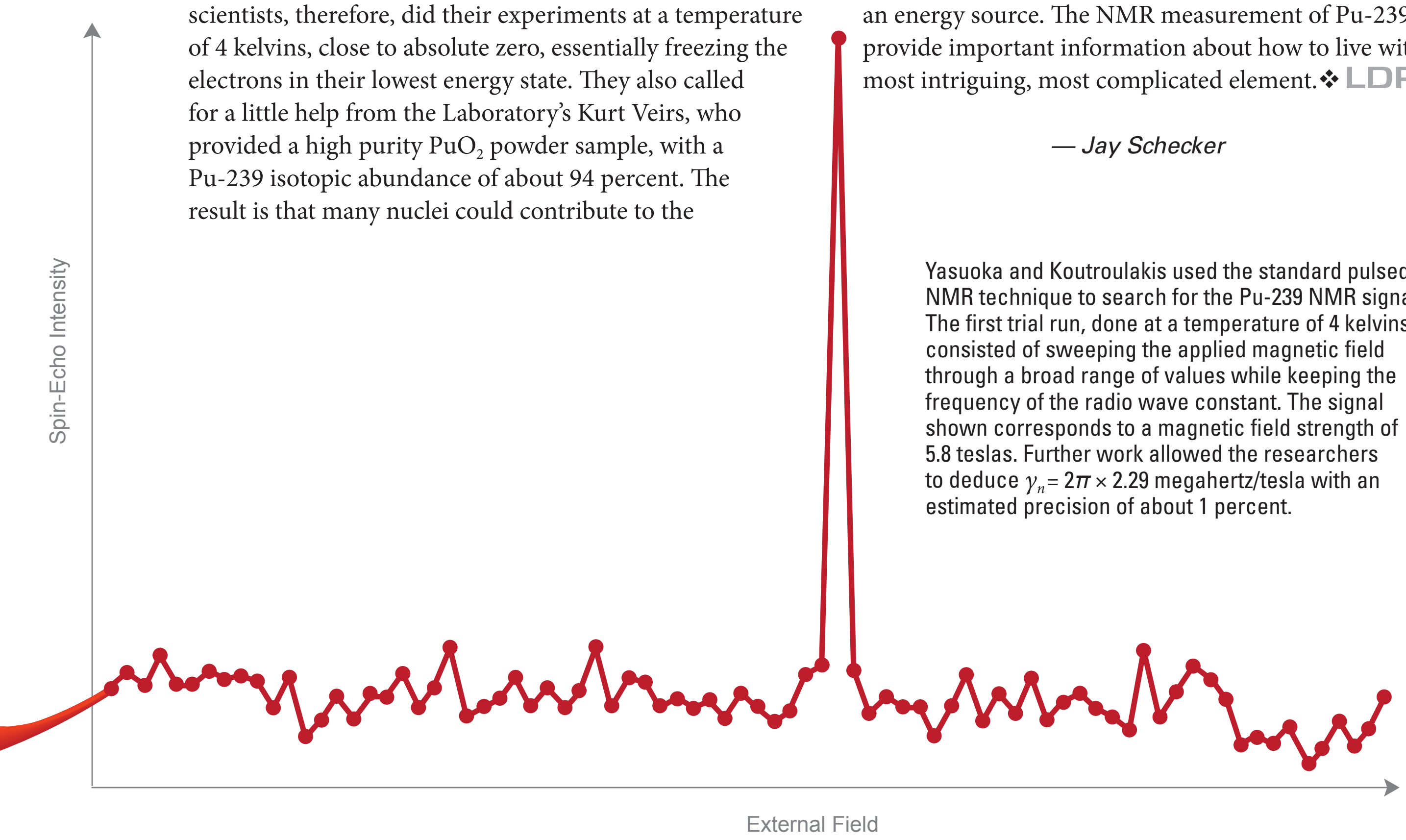
"I remember they were doing the experiment and Hiroshi said they see a small signal," says Bauer. "Well, he must have remarkable intuition because I looked and couldn't see anything, but that's where the signal proved to be. Once you have even the slightest hint of the signal you can optimize the NMR parameters and enhance it."

## What Now?

The finding of the Pu-239 NMR signal in $PuO_2$ is an important milestone that couldn't have come at a better time, but the work is just beginning, since scientists will need to find and study the signals in a range of materials and under a range of conditions. Hopefully, the signals can be observed under conditions that are less expensive, less time-consuming, and less technically challenging to achieve. It's likely, though, that each measurement will present some obstacle that will require the wiles and talents of the experimenters to overcome.

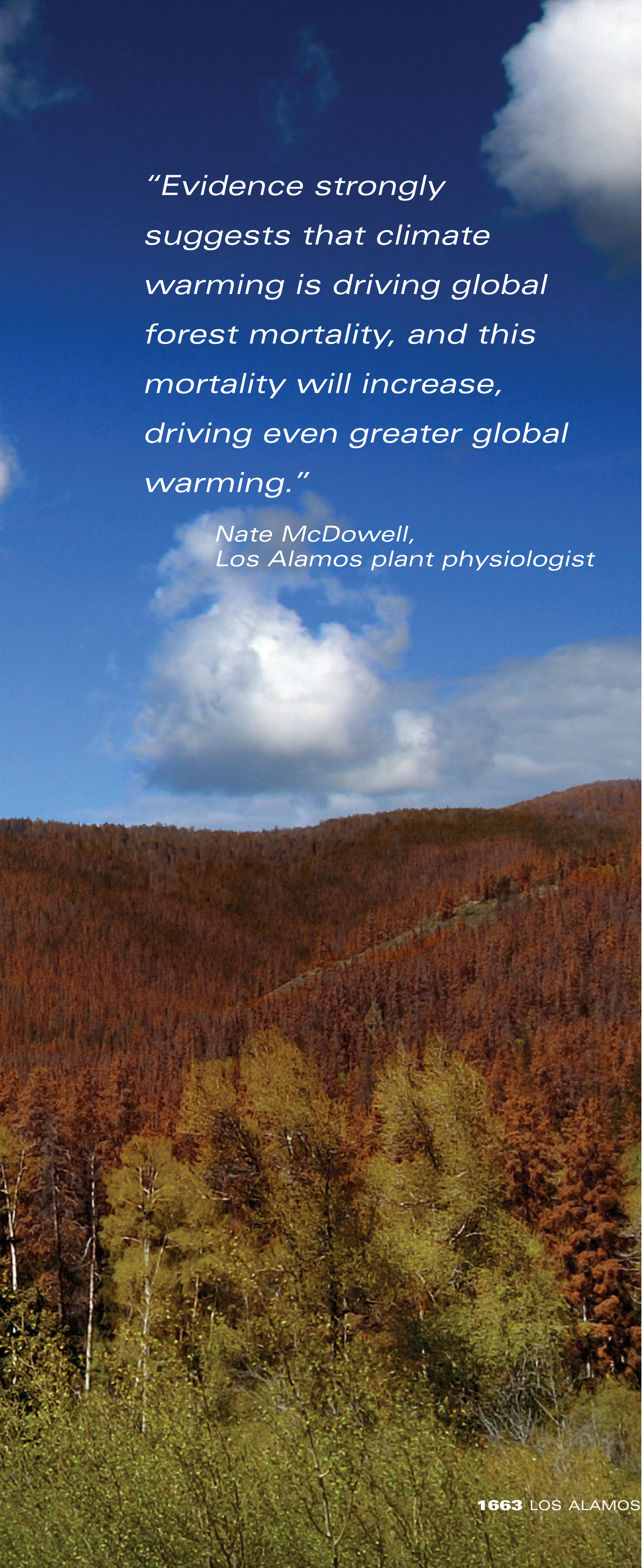
Regardless of its application, plutonium poses the same problem—the element responds in complex, unexpected ways to changes in its environment. The inability to mitigate those responses, or redirect them to favorable outcomes, in part prevents the nation from embracing plutonium as an energy source. The NMR measurement of Pu-239 could provide important information about how to live with this most intriguing, most complicated element.❖ LDRD

*— Jay Schecker*



Yasuoka and Koutroulakis used the standard pulsed NMR technique to search for the Pu-239 NMR signal. The first trial run, done at a temperature of 4 kelvins, consisted of sweeping the applied magnetic field through a broad range of values while keeping the frequency of the radio wave constant. The signal shown corresponds to a magnetic field strength of 5.8 teslas. Further work allowed the researchers to deduce $\gamma_n = 2\pi \times 2.29$ megahertz/tesla with an estimated precision of about 1 percent.

# OUR DYING Global Forests



> “Evidence strongly suggests that climate warming is driving global forest mortality, and this mortality will increase, driving even greater global warming.”
>
> Nate McDowell,
> Los Alamos plant physiologist

**Trees dotted this planet** more than 400 million years before we did. They have adapted slowly, developing unique attributes that allowed them to thrive despite the stress of changing environmental conditions. They are famously long lived—some living more than a millennium—but now they are dying at alarming rates, with mortality doubling across a wide variety of forest types, at all elevations, in trees of many different sizes and species.

According to scientists, the most probable cause of this death is warming due to climate change, for which the health of trees is an important factor. Living trees soak up the greenhouse gas carbon dioxide ($CO_2$), but dying trees return $CO_2$ to the atmosphere, accelerating global warming. Since warming begets tree death and tree death begets warming, it’s important to know how soon and how severe this runaway effect will be. And the only way to know that is to find out exactly what causes trees to die, so that those deaths can be figured into climate models.

Los Alamos forest ecologist and plant physiologist Nate McDowell has been preparing his entire life to answer this question. Raised in the maritime climate of Washington’s Puget Sound, he examined how the cool coastal clouds nurtured the rainforest in his backyard. After learning more about those trees while acquiring his Ph.D., he moved to Los Alamos, attracted by the world-class science as well as the high-altitude, tree-covered slopes that harbor his two favorite pastimes, skiing and trail running. Now, just a decade later, 97 percent of the formerly prevalent piñon trees outside his office window have died, and not by fire.

McDowell recently launched the world’s two largest drought experiments, both based in New Mexico, with the goal of determining specifically why trees are dying. It may seem like common sense that too much heat or too little water would kill a tree, but the trees do not always die in predictable ways. For example, trees died during a 2008 drought experiment, but not during a longer and drier drought experiment in 2011. Why? It may be because the latter study followed a particularly cold winter, which led to a reduced population of tree-harming insects. Scientists believe that severe drought compounded by warmer temperatures hinders trees’ ability to fend off insects and pathogens, but the details remain uncertain.

“Everyone knows that when you have a drought, insects can show up and trees can die, but nobody can yet model it with accuracy,” McDowell says.

In addition to studying *why* trees are dying, McDowell's large Los Alamos team of staff scientists, postdoctoral researchers, and students is working to create a global monitoring system to determine *where* trees are dying, in order to improve predictions of future tree mortality. In addition, his team seeks to put their predictive capability to work determining how rapidly the death of these trees—long-term carbon reservoirs—might create a significant new carbon source that could exacerbate the very climate change that's driving the accelerated pace of forest mortality in the first place.

## Hunger Strike

A tree's structure and functions are not entirely dissimilar from a human's. It must drink and, in a sense, breathe, and it has a vascular system for transporting water and vital nutrients. A key difference is that it can make its own food, but it must first take in the elements necessary to make that food. All organisms need carbon, and trees obtain their carbon from atmospheric $CO_2$, absorbed through small pores on the leaves. These pores, called stomata, open and close to allow the transfer of gases such as $CO_2$, water vapor, and oxygen. During photosynthesis, the tree uses the energy from sunlight to combine the $CO_2$ with stored water to form carbohydrates. These carbohydrates are distributed throughout the tree by a cellular duct system called the phloem to be used for growth and metabolism. They are also converted into other forms needed by the tree, including a thick resin that the tree secretes to surround and kill attacking insects and fungi and to support wound repair.

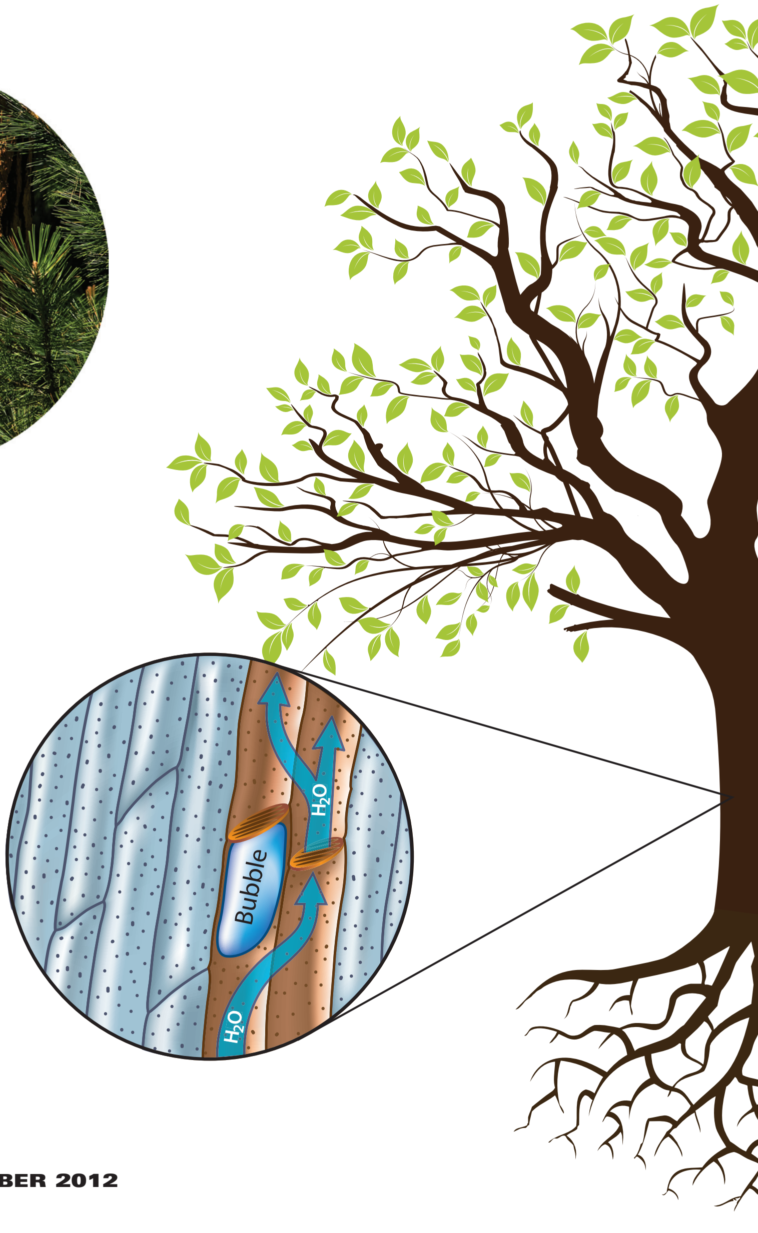
All of this activity requires water. Trees obtain most of their water through their roots, which also absorb minerals. This mixture is transported from the roots to a tubal system

## *Evil Weevil*

As if trees don't have enough struggles, those suffering from heat and drought become defenseless against bark beetles, which have killed more than 41 million acres of trees in the Western U.S. since 1997 in some of the most severe outbreaks in recorded history. Warmer temperatures have aided the cyclical outbreaks of these insects, increasing their reproduction and decreasing their deaths, which are normally caused by cold winters.

Bark beetles burrow through the outer bark and consume the inner bark of conifers, where they introduce a parasitic fungus and lay their eggs. The larvae eat through the vascular system that provides nutrients to the tree. Healthy trees fend off beetles by secreting a thick resin (right) that repels invaders and prevents their entry into the tree, but producing this resin requires a lot of energy, and unhealthy trees are incapable of this defense. When their population skyrockets, the beetles conduct mass attacks; even healthy trees are at risk then, overwhelmed by sheer numbers. Los Alamos's Nate McDowell links these beetle outbreaks to the recent widespread droughts in North America.

Wildfires have been fueled by the stands of trees recently killed by beetles, kindling ripe to rage. This fuel exacerbates difficult-to-suppress crown fires and might be leading to hotter, faster fires that are extremely harmful to ecosystems and the economy.



in the trunk and leaves known as the xylem, which uses the pressure difference between the outside air and the fluid in the leaf, often called tension, to suck the water and nutrients upwards throughout the tree in a solution called xylem sap. Once the water reaches the surface of the leaves (or needles, which function similarly), it is allowed to evaporate into the atmosphere through the stomata in a process called transpiration. Normally, 95 percent of the absorbed water is released this way. This water loss contributes to the pressure difference, pulling up more water from the roots—but only if there is enough water in the soil.

When facing drought, trees close their stomata to avoid water loss. If the retention of water is insufficient, hydraulic failure can ensue: the tree quits transporting water and becomes desiccated. Simultaneously, closing the stomata prevents the foliage from obtaining $CO_2$, thereby curtailing photosynthesis. As a result, carbon starvation can ensue: the tree consumes its carbohydrate stores in order to maintain its metabolism, leading to death by outright starvation or inability to defend against pests.

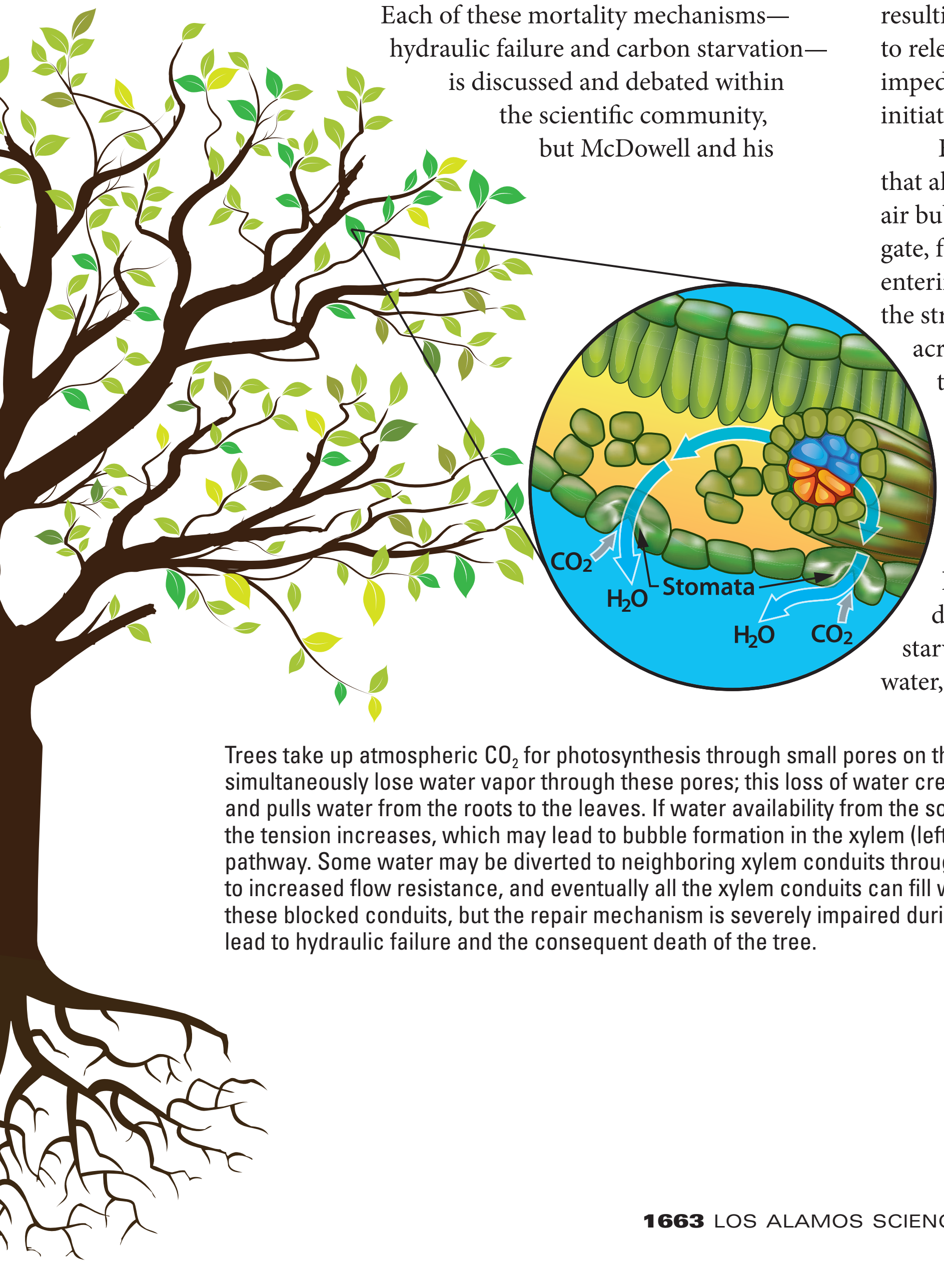
Each of these mortality mechanisms—hydraulic failure and carbon starvation—is discussed and debated within the scientific community, but McDowell and his colleagues hypothesized that the two are coupled in multiple interactions, perhaps akin to a starving human becoming too weak to drink. The preservation or failure of one function may destroy another, and under stress, the coupled processes can drive each other towards death.

## The Last Straw

During the early stages of drought, the tree attempts to preserve its carbohydrates by decreasing its own growth rates so that newly acquired photosynthate can be allocated only to basic functions to maintain life or stored in anticipation of a long-term drought. (This survival mechanism is not too different than the human body's response to a diet: fearing starvation, the metabolism adjusts and becomes more efficient to protect fat storage.) The supply of carbohydrates available to perform other important tasks—including fixing hydraulic failure—is sharply limited.

When the air becomes particularly hot and dry, as during severe droughts, the subsequent pressure change pulls more water from the roots than can be supplied. The resulting rise in water tension may cause water in the xylem to release dissolved air, creating gas bubbles that expand and impede the flow of water and nutrients throughout the tree, initiating hydraulic failure.

Each xylem is broken into sections by porous gates that allow water to flow from one section to the next. An air bubble creates a force that pushes against the closest gate, forcing it to slam shut and preventing the bubble from entering the next section of the xylem. Since a portion of the straw-like water column is blocked, the tree sends water across xylem membranes into a parallel straw to continue the flow. However, continued drought will cause more bubbles to form, and eventually the tree will die unless it repairs the damage. Such a repair is possible if the damaged xylem section can be refilled, causing the air bubbles to re-dissolve in the xylem sap. But McDowell hypothesizes that in some trees, the repair of the hydraulically impaired xylem costs a lot of energy, derived from carbohydrates that may be depleted by starvation. Here again, the plant needs food to obtain water, and vice versa.



Trees take up atmospheric $CO_2$ for photosynthesis through small pores on the leaves called stomata (right inset) but simultaneously lose water vapor through these pores; this loss of water creates a tension inside the water-conducting xylem and pulls water from the roots to the leaves. If water availability from the soil does not match the loss through the stomata, the tension increases, which may lead to bubble formation in the xylem (left inset). The bubbles expand and block the water pathway. Some water may be diverted to neighboring xylem conduits through pits in the xylem walls, but this is inefficient due to increased flow resistance, and eventually all the xylem conduits can fill with bubbles. In moist conditions, trees can repair these blocked conduits, but the repair mechanism is severely impaired during drought. Excessive formation of bubbles may lead to hydraulic failure and the consequent death of the tree.

*Sanna Sevanto, a member of McDowell's team and an expert in water and carbohydrate transport, monitors a piñon tree at one of the field sites she oversees. Sevanto is combining her field measurement analysis with nuclear magnetic resonance imaging to accurately quantify water and carbon dynamics to understand tree mortality.*

## Microcosms of Mortality

The current U.S. drought is coupled with high temperatures, and the previous decade was the warmest on record. Multiple scientific and government agencies report that global average annual temperatures are expected to increase between 1.4 and 4.1°C, and potentially up to 6.4°C, before the end of this century. (These estimates depend on factors such as population patterns, economic development, technological progress, and renewable energy use.) But McDowell isn't about to wait that long: one of his field research sites, called SUMO (SUrvival MOrtality experiment), subjects trees to future temperatures today.

"Our goal with SUMO is to test our theories regarding how trees die during both current droughts and the warmer droughts of the future," he says.

The SUMO site in Los Alamos contains 80 trees, many of which are enclosed in an acrylic chamber intended to simulate future temperatures approximately 5°C higher than they are today (see photograph on page 14). In addition, a large drought plot was installed that removes nearly half of the natural precipitation, enabling scientists to test the impacts of heat and drought, either individually or combined. The trees oddly resemble hospital patients, attached to probes and tubes. In each chamber, researchers create novel systems to control water and $CO_2$ inputs and manipulate temperature, closely monitoring the tree's reaction to these environmental changes. The team records a variety of measurable properties in order to test their hypotheses, including photosynthesis rates, growth, water flux, carbohydrate stores and transport, and respiration levels throughout the tree and soil.

A challenge for field research is identifying where and when changes are occurring inside the tree without excessively damaging the tree (e.g., cutting into it or draining sap from it). To better "see" inside the tree, McDowell recruited Sanna Sevanto, an expert on the tricky measurement of phloem transport, to Los Alamos, where they teamed up with colleague Michelle Espy. Espy, an expert in ultra-low field nuclear magnetic resonance (NMR) imaging technology, developed a portable field instrument that uses NMR to obtain evidence about what's going on inside a tree without actually penetrating it. This is the first-ever noninvasive study of a plant's function and mortality using NMR (see "New Tool of the Tree Trade" on this page).

At another field site, the Sevilletta long-term ecological research station in Central New Mexico, McDowell's team conducts more experiments on rainfall and sap flow to test the physiological limits of pine and juniper during

## *New Tool of the Tree Trade*

Seeing what's happening deep within a tree requires it be opened up in some fashion at many locations on the tree—sometimes even killing it. But apart from harming the tree, such methods fail to capture critical processes, including carbon and water flows in the xylem and phloem. Furthermore, such invasive methods employ relatively unreliable measurements, limited to the spot(s) where the tree is cut.

McDowell and Sanna Sevanto, a scientist on McDowell's team, teamed up with Los Alamos physicist Michelle Espy to develop a better way to continuously quantify the content and flow of water and carbon within a tree. Renowned for her work with nuclear magnetic resonance (NMR) imaging that has been applied to improving brain scans and security screening for airline passengers, Espy helped engineer a way to scan intact trees using ultra-low field NMR. The tree is immersed in a magnetic field and hit with radio waves, which activate particular elements in the tree (such as carbon) to send out a signal. (For more on NMR and its applications, see "A Plutonium Resonance" on page 2.)

The team's portable system has been successfully tested in a pilot study on an aspen tree. During two weeks of continuously monitoring this aspen, the researchers saw evidence of changes in water content between day and night, as well as an overall decline in water content as the tree dehydrated during an imposed drought treatment. The team observed the first noninvasive test of dehydration during drought-induced mortality.

According to McDowell, the ability to nondestructively monitor a plant's internal functions—especially with portable technology that's easy to use in the field—will be a game-changer for plant physiology and may also benefit other areas of research, such as bioenergy and carbon sequestration.

prolonged drought and to determine why some trees die while others do not in similar environments. This is the first and largest study of its kind. The team uses data obtained from this study to create carbon assimilation, water-use, and tree-death models to predict larger ecosystem changes.

During drought at the Sevilleta plots, the researchers observed that pines died before juniper and with much higher rates of hydraulic failure. They also noted that the trees that lose carbohydrates fastest are also the first to die, lending support to McDowell's hypothesis regarding feedbacks between hydraulic failure and carbon starvation. Despite the pines' earlier deaths, they found strong evidence for carbon starvation in both pine and juniper, and the hardy juniper is now dying after three years of induced drought. If the broader region encounters a similarly severe natural drought that lasts three years, its juniper could also disappear.

"This would be a big blow because there would be no woody species available to provide habitat for animals or to maintain the woodland ecosystem. This would have numerous downstream consequences," says McDowell. "In 2002, much of the Southwest U.S. transformed from piñon-juniper woodlands to juniper savannas. When will we have a three-year drought that pushes these juniper savannas to grasslands?"

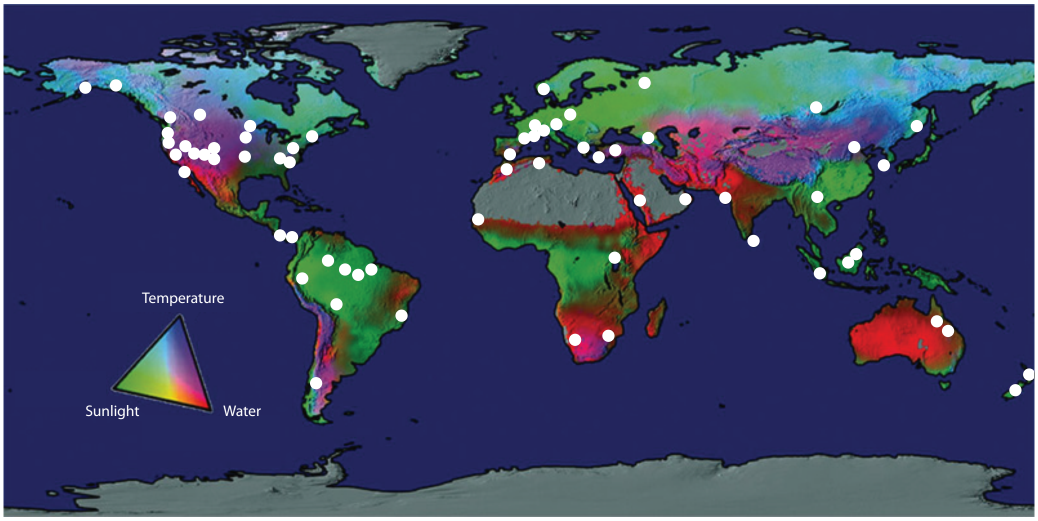
## Hitting Close to Home—Any Home

Once McDowell's team studies the physical effects that a changing climate has on trees at the local level, it combines that data with information obtained from remote sensing into a global climate model to monitor and forecast forest death and climate repercussions locally and worldwide. His team is currently creating the first globally comprehensive data set of tree mortality so that models can be tested, which has been impossible until now due to a lack of data about what is happening both within the tree and around the world.

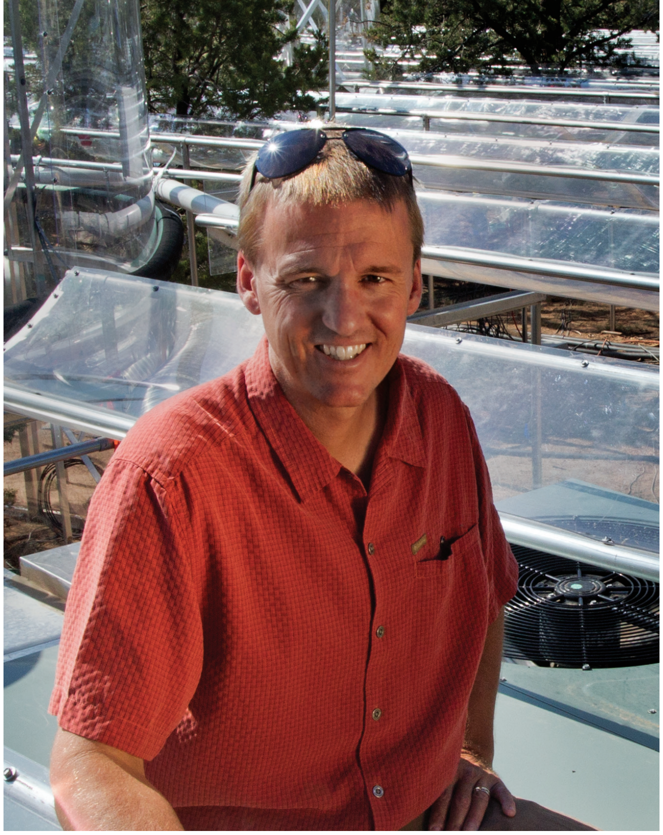
McDowell works with Los Alamos colleague Park Williams, a climate-impacts expert, whose projections reveal that a continued increase in warm-season drought conditions will likely force forests in the Southwest into persistent megadrought conditions—beyond the most severe levels experienced in more than 1000 years—by 2050. Williams, McDowell, and their colleagues showed that drought impacts on forests have been particularly severe during the last two decades, with large bark beetle outbreaks and increasingly large wildfires. Their predictions foreshadow major changes starting with all water-limited forests globally. The forests of the Southwest, and similar forests around the world, will look quite different in the near future—and in fact, across large swaths, they already do.

"Even if precipitation remains unchanged, these results reveal that rising temperature alone will result in far more drought stress, fire, and bark beetle-mediated mortality in future decades," notes McDowell. "Add periods of low precipitation to that scenario, and it's clear that the forests of the Southwest are in trouble."

McDowell is quick to point out, however, that the increase in forest mortality is a global phenomenon. He coauthored a paper—the first global assessment of recent tree mortality attributed to drought and heat stress—that details 88 cases of significant tree mortality associated with heat and



White dots indicate forest mortality related to climatic stress from drought and high temperatures. While drought- and heat-driven forest mortality is more frequently documented in relatively dry regions (red, orange, pink), it is also occurring outside these regions at an accelerating rate.
CREDIT: CRAIG D. ALLEN ET AL./USGS



Nate McDowell launched the world's two largest drought studies at field sites in New Mexico. Here, McDowell stands between plastic channels installed to divert rainwater away from trees so his team can monitor the effects of drought.

drought since 1970 on every continent except Antarctica. Although some forests are faring better than others, trees are dying across all biomes and dying faster in response to climate change.

Steve Garrity, a postdoctoral researcher who works with McDowell, has been developing new techniques for interpreting satellite data in terms of forest function. One striking discovery to come out of this work is that forest mortality does not appear to diminish with elevation, even though higher elevation forests are considerably wetter. Garrity, McDowell, and their colleagues observed a dramatic rise in mortality over the last two decades that has increased at equal rates across forests of all elevations. This somewhat surprising result has significant implications because it suggests that no forest is immune from drought-induced mortality. Perhaps more concerning is the fact that the death of the high-elevation forests releases vastly more carbon to the atmosphere than that of the sparsely-populated, low-elevation woodlands, leading to more warming. They are now extending this work to study two other major forest systems in order to check for global consistency: the tropical Amazon rainforest and the boreal forest, which encircles the Earth at far-north latitudes.

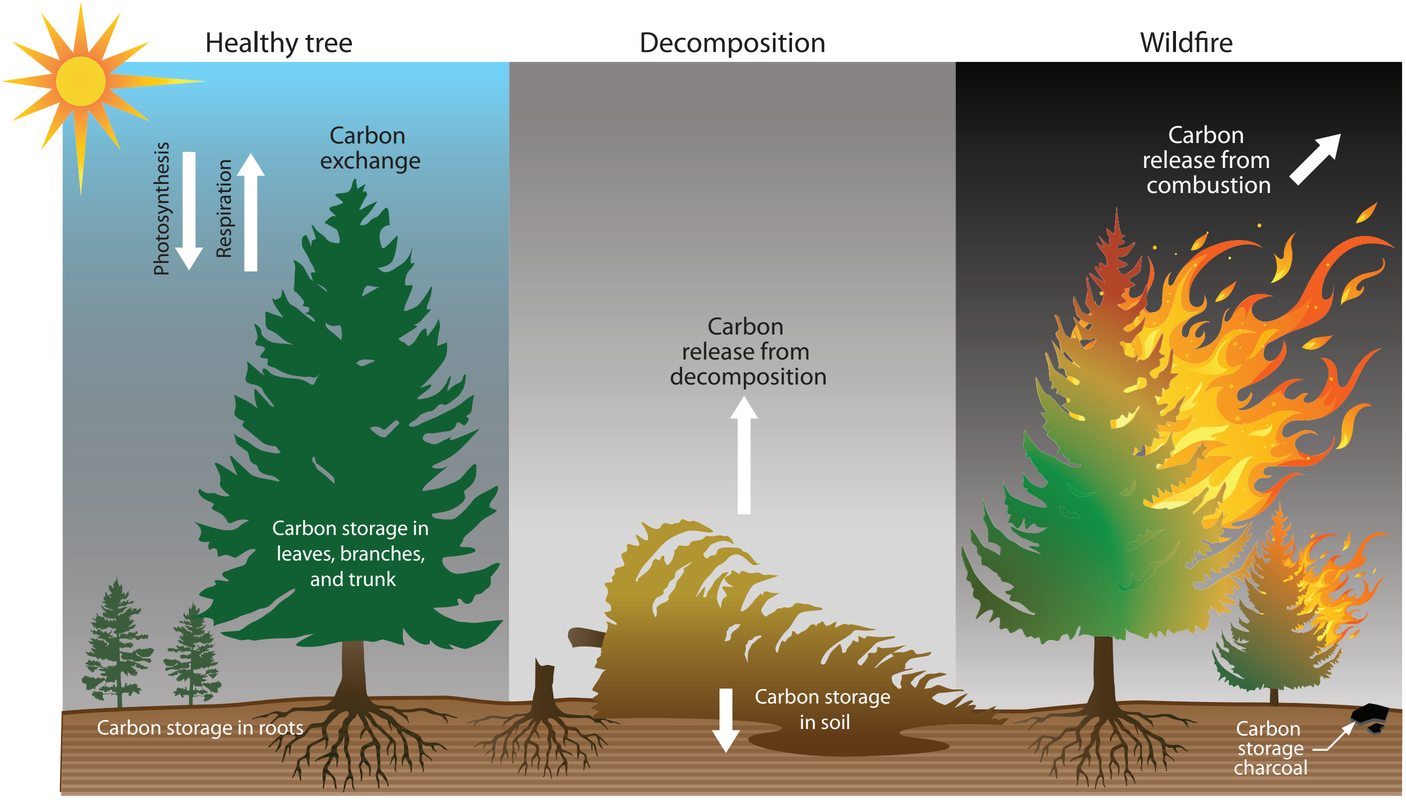
Such efforts to expand beyond the local are important, according to McDowell, because existing international forecasts of future climate have gaps. The gaps stem from an inability to accurately simulate vegetation changes and their feedback effects on climate due to incomplete information, such as knowledge of what vegetation dies and how much carbon is released. Observational data are incomplete as well; for instance, little is known about tree mortality patterns throughout Asia. A globally coordinated observation system is necessary for a more complete picture, he says.

## The Tree of Life

The loss of trees is no small concern. Trees filter Earth's freshwater, from root to xylem to leaf to air. They provide shade, shelter, and food to humans and other animals alike. They provide fuel, building materials, and other products used every day. They protect soils against erosion. They anchor entire ecosystems. And, of course, they keep carbon out of the atmosphere.

Enclosed in an acrylic chamber, a piñon tree and a juniper tree at the Los Alamos SUMO field site are introduced to increased temperature and decreased water to simulate the effects of climate change and determine how trees die.

CREDIT: JOSH SMITH/LANL



Forests play a major role in the carbon cycle, covering 30 percent of the world's land surface and sequestering more carbon dioxide ($CO_2$)—about 8.8 billion tons annually—than other types of vegetation. During its life cycle, a tree removes $CO_2$ from the atmosphere via photosynthesis, converting this gas into the carbon that constitutes the tree's tissues. At night, the tree releases small amounts of $CO_2$ through respiration, but during its life, the tree takes in more $CO_2$ to support growth and repair than it releases (although respiration increases in response to rising temperatures so climate change may alter this ratio). When the tree dies or its leaves and branches fall and decompose—or when the tree is burned—most of the stored $CO_2$ is returned to the atmosphere. Microbes in the soil that digest the dead tree respire $CO_2$, although some carbon remains within the soil for geological timescales.

Could this carbon sink become a carbon source? A new federal report states that trees are the most significant terrestrial carbon sink, absorbing 8.8 billion tons of $CO_2$ annually—about one third of all human $CO_2$ emissions—and storing it in their wood. But a tree does not remove $CO_2$ from the air forever. Once it dies, the wood decays, slowly releasing $CO_2$ in the process. Forests full of trees that took hundreds or thousands of years to grow may be killed by severe drought within a few months, simultaneously initiating a large-scale release of greenhouse gases.

McDowell points to the positive feedback between warming and tree death and more warming, noting how critical it is to find out how strong this feedback is. "You lose all the green material for $CO_2$ uptake," he says. "It's potentially a very big number."

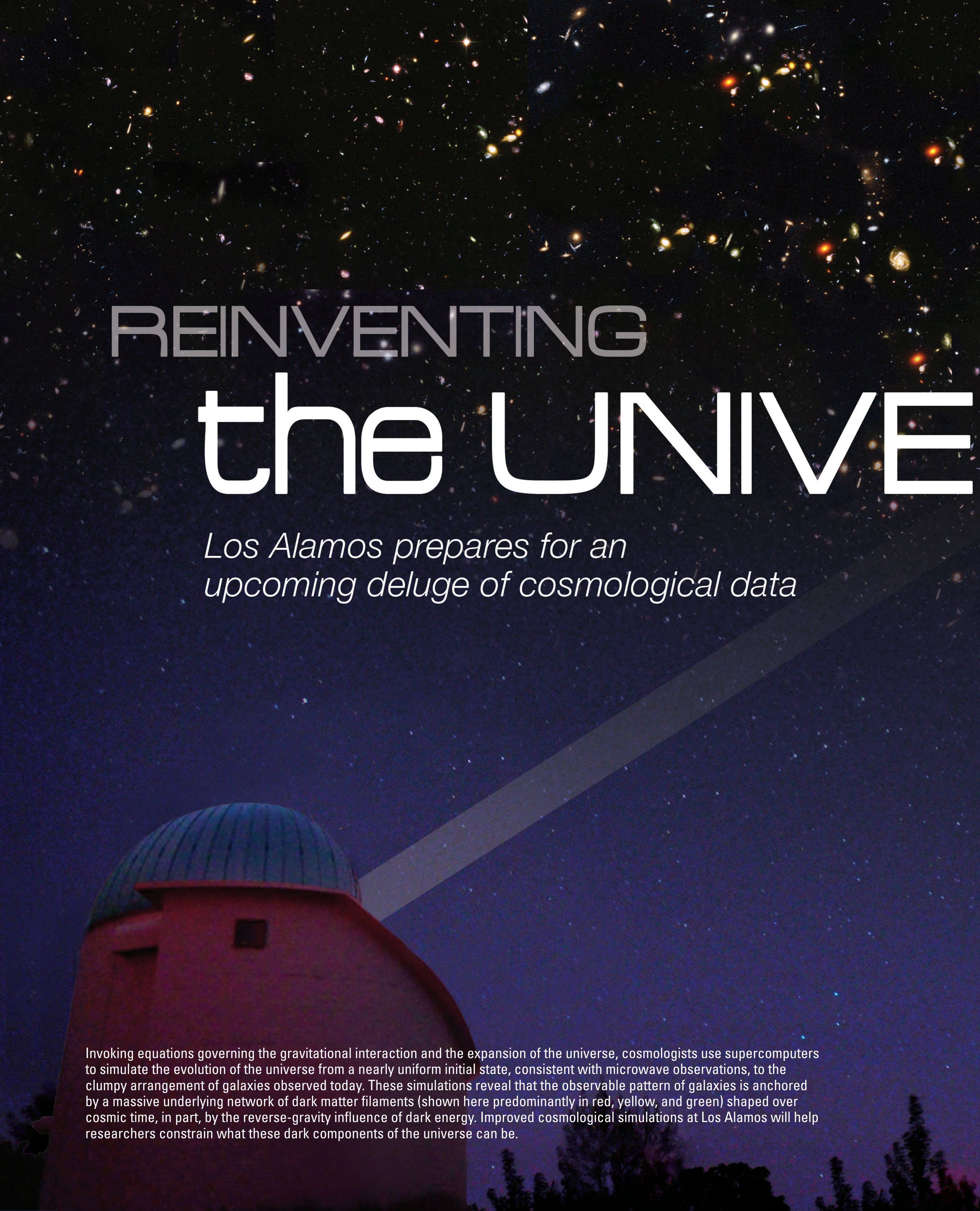
But is there a clear-cut solution to remedy this trend? Maybe forests could be managed differently. McDowell suggests that a sustainable thinning and prescribed burning of arid and moderately arid forests, which cover most of the Rocky Mountains, might mitigate the problem. More accurate modeling should make it possible to assess the extent to which such an approach is likely to succeed. Until then, he says the best solution is to put a lid on humanity's carbon output.

In the meantime, McDowell is working hard to isolate the mechanisms of mortality, engage large-scale global monitoring, and construct an accurate prediction capability in coordination with climate models. Finding a cure, if there is one, requires first understanding the disease.❖ LDRD

*— Kirsten Fox*

# REINVENTING the UNIVE

## *Los Alamos prepares for an upcoming deluge of cosmological data*



Invoking equations governing the gravitational interaction and the expansion of the universe, cosmologists use supercomputers to simulate the evolution of the universe from a nearly uniform initial state, consistent with microwave observations, to the clumpy arrangement of galaxies observed today. These simulations reveal that the observable pattern of galaxies is anchored by a massive underlying network of dark matter filaments (shown here predominantly in red, yellow, and green) shaped over cosmic time, in part, by the reverse-gravity influence of dark energy. Improved cosmological simulations at Los Alamos will help researchers constrain what these dark components of the universe can be.

# RSE

**IT WAS NEARLY A HUNDRED YEARS AGO** when scientists began to contemplate the expansion of the universe. It was nearly fifty years ago when scientists first observed what is now frequently considered to be the primary line of evidence for the big bang. But only in recent decades has cosmology, the science concerned with the origin and evolution of the universe, come into its own. Data from a variety of telescopes and satellites, observing visible and nonvisible forms of electromagnetic radiation, have transformed cosmology from a somewhat speculative field into a precision science. Cosmologists today refer to the widely agreed-upon "standard model of cosmology" without batting an eye. But that well-tested and highly successful standard model includes two as-yet unidentified components—dark matter and dark energy—which, taken together, account for 95 percent of the energy in the universe.

**DARK MATTER** refers to an unseen source whose gravitational influence is observed in galaxies and galaxy clusters throughout the universe. It comes in two varieties: baryonic dark matter, which is made from normal matter particles—protons, neutrons, and electrons—and nonbaryonic dark matter, which is made from something as yet undiscovered. The vast majority of dark matter (and therefore the variety of dark matter discussed in this article) is nonbaryonic. Whatever comprises it does not emit, absorb, or obscure light. And if it interacts nongravitationally with other matter (including itself), it does so extremely weakly, such that normal-matter interactions like magnetism and pressure are not present. Multiple independent observations constrain the total amount of matter, whether normal or dark, based on its gravitational effect. Similarly, multiple independent observations constrain the total amount of normal matter, based on the nuclear and electromagnetic interactions it does not share with dark matter. Comparing the two totals in terms of mass reveals that the universe contains five times more nonbaryonic dark matter than normal matter.

### Identity Crisis

The difficulty with both unidentified components began in the first half of the 20th century. In 1933, an astronomer named Fritz Zwicky reported that galaxies orbiting one another in a giant galaxy cluster appeared to move too quickly—so quickly, in fact, that the gravitational force created by the thousands of galaxies in the cluster would need to be more than a hundred times stronger to keep the galaxies from flying away. So there shouldn't have been a cluster at all, yet there it was. He proposed there must be a large amount of "dark" matter hidden in the cluster to provide the needed gravity. It was a bold proposal, and yet it went largely ignored until the 1970s, when it became evident that the same problem plagued individual galaxies: their stars and gas clouds move too quickly to be bound by the gravity of the galaxy's visible matter. Dark matter would be needed to keep galaxies from flying apart too.

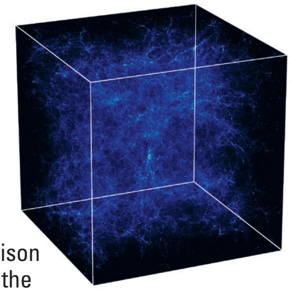
Shortly before Zwicky discovered trouble in galaxy clusters, Albert Einstein discovered trouble for the whole universe. The equations of his own theory of spacetime and gravity, known as general relativity, predicted that the universe should expand (or contract) rather than sit still. Finding a static universe to be more likely, he added an additional term to his equations in order to make the universe stay the same size and called the additional term the cosmological constant. But in 1929, when astronomer Edwin Hubble published observations of galaxies moving outward, Einstein realized the universe was expanding just as his original theoretical work had predicted, and he subsequently rescinded his cosmological constant because it was no longer needed. That settled the issue for much of the scientific community until 1998 when observations of extremely distant supernova explosions allowed scientists to characterize the effect of the expanding universe on the supernova light during its long journey to reach Earth. The data showed that the universe hasn't been expanding steadily; rather, the expansion has been accelerating, which requires a modification to Einstein's equations. The cosmological constant, or something like it, was back. The general term for "something like the cosmological constant" is dark energy.

Both dark matter and dark energy are referred to as "dark" for a reason: they cannot be seen or directly observed—not easily and not yet, anyway. Instead, researchers must observe their effects to figure out exactly what they do, in order to slowly zero in on what they are. And knowing what the dark components do makes possible a powerful way to study them: calculate their effects in various simulated universes and then compare those simulated universes with the real one.

### Universe in a Box

Mike Warren is a cosmologist and computational scientist at Los Alamos National Laboratory. He develops supercomputer codes to simulate the evolution of the universe, and in so doing, he probes our nation's supercomputing capabilities. At the heart of his cosmological simulations is the hashed oct-tree (HOT) computational code he authored as a graduate student in the 1990s in order to take advantage of the new parallel computing systems being

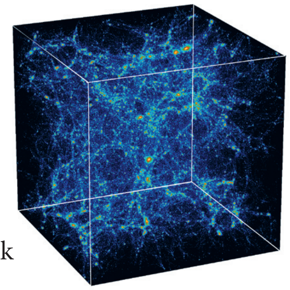
**DARK ENERGY** refers to an unseen agent responsible for inducing an expansionary pressure on the universe. The effect is like antigravity and is observed as an acceleration in the expansion of the universe. This phenomenon is only seen at very large distances; otherwise, the inward force of gravity would overwhelm the outward force of dark energy. Hence, its effect might be observed between very distant galaxies, for example, but not between the Earth and the Moon. Multiple independent measurements agree that the universe contains nearly three times more dark energy than all other forms of energy combined, including that in the form of normal and dark matter.



Simulated universes are built within cubes of simulated space. Differences in the input parameters yield differences in the properties of the resulting universe, allowing cosmologists to narrow down the parameters of our universe by comparison with the simulated ones. For example, the box near the center of the page shows a “standard model” universe, including normal matter, dark matter, and dark energy. The lower box shows the same universe without dark energy, causing it to exhibit tighter matter clustering for lack of dark energy’s additional expansionary influence. The upper box shows a universe with less matter, both normal and dark, and more dark energy than the universe we actually inhabit, leading to greater uniformity and less gravitational clustering.

invented then. His HOT code, which has three times won the annual Gordon Bell Prize for high-performance computing, must once again earn its stripes: Warren is currently getting it geared up for a record-setting, trillion-particle cosmological simulation of the evolution of structure in the universe in anticipation of ever-greater data sets from upcoming astronomical observations.

“We’re stress-testing the biggest computers in the world with these codes,” says Warren. And what better test could there be for a high-performance computing system than a simulation of something as grand as the universe?



The universe, real and simulated, contains particles of dark matter and normal matter tugging on one another by the force of their mutual gravity and, on the largest scales, pushing away from each other by the expansion-accelerating force of dark energy. For particles of dark matter, the competing forces of gravity and accelerated expansion are the whole story. Particles of normal matter, by contrast, are capable of much more—including interacting with each other by electromagnetic forces, exerting pressure, forming simple molecules, and radiating away energy in the form of photons. The simulations must, therefore, combine separate routines for dark and normal matter. Fortunately, however, the nongravitational interactions of normal matter tend to be short-ranged, rendering them unimportant on large scales.

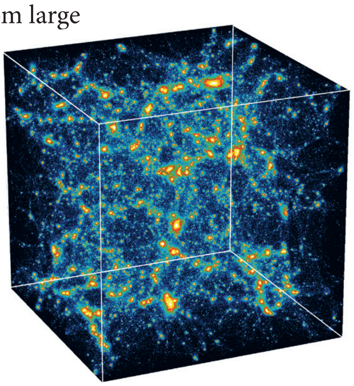
From a computational perspective, designing a large-scale, high-resolution simulation to track only the dark matter is challenge enough. Recent simulations conducted on Los Alamos’s Mustang supercomputer, for example, included more than 69 billion dark matter particles occupying imaginary cubes that range from 750 million to 12 billion light-years on a side. (For comparison, the distance from our Milky Way galaxy to the nearest comparable galaxy is about 2.5 million light-years.) Mustang is capable of resolving gravitational interactions at scales down to approximately one-hundred-thousandth of each cube’s side length, calculating all such forces acting on each particle—from all the other particles in the simulation combined—in just 10 nanoseconds before moving on to the next particle. And once it finishes determining all the forces on all the particles, it moves each one as needed to satisfy the particular forces acting on it and then starts over, calculating all the forces arising from the new arrangement of particles.

Even at supercomputer speeds, it’s a big job. There are a lot of particles and a lot of iterations needed to carry the simulation forward through the 13.7-billion-year span of cosmic history since the big bang. So scientists in this field are always working to find bigger computers and develop more efficient codes by exploiting clever computational shortcuts. Recently, the HOT code performed a dark matter simulation with more than a trillion particles while sustaining a processing speed that exceeded 1.5 petaflops ($10^{15}$ arithmetical floating-point operations per second) at 90 percent parallel efficiency during scaling studies on the Jaguar supercomputer at Oak Ridge National Laboratory. This represents a major milestone in that only a handful of scientific codes of any type have achieved petaflop performance so far.

Warren likes to compare this performance to that of his first dark matter simulations in 1990, with just 1.1 million particles, a speed of 160 megaflops ($10^{6}$ floating-point operations per second), and 85 percent parallel efficiency. “The problem size has increased by a factor of a million and performance by a factor of ten million,” he says. “Increasing the performance of an automobile by a factor of ten million would make it travel at the speed of light.”

## Virtual Voids

When a simulation finishes, the computer outputs the positions and velocities of all the simulated particles for the duration of the simulated time period, right up to the final state. If the parameters used to set up the simulation are realistic, the thinking goes, then the output final state should look like the real universe, with arrangements of dark matter matching the sizes, shapes, and numbers of gravitational sources we observe. The gravity from large clumps of dark matter should end up anchoring large clumps of normal matter, partially allowing astrophysicists to match up the features of the observed distributions of galaxies and galaxy clusters with those of simulated clumps of dark matter.



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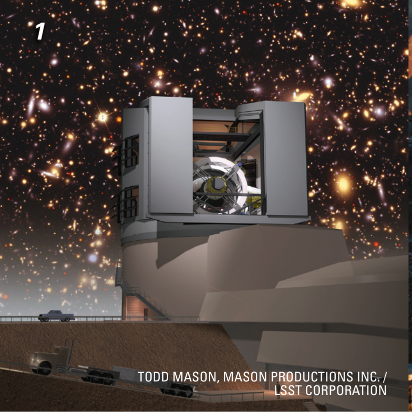

TODD MASON, MASON PRODUCTIONS INC. / LSST CORPORATION

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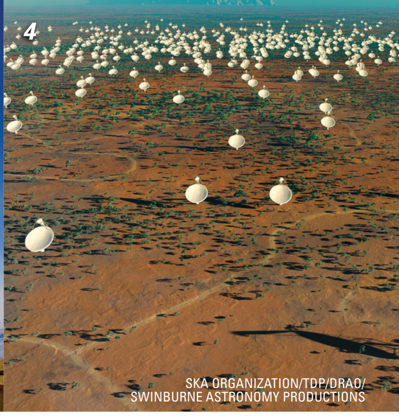


SKA ORGANIZATION/TDP/DRAO/ SWINBURNE ASTRONOMY PRODUCTIONS

# THE GREAT SURVEYS

Various large-scale survey programs, in operation now or set to begin within a decade, will obtain vastly more astronomical data than has been collected in all prior human history, allowing researchers to discriminate between alternative features of our universe, such as different types of dark matter or dark energy. Four such programs of particular relevance to cosmology are described below; each description corresponds to a numbered image above.

**1** - The proposed Large Synoptic Survey Telescope (LSST) is planned to be operational within a decade, observing from a Chilean mountaintop a sky full of distant galaxies similar to the simulated sky shown. Among other things, LSST will "see" the 3-D distribution of dark matter, the action of dark energy, and starlight from some of the first stars and galaxies to form in the universe. LSST is a nonprofit collaboration funded by the National Science Foundation, private foundations, grants to universities, Department of Energy (DOE) laboratories, and other member institutions.

**2** - At the Cerro Tololo Inter-American Observatory, also in the Andes Mountains, the Blanco telescope (largest dome) is being fitted with a new camera system to carry out the Dark Energy Survey (DES), which will combine four different methods of observation to isolate and quantify the influence of dark energy on the expansion of the universe and the formation of large gravitational structures, such as galaxy clusters. DES is scheduled to take data for five years, beginning this fall.

**3** - The South Pole Telescope (SPT) surveys the cosmic microwave background radiation—the glow left over from the hot, early universe—in the southern sky. Among other research benefits, SPT can identify distortions in the microwave radiation caused by its passage through a galaxy cluster along its path to Earth. Hot gas that pervades the cluster boosts the microwaves' energy. Much can be learned about the cluster itself, including its mass and its distance from Earth, when the SPT microwave distortions are combined with other x-ray, optical, and infrared observations. Since the very process of clustering is governed by gravitation from normal and dark matter, together with the expansion and the expansion-accelerating effect of dark energy, galaxy clusters make a valuable target for studying the major unknown agents of cosmology. SPT, already in operation for several years and shown here during construction in 2007, will eventually capture this effect in thousands of clusters, creating an important new cosmological data set.

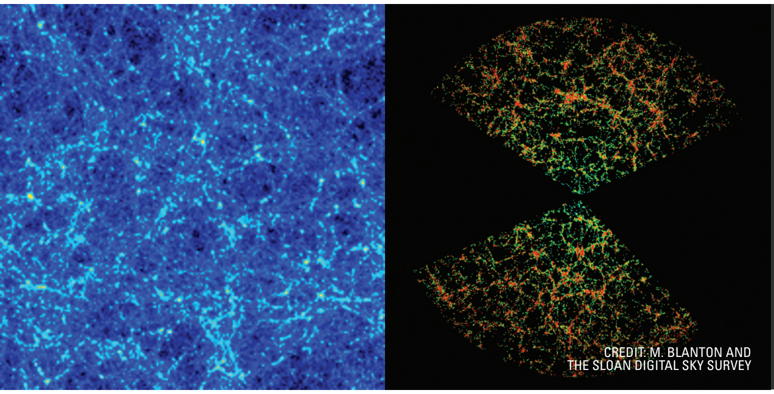
**4** - The Square Kilometre Array (SKA), shown here as an artist's impression and scheduled to begin construction in 2016, will be a vast network of 3,000 radio dishes spread throughout parts of Australia, New Zealand, and Southern Africa, with a combined collecting surface area totaling approximately one square kilometer. The result of an international partnership of 67 organizations from 20 countries, SKA will be able to detect the radio emissions from the hydrogen gas that pervades galaxies, galaxy clusters, and the clouds of matter that seed the formation of both. And because it will be able to see the otherwise invisible precursors of galaxies, it will give astrophysicists access to a previously undetected period in cosmic history: after the glow of the big bang had faded but before there were any stars or galaxies to produce light—a period known to cosmologists as the dark ages.

The most revealing source of cosmological data available today, the cosmic microwave background, is essentially a snapshot of the universe when it was about 400,000 years old, shortly before the dark ages began. Hundreds of millions of years of darkness ensued, and SKA is expected to provide access to all of it. Because the wavelengths of electromagnetic radiation (including light and radio) expand as the universe expands, astrophysicists will be able to separate the hydrogen emissions—which have a single, characteristic wavelength—according to how much their wavelengths have expanded. The longer the wavelength, the more time the light spent traveling through the expanding universe, and therefore the older the signal. That is, the SKA data will not just be a snapshot of one moment of cosmic history, but rather a nearly billion-year, 3-D movie.

"The volume of data SKA will generate from galaxies forming during the dark ages will dwarf everything we currently have about the formation of galaxies," Los Alamos cosmologist Mike Warren explains. "No existing simulations are equipped to make sense of it." That's one reason his work is vital to the future of cosmological science.

This match-up has been encouraging so far (see figure below). Current observational programs known as galaxy surveys locate up to a million galaxies in order to discover how they are arranged over large distances. The largest such survey to date, the Sloan Digital Sky Survey (SDSS), presents slices of the universe, showing galaxies arranged in clusters and long rows called walls surrounding relatively empty regions called voids. Meanwhile, simulations from Los Alamos and elsewhere reveal a universe laced with a web-like network of dark matter arranged in filaments. The filaments (strands of the web) have enough gravity to pull in normal matter and, therefore, host strings of galaxies resembling the walls seen in galaxy surveys. And the most dense dark matter regions—vertices where filaments converge—attract enough normal matter to form massive galaxy clusters. The spaces between filaments are thus depleted of normal matter, leaving behind empty voids. Evidently the simulations are on the right track.

The fact that theoreticians can construct a simulated universe from known particles and forces—even poorly known ones like dark matter and dark energy—and watch it self-arrange to exhibit the same types of large-scale structures that experimentalists observe via major telescope initiatives is an impressive success. This type of qualitative agreement implies that the ingredients are correct: an expanding universe populated by normal and dark matter, under the influence of gravity and dark energy, for 13.7 billion years. (Other lines of observational evidence corroborate this scenario as well.) In order to make progress at this point, researchers must ask more specific questions: What specific kind of dark matter is it, and exactly how much is out there? Does the force of gravity ever depart from Einstein's equations for general relativity and, if so, in what way? Does the dark energy uniformly occupy space, or are there regions where it has greater influence? And has its strength been constant over the entire history of the universe?


CREDIT: M. BLANTON AND THE SLOAN DIGITAL SKY SURVEY

One of Warren's simulated universes (blue, left) shows a large-scale structure—a web-like arrangement of walls (lines containing many galaxies) and voids (dark spaces in between)—similar to that seen in galaxy survey data from the Sloan Digital Sky Survey (pie-shaped slices, left). In the SDSS image, each tiny dot represents the location of a single galaxy. The pie-shaped slices range outward two billion light years (outer circumference) from Earth at the center. (The shapes of the two images are different because simulated regions are cubical, while observed regions come from arcing telescope sweeps across the sky.) The simulation-generated image includes dark matter, while the SDSS image shows only observably luminous galaxies. Yet, as seen by comparing the two, the arrangement of galaxies traces the underlying dark matter distribution.

Answering questions such as these requires more detailed observations capable of capturing subtle bits of evidence concerning the gravitational and expansion-related histories hidden in the spatial distribution of galaxies. It also requires more detailed simulations capable of generating observably distinct structural features in response to any subtle deviations in the behavior of the particles and forces present. For example, researchers need to be able to predict how observations of the universe would differ if dark matter particles were a little bit more massive, or if the first galaxies looked a little different or formed a little later.

"The detailed observational data needed to address these questions is on its way," Warren says. "Our simulations need to be ready for it."

## Information Overload

Recent successes in large-scale observations of galaxies (including SDSS) and observations of the cosmic microwaves also seem to validate the expansion of such survey programs to ever-larger regions of space with ever-higher resolution imaging. And because cosmological physics and the parameters that govern it, such as the density of dark matter, tend to reveal themselves in observations covering vast regions, upcoming observational cosmology programs include several so-called "great surveys" (see "The Great Surveys," facing page). For example, the large synoptic survey telescope (LSST), currently in design and set for construction on a high mountaintop in Chile later this decade, will capture the entire southern sky and do so faster and in far greater detail than the SDSS telescope (located in New Mexico with a view of more of the northern sky). But with observations conducted on such an unprecedented scale comes an unprecedented challenge in analyzing them: scientists must be able to draw meaning from statistical patterns hidden in the flood of data.

"During the next decade," Warren points out, "large astronomical observing projects will gather more than a thousand times as much astronomical data as has been gathered in all prior human history." According to Warren, these data will add up to hundreds or thousands of petabytes (a thousand gigabytes, or $10^{15}$ bytes), leading him to refer to the era of “petascale cosmology.” Therefore, simulations capable of analyzing great survey data must be on the petascale as well. Analysis of dark matter and dark energy in particular—both unobservable apart from their effects on luminous objects—can be obtained from great survey data by comparison with simulation-based predictions of, for example, galaxy positions and velocities.

## PETASCALE COSMOLOGY PROJECT

*Our scientific aims are to use computer simulations to better understand the fundamental properties of the large-scale universe. These questions at the frontier of science include: How do cosmic structures form and evolve? What is dark matter? Why is the universe accelerating?*

*Computer simulations enable discovery. In the words of the National Research Council’s astronomy and astrophysics decadal survey, “Through computer modeling, we understand the deep implications of our very detailed observational data and formulate new theories to stimulate further observations.” The only way to accurately model the evolution of dark matter in the universe is through the use of advanced algorithms on massively parallel computers.*

*Over the coming years, a large investment will be made in observational projects probing for signatures of dark matter and dark energy. The return on this investment depends a great deal on having a robust and accurate suite of simulations to interpret these observations in the light of our theoretical models. In order to achieve the scale and accuracy necessary, these simulations require a computer with hundreds of terabytes ($10^{12}$ bytes) of memory and petascale performance. Our research goal is to produce simulation data accurate at the 1-percent level, and to analyze and compare this data with that from current and upcoming observational probes.*

— M. Warren

The following research objectives of Warren’s petascale cosmology program have been rank-ordered by him according to significance:

- Constrain the nature of dark energy: Identify signatures of different manifestations of dark energy, including those that vary with time or location. Predict the effects of dark energy in detail as a function of its expansionary pressure on the universe.
- Distinguish between dark matter candidates: Determine the identifying features for each of many different types of dark matter particle (such as those with different masses), including combinations of multiple dark matter particles in the same universe.
- Extract cosmological parameters: Explore the nature of different universes by generating new ways to measure and convey the statistical properties inherent in the spacing, clustering, and motion of galaxies and other objects. Use simulations to determine which of these parameters offer the most insight into different scientific questions.
- Generate mock skies: Create a rich suite of expected observables by generating artificial arrangements of galaxies resulting in universes with different physical inputs. Use these “mock skies” to practice interpreting future observations to be made by the great surveys.
- Calibrate simulations to observables: Develop techniques to directly and accurately compare simulated results with many specific types of observations (such as galaxy survey data, radio signals from the dark ages, and expansion measurements obtained from supernova observations), accounting for systematic errors. Optimize observation strategies (i.e., what to look for and in what order) based on this calibration.

## Simulated Signatures

One of Warren’s major objectives is to use his simulations to predict a variety of observable outcomes representing different cosmological conditions. For example, suppose that dark energy is relatively straightforward—e.g., Einstein’s cosmological constant, uniform in space and time—but dark matter comes in three different varieties and general relativity theory needs a particular modification to correctly explain gravity on the scale of galaxy clusters. How would these characteristics reveal themselves in observations made by the great surveys? Which parameters (or combination of parameters), when extracted from great survey data, will distinguish this particular model universe from alternative ones? What would the sky images look like, and what is the most efficient pattern of observations to follow to obtain evidence of this universe?

Warren is not only trying to simulate the outcomes of different input physics, but also recast simulation results to generate very specific predictions that can be readily compared against astronomical observations and characterize the associated uncertainties.

It’s a question of comparing apples to apples: Simulations and observational surveys provide similar information, but not the same information. For one thing, observations generally see only the normal matter, not the dark matter. (One exception is an effect called gravitational lensing, which allows researchers to infer the presence of matter from its distorting effect on background light, but it does not differentiate between normal and dark matter.) And observations of normal matter can determine, within experimental and other uncertainties, where a galaxy (for example) is located, but cannot determine its three-dimensional velocity (as it orbits within a galaxy cluster, perhaps). Rather, observations are limited to the component of velocity along the line-of-sight to Earth. Simulations, conversely, can provide exact positions and three-dimensional velocities—but only for a hypothetical universe. It's no simple thing to compare a billion different simulated positions and velocities with a billion partially observed ones and draw definitive conclusions, but that's precisely the capability that Warren seeks to enable.

## The Prize in the Skies

In the last fifteen years or so, computer simulations have proven to be an invaluable tool for cosmological research, and much of this simulation science capability was developed at Los Alamos. Looking forward, it is Warren's goal that Los Alamos go on to become a national center for computational cosmology, with scientists throughout the astrophysics community seeking out the Lab's resources and expertise.

So far, cosmological simulations have provided strong supporting evidence to complement the body of observational data indicating that scientists' overall picture of the universe—one of dark energy and dark matter, peppered by normal energy and normal matter—is correct. Scientists now have a proof of concept that it is possible to learn about the nature of the universe by adjusting key parameters in a virtual universe to obtain consistency with large-scale observations. "The scientific merit of simulating universes is now well known," says Warren. "It's time to take it to the next level."

The next level means bigger and higher resolution simulations, grounded by more (and more detailed) data. It means being able to query a simulation for specific predictions that can be directly tested with prescribed telescopic observations. And it means identifying telltale signatures of particular varieties of dark matter and dark energy, advancing our understanding of the universe beyond what's possible with observations alone.

But even outside of astronomy, Los Alamos's advances in cosmological simulation science offer the prospect of furthering the world's knowledge of fundamental physics. For example, any information obtained about the properties of the dark matter particle is likely to constrain a variety of theories of high-energy physics by eliminating (or at least modifying) all those that do not predict the existence of a particle with those properties. Today, one of the most promising ways to pursue hard-nosed, rigorous, and exacting physics relies on experimenting with nonphysical universes that occupy virtual spaces, contain hypothetical ingredients, and evolve according to adjustable physical laws.

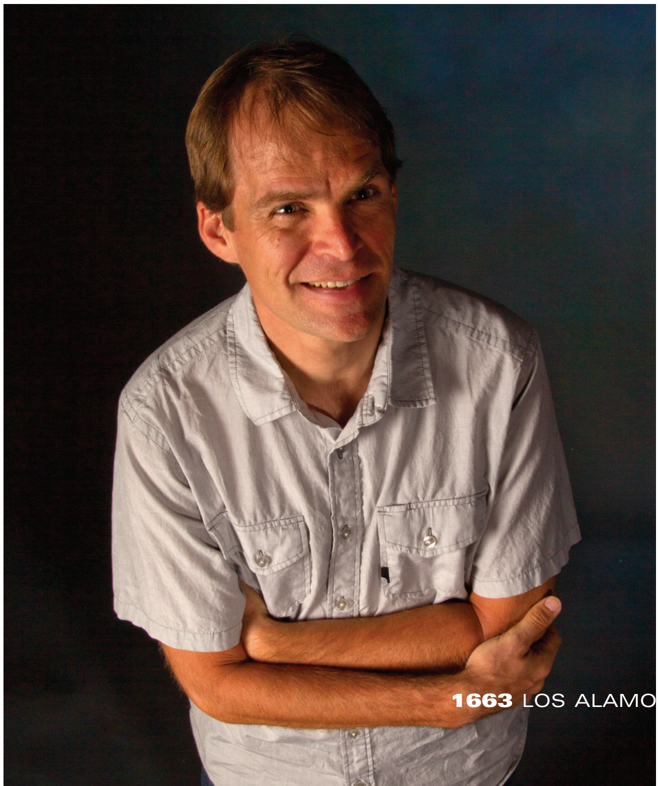
In other words, imagining how the universe might be has become one of the best ways to find out how the universe actually is—as long as you've got the right tools to flesh out every observable detail of your imaginary world. ❖ LDRD

— *Craig Tyler*


CREDIT: HIGH-Z SUPERNOVA SEARCH TEAM, HST, NASA

In 1994, a supernova (bright spot, lower left) was observed in the outskirts of spiral galaxy NGC 4526. Nearly as bright as its entire galaxy, this type of supernova—known as type Ia—can be seen at great distances, making it a useful indicator of dark energy's accelerating effect on the expansion of the universe. By comparing the supernova's observed distance from Earth and how much the wavelengths of its light have stretched with the expanding universe, astrophysicists obtain the expansion rate at different times in the past. The Dark Energy Survey will scan for type Ia supernovae like this one in addition to other indicators of dark energy.

Master of the universe—the simulated universe anyway—Mike Warren uses Los Alamos supercomputers to advance modern cosmology.



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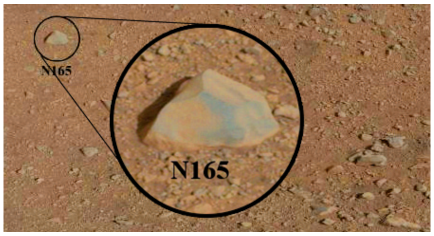


*ChemCam's first study target: Coronation Rock on Mars.*
CREDIT: NASA/JPL-CALTECH/MSSS/LANL

## Los Alamos in Space

Two Los Alamos experiments described in recent editions of *1663* just arrived at their extraterrestrial destinations in August. The ChemCam instrument aboard the Mars Science Laboratory's Curiosity rover landed on Mars on August 5 (See "Shooting Rocks on Mars" in the November 2010 issue of *1663*), and the HOPE spectrometers aboard the Radiation Belt Storm Probes (RBSP) mission was launched for the Van Allen radiation belt surrounding Earth on August 30 (see "The Stuff That DREAM Is Made Of" in the June 2012 issue of *1663*). ChemCam is alive and well on Mars, and the RBSP satellites have arrived in their proper orbit and begun a 60-day period of instrument and satellite subsystem testing before beginning full science operations.

Since its arrival on Mars, ChemCam has been drilling into rocks with a laser, vaporizing small portions of them to create a bit of glowing plasma. A telescope on Curiosity's mast captures the glow and sends it through a fiber-optic cable to a spectrometer, which resolves the light into different wavelengths to reveal what chemical elements are present in the rock. This information will help determine key aspects of Martian history, such as timescales for the presence of liquid water and the overall habitability, past and present, of Mars's surface. According to Los Alamos scientist and ChemCam team leader Roger Wiens, both the Curiosity rover and the ChemCam instrument are working perfectly.

The Helium Oxygen Proton Electron, or HOPE, spectrometers on the two RBSP satellites are part of a suite of instruments that Los Alamos is using to understand the acceleration, global distribution, and variability of radiation belt particles. The new observations will help researchers to better model and predict space weather—and protect satellites from the worst of it. HOPE measures its namesake ions and electrons, which initiate the processes that control the radiation belt structure and dynamics. According to Los Alamos team lead Geoffrey Reeves, if all goes as planned, HOPE will be producing continuous science data by Halloween. LDRD

— *Craig Tyler*

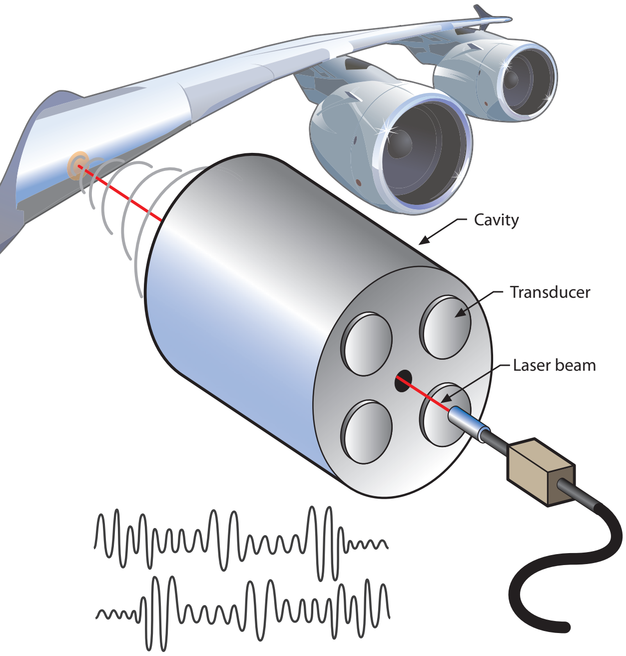
## Structurally Sound

How do you know there isn't a dangerous, microscopic crack hidden inside a bridge's support beam when you drive across or in an aircraft wing when you fly? Fortunately, structures like these can be tested for internal damage with acoustic waves, with material defects causing detectable changes in the waves. But unfortunately, this technique normally requires physically attaching to the surface of the structure a transducer that produces ultrasound (higher pitched sound than can be perceived by human hearing) and gathers data from its immediate vicinity only. It is economically impractical to cover and test every structure with such transducers, and in some cases it is impossible to use them: objects being tested may contain hazardous materials or may be too small to attach a transducer.

The natural alternative to attaching an acoustic source to a structure is to broadcast a sound *near* the structure. Then the source could be moved around to scan for defects everywhere. But this approach has been unsuccessful because noncontact sources do not induce waves with sufficient amplitude in the material being tested, so the telltale sound of internal damage goes unheard. When a sound wave encounters a discontinuity inside the material, such as a crack, it naturally "echoes" with the original frequency plus several harmonic frequencies, and these harmonic frequencies indicate internal damage. But existing noncontact acoustic wave sources simply do not cause the material to produce these harmonics at a detectable level—until now.

Pierre-Yves Le Bas, T. J. Ulrich, and Brian Anderson of the Laboratory's Geophysics Group recently discovered how to generate and detect high-amplitude sound waves in a solid material without physical contact. First, they broadcast a pulse of ultrasonic waves with a chosen frequency into a cavity as "loudly" as their equipment allows without distortion. This original pulse is only a few tenths of a millisecond long, but it bounces around inside the cavity in a complex manner before escaping the cavity through a small hole centered over the material being tested. The bouncing waves escape in succession, causing the material's surface to vibrate in a complex pattern of fluctuating amplitudes lasting several milliseconds. This long-duration vibration still lacks sufficient overall amplitude to reveal the internal structure of the material, but the Los Alamos team uses it for a different purpose.

With a laser vibrometer, the team records a signal detailing the vibration of the material's surface. They then program their acoustic source to broadcast the exact same signal, but reversed in time. (For example, if the observed signal was "loud then quiet," they would broadcast "quiet then loud," but a real signal would be more complex.) This causes the cavity to produce the exact time-reverse of its original motion: Instead of the cavity converting a brief pulse into a long, fluctuating, low-amplitude signal that causes a ringing of the material's surface, it does the opposite. It concentrates the longer and more complicated signal into a short, intense burst. Each time the team broadcasts, they amplify their source



*Listen carefully: In order to test for structural defects in an important material (an aircraft wing in the example shown), several transducers generate ultrasound waves that bounce around inside a cavity, transforming a brief, simple tone into a complex set of echo-like pulses. The wave pulses eventually emerge from a small opening and cause a vibration on the surface of the wing, and a laser records that vibration (upper waveform). Then the transducers are made to amplify and play the time reverse (lower waveform) of the previous laser-recorded sound. This time, the bounces within the cavity merge the complex pulses into a single burst powerful enough to reveal any hidden defects.*

as much as possible. But while the first time they get a lower-amplitude response from the cavity, the second time they get a higher-amplitude response. That latter vibration is once again recorded by a laser vibrometer pointed at the material's surface. This time it contains the detectable harmonics that reveal internal defects.

The noncontact acoustic source capable of producing evidence of internal defects is revolutionary, yet in one important respect, it almost designed itself: The cavity does not need to be exquisitely designed or constructed with exacting tolerances. Rather, a complex and misshapen cavity is ideal because it generates a convoluted and stretched-out ringing signal—one that becomes a concentrated burst with time reversal. As project leader Le Bas explains it, "In a sense, the more imperfect our cavity design, the better the results." LDRD

*— Craig Tyler*

## The Other Left Hand

It's a case of technology imitating nature, only doing it one better. A team led by Los Alamos researchers Antoinette Taylor and Hou-Tong Chen, collaborating with a group from UC Berkeley, took the concept of molecular chirality, or molecular handedness, and created a novel polarizer that can be dynamically switched to transmit either left- or right-circularly polarized radiation. There's nothing quite like it, either in nature or in industry.

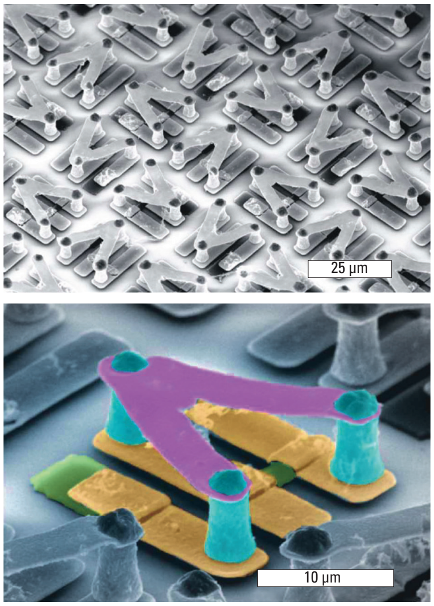
Chirality refers to a lack of symmetry between an object and its mirror image. Your hands, for example, are chiral; while mirror images of each other, to make your left hand resemble your right (not recommended) you have to remove your left thumb and reattach it to the base of the palm below the pinky, then remove and reattach your fingers in reverse order. Similarly, chiral molecules—those lacking any mirror symmetry planes—would require some rearrangement of atoms to be identical to their mirror images. They are of particular interest because they are optically active. A chiral molecule will rotate linearly polarized light in one direction, while its mirror image will rotate the light the opposite way. Chiral molecules may also absorb one type of circularly polarized light more than the other.

Taylor and Chen were looking to mimic this effect in metamaterials. Typically fabricated on a silicon-on-sapphire wafer, a metamaterial consists of tiny, custom-designed metal and silicon structures arranged in a pattern on the wafer's surface. It is the interaction of those structures with electromagnetic waves that determines the metamaterial's electromagnetic properties. The materials work particularly well for terahertz-frequency waves (THz), which occupy the portion of the electromagnetic spectrum between the microwave and far infrared. THz waves have been earmarked for several types of imaging applications, but many of the components needed to fully exploit the radiations—lenses, polarizers, amplifiers, switches, etc.—have yet to be developed.

Chen and colleagues designed a metamaterial structure that was inherently chiral and created a surface pattern such that the metamaterial transmitted left-circularly polarized THz waves. Each structure contained two silicon pads that when illuminated by an infrared laser switched from being insulators to conductors. This effectively switched the structure to its opposite chirality, so the metamaterial transmitted right-circularly polarized radiation. By pulsing the laser on and off, the transmitted THz waves would switch between polarizations or, if the incoming radiation was elliptically polarized, rotate its polarization axis.

One possible application would be to probe biological systems and measure the relative abundance of right- versus left-chiral molecules. But says Chen, "We've never had this capability before. It opens up entirely new avenues of research." And that deserves a hand.

*— Jay Schecker*



*(Top) Scanning electron microscope image of the chiral structure of the fabricated metamaterial. (Bottom) The purple, blue, and yellow colors represent gold structures; the silicon pads (see text) are shown in green.*

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Balloons aglow in autumn at the Albuquerque International Balloon Fiesta, the world's largest hot-air balloon event.

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