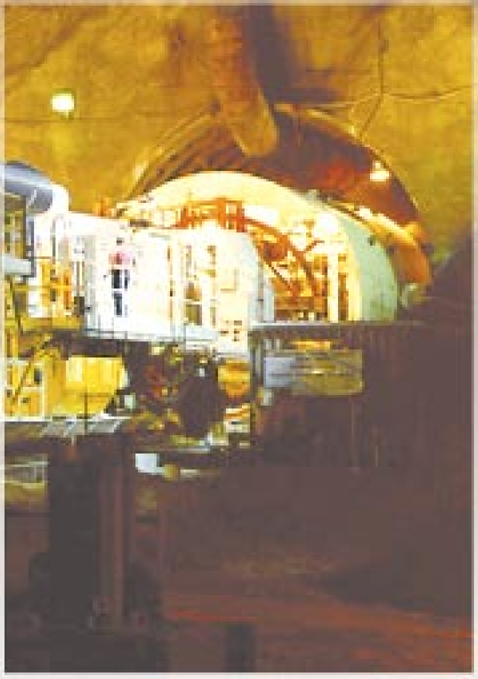
Building a Virtual Time Machine



A new computer code taps the world's most powerful computers to show how buried nuclear wastes would affect the geology of Yucca Mountain.

ONE of the most nagging technical challenges facing America's nuclear power industry is the disposal of its nuclear wastes. Likewise, the long-term success of many programs in the U.S. defense complex ultimately depends on the safe and secure disposal of high-level nuclear waste. Currently, both the civilian and defense sectors maintain their waste at locations across the country while the Department of Energy works to establish a permanent underground repository.

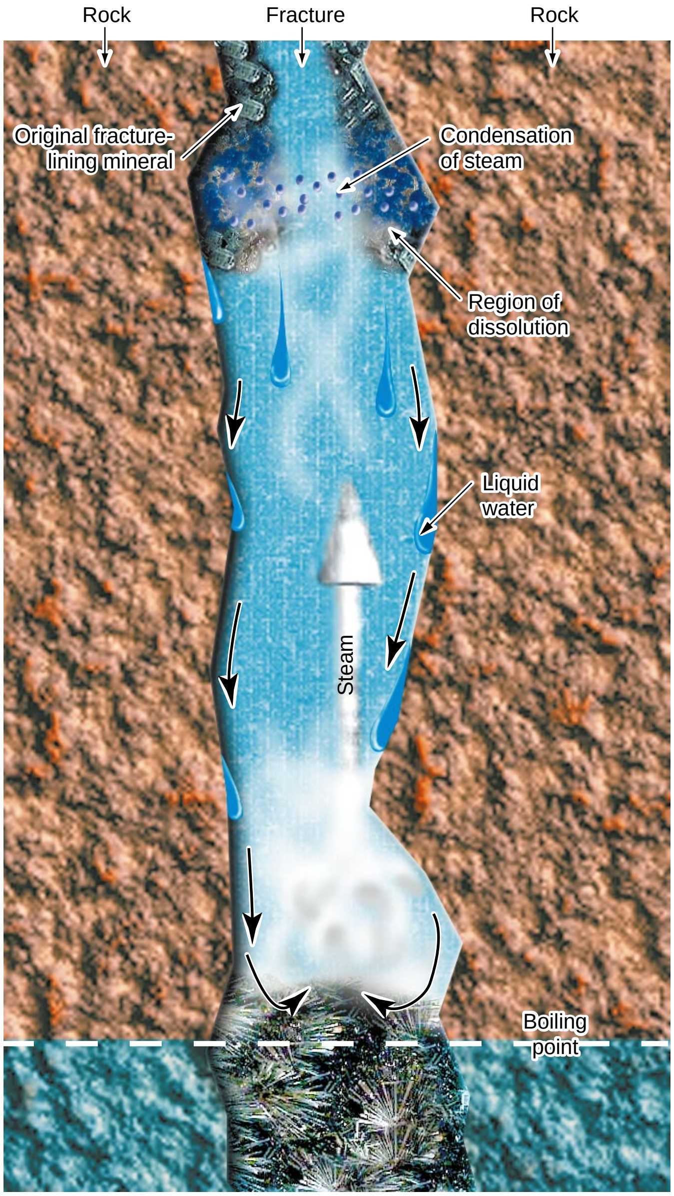
The only candidate site for a national high-level nuclear repository is Yucca Mountain, Nevada. (See box on p. 16.) The DOE has spent about $7 billion to date assessing the characteristics of this arid terrain for its suitability as a repository. This effort involves more than a thousand experts, including teams of geologists, materials scientists, engineers, and computer scientists from Lawrence Livermore, who are researching the site's geology and testing materials for making waste storage containers to be buried in underground tunnels. (See *S&TR*, July/August 1997, pp. 8–9, and *S&TR*, March 1996, pp. 6–16.)

While this work proceeds, scientists also need a way to accurately predict the potential repository's likely evolution over a lifetime of 100,000 years or more, including the Performance Confirmation Period of the first 100 years. "One of the biggest challenges of the Yucca Mountain project is determining how the mountain will respond to the tremendous amount of heat generated by the buried waste and if any of those geologic responses will result in the waste packages getting wet," says Livermore geochemist Bill Glassley.

Constructing a code to simulate the geologic evolution of a nuclear waste repository has long seemed an impossible task, for two reasons. The required computer horsepower was unavailable, even in the most powerful computers. And the software to accurately reflect all of the interweaving and evolving physical and chemical reactions of a repository also did not exist.

But now a 10-person team, supported by Laboratory Directed Research and Development funds and taking advantage of a new generation of DOE supercomputers, has constructed a code that models in unprecedented detail the likely evolution of the geochemistry and hydrology of a repository at Yucca Mountain. The Livermore team, headed by Glassley and applied mathematician John Nitao, is composed of geochemists, computer scientists, a physicist, and an ecologist. Together, the researchers have in essence developed a virtual time machine to simulate the extraordinarily complex interaction of the heat from nuclear wastes with the subsurface environment over thousands of years.

The preliminary results from dozens of simulations show how the code provides a rigorous tool for tracking the interplay of water (both liquid and vapor), heat, carbon dioxide, and chemical reactions within the repository's fractured rock. The simulations also show how the code can help determine the effect of



Water vapor or steam in the vicinity of buried wastes will likely travel tens of meters before condensing on fractures in cooler areas. The condensed water may dissolve small quantities of the minerals lining the rock's pores and fractures (see upper part of fracture). As the water flows down toward the waste, it may also precipitate other dissolved minerals. Over time, the precipitated minerals may accumulate and seal the fracture (see lower part of fracture). The scale of this reaction process could range from a few centimeters to tens of meters.

different strategies for arranging waste packages in tunnels and whether they will come into contact with water.

Desert Rock Is 10 Percent Water

At first glance, it may seem strange that scientists are concerned about the flow of water in a desolate desert that experiences summer temperatures up to 50°C. However, Yucca Mountain is formed from volcanic rock called tuff, whose principal chemical constituent is silicon dioxide. Like virtually all rocks, the tuff contains water in its microscopic pores, in this case about 10 percent by volume. What eventually happens to this water is of intense interest because the waste packages must remain as dry as possible to help avoid corrosion and prevent their contents from leaching out. Scientists are particularly concerned about the changes in the vicinity of waste-emplacement tunnels because fractures in the rock are the principal pathways for water to enter—and leave—the tunnels.

Glassley says that it is a certainty that the intense heat from the waste will evaporate or boil off the water trapped in the rock immediately surrounding the waste packages. The water vapor or steam will likely travel up to tens of meters before condensing on fractures in cooler areas. The condensed water may dissolve small quantities of the minerals lining the rock's pores and fractures.

Gravity will likely cause some of the water to flow back down toward the emplaced waste, where it will evaporate or boil off once again. On its downward journey, the water may also precipitate other dissolved minerals if their concentrations are sufficiently high. This cycling may be repeated hundreds or thousands of times. The structure of the rock's pores and fractures will thus be modified by steam and liquid water moving through them, as well as by simple expansion and contraction in response to the intense waste heat. These changes, in turn, will alter the rate at which water moves through the rock.

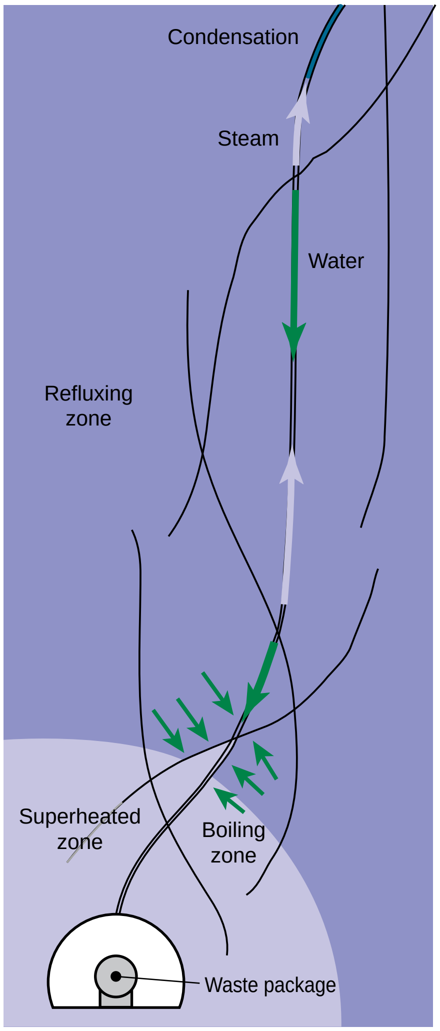
"You end up with the water changing the rock chemistry, which changes where the water moves, which changes the chemistry again. It's a strongly coupled system," says Glassley.

Over hundreds and thousands of years, some of the continuing processes could seal fractures in the rock. Or the continuing reactions could increase the opening of the cracks, producing a natural drainage system to any water and eventually leading to the water table far below.

"The two possibilities have very different implications important to waste package leakage, although the probability of such a failure is very low," says Glassley. If the water sealed the rock fractures above a tunnel, it could increase the probability that radionuclides from a leaking waste package would not leave the immediate environment, because water would be prevented from getting into tunnels. Sealed fractures below a tunnel could lead to ponding of water in the tunnel itself. If the fractures were enlarged below the tunnel, the contents of a leaking package could, over thousands of years, make their way to the water table several hundred meters below, assuming water were to enter the package. Or, depending on where the major cracks formed, they might provide a throughway for condensed or percolating water to escape the surrounding area without contacting a waste package.

All Processes Must Be Coupled

Without a realistic simulation of a nuclear repository, it is difficult to predict if water is likely to reach waste packages, and if so, when during the repository's lifetime and exactly where in the tunnels it would likely do so. A detailed simulation requires the ability



Gravity will likely cause some of the condensed water to flow back down toward the emplaced waste, where it will evaporate or boil off once again. Such cycling may be repeated hundreds or thousands of times over many centuries.

to calculate how heat and water (and steam) migrate, and how chemical reactions occur over thousands of years. It requires simultaneously calculating hundreds of independent chemical, mechanical, and physical variables at millions of locations. The calculations must be repeated hundreds to thousands of times to track changes that occur over time.

"Until recently, we couldn't even begin to think about simulating what will go on at the mountain because we'd first need a code that integrated chemistry, hydrology, and heat," says Glassley. "These processes cannot be studied individually; they must be studied together to understand the

All Roads Lead to Yucca Mountain

Experts agree that the best method for disposing of highly radioactive materials is to place them deep underground. For almost two decades, the search for an underground disposal site for nuclear waste has focused on the scorching Nevada desert, specifically, a place called Yucca Mountain. If it proves suitable, and if approved by federal agencies, Yucca Mountain will be the nation's first geologic repository for the permanent disposal of both spent nuclear fuel from nuclear power plants and high-level radioactive waste from nuclear weapons production.

Yucca Mountain is located about 145 kilometers northwest of Las Vegas on federally owned land on the western edge of the Department of Energy's Nevada Test Site. Currently, it is the only site being evaluated for suitability as a potential underground repository. It is a candidate because of its long distance from any large population center, its dry climate, its deep water table, and the geochemical and hydrologic properties of its rock, mainly compressed volcanic ash called tuff.

Scientists are trying to determine whether radioactive waste stored in highly corrosion-resistant containers deep within the mountain and 300 meters above groundwater can be considered to be reliably isolated from the environment accessible to humans. This consideration includes the migration pathways that might be followed by any escaping radionuclides—should a waste container ever fail—the ability of the rock to trap radionuclides along these pathways, and the persistence of radionuclide migration.

Yucca Mountain in the Nevada desert is a potential location for the storage of high-level nuclear wastes.

Cylindrical waste packages, measuring 3 to 6 meters long and weighing about 50 tons apiece, would be placed lengthwise along about 50 horizontal tunnels, called drifts, each stretching about 1 kilometer. During the repository's first century of operation, called the Performance Confirmation Period, scientists would track the short-term changes in the repository and test their ability to predict the behavior of the repository, including the movement of water and gases in response to heat. The results of this monitoring would provide a database against which refinements in predictions and simulations would be measured.

Three federal agencies are involved in the project. The DOE is responsible for the site evaluation, construction, management, and operation of the potential geologic repository; the Environmental Protection Agency is responsible for developing standards to protect public health and the environment; and the Nuclear Regulatory Commission is responsible for issuing the required licenses to dispose of the waste.

More than 15 years of research has gone into characterizing the site to determine its suitability as a repository. Lawrence Livermore scientists, who have been involved in the nation's nuclear waste disposal programs since the late 1970s, have participated in the Yucca Mountain project from the start. Livermore scientists have the responsibility for determining the Engineered Barrier System materials that comprise the waste package, drip shield, and backfill. They are also responsible for defining the environment that the barrier system will experience over time, including the effects of heat on that environment.

In December 1998, DOE issued a Viability Assessment, stating that the agency believes Yucca Mountain remains a promising site for a geologic repository. The overview acknowledges that uncertainties remain about key natural processes, the preliminary design, and how the site and design would interact. When the characterization work is completed next year, the Secretary of Energy will decide whether to recommend the site to the President.

With adequate funding for completion of scientific and engineering work needed to support the licensing process, the first waste could be placed in a repository by 2010. Future generations will decide when it should be closed and sealed.

evolution of the repository." Such a code did not exist, although several institutions were working on one.

Furthermore, the raw computational power to run such a complex code did not exist. But the Accelerated Strategic Computing Initiative (ASCI)—supporting DOE's Stockpile Stewardship Program to keep the U.S. nuclear stockpile viable—brought about a new generation of computers. These computers made running such a code feasible for the first time.

Livermore's Blue Pacific supercomputer, one of the key ASCI machines, uses 1,464 nodes or individual computers, each of which has four processors, for classified applications. Blue Pacific's separate unclassified platform, which the Yucca Mountain team uses, houses an additional 352 nodes containing 1,408 microprocessors. By tying the microprocessors together, Blue Pacific drastically reduces processing time to solve formerly intractable problems from months or even years (on a typical workstation) to several hours or less. "The machine was a big motivator to develop a comprehensive code," says Glassley.

They Started with NUFT

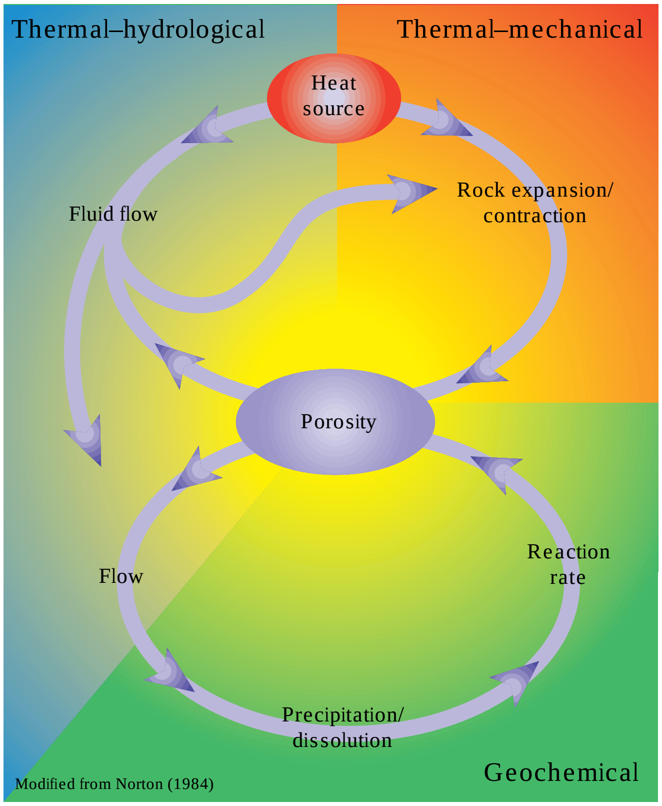
Beginning in 1998, the team embarked on writing a code that would couple heat, water, and chemical processes and take advantage of Blue Pacific's processing ability. They chose a well-regarded program called NUFT (non-isothermal unsaturated flow and transport) that was developed in the early 1990s by Nitao.

A particularly flexible code, NUFT was used during an experiment at the Nevada Test Site in 1994 to determine if a clandestine nuclear test could be detected by gases moving toward the surface. (See *S&TR*, Jan/Feb 1997, pp. 24–26.) It was also used to simulate the cleanup of underground wastes at Visalia, California, where it made accurate predictions about the success of Livermore's promising dynamic stripping cleanup technology. (See *S&TR*, May 1998, pp. 4–11.)

The code is currently being used by Yucca Mountain researchers to predict the temperature evolution surrounding buried waste and to predict how water will likely enter tunnels over the eons. While NUFT does an excellent job simulating the temperature and physics of water flow, it does not account for chemical reactions and how they modify rock fractures and pores. Nitao and computer scientist colleagues spent two years upgrading the code to reflect chemical reactions and linking chemical reactions to equations describing the transport of heat and water.

In the earth sciences community, observes Glassley, simulating chemical reactions, heat transport, and flow of liquids and gases is "a big deal" because it depends on a host of environmental factors. Simulating chemical reactions is particularly important for the Yucca Mountain project because a host of chemical reactions can take place in the tuff and its fissures, cracks, and pores that determine the flow of water. Furthermore, the waste packages will employ highly corrosion-resistant alloys, and each alloy will have different reactions with water and dissolved rock minerals. Understanding what minerals will be present to react with the waste packages is essential in predicting a response.

Simulating the likely chemical reactions at Yucca Mountain was a particular challenge. The most difficult problem was representing the kinetics of mineral precipitation in the region where boiling occurs, because large



Modified from Norton (1984)

Realistically simulating a nuclear repository requires the ability to couple the continuous interplay of heat, chemistry, water flow, and rock mechanics. Porosity and permeability are the fundamental variables that link these processes.

chemical changes can occur there in very short time periods. Standard reference data about chemical reaction rates are not applicable for conditions at the boiling point of water, which may be the conditions near buried waste packages. “We spent a lot of time figuring out how to write equations that would accurately describe reactions in these extreme environments,” Glassley says.

Fractures Made More Real

Another challenge was making sure the code simulated minerals dissolving and precipitating along the insides of fractures within the rock. A typical code represents a rock fracture as two smooth plates separated by some space. But real fractures are rough, twist around, and directly affect the rate of water movement and the consequent mineral dissolution. The team’s code incorporated a more realistic representation of fractures.

With code writing complete, the team compared the code’s chemistry predictions to results from experiments conducted at Livermore. “We needed to check how we represented water interacting with the rock to make sure we were getting the chemistry right,” says Glassley. “We found the code to be very accurate.”

The team had to adapt the program to run on Blue Pacific. Fortunately, Livermore computer scientists have extensive experience adapting codes to run efficiently on enormously powerful supercomputers. The code can also be run on workstations, and the team is particularly eager to distribute it to other geochemists when it is complete. Glassley cautions recipients, however, that particularly complex problems will take a very long time on anything short of a supercomputer.

Glassley expects that the code will prove highly useful in evaluating Yucca Mountain in its Performance Confirmation Period. The code can be tested easily as it simulates specific changes that are likely to occur during the first 100 years. Early changes include a rise in the rock temperature surrounding the tunnels and an increase in carbon dioxide in rock pores associated with steam traveling through them. “The Yucca Mountain project wants to make sure what is seen in the first several decades of repository operation is consistent with our code and others that scientists plan to use,” says Glassley.

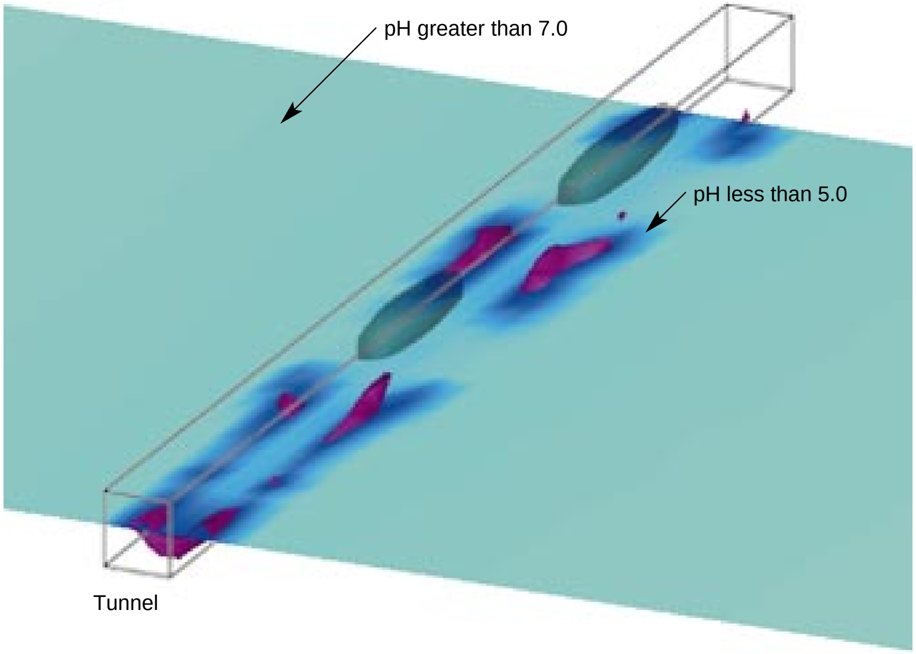
Complex Interplays

Most of the preliminary simulations conducted with the code have focused on a hypothetical waste emplacement tunnel more than 200 meters below the surface. This virtual tunnel contains separate packages of nuclear power plant wastes that are as hot as 200°C and nuclear weapon production wastes that are relatively cool at 60° to 90°C.

After about 500 years, significant and irreversible changes to the rock near the waste are apparent. Water that has condensed above the upper parts of the tunnel cause the formation of a dome that partially seals the rock fractures. The hotter waste packages cause more extensive sealing than the cooler packages. What’s more, the partially sealed domes occur farther away from the hot waste than from the cooler waste.

“The code is really giving us snapshots in time of the openings and

Three-dimensional simulations depict chemical changes after more than 1,000 years in the vicinity of waste packages. In this case, two emplacement tunnels, each with eight waste packages with different heat outputs, were represented. The red volumes enclose those regions in which the pore and fracture waters are somewhat acidic (pH less than 5.0). The blue areas indicate regions where the water is neutral to slightly alkaline (pH greater than 7.0).



closings of rock fractures," explains Glassley. Many findings, such as the complexity of the partially sealed regions, are surprising. Also unexpected is the finding that after about 3,000 years, the domes are still present, but a film of liquid water covers the cool waste packages. Presumably, the water has been driven off slowly from near the hot waste and has come to settle over the cooler waste. "Discovering this water shows how difficult it is to make accurate predictions without a strong simulation tool," Glassley says.

Additional simulations show that the extent of fracture sealing and the occurrence of moisture near the cooler packages depend on the exact placement of the waste packages. Numerous strategies are possible to minimize moisture near the cooler waste packages, including combining civilian and defense waste so the temperature is roughly the same above all waste packages and placing the packages closer together to boil off any water that might collect on the cooler ones.

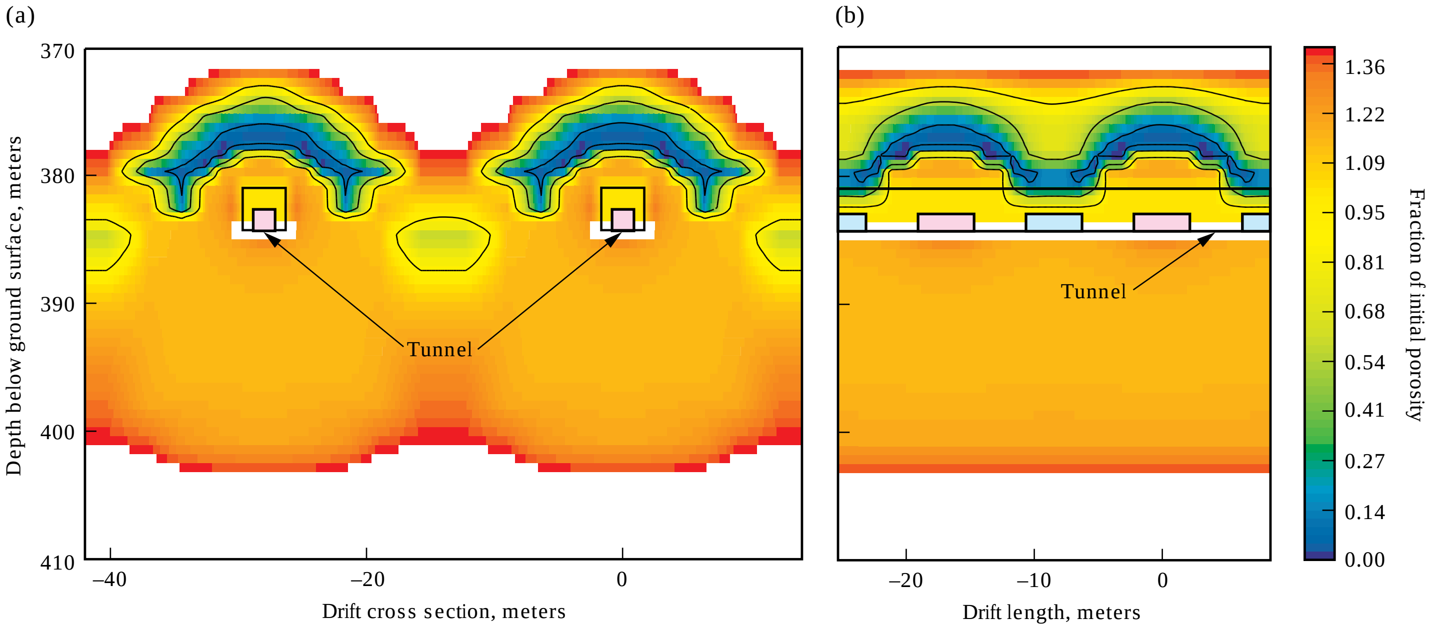
Looking to the Future

The team has conducted short simulations using more than a thousand of the 1,408 microprocessors on the Blue Pacific's unclassified platform. A new series of simulations, scheduled to begin this summer, will require all of the machine's unclassified capacity for extended times. The new simulations will depict multiple tunnels, with each tunnel containing waste packages generating different amounts of heat. The simulations will examine the effects over time of interaction among arrays of waste packages.

The team also plans to increase the number of chemical reactions the code mimics, including those involving radionuclides that could possibly leach out of containers—should there be a breach of the container—over thousands of years. Scientists believe that minerals in the rock could retard the movement of radionuclides dissolved in water, either through chemical reactions or by adsorption onto the rock surface.

Obtaining access to more powerful visualization capabilities is also high on the to-do list. "A thousand processors working for several hours will produce far too much information to contain on a single computer screen," says Glassley. The team hopes to use a power wall, which is an array of monitors pieced together into one giant monitor, to project the true wealth of detail generated by the code.

But viewing even a multitude of computer screens remains a two-dimensional experience. The team also hopes to use three-dimensional visualization tools currently being acquired at Livermore. "With 3D glasses, we'll be able to seemingly fly into the tunnels and look around at the waste packages," says Glassley.



(a) Two-dimensional cross section through two tunnels shows the formation of domes overlying the "hot" (pink) waste packages from spent nuclear power plants. (b) A lengthwise cross section of a single tunnel simulates both "cool" (blue) waste packages from defense production and hot waste packages. The hot waste clearly causes more extensive sealing than does the cool waste. Also, the domes occur farther away from the hot waste. After about 3,000 years, the domes are still present, but a film of liquid water covers the cool packages.

The future may bring other important assignments for the code. Two obvious applications are in helping to manage underground aquifers and cleaning up contaminated groundwater. The team is also in discussion with a U.S. petroleum company to use the code for oil exploration. Adapting the code for the oil industry should not be particularly difficult because it only requires adding an additional liquid—oil—with its different properties and tracking it as it moves through underground strata. The code is currently structured to do exactly this kind of simulation.

One intriguing application is for advancing the understanding of how earthquakes are triggered. Some geologists believe that fluids, specifically deep underground water, play an important role in fault rupture. "We think the code will be able to test this theory," says Glassley.

In the near term, however, the team is focusing its efforts on strengthening the scientific understanding of how America's potential first underground nuclear waste repository will perform in the near—and far—future.

—Arnie Heller

Key Words: Accelerated Strategic Computing Initiative (ASCI), Blue Pacific, computer simulation, Engineered Barrier System, Nevada Test Site, nuclear waste repository, NUFT (non-isothermal unsaturated flow and transport), Performance Confirmation Period, power wall, Yucca Mountain.

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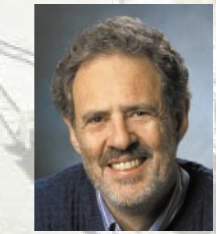
About the Scientist



BILL GLASSLEY received his B.A. in earth science from the University of California at San Diego and his M.S. and Ph.D. in geochemistry from the University of Washington, Seattle. For ten years, he was a professor and researcher at Middlebury College in Vermont. He joined Lawrence Livermore in 1986, where he is a geochemist in the Earth and Environmental Sciences Directorate.

For the modeling and simulation work on the Yucca Mountain project, Glassley and Livermore applied mathematician John Nitao led a multidisciplinary team of scientists and engineers that included Thomas Boulos, Mary Gokoffski, Charles Grant, James Johnson, James Kercher, Jo Anne Levatin, and Carl Steefel.