Water resource management has become a critical issue worldwide, the result of dwindling potable water supplies and expanding populations into regions with limited water reserves. In the United States, it is critical for national security and a strong economy that we ensure safe, dependable water supplies can meet the country's changing population demographics. For several years, Los Alamos National Laboratory has focused efforts to resolve risks and problems to water resources through its research in atmospheric, surface, and subsurface water. The Laboratory has also guided technology developments to ensure dependable water resources and to protect human health and the environment.

With a cohesive strategy the Laboratory pursues water issues on multiple scales, from atoms to oceans, while embracing a variety of identified scientific challenges. These challenges encompass multiple water resource issues, from ensuring clean, adequate water supplies to assessing water security risks to understanding the effect of societal shifts on water demands.

Current Scientific Challenges in Water Resources Research

- Advanced modeling, simulation, and prediction
  Creating integrated models based on acquired data is necessary to gain insight into water resource issues and to assist with trend prediction.
- Predictive decision analysis
  Analyzing uncertainties, decision analysis techniques help researchers to understand trade-offs, predict scenarios, and implement optimized solutions.
- Precise technical solutions and water resource education
  Applying research results to real-world situations, delivering protection and conservation solutions to the nation, and educating both policymakers and the general public about water issues are the final challenges for water research activities.

Problem-Solving Capabilities in Water Research

- Modeling and Simulation
  Los Alamos National Laboratory has expertise in modeling water on all scales, from models of atomic and molecular interactions to coupled models of river basins to integrated models of ocean currents and ice flow patterns.
- High-Performance Computing
  Los Alamos researchers have high-performance computing facilities to execute complex simulations.
- Observational and Experimental Methods
  The Laboratory has extraordinarily sophisticated observational and experimental methods, and has gathered data on atmospheric water, sediment, surface water, and groundwater.
- Analytical Chemistry
  The Laboratory has the analytical chemistry expertise to solve key water quality issues.
- Multidisciplinary Approaches to Complex Systems
  Exceptionally diverse multidisciplinary teams solve scientific and engineering challenges.
- Data Management and Analysis
  Legacy databases are valuable resources to water quantity, quality, and interaction research.
Water Research at Los Alamos National Laboratory

• Pollution Prevention
  Scientists and engineers at Los Alamos National Laboratory have long been involved in green chemistry activities and experiments involving various chemical and radioactive species, allowing them to develop expertise in minimizing the impact of these species on the environment.

• Decision Analysis
  Procedures developed by the Laboratory to support military and national security decisions can be applied to allow researchers and policymakers alike to make more informed decisions regarding water issues.

• Security and Threat Analysis
  The Los Alamos team has decades of experience in providing national and international nuclear security to protect the civilian water supply.

Water Initiatives and Projects at Los Alamos National Laboratory

National Focus Thrust Area
DOE Water Cycle Research Strategy ........................................... W3
DOE Water Cycle Pilot Study ..................................................... W4
BOR Evapotranspiration Mapping and Riparian Consumptive Use .......... W5
SAHRA - NSF National Science and Technology Center ....................... W6

State and Regional Focus Thrust Area
Española Basin Aquifer Model .................................................... W7
Jemez y Sangre Water Planning Council ....................................... W8
Governor’s Blue Ribbon Task Force on Water .................................. W9

LANL Site and Local Focus Thrust Area
Los Alamos Hydrogeologic Workplan ......................................... W10
Hydrogeologic Model of Pajarito Plateau ....................................... W11

Basic and Applied Sciences Thrust Area
Understanding Uncertainty in Water Resource Predictions .................. W12
Plant Cover Effects on Water Resources ....................................... W13
Improved Water Conservation with Waste Materials ........................ W14
Plants with Improved Water Use Efficiency Project .......................... W15

Remediation, Conservation, and Monitoring Techniques
SCORR: Supercritical CO₂ ........................................................... W16
Groundwater Remediation ............................................................ W17
Scanning Raman Lidar ................................................................. W18
DOE Water Cycle Research Strategy

Thrust Area: National Focus

KEY CAPABILITIES

- High-Performance Computing
- Multidisciplinary Approaches
- Observational and Experimental Methods
- Modeling and Simulation

SITUATION

Assessing and Predicting the Effects of Climate Variability and Land Use Change on Water Represents an Important Societal Concern

The United States Global Change Research Program (USGCRP) has identified the water cycle as a national research priority for the next 10 years. As a member of the USGCRP, the Department of Energy (DOE) tasked a committee to develop the research strategy for a program that uses DOE capabilities and facilities to respond to this priority. Cochaired by Los Alamos and Berkeley National Laboratories, the committee included members from 7 national laboratories and 12 universities.

INNOVATION

Understanding that “Without the Plan, There will be No Projects”

Collaborating to devise the DOE research strategy highlighted the Laboratory's ability to develop a large interdisciplinary program. The components that were recognized as essential to the project success were:

- Sustaining the overall DOE goal through frequent communications between the Los Alamos project manager and the DOE program manager;
- Exchanging scientific insights;
- Fostering the cooperative team atmosphere; and
- Emphasizing negotiated compromises.

APPLICATION

Improving Predictions of Seasonal to Decadal Variability in the Water Cycle at the Regional Scale

With the contribution of its strengths in high-performance computing, modeling and theory, and operations of large field operations to collect data, the collaborative efforts of Los Alamos and the larger team produced the DOE Water Cycle Initiative Research Strategy. This document achieved three pivotal results necessary for future DOE programs in Water Cycle Research:

1. Creating the basis for a program if DOE is to fund an effort;
2. Defining the DOE role in the USGCRP Water Cycle Study; and
3. Identifying and addressing the science issues relative to water cycle predictions.

Implementing the strategy will:

- Initiate process studies to improve model parameterizations and enhance physical understanding of the water cycle;
- Develop observational methods and field sites that provide continuous long-term data streams;
- Create coupled models in a high-performance computing environment;
- Link domain models across processes (physical, chemical, geological, and biological) and scales (global, regional, and local); and
- Provide a modeling and testing environment for DOE and all USGCRP research efforts.
SITUATION | Integrating Multidisciplinary Teams to Develop Projects

Los Alamos National Laboratory cochaired the committee that produced the DOE Water Cycle Initiative Research Strategy, which defined the DOE role in the USGCRP Water Cycle Study. The successful collaboration between Los Alamos and the larger team led to a pilot study that was funded by the DOE. The Water Cycle Pilot Study is focused on the Whitewater River basin in Kansas, which is part of the DOE ARM Southern Great Plains site; it began in Fiscal Year 2001. The goals of the Pilot Study are to:

1. Improve model parameterizations and physical understanding of the water cycle through process studies, develop observational methods, and establish field sites that provide continuous long-term data streams.
2. Couple models in a high-performance computing environment, link domain models across processes (physical, chemical, geological, and biological) and scales (global, regional, local), and provide a modeling and testing environment for DOE and all USGCRP.

INNOVATION | Contributing Key Capabilities to Ensure Success

The Pilot Study was built upon the complementary abilities of the larger team. With each team member's contributions corresponding to their strengths, the Laboratory contributed its high-performance computing and existing capabilities in coupling regional atmospheric and hydrologic models.

APPLICATION | Achieving Results to Advance Understanding

Over the course of the Pilot Study, researchers are collecting and analyzing data to assess and predict the effects of climate variability and land use change on water resources. The science that will be performed and in particular the high-performance computing aspects of the Pilot Study will:

- Assert Los Alamos achievements in the water resources area with journal articles and presentations;
- Apply Los Alamos codes to different conditions to further develop coupled modeling capabilities; and
- Augment Los Alamos capabilities in solving complex nonlinear problems in an open environment.

When the pilot study is completed, it will have:

- Created coupled models in a high-performance computing environment; and
- Demonstrated the capability of integrated teams to addressing complex problems.
BOR Evapotranspiration Mapping and Riparian Consumptive Use

KEY CAPABILITIES
High-Performance Computing • Observational and Experimental Methods Modeling and Simulation

SITUATION Addressing the Critical Unknown Variable of Riparian Vegetation Water Use

Complementing the United States Global Change Research Program (USGCRP) identification of the water cycle as a national research priority for the next 10 years, the Bureau of Reclamation (BOR) has identified riparian vegetation consumptive use of water as a critical unknown variable for river management in understanding surface and subsurface water resources on watersheds such as the Rio Grande. Previous studies have used point sensors to make these evapotranspiration measurements, but uncertainty in the spatial variability precluded definitive results. To overcome this problem, the BOR in Albuquerque funded a Water Flux Mapping Study and requested Los Alamos participation.

INNOVATION Developing Tools to Measure the Water Use of Riparian Vegetation

The laboratory is part of a team that is measuring evapotranspiration in time and space. In coordination with universities in New Mexico and nationwide, the laboratory has developed an interdisciplinary measurement and analysis team to field, operate, and analyze data from its mobile scanning Raman water vapor lidar. The ongoing research is to measure the water use of two common tree species - salt cedar and cottonwood - to riparian zones in the southwest in order to:
- Determine if the two species differ in their water use; and
- Help develop a plan to improve water use on the Rio Grande.

APPLICATION Using the Unique Scanning Raman Lidar and Spatial Analysis Methods to Analyze the Combined Array of Point Sensors and Remote Sensing Platforms

Operating the lidar as part of a larger team headed by BOR, the Laboratory has maintained a leadership role in the planning and execution of field logistics, equipment, and personnel for the entire team. The Laboratory also evaluated resources for field deployment. The collaboration will help to:
- Better understand evapotranspiration at selected riparian sites along the Rio Grande;
- Create spatial maps of evapotranspiration over the Bosque del Apache study site to represent selected phonological periods in the riparian vegetation growth patterns;
- Quantify the spatial and temporal variability in evapotranspiration on local micro-scales; and
- Translate spatial and temporal variability terms to a BOR-operated evapotranspiration model for sub-sections of the Rio Grande.
In 2001 the National Science Foundation (NSF) Science and Technology Center for Sustainability of semi-Arid Hydrology and Riparian Areas (SAHRA) began operations with a mission to promote sustainable management of water resources in semi-arid regions. Led by the University of Arizona, participants include other southwestern universities and government agencies. Los Alamos National Laboratory is a partner in the SAHRA multidisciplinary team and leads Thrust Area 4: Multi-Resolution Integrated Modeling of Basin-Scale Processes.

Los Alamos was requested to participate because of their unique capabilities in high-performance computing and modeling, which have:

- Created an integrated, high-resolution model to understand and predict the effects of climate variability and land use change on the water balance;
- Allowed for rapidly integrated computer codes that simulate atmosphere, surface, and groundwater components; and
- Used the Parallel Applications Workspace - developed at Los Alamos - to couple the Regional Atmospheric Modeling System and the Los Alamos Distributed Hydrologic System with minimal changes to the two application codes.

This model simulated the Rio Grande Basin, where it is now being tested.

One major interface that has not been exploited in the past is the socio-economic modules. This interface is challenging, but necessary for models to be successful in supporting decisions. Without it, policymakers fail to see the strong personal and politically-sensitive reasons behind studying and protecting the hydrology of semi-arid riparian areas.

### APPLICATION

**Developing Approaches for Real-World Problems**

The project manager's ability to foster close collaboration with the diverse partners involved in SAHRA ensures that the correct products are delivered. SAHRA is a high-visibility NSF center, and Los Alamos participation:

- Provides the Laboratory with an opportunity to address critical water resource problems in the southwestern United States, and
- Demonstrates the capability of Los Alamos to solve such problems.
Espeñola Basin Aquifer Model  
**Thrust Area:** State and Regional Focus

| KEY CAPABILITIES | Modeling and Simulation • High-Performance Computing  
High-Precision Geophysical Measurements |

**SITUATION**  Investigating Groundwater Quantity and Quality to Ensure Sustainable Water Supplies

Maintaining a dependable and high-quality water supply in arid and semi-arid regions is a growing national concern, particularly because of prolonged drought conditions. In New Mexico, where groundwater provides more than 80 percent of public water supplies, Los Alamos National Laboratory and the surrounding area (Los Alamos, Espeñola, Santa Fe, and numerous pueblos) rely on the Espeñola Basin Aquifer. Declining water levels in the basin are of great importance to the Laboratory because of the implications for a sustainable water supply and because of the potential decline in groundwater quality.

**INNOVATION**  Using Multidisciplinary Teams to Address Hydrologic Questions

With an on-site technical team of geologists, geophysicists, geochemists, and hydrologists, Los Alamos is developing a unique, multidisciplinary approach to address basin-scale hydrologic questions, such as:

- How much high-quality water is in storage in the regional aquifer and how rapidly is this reservoir being depleted?
- What impact do aquifer withdrawals have on surface water flow?
- How will the drought affect groundwater supplies?

Answering these questions requires developing a simulation model that is sufficiently large in scale to encompasses the entire aquifer (approximately 100 square kilometers) but also sufficiently detailed as to capture small-scale variations in hydrostratigraphy and stresses on the aquifer because of pumping. The high-performance computing facilities and flow and transport codes at Los Alamos provide a cornerstone for developing models with high resolution and tight coupling between hydrologic and geochemical processes. Using these tools, a large body of geologic, geophysical, and geochemical data has been integrated into a sophisticated 3-D model of the basin aquifer. Los Alamos has also developed and applied statistical methodologies for applying model predictions in decision-making contexts. The modeling and analysis tools can:

- Predict the rate of future water level declines due to pumping;
- Predict the ultimate fate of contaminants in the regional aquifer;
- Optimize data collection in deep boreholes being drilled at the Los Alamos site;
- Evaluate the adequacy of groundwater monitoring strategies;
- Estimate the uncertainty of model predictions; and
- Visualize flow paths and aquifer characteristics in 3-D.

**APPLICATION**  Realizing Benefits on Local, Regional, National, and Global Levels

Detailed analysis of these problems is important not only for the study area, but also regionally and globally. Benefits of the modeling include:

- Assisting Los Alamos National Laboratory and surrounding communities in evaluating potential threats to water quality and rates of aquifer depletion;
- Assisting communities in the region with water resource planning; and
- Making new methodologies for groundwater resource evaluation available to the wider scientific community via publications in peer-reviewed journals.
Jemez y Sangre Water Planning Council  
Thrust Area: State and Regional Focus

**KEY CAPABILITIES**  
Modeling and Simulation • Data Collection  
Hydrogeology

**SITUATION**  
Chairing the Council to Develop the Water Plan

In 1987 the New Mexico legislature enacted a statute enabling regions in the state to plan their water future, and in 1998 the Jemez y Sangre Water Planning Area was established. Water planning was initiated at the regional level so that unique characteristics of each region would be equally protected. As a major water user in the planning region, Los Alamos National Laboratory is actively participating in developing the Jemez y Sangre Regional Water Plan.

**INNOVATION**  
Understanding and Addressing Water Resource Issues

The Laboratory chairs the Water Planning Council, and also has representatives on the subcommittees for water supply, water supply alternatives, the legal subcommittee, and the executive committee. Los Alamos participation in the Jemez y Sangre Council:

- Provides additional insight into New Mexico water resources issues; and
- Provides opportunities to use its capabilities to understand and address water resource issues of the state and region.

**APPLICATION**  
Securing Water Supplies for the Next 60 Years

The regional water planning efforts of the Jemez y Sangre Council:

- Developed and inventory of the quantity and quality of water resources in the Jemez y Sangre Region (completed January 2001);  
- Projected water resource demands responding to a range of conditions (completed January 2001);  
- Is determining methods to meet projected water demands through 2060 by managing and conserving the region's available water supplies under existing rights, water supplies, interstate agreements, and court decrees (to be completed and documented in the Jemez y Sangre Regional Water Plan in early calendar year 2003); and  
- Will help secure a sustainable water supply for future generations.
Governor’s Blue Ribbon Task Force on Water

**KEY CAPABILITIES**

Science-Based Understanding

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**SITUATION**

Investigating the Current Water Policies and Laws of New Mexico

New Mexico is an arid state with a limited amount of water available for use by its citizens. To ensure an adequate water supply for generations of New Mexicans to come, long-range planning relating the State water use and policies is necessary. To meet New Mexico’s planning needs, the Blue Ribbon Task Force was established through Executive Order 99-35.

**INNOVATION**

Providing Insight and Laboratory Capabilities to Understand and Address the State’s Water Resource Issues

As requested by Governor Gary Johnson, Los Alamos National Laboratory chairs this Task Force, which will be in existence until December 2002. Emphasizing long-range planning related to water use within New Mexico, the Task Force:

- Recommends changes to existing water policies and laws; and
- Proposes new policies and laws to the Office of the Governor.

**APPLICATION**

Advising the State of Appropriate Actions

Task Force recommendations to the Governor include:

- Watershed restoration and management - To reduce the depletion of potential water supplies and the potential for catastrophic wildfires, State efforts must ensure water resources stewardship at the watershed level by working with Federal and private entities.
- Domestic well management - To answer the problems created by more than 5,000 new domestic wells being drilled each year, more stringent domestic well management is needed, which could include inventorying and metering, constraining development, and limiting pumping.
- Water conservation and banking - To relieve the burden on what is already a fully appropriated water supply, water marketing and banking must connect willing buyers together with willing sellers to maximize use of New Mexico water without fear of forfeiture.
- NM/Mexico border development - To ensure the economic vitality of New Mexico, sustainable water supplies must be secured as development occurs.
- Water trust fund - To provide necessary funding for capital outlay projects for storage, conveyance, and delivery of water in New Mexico, the State must invest in effective water planning for the welfare of its citizens.
Los Alamos Hydrogeologic Workplan  

**Thrust Area:** Los Alamos and Local Focus

**KEY CAPABILITIES**  
High-Performance Computing  
Modeling and Simulation  
Observational and Experimental Methods

**SITUATION**  
Recognizing Insufficient Understanding of the Los Alamos Hydrogeologic Setting

In response to a 1995 request from the New Mexico Environment Department, the Laboratory developed a Hydrogeologic Workplan that details the activities to be performed over a 7-year schedule for a site-wide hydrogeologic characterization. Implementing the Workplan would provide sufficient information to adequately design and install additions to the groundwater monitoring network for the site. Los Alamos based the Hydrogeologic Workplan on the application of the Environmental Protection Agency Data Quality Objective (DQO) process to optimize the data collection design. The Workplan depends on an iterative approach—collecting data from a specific borehole and well that will be analyzed and interpreted for sound decision-making on future data collection activities, thereby allowing for project economies and selection of appropriate DQOs.

**INNOVATION**  
Producing Sophisticated Models to Understand Site Hydrogeology

The Laboratory develops discrete sampling and analysis plans for each well; these plans detail the DQOs and well design. The completed wells are typically constructed with multiple screens, where Westbay Instruments, Inc. instrumentation is used to allow discrete sampling and pressure measurements to be made at different depths in the well. During borehole construction of the 32 regional aquifer wells, at depths near 2,000 feet, the Laboratory has collected:

- Geologic samples (cuttings and core) for laboratory analysis;
- A complete suite of geophysical and video logs in the borehole; and
- Water samples for contaminant screening.

Each well is sampled 4 times during an 18-month period. The high-performance computing and modeling capabilities at Los Alamos are used to produce sophisticated models of the vadose zone and saturated zone. As a result, the Laboratory has derived a comprehensive understanding of the site hydrogeologic setting.

**APPLICATION**  
Applying Advanced Techniques to Solve Groundwater Resources Problems

After 4 years of implementing the Hydrogeologic Workplan, Los Alamos has been able to:

- Refine and validate the conceptual model of the Pajarito Plateau hydrogeologic setting;
- Increase the efficiency and cost-effectiveness of the drilling process based on experience;
- Enhance data collection activities through the iterative DQO process; and
- Enable the development of useful tools for performing risk assessments and protecting groundwater resources.

Collaborating with regional government agencies and interested parties, the Laboratory is contributing its expertise and knowledge to solve problems on a regional basis in the Espanola Basin. Additionally, the experience gained by the Laboratory in conducting such a large-scale site investigation is directly transferable to other sites and locations, where it can be used to develop solutions for related groundwater resource management questions and problems.
Hydrogeologic Model of the Pajarito Plateau  
Thrust Area: Los Alamos and Local Focus

KEY CAPABILITIES  Modeling and Simulation

SITUATION  Collecting Data on the Pajarito Plateau Aquifer

Research on the hydrogeology of the Pajarito Plateau began in 1998 as an outgrowth of the Rio Grande Project and the implementation of the Hydrogeologic Workplan for the Laboratory site. Driven by the need for a sound scientific basis to assess and manage groundwater resources, the Laboratory is conducting analyses of groundwater resources based on data collected from 32 deep monitoring (characterization) wells in the regional aquifer across the Pajarito Plateau, and numerous existing wells located throughout the region.

INNOVATION  Creating a Basin-Wide Model for Testing, Analysis, and Prediction

With its capabilities in geoscience, hydrology, modeling, risk management, and computational analysis, the Laboratory is well-suited to create a 3-D model of the geologic framework and a sophisticated hydrologic model of the aquifer. The hydrologic model encompasses the entire Española Basin and includes:

- Major stratigraphic units;
- Major water-cycle components;
- Topographic control on the watershed boundaries;
- Flow and transport components for both the vadose zone and the regional aquifer; and
- Accurate predictions of the combined impact of groundwater withdrawals from water users in the basin.

To maintain consistency in scientific approaches and provide technical recommendations to principal investigators and project managers, a Laboratory-wide Groundwater Integration Team (GIT) has been organized to serve as a technical peer review board and a collaborative configuration control board for technical information.

APPLICATION  Providing Insight on Issues of Groundwater Resources

Enhancing the understanding of the regional groundwater resources and the hydrogeologic setting of the Pajarito Plateau in northern New Mexico, Los Alamos modeling of the basin is:

- Performing characterizations and predictions regarding the hydrogeologic setting of the Laboratory, as well as of regional groundwater resources;
- Helping site environmental programs comply with regulations;
- Estimating the fate of dissolved high explosives discovered at TA-16;
- Siting sentry wells near water supply wells at risk of future contamination;
- Providing insight into impacts of pumping municipal supply wells on the Pajarito Plateau and other existing wells in the basin; and
- Serving surrounding communities and Pueblos by illustrating and communicating water resource information and providing a tool for making water resource management decisions.
Understanding Uncertainty in Water Resource Prediction

Thrust Area: Basic and Applied Sciences

KEY CAPABILITIES
Numerical Modeling • Uncertainty Analysis • Inverse Analysis
High-Performance Computing • Code Development

SITUATION  Estimating Predictive Uncertainty in Water Resources Modeling

Models are widely used to understand and analyze behavior of physical systems and are particularly crucial to water resources research. Significant improvements in groundwater modeling capabilities have allowed for predictions based on more accurate simulations of complex processes. Relatively little attention, however, has been paid to a key aspect of model application: estimating predictive uncertainty. The uncertainty in predictions can be significant when models depend on uncertain knowledge about the modeled system and its governing processes. Los Alamos is developing new methodologies to provide not only water resource predictions, but also robust estimates of prediction uncertainty. Since models and their predictions are used widely in any decision-making process, careful analysis of model predictions and their uncertainty is of great importance to facilitate this process.

INNOVATION  Developing Forward and Inverse Models to Predict Water Behavior

Los Alamos has developed complex forward models, which predict system behavior given a set of model parameters, and complex inverse models, which estimate the model parameters (recharge rates, aquifer permeability) given a set of system measurements, i.e. calibration data (water levels in wells, streamflow measurements). To quantify the sensitivity and uncertainty in the calibrated inverse model is computationally intensive. Therefore, these models require robust information systems and complex coding, both of which are available and were developed at the Laboratory.

Los Alamos uses two analytical approaches to the inverse model to quantify uncertainty. In constrained nonlinear optimization, plausible solutions are sought that maximize and minimize given model predictions, allowing prediction uncertainty to be quantified. In inverse-inverse analysis, which Los Alamos is developing, the set of calibration data required to produce a given model prediction with a specified degree of uncertainty:

- Overcomes limitations associated with non-linearity of the forward model and non-normality and non-linear correlation of the errors;
- Reveals the sensitivity of model parameters and predictions to the calibration data;
- Illuminates the impact of measurement error in calibration data on the inverse estimates and predictions, and
- Extends to quantify the sensitivity of inverse model estimates relevant to general system knowledge that can include the uncertainty caused by measurement or conceptual errors.

APPLICATION  Improving Diverse Modeling Efforts with Los Alamos Methodologies

The methodologies developed under this project estimate prediction uncertainties and identify key areas where improvements in our understanding of studied systems would decrease the uncertainty in the model predictions. The approaches developed under this project apply to a wide range of problems, including the Los Alamos's Española Basin study, which deals with the aquifer in the Los Alamos region.

Most of the national laboratories undertake projects that focus on developing models and making important predictions and conclusions using these models. As a result, the Los Alamos project is essential for the future of the laboratories as they work toward the future of the nation.
SITUATION  Focusing on an Overall Strategy for Addressing Climate Change and Energy Issues

The United States Global Change Research Program (USGCRP) has identified the water and carbon cycles as national research priorities for the next 10 years. Within the water cycle, hydrological and ecological processes of dry land ecosystems are tightly interrelated. Many important relationships center on the effects that plant cover has on the water budget; for instance, changes in plant cover can trigger high rates of soil erosion. The Laboratory involvement stems from addressing local environmental restoration needs, obtaining competitive grants within Los Alamos and DOE, and developing a terrestrial carbon sequestration program with the National Technology Energy Laboratory.

INNOVATION  Adopting a Suite of Projects to Address the Interrelationships between Plant Cover and Water Budget

Los Alamos activities include field experiments; long-term monitoring of soil moisture, runoff, plant water stress, and ground cover; simulation modeling; analysis of historical aerial imagery; and theory development. The goal is to better quantify the interrelationships between vegetation pattern and dynamics with hydrological pattern and dynamics.

To achieve this goal, the Laboratory is applying its strengths in the area of plant cover and water budget relations. In conjunction with its capabilities in high-resolution hydrological modeling, the Laboratory offers:

- The longest-term soil moisture data set for a semi-arid woodland;
- The best-documented example of a drought-induced ecotone shift;
- An experimental drought plot;
- The most intensely studied pinyon-juniper woodland site; and
- Biophysical scaling relationships.

APPLICATION  Building the Base for Real-World Applications

These projects generate a high level of visibility and credibility for the Laboratory from the scientific community. As a result, the Laboratory can use a variety of data in addressing diverse issues that include:

- Contaminant transport;
- Drought impacts management;
- Land use in semiarid environments;
- Global change impacts; and
- Terrestrial carbon management and sequestration.
Improved Water Conservation with Waste Materials

**KEY CAPABILITIES**
- Multidisciplinary Approaches
- Stable Isotope Technology

**SITUATION**
**Linking Water Conservation and the Energy and Agriculture Industries**

The two major users of water in the United States are energy and agriculture. An important connection between these different areas is the importance of fostering the growth of plants with optimal water efficiency: in agriculture, for crop production; in energy, for mine site reclamation and carbon sequestration. (Comprising our terrestrial biosphere, plants are responsible for capturing the CO2 of greenhouse gas emissions in the sequestration process.)

Following the United States Global Change Research Program identification of the carbon and water cycles as national research priorities, the DOE Office of Fossil Energy, with its history of programs in water management, has prioritized using energy production waste to the greatest extent feasible. Therefore, a multidisciplinary team of Los Alamos researchers collaborated with site reclamation experts from the State of New Mexico Abandoned Mine Bureau and examined the potential of using coal mine site spoil and other waste materials to achieve improved vegetative growth and productivity.

**INNOVATION**
**Using Mine Site Waste Material as a Beneficial Soil Amendment**

As Los Alamos researchers have pursued reclaiming western mine sites for vegetative growth, they have found that:
- Waste from western mine sites is high in nitrogen, but does not hold water well, making it a poor vegetation producer; and
- Native western soil contains clay and holds water well, but is low in nitrogen, making it a poor vegetation supporter.

With its expertise in isotopic signatures and multidisciplinary approaches, the Laboratory has been able to:
- Distinguish carbon from coal from that derived from plants at mine sites;
- Address the potential of using western mine site material to stabilize native alkaline soil to establish vegetative cover; and
- Combine native soil and mine site spoil to test its ability to support plant growth in water-limited regions.

**APPLICATION:**
**Supporting Plant Growth in Water-Limited Growth Systems**

Results of this study reveal that native plants grown in combinations of coal mine spoil and native soil are outperforming those grown solely in native soil or solely in mine spoil. With further work, results of this project will be able to:
- Reduce the initial cost of mine site reclamation;
- Contribute to more efficient use of water when stabilizing recently reclaimed mine sites;
- More effectively manage water in dry lands, where nitrogen is sparse; and
- Use materials now considered to be waste and eliminate the cost of waste disposal.
Plants with Improved Water Use Efficiency Project

SITUATION: Recognizing the Importance of Water-Efficient Plants in Carbon Sequestration

Following the United States Global Change Research Program identification of the carbon and water cycles as national research priorities, Los Alamos has adopted a project to optimize the water efficiency of plants. This project is of special interest to two major American industries: energy and agriculture. In addition to being the nation's largest users of water, the two industries are acutely interested in hardy, easily sustained plants for separate reasons. While agriculture has a keen financial interest in more water-efficient plants, the energy industry's particular interest is based on the role of plants in carbon sequestration. In the arid and semi-arid western United States, where precipitation is scarce, improving water efficiency is essential to using the natural ability of plants to capture CO₂ from greenhouse gas emissions.

INNOVATION Using a Unique Approach to Affect the Water Use Efficiency of Plants

Los Alamos has collaborated with a plant physiologist to develop and patent a unique approach to impacting the water use efficiency of plants. Because well-nourished plants require less water, the Laboratory has focused on developing plants that take up and use nutrients more efficiently. Using its strengths in DNA sequence-based techniques in combination with isotope-assisted metabolic analysis, the Laboratory has developed the ability to manipulate plant growth by influencing the plant’s own metabolic coordination of carbon and nitrogen.

The Laboratory:
- Characterized the nutrient-use systems of a set of experimental plant systems; and
- Developed a prototype plant with improved nitrogen use and water use efficiencies.

APPLICATION Manipulating Plant Growth and Water Use Efficiency

With results far beyond the original goals of the project and with the technical approaches applicable to both traditional and modern biotechnology, the generation of even more water efficient plants is possible. These plants could be expected to:
- Be a valuable part of carbon sequestration in the biosphere; and
- Contribute to more water-efficient agricultural production.
Supercritical CO₂ Resist Removal (SCORR)  
T rust Area: Remediation, Conservation, and Monitoring Techniques

**KEY CAPABILITIES**  
- Supercritical Fluid Facility (SCRUB)  
- Scale-Up to Pilot  
- Supercritical CO₂ Research Expertise

**SITUATION**  
**Addressing Inefficiencies in Integrated Circuit Manufacturing**

An integral step in integrated circuit (IC) manufacturing is photolithography. This step requires large amounts of hazardous solvents and vast amounts of ultra-pure deionized water. Along with 100,000 gallons of solvents, a single fabrication plant may use up to 4 million gallons of water per day to ensure that all traces of organic solvents and sulfates are removed from the wafer surface. Ironically, many of the largest plants in this country are located in states already plagued with chronic water and occasional energy shortages: New Mexico, California, Texas, and Arizona. In 1998, responding to a technical request from Hewlett Packard (now Agilent Technology), Los Alamos began developing the SCORR technology to address this problem.

**INNOVATION**  
**Initiating the Use of SCORR as a Replacement Solvent**

Reflecting the urgency of the problem facing the IC manufacturing industry, since 1998 SCORR has rapidly evolved from a business question to its commercial applications. Meeting performance goals outlined in the International Technology Roadmap for Semiconductors (ITRS), supercritical carbon dioxide as a replacement solvent for the IC manufacturing process:
- Reduces or eliminates the use of water;
- Eliminates energy requirements for drying wafers and purifying water; and
- Reduces, by 95 to 99 percent, the use of hazardous chemicals (chlorofluorocarbon compounds, hydrogen peroxide, sulfuric acid, acetone, methyl-ethyl ketone and isopropyl alcohol.)

SCORR is a technically-enabling green process that is not only accepted but driven by leading semiconductor and IC manufacturers, as well as equipment and material suppliers.

**APPLICATION**  
**Keeping Pace with IC Advancements through SCORR Technology**

To continue on its astounding growth curve, ICs must become smaller, faster and cheaper. The ITRS details the technological barriers that need to be overcome in order to fabricate ICs with diminishing feature sizes. Because of their high viscosity, the traditional liquid solvents presently being used will not be able to clean these small features. With SCORR, the smallest features present no barriers because supercritical fluids have zero surface tension and a gaslike viscosity, which allows them to remove particles smaller than 100 nanometers from IC features.

The Laboratory developments in SCORR technology:
- Enable industry to advance to increasingly finer architecture by removing a rate-limiting technical hurdle for the IC industry while cutting cost and nearly eliminating environmental liabilities; and
- Allow for the use of supercritical fluids to expand into many other fabrication processes and into other areas of nano-technology such as flat panel displays, micro-electro-mechanical (MEM) devices, and memory.
Groundwater Remediation

Thrusted Area: Remediation, Conservation, and Monitoring Techniques

KEY CAPABILITIES
Innovative Technologies • Computer Modeling • Experimental Methods
Characterization of Groundwater Systems

SITUATION
Identifying and Addressing Groundwater Pollution

Groundwater is a precious resource in New Mexico and elsewhere. After 50 years of serving the nation, Los Alamos National Laboratory discovered that the alluvial (shallow) groundwater within Mortandad Canyon has been contaminated with radionuclides, perchlorate, nitrate, and other inorganic chemicals. Los Alamos developed the concept of multipermeable reactive barriers, which are designed to remove a variety of inorganic chemicals and radionuclides using natural materials. The materials were tested in the laboratory prior to designing the permeable reactive barrier (PRB) to be installed in Mortandad Canyon during the fall and winter of 2002. The Mortandad Canyon field site was selected based on the nature and distribution of contaminants found in alluvial groundwater.

INNOVATION
Combining Natural Materials to Remove Inorganic Pollution

To maximize the technical defensibility and success of the project, a multidisciplinary team was selected to work on the PRB project, integrating Los Alamos capabilities in hydrology, geochemistry, geology, engineering, regulatory compliance, and computer modeling. The PRB is a passive system that:

- Eliminates the need to pump and treat contaminated alluvial groundwater, which is costly and ineffective for most inorganic chemicals and radionuclides;
- Removes contaminants through adsorption, biodegradation, and precipitation; and
- Consists of natural materials (calcium hydroxyl phosphate, cottonseed meal, pecan shells, and calcium carbonate) that achieve desired reactions with specific contaminants:
  - Radionuclides are removed by adsorbing onto calcium phosphate and coprecipitating with other metals and phosphate;
  - Perchlorate is biochemically reduced to chloride by cottonseed meal;
  - Nitrate is reduced to nitrogen gas under anaerobic conditions enhanced by cottonseed meal; and
  - Carbonate, with a pH range between 7 and 8, neutralizes groundwater within the PRB.

APPLICATION
Developing Technologies for Pollution Cleanup Efforts

Since contaminated alluvial groundwater migrates through the subsurface and impacts deeper groundwater within Mortandad Canyon, removing perchlorate, nitrate, strontium-90, and other chemicals and radionuclides from alluvial groundwater within the canyon is most desirable. Installing the PRB will help to:

- Remediate alluvial groundwater, including the regional aquifer;
- Reduce the volume of contaminated groundwater migrating through the subsurface; and
- Reinforce the Laboratory dedication to groundwater remediation and protection.

This technology undoubtedly will be applied at other sites contaminated with metals, perchlorate, nitrate, radionuclides, and other inorganic contaminants.
Scanning Raman Lidar

Thrust Area: Remediation, Conservation, and Monitoring Techniques

KEY CAPABILITIES

- High-Performance Computing
- Observational and Experimental Methods
- Data Management and Analysis
- Multidisciplinary Approaches

SITUATION

Using Design, Fabrication, and Field Capabilities Originally Developed for the Weapons Program

In the late 1980s, the US Department of Defense requested that Los Alamos develop scanning lidars to detect and monitor biological and chemical agents released into the atmosphere. An outgrowth of this program was the development of a scanning Raman water vapor lidar. Los Alamos built, tested, and fielded the scanning Raman lidar in an unprecedented 6 weeks.

INNOVATION

Using the World's Only Mobile Raman Lidar

Backed by Los Alamos capabilities in high-performance computing, observational and experimental methods, data management and analysis, and multidisciplinary approaches, applications of the scanning lidar include:

- 1993: Los Alamos fielded a scanning Raman lidar aboard a ship for the Central Equatorial Project (CEPEX) at the request of the Scripps Oceanographic Institute and the National Science Foundation (NSF);
- 1997: Los Alamos developed a program plan for lidar water vapor and flux measurements for the Bureau of Reclamation (BOR), which continues to this date; and
- 1999: The Laboratory's effort in the Vertical Mixing and Transport Experiment (VTMx) has received support from the Department of Energy, which is still ongoing.

APPLICATION

Solving Complex Nonlinear Data Collection Problems in an Open Environment

The scanning lidar is an ideal tool for:

- Measuring eco-physiological parameters in the atmosphere, including the fate and transport of water vapor over agricultural and forested sites; and
- Forming the field support basis of integrated water/carbon cycle programs that will involve measurements and observations of water vapor and flux.

Ultimately, the Laboratory's ongoing lidar research will help:

- Explain the spatial distribution of water vapor and flux in the atmosphere boundary layer (the region extending 1 kilometer into the atmosphere); and
- Develop a water vapor and flux mapping system at an extremely high resolution in space.
Future Directions

Trends and Challenges in Water Management

Our nation and the world face increasingly difficult challenges in water resource management. The Earth’s abundance of water gives many a false sense of confidence in its continued availability. But while two-thirds of the planet is covered in water, only 2.5 percent of that is fresh water, and only 1 percent is readily accessible. Pollution could reduce this percentage to even less, and projected increases in population mean increases in demand for an already strained resource. Any comprehensive water research program that seeks to enhance national security and global stability must identify current and future needs and trends in water availability and use. Los Alamos National Laboratory has identified these needs and trends and strategically aligned them with its scientific and technical strengths.

Los Alamos National Laboratory Water Program Strategic Goals

Water for Energy
Water has received too little attention as a potential energy producer. Water and energy are intertwined from the extraction and refinement of fuels to the cooling of power plants, making the energy industry second only to agriculture in water use. As a result, population growth will not only strain water resources through direct use, but also indirectly through increased demand for energy. Los Alamos is leading the way in identifying the key technical challenges that must be addressed if we are to enjoy reliable supplies of energy and water in the future. The Laboratory has engaged industry and water regulators across the country and has performed in-depth economic and technical analyses to identify real-world problems. The Water Portfolio is now poised to develop effective solutions that will include decision support tools for water and energy policy makers, technologies to reduce water use, access untapped resources, and ensure water quality. Ongoing collaborations with industry and all levels of government will facilitate moving solutions into the marketplace and planning community where they can make a difference.

Water Security
As the events of September 11 have illustrated, the nation must be vigilant if it is to preserve its quality of life. Because our continued health and economic development depend heavily on an adequate quantity and sufficient quality of water resources, the protection of those resources must be a key focus for the national security community. As part of that community, Los Alamos National Laboratory is already applying its scientific and technical expertise to issues of homeland defense and is evolving to address the new threats of a rapidly changing world. The Laboratory is working to improve its ability to predict, prevent, and rapidly respond to attacks on the nation’s water supplies.

Global Climate Change
Rising concentrations of greenhouse gases, especially carbon dioxide, and the resulting changes in climate have been recognized nationally and worldwide as an issue requiring urgent attention. Understanding the interconnections between the carbon and water cycles and the effects of climate change on water supply and distribution is critical to planning for the future. Through the Water Cycle Initiative, Los Alamos National Laboratory and the nation can gain a detailed understanding of how water resources, from the deepest aquifer to atmospheric vapor, might change in coming years. The effects of climate change would vary greatly by region, some becoming far drier and some far wetter. Therefore, a practical understanding of the issue (that is, one that can be implemented in the real world) requires the ability to predict not just globally, but at the regional level. Such a finely resolved understanding of the water cycle does not yet exist and is the primary goal of the Water Cycle Initiative. The fundamental understanding gained by this initiative would also have applications far beyond the climate change issue.

Los Alamos National Laboratory Capabilities

The challenges facing water management are highly complex and involve interactions between many natural systems and human-made infrastructures. Addressing them will require diverse expertise. The key strength of Los Alamos National Laboratory is its multidisciplinary approach to complex systems. Our expertise in the following areas is especially relevant to water issues:

- Hydrology/hydrogeology
- Observational and experimental methods
- Analytical chemistry
- Remediation, conservation, and monitoring technologies
- Security and threat analysis
- Modeling and simulation
- High-performance computing
- Data management and analysis
- Decision analysis

In addition, Los Alamos has years of experience managing interactions between industry, government agencies, universities, and other national laboratories, which is critical to implementing solutions.