Jefferson Lab's Maud Baylac.

Page 2

DOE Pulse
Science and Technology Highlights from the DOE National Laboratories
Number 92 October 22, 2001

Research Highlights . . .

Evidence for the onset of quark effects

Evidence for the onset of quark effects in a nuclear reaction has been observed for the first time at DOE's Jefferson Lab. Just as urbanologists strive to locate where a city truly ends and its suburbs begin, physicists wish to find the boundary at which nucleon-based descriptions give way to quark-based ones. JLab researchers have studied the behavior of the deuteron, the simplest nucleus, one proton and one neutron. The experiment fired an electron beam at a copper target, creating high-energy photons that impinged upon a deuterium target, and broke the deuterons into their constituent protons and neutrons. The results were surprising since they disagreed with many current theoretical expectations for the onset of quark-counting-rule behavior.

[Linda Ware, 757/269-7689, ware@jlab.org]

Lead detection instruments get field test

Instruments and methods to detect lead in housedust will get a field tryout next month in tests conducted by DOE's Oak Ridge National Laboratory.
Representatives from six companies will participate in the test, which will help them assess how well their field-portable gear detects lead in dust. Better and less expensive instruments can help speed the identification and cleanup of lead-laden dust in homes. "In the past, the focus was on lead chips, but the Environmental Protection Agency has been expanding its scope to look at lead dust," says researcher Roger Jenkins. The evaluation is part of the EPA's Environmental Technology Verification program to accelerate the use of innovative technologies in the field.

[Ron Walli, 865/576-0226, wallira@ornl.gov]

Scientists advance seed production, oil remediation

A plant growth stimulator, developed with the aid of Russian scientists through a DOE program, could increase the growth rate of grasses and many broad-leaf plants by 40 percent under controlled conditions. Dye Seed Ranch of Pomeroy, Wash., recently sought technical expertise for its turf grass operation from DOE's Pacific Northwest National Laboratory. The Lab linked them with Russian scientists who had developed a plant growth stimulator and an oil remediation biotechnology. The work, funded by DOE's Initiatives for Proliferation Prevention program, could shorten the current 18 months seed producers wait between planting and harvesting their first crop. Also, a microbe capable of remediation of oil-contaminated fields also may hold promise for industries looking for new methods to clean up agrochemicals.

[Staci Maloof, 509/372-6313, staci.Maloof@pnl.gov]

Water surety study gains new urgency

A project Jeffrey Danneels has had under way as manager of Civilian Surety Programs at the Department of Energy's Sandia National Laboratories became dramatically more urgent after the Sept. 11 terror attacks on New York and Washington. His work with the Environmental Protection Agency and the American Water Works Association Research Foundation sent him recently to testify before Congress on the vulnerabilities of water systems. The potential damage that could be done by attacks on water systems became more obvious with the rising concern over the discovery of anthrax infections in different parts of the country. Danneels is now planning workshops on the issue, scheduled to begin in November.

[Howard Kercheval, 505/844-7842, hckerch@sandia.gov]

DOE Pulse highlights work being done at the Department of Energy's national laboratories. DOE's laboratories house world-class facilities where more than 30,000 scientists and engineers perform cutting-edge research spanning DOE's science, energy, national security and environmental quality missions. ***DOE Pulse*** (www.ornl.gov/news/pulse/) is distributed every two weeks. For more information, please contact Jeff Sherwood (jeff.sherwood@hq.doe.gov, 202-586-5806).

Code crafters

With funding from DOE's Scientific Discovery through Advanced Computing initiative, DOE's Ames Laboratory researchers are scaling up efforts to improve software for high-performance computing systems—terascale computers that are capable of doing trillions of calculations per second.

The Ames Laboratory team will be combining their talents with collaborators from Michigan State University and DOE's Pacific Northwest National Laboratory to develop scientific simulation codes that can take advantage of today's extraordinary advances in computing technology—a major thrust of the SciDAC program.

Increasing the performance of the scientific simulation codes used to model physical, chemical and biological systems is essential to scientists' efforts to address ever-larger and more complex problems. Issues to be explored include, among other things, expanding our knowledge base on the structure of matter from simple molecules to the building blocks of life and gaining better insights into the energy-related processes of combustion, catalysis and photochemical energy conversion.

The Ames Laboratory researchers, led by Mark Gordon, the Lab's program director of Applied Mathematics and Computational Sciences, Jim Evans and Klaus Ruedenberg, will work with Piotr Piecuch of Michigan State to develop highly scalable computational chemistry simulation codes that are capable of predicting potential energy surfaces of very high accuracy in both ground and excited states. (Scalable refers to the ability to increase, or "scale up" computer processing power to run the same job in less time.) The codes will be interfaced with and then integrated into GAMESS, a quantum chemistry software package developed by Gordon and Ames Laboratory associate Mike Schmidt. The package contains a popular suite of electronic structure programs that are free to any user.

"The advances in computational chemistry tie together with advances in scalable computing—they really feed off one another, so our project will also include a lot of interaction with Ames Laboratory's Scalable Computing Lab," said Gordon.

Another collaborator, the PNNL Theory, Modeling and Simulation Group, will develop new simulation codes for cluster computers that will also predict ground and excited potential energy surfaces. The codes developed by the Ames Laboratory researchers will be made available to the PNNL developers of NWChem, a highly scalable quantum chemistry program that has much in common with GAMESS. New computational chemistry codes developed for NWChem and GAMESS will be shared between PNNL and Ames Laboratory.

"These collaborations will serve to strengthen the overall effort to develop extremely high levels of theory into scalable code for new theoretical and computational models," said Gordon. "Improving the performance of scientific simulation codes will allow scientists to do very accurate calculations on much larger chemical systems. And that means we'll be able to attack more complicated problems."

Submitted by DOE's Ames Laboratory

New scientist getting her feet wet

Jefferson Lab's Maud Baylac in the lab.

Maud Baylac grew up in the French Alps far away from Newport News, Virginia, and knew from junior high school she wanted to be in science. During her first taste of sub-atomic physics in college she was hooked. But a long way from joining the DOE's Thomas Jefferson National Accelerator Facility in January 2001, as an injector group staff scientist prepared to study lasers, optics and electronics.

Maud's studies led her to become an exchange student for the University of California at Berkeley for her undergraduate senior year in college where she learned about life in the US. Her graduate work in France pulled her back to the United States to Jefferson Lab, where she worked for three years while completing her studies.

Maud's experience as a graduate student at Jefferson Lab mirrors that of other graduate students. She built, installed, commissioned special equipment and took experimental data using that equipment during her tenure. But she went beyond that and so impressed Jefferson Lab that she was awarded a prize for outstanding thesis work. The committee was impressed with her clarity of writing, depth of undertsanding and the lasting legacy of her work in polarized experiments.

So how does one go from being a dedicated graduate student to a dedicated injector scientist? Her same dedication works only the time scale changes. Nuclear experiments take years to plan and involve large groups of people willing to dedicate those years of work to an experiment. Now the group is small and still dedicated to a goal but the work has to be done quickly for the users of the Lab.

Do people think it is unusual to for a woman to be in this field?

Maud says, "Science does not care whether you are a man or a woman. The bottom line is that we are all scientists."

Submitted by DOE's Thomas Jefferson National Accelerator Facility