Research Highlights . . .

How DNA gets the bends
The most detailed computer model of damaged DNA to date shows that banged up DNA becomes flexible. Further, this flexibility explains how the body’s enzymes recognize and fix damaged DNA. The model surveyed a DNA fragment made up of 350 atoms, a large complex simulated on the supercomputer at DOE’s W.R. Wiley Environmental Molecular Sciences Laboratory on the Pacific Northwest National Laboratory campus. In the model, damage triggered a re-organization of the sugar-phosphate in the DNA’s backbone, causing the DNA to thin and become bendable. This difference in flexibility between damaged and intact DNA is apparently what the repair enzymes zero in on. The results were reported at the American Chemical Society national meeting in Philadelphia.

[Bill Cannon, 509/375-3732; cannon@pnl.gov]

BaBar produces penguin mode
Asymmetry in “penguin modes” is an intriguing result from the incredible 64 papers the BaBar collaboration presented at the International Conference on High Energy Physics in Beijing this summer. The BaBar experiment at DOE’s Stanford Linear Accelerator Center is pursuing hints that penguin modes—a rare class of decay from B mesons to other particles—reveal new physics beyond the Standard Model, perhaps supersymmetry. If the Standard Model is correct, penguin modes should have the same amount of asymmetry as in another, well-studied decay process. But experimental data from BaBar and Belle in Japan show the penguin modes appear to have less asymmetry. To be statistically convincing, BaBar will collect two more years of data, starting with a new run Oct. 15.

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Trimming water needs, adding solar power sources
A method that uses about one percent of the fresh water needed to grow forage for livestock may leave much more water for human consumption and help avert future wars. A method being overseen by DOE’s Sandia National Laboratories at a greenhouse near the US-Mexican border also may add untapped solar energy to the electrical grid. Peter Davies, director of Sandia’s Geoscience and Environment Center, says, “A large proportion of freshwater usage around the world is agricultural. Reducing the amount of water needed for it and, thus, lessening the possibility of international conflict is important to the security of the United States and the world.”

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Protein-fishing at PNNL
Proteins pass messages to other proteins much like fly-fishermen flicker their lines against water. The weak slapping of protein surfaces against each other is the critical first step in a chain of events that rule all subsequent cellular behavior. But this vital exchange between single molecules has defied direct observation because that line-flicking and message-passing happen randomly at such a small scale. Now, a technique called single-molecule photon stamping spectroscopy, developed at DOE’s Pacific Northwest National Laboratory, reveals real-time interactions of single proteins and supports the fly-fishing theory of protein communication. Each peak seen here depicts a fluorescing protein interacting with another protein. An analysis of the intensity, duration and other physical properties of the photon peaks provides a sequence of subtle and sublime communication between cellular proteins.

[Bill Cannon, 509/375-3732; cannon@pnl.gov]
New Idaho facilities help safeguard critical infrastructure

Across the country, a fleet of aging and unprotected computer-aided control systems operates critical infrastructures such as electric power grids, oil and gas refineries and telecommunications systems. These control systems, originally designed for efficiency and reliability, are today susceptible to cyber attacks by hackers, virus writers and adversaries looking to disrupt our way of life.

To counter these threats, the U.S. departments of Energy and Homeland Security selected the Idaho National Engineering and Environmental Laboratory (INEEL) to support their efforts to reduce the vulnerabilities associated with supervisory control and data acquisition (SCADA) and other control systems. This designation creates a centralized location and state-of-the-art testing facility at the DOE’s INEEL, which allows utility companies, equipment manufacturers and government agencies to find practical solutions to this growing problem.

Last month, the INEEL officially opened the National SCADA Test Bed and the Control System Security and Test Center (CSSTC). The National SCADA Test Bed, sponsored by DOE, is operated in collaboration with Sandia National Laboratory. SCADA systems are a type of control system commonly used within electrical power distribution. The Department of Homeland Security is sponsoring the CSSTC to take action to reduce vulnerabilities in control systems that operate the nation’s critical infrastructures. Housed within the center are functioning control systems from national and international manufacturers, a multi-functional cyber security test bed that is capable of performing cyber attacks and mock scenarios on various control systems, and an operational war room used for training and emergency management response.

The INEEL testing facilities leverage research capabilities from other test beds located within its 890 square-mile complex – including a wireless telecommunication system and a power transmission structure – and at other DOE labs nationwide. These test beds will allow customers to visualize the effects of a cyber attack on a control system without the resulting consequences.

Currently, the INEEL has working relationships established with over 30 utility companies and equipment manufacturers.

Submitted by DOE’s Idaho National Engineering and Environmental Laboratory

Numbers for Real World Applications

Developing numerical methods to solve real-world problems is the forte of Alston S. Householder Fellow Jennifer K. Ryan, the latest in a line of outstanding mathematics researchers at DOE’s Oak Ridge National Laboratory.

Ryan, a native of Houston, Texas, is an applied mathematician working on numerical algorithms. Her primary research focuses on developing accurate numerical solutions to physical and chemical models represented by partial differential equations.

Ryan’s current research is on accuracy enhancement techniques and higher order numerical methods such as the discontinuous Galerkin method. Using those methods, she has investigated real-world issues in areas such as computational fluid dynamics, computational chemistry, aeroacoustics, and climate modeling.

Previously a graduate fellow at NASA-Langley, at ORNL, Ryan collaborates with a number of researchers, mostly in the area of computational chemistry. Recently, she completed three scientific papers as lead author.

Originally destined to be an engineer, Ryan’s interest in math emerged with higher level math courses and a computer programming class during her last years at Rutgers University. She went on to receive her master’s degree from New York University’s Courant Institute for Mathematical Sciences and her doctorate from the Division of Applied Mathematics at Brown University, where she earned the Stella Dafermos Award for excellence in graduate studies.

The Householder Fellowship is named for a renowned pioneer in the field of linear algebra who was also the founder of what is now the Computer Science and Mathematics Division at ORNL. Ryan is well aware of the reputation for excellence her fellowship represents.

"Alston Householder made many important contributions to the field of Linear Algebra. As an applied mathematician I am well aware of his legacy," Ryan says. "Coming to ORNL on this fellowship is a privilege."

Submitted by DOE’s Oak Ridge National Laboratory