BIG-PICTURE ENGINEERING

School of Engineering and Applied Sciences

University at Buffalo *The State University of New York*

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FROM THE DEAN

Mark H. Karwan
Professor and Dean

This publication, *Visualization, Simulation, and Modeling*, is the sixth in a six-issue Igniting Ideas series explaining our school's research focus areas. The others have been:

- ***Bio Research***
- ***Infrastructure and Environment***
- ***Photonics, Microelectronics, and Nanotechnology***
- ***Computing and IT***
- ***Energy, Flows, and Materials Processing***

Each area contributes to our strategic objective of performing high-quality research while preparing future researchers for industrial, academic, and government positions.

Presented in this issue is research that helps us visualize unseen things and create items that don't yet exist. Also included are key happenings in the life of our school:

- **Distinguished Professor Eli Ruckenstein's National Academy of Engineering's Founders Award**
- **The grand opening of our National Science Foundation node of the Network for Earthquake Engineering Simulation facility**

I trust that you will find *Visualization, Simulation, and Modeling* indicative of the research being conducted and the recognition being received at UB SEAS.

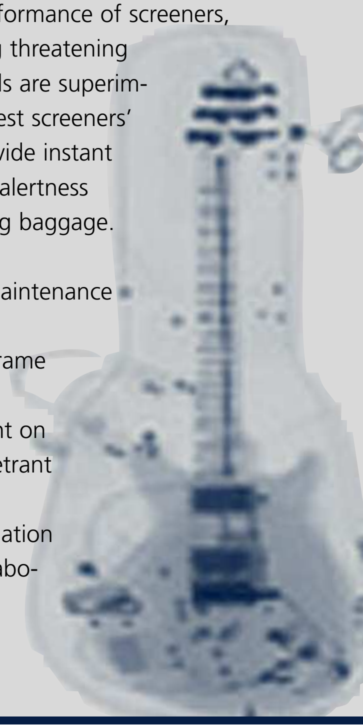
Overview and past issues available at: www.eng.buffalo.edu/IgnitingIdeas

Produced by the University at Buffalo Office of Creative Services, University Communications. June 2005. 05-EAS-002.

Keeping Airlines Safe

UB researchers are working hard to make air travel safer. Colin Drury, chair and UB Distinguished Professor of Industrial Engineering, recently received a grant from the Transportation Security Administration (TSA) to found and direct the UB Research Institute for Safety and Security in Transportation (RISST). RISST builds on Drury's 15-plus years of research and development leadership in aviation inspection and maintenance.

The objective of one study, the Error Analysis Screening of Carry-on Baggage, is to increase the performance of screeners, making them more effective at detecting threatening materials. Images of contraband materials are superimposed on X-rayed carry-on baggage to test screeners' abilities to find targets. False targets provide instant feedback about screeners' vigilance and alertness through the repetitious work of screening baggage.



RISST's other projects include:

- Language-Related Errors in Aviation Maintenance Outsourced to Foreign Countries
- Handbook of System Reliability in Airframe and Engine Inspection
- Effects of Fatigue/Vigilance/Environment on Inspectors Performing Fluorescent Penetrant and/or Magnetic Particle Inspection

Funding comes from the Federal Aviation Administration and the TSA. Recent collaborators include Delta Airlines, Northwest Airlines, and US Airways.

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Visualizing

NEW TECHNOLOGIES AT NYSCEDII

At the New York State Center for Engineering Design and Industrial Innovation (NYSCEDII), engineers and applied scientists are using cutting-edge techniques—from visualization to simulation to optimization—to transform industries and pioneer new research.

Established in 2000 and headed by Christina Bloebaum, professor of competitive product and process design in the Department of Mechanical and Aerospace Engineering, NYSCEDII is one of only a handful of engineering-oriented visualization centers in the country.

NYSCEDII has become a leading center for the application and development of high-end visualization, simulation, and optimization technologies to address complex analysis and design problems, such as those found in product research, design, and manufacturing. The center's emphasis on visualization, haptics, data analysis, and collaborative tools complement economic development and training activities in the Western New York region and across the state.

The center's breadth of applications makes its research particularly important. From plant design to product optimization to prototype visualization, the center has worked to make all phases of industry more efficient. In a project with Praxair, a top-ten industrial gases company, NYSCEDII has been using optimization and visualization techniques to find an optimal layout for an air-separation-plant cold box. The tool developed has the potential to reduce design time on one product from a few months to a few days.

In another project, a team of researchers led by Kemper Lewis, associate professor of mechanical and aerospace engineering, and including Bloebaum, Kenneth English, Aidong Zhang, Ann Bisantz, and Eliot Winer is developing new visualization techniques for the design and prototyping of complex systems. The developed techniques allow users to make trade-off decisions about product development with a greater amount of knowledge than in traditional processes. Rapid Virtual Prototyping facilitates compromises by allowing geographically distributed participants to make decisions that take into account various degrees of uncertainty in product development.

NYSCEDII's advanced imaging capabilities have resulted in benefits in health care and safety. Working with the Toshiba Stroke Research Center, UB Center for Advanced Biomedical and Bioengineering Technology, Clarix Technologies, and SGI Inc., researchers at NYSCEDII have developed a multipurpose medical image analysis and visualization programming interface. The program is able to obtain information from digital medical files, parse this information into standard formatted image files, analyze the image to generate a 3-D surface model, manipulate the image to increase visual clarity, and extract particular features or objects from the image. The program will help medical professionals to better examine and diagnose patients.

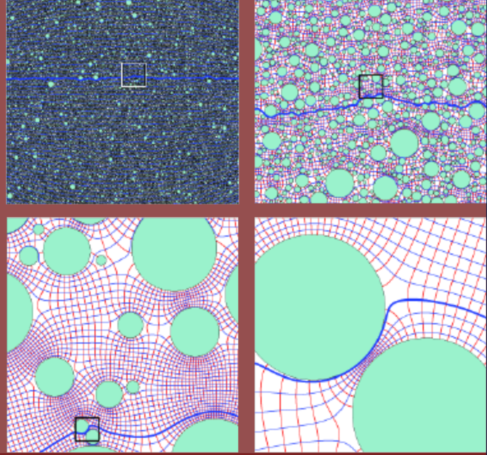
The center also has paired with Dr. J. Gayle Beck from the UB Center for Anxiety Research to develop the first real-time virtual-reality driving simulator to treat car-accident victims suffering from post-traumatic stress disorder. The driving simulator includes a steering wheel and pedals, a six-degrees-of-freedom electric motion base, and a stereoscopic projector display, creating a system that is extremely customizable and realistic. Patients are slowly acclimated to driving again by working from a safe environment to one that is reminiscent of the original accident, including weather and particular road conditions.

In biological research, simulation has also been used to investigate the mechanical behavior of extinct animals, such as the saber-toothed cat *Smilodon fatalis*. By creating anatomically and biomechanically accurate virtual models of modern animals, researchers have established how various bones move and what muscular forces are needed to create movements during activities, such as biting. This baseline allows the virtual reconstruction of fossilized remains. This same technology can be used for human studies.

Currently, NYSCEDII is working on further developing a fire egress simulation system, called Vacate, that surpasses the leading tool available. Researchers have also filed for a patent on a visualization tool that gives users new ways to display complex data sets in such fields as economics.

The range of projects supported by NYSCEDII gives clear testimony to the breadth of the center's capabilities. As this work demonstrates, visualization, simulation, and modeling let UB researchers see the future of industrial innovation, bringing virtual ideas into the real world of industry and research.

Simulating Groundwater Contaminants



Developed through the collaboration of researchers from UB and around the world, Virtual Porous Medium (VPM) is a numerical laboratory designed for modeling groundwater contaminants in heterogeneous aquifer formations. Using VPM at UB's Center for Computational Research, tens of thousands of simulations have been carried out, ultimately relating the rates of contaminant spreading to heterogeneity structures and contributing to the development of a contaminant-spreading theory. Unlike other theories of contaminant spreading, the VPM-produced theory is applicable regardless of heterogeneity levels.

The laboratory also has been used to investigate the general effective properties of heterogeneous materials, which is an area of inquiry relevant to many branches of physics. These effective properties, investigated for over a century, are a central problem for at least eight different physical processes. Applications range from electrical and thermal conduction to the design of carbon nanotubes to remote sensing.

In a paper published in the journal *Multiscale Modeling, Analysis, and Simulation*, VPM researchers were able to disprove a famous formula for effective properties that was conjectured by Lev Davidovich Landau, the 1962 Nobel Prize laureate for physics. Following these results, a new analytical formula was derived that can predict effective properties for a wide range of problems.

The VPM model was developed by Igor Jankovic, assistant professor, Civil, Structural, and Environmental Engineering, and colleagues Gedeon Dagan, professor, Department of Fluid Mechanics and Heat Transfer, Tel Aviv University, Israel; Aldo Fiori, associate professor, Department of Civil Engineering–Water Resources Unit, University of Roma Tre, Italy; and Eliot Winer, now assistant professor, Mechanical Engineering, Iowa State University. Much of the work is funded by a three-year grant from the National Science Foundation.

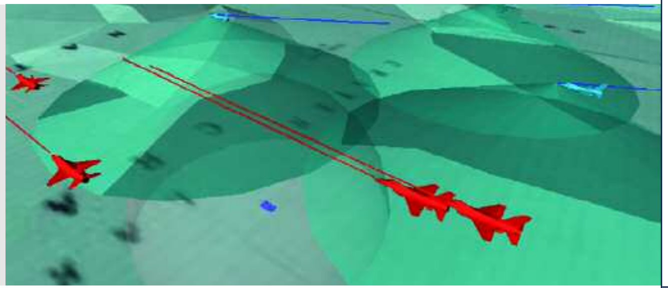
Lifting the Fog of War

A UB-developed software package promises to give military decisionmakers a clearer look at their battlefield operations. Using technology referred to as "network-centric warfare," the software connects a multiplicity of platforms and sensors to observe and track targets.

In a warfare setting, military leaders require the unambiguous integration of intelligence information sources. In response, researchers in the School of Engineering and Applied Sciences have focused on the development of an integrated, simulation-based software package capable of aiding in the design and analysis of fusion-based tracking systems that are agile, adaptive, and decentralized.

New technologies used in the package include a circular filter for maneuvering air targets and a particle filter for maneuvering ground targets, where data from disparate sensors are processed and fused to exploit information from all sources. Researchers have also developed a dynamic expected-coverage model and solution algorithm for ad hoc sensor networking. The result is a network topology that responds to perceived threats as targets are identified by sensors.

Researchers working on the project also have explored novel methods for information visualization and simulation steering. The software system has been developed with a modular architecture using C++ on the Linux platform. The easy-to-use interface allows the user to adaptively extract and visualize pertinent information related to complex simulation environments.



Contributors to the project include Tarunraj Singh and Thenkurussi Kesavadas, Department of Mechanical and Aerospace Engineering; Rajan Batta and Rakesh Nagi, Department of Industrial Engineering; and Bharat Jayaraman, Department of Computer Science and Engineering. The UB centers for Multisource Information Fusion and Computational Research collaborate on the project. Funding for the research is provided by Rosettex Technology and Ventures Group, and the National Technology Alliance.

UB Engineers Reimagine the OR

In recent years, computer simulation has become an essential tool for improving the efficiency of businesses of nearly every imaginable shape and size. However, until very recently, the world of health care remained a new frontier for industrial engineers anxious to improve the way we work. Today, industrial engineers at UB are taking their expertise to the hospital, rethinking how to design and run operating rooms (ORs).

"Increasingly, hospital executives are becoming very keen in understanding the enterprise aspect of their business," says Li Lin, professor of industrial engineering and director of UB's Center for Excellence in Global Enterprise Management. "We have helped several Western New York hospitals in streamlining their operations using animated computer simulation."

In the last three years, Lin has helped the Erie County Medical Center and Mercy Hospital of Buffalo design their OR suites and surgical recovery centers. At Mercy Hospital, Lin's team worked closely with an architect to design four new ORs, with a special emphasis on the efficient accommodation of patients' needs in limited spaces. Hospital management was integral to the design-selection process, which included computer simulations of each design alternative. The new ORs are open for surgeries in 2005.

Learning Thermodynamics on the Web

Chemical engineering students around the United States are using a suite of Web-based materials to learn thermodynamic and transport concepts. The materials were prepared by David A. Kofke, UB Distinguished Professor of Chemical and Biological Engineering, and colleagues.

Kofke hopes to advance the understanding of free energy calculations, which are prone to inaccuracy. Free energy molecular simulation is critical to the study of many behaviors, from simple study phenomena, such as boiling, freezing, and immiscibility, to more complicated behaviors, such as protein folding and molecular binding.

The work is promoted by CACHE, a national consortium that develops and distributes computer-based tools for chemical engineering curricula. Funding comes from the U.S. Department of Energy and the National Science Foundation. It is also supported by the UB Center for Computational Research and an IBM Eclipse Innovation Grant.

Advanced Nanoscale Simulations

In recent years, there has been enormous interest in single photons and phonons interacting with nanoscale objects. This interest has been driven in part by promising applications of nanosensors and nanoemitters in such areas as precise medical diagnostics, quantum information technologies, and macromolecular engineering.

Recognizing the importance of such applications, Vladimir Mitin, professor and chair of Electrical Engineering (EE), established the Materials, Device, and Circuit Simulations Laboratory, which focuses on modeling nanodevices with single-quantum sensitivity. Lab studies involve investigations of fundamental processes in nanostructures, multiscale simulations, and the design and optimization of novel nanodevices. Because the experimental tools for nanoscale manipulations are expensive and resources are limited, the theoretical research being done in Mitin's lab plays a critical role in the expansion of the field.

Mitin, together with Andrei Sergeev, EE research associate professor, looks at fundamental problems in transport phenomena, investigating how the quantum interference of various scattering mechanisms modifies kinetics processes. For example, in metallic nanostructures, the interference between electron-phonon and electron scattering has a dramatic effect on the electro-cooling rate; the rate can be increased or decreased by a few orders of magnitude depending on impurities and boundaries. Very recently, measurements by Jonathan Bird, professor of electrical engineering, demonstrated that the interference phenomena in electrical resistivity of nanocomposite materials can dominate traditional mechanisms even at room temperatures.

With Nizami Vagidov, EE research assistant professor, Mitin investigates solid-state nanoemitting devices for applications in medical diagnostics and single-molecule spectroscopy. The nanoemitters radiate in the wide range of electromagnetic spectrum, from terahertz to infrared. The researchers moved from modeling structures on the order of hundreds of nanometers to tens of nanometer structures. Their work takes into account the atomistic nature of the structure using advanced simulation techniques, such as a tight-binding model that takes into account each single atom or each layer of atoms.

The results of modeling are used by experimental groups to construct novel nanosensors with ultimate quantum sensitivity. One long-term project is a joint effort with Boris Karasik of the Jet Propulsion Laboratory, California Institute of Technology, to build an ultrasensitive detector of submillimeter photons for future NASA astronomy missions.

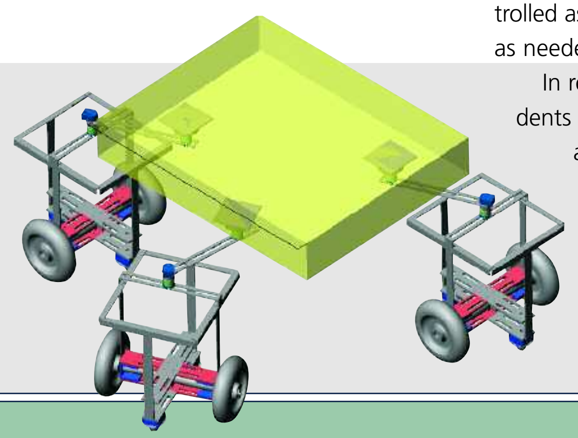
Funding groups include NSF, NASA, ONR, and the American Chemical Society.

Cooperative Payload Transport

A research team led by Venkat N. Krovi, assistant professor of mechanical and aerospace engineering and director of the Automation Robotics and Mechatronics (ARM) Laboratory, is applying lessons about cooperation in biological collectives (e.g., armies of ants) to models of automated systems. In one project, Krovi's team is creating a framework for payload transport by a fleet of semi-autonomous wheeled mobile modules. The modules are combined to create a flexible variable-topology composite system and can be controlled as a collective and reconfigured as needed to enhance performance.

In recent work, Krovi and his students investigated the development and implementation of two variants of kinematic cooperation—leader-follower and decentralized—in a system of wheeled mobile manipulators. They tested the framework for optimal configuration of the articulations to maximize manipulability of the payload. In a parallel effort, they examined the development of decentralized motion planning within a geometric framework to determine the best formation for given tasks. Another student examined the creation of distributed dynamic simulations for multi-body systems with multiple closed kinematic loops. The work employed novel recursive forward and inverse dynamics algorithms for parallel architecture systems based on the decoupled natural-orthogonal complement.

The remotely controlled frameworks created by the ARM Lab have numerous applications. In particular, their unique non-odometric dead-reckoning accuracy and active-reconfigurability has reinvigorated interest in distributed physical collaboration between systems of systems. The emergent applications, civilian and military, range from material handling on the shop floor to terrestrial and extraterrestrial uneven terrain locomotion. Principal funding comes from Krovi's National Science Foundation CAREER Award. Many aspects of the research are conducted in cooperation with the New York State Center for Engineering Design and Industrial Innovation.



UB's Ground-Shaking Laboratory

A new era in earthquake-engineering research was ushered in at UB with the grand opening of the National Science Foundation's George E. Brown Jr. Network for Earthquake Engineering Simulation (NEES) facility within the Department of Civil, Structural, and Environmental Engineering (CSEE). The $21.2 million NEES facility is the largest investment in the NSF's $81.9 million project to improve the understanding of earthquakes and their effects on buildings, bridges, roads, and other forms of infrastructure.

The facility is a key node in a nationwide earthquake-engineering "collaboratory"—a network of 15 state-of-the-art laboratories at universities throughout the United States that will allow earthquake engineers and students to share resources, collaborate on testing, and exploit new computational technologies.

The centerpieces of the facility are dual movable, six-degree-of-freedom shake tables that can be repositioned for real-time seismic testing of structures up to 120 feet long and 30 feet high. The tables will enable earthquake engineers to conduct real-time dynamic hybrid testing, a form of testing being pioneered by UB researchers that sets new standards in earthquake-engineering research. The approach combines shake-table tests with real-time computer simulations, providing a more complete picture of the effects of earthquakes without having to test entire structures.

The UB NEES principal investigators are CSEE professors Andrei Reinhorn and Michel Bruneau; coprincipal investigators are CSEE professors Michael Constantinou, Andrew Whittaker, and Sabayanagam Thevanayagam.

Virtual Environments with Real-World Applications

At UB, researchers and students are reconstructing ancient archeological sites, developing noninvasive medical techniques, and automating industrial processes—and they're doing it all without leaving the lab. It's all happeing in UB's Virtual Reality Lab (VRL).

Headed by Thenkurussi Kesavadas, associate professor of mechanical and aerospace engineering, the lab specializes in VR applications related to manufacturing, data visualization, and medicine. Specifically, projects at the VRL have included:

The Virtual Site Museum. Using data from archeological sites, researchers meticulously constructed a highly detailed—and fully explorable—digital model of an ancient Assyrian palace. The project, which received CNN coverage, resulted in a multimedia model suitable for both educational and research applications.

Virtual Clay. The system enables users to replicate in real time on a personal computer the physical act of sculpting a block of clay or other malleable material.

The Virtual Factory Project. VRL researchers developed a VR-based factory-development software package useful for exploring new techniques in industrial automation.

Medical Diagnostics. Kesavadas and his colleagues developed a VR-based diagnostic system for medical examination of the human abdomen. The system could be used in conjunction with telemedicine systems for remote applications.

Corporate support has come from Praxair, American Axle, Roadgard, and Honda; the National Science Foundation, the National Institutes of Health, and the National Highway Traffic Safety Administration also provide support.

Detecting Leaks in the ISS

New software developed from a UB-NASA collaboration promises to help detect leaks aboard the International Space Station (ISS). Created by John L. Crassidis, associate professor of mechanical and aerospace engineering, graduate student Jong-Woo Kim, and Adam L. Dershowitz, an engineer with United Space Alliance, the software is able to quickly locate and calculate the size of holes in the station.

The software continuously monitors the space station for leaks by detecting disturbances in the spacecraft's behavior. The software correlates the effects of this behavior with the geometric structure of the space station to predict leak location and the size of the hole causing the leak, all in less than a minute. Using the software, NASA is able to locate holes with diameters of .4 inches and smaller.

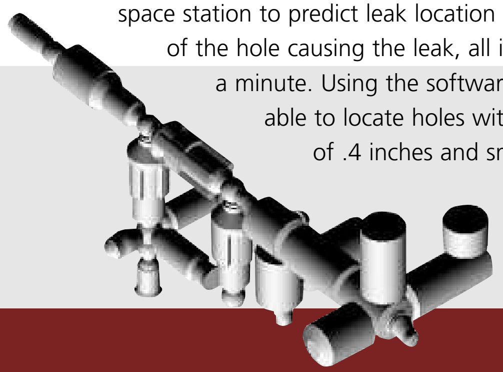
"Other disturbances are always present, such as drag and solar wind," Crassidis explains. "We've developed very detailed models of these other disturbances, which are used to separate out these effects from the leak, thus isolating the leak disturbance."

Although the space station is equipped with a shield designed to catch debris and micrometeoroids, leaks from even small collisions can cause great damage. Currently, NASA tracks debris from the ground, and the station is capable of maneuvering to avoid collisions; however, NASA is only able to track debris .5 inches or greater.

"The idea is to localize the leak," Crassidis says. "It's a time saver for the astronauts and is a life saver, in a sense, because time is crucial when you're dealing with a leak."

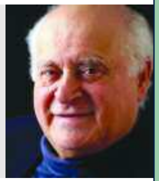
The software will be installed in NASA's mission control when the space station is expanded from its current eight-module configuration to its final 15-module configuration.

NASA funds the work.



Surface model of pressurized modules for ISS assembly stage 16A.

Ruckenstein Receives Founders Award



Eli Ruckenstein, SUNY Distinguished Professor of chemical and biological engineering, was honored with the National Academy of Engineering's (NAE's) Founders Award, and cited for leadership in modernizing research and development in key areas of chemical engineering. The award honors outstanding members who have upheld the ideals and principles of the NAE and who are "the elite" of the organization—those individuals who have proven their worth to the engineering community and demonstrated dedication to NAE.

Ruckenstein conducts both theoretical and experimental research that has changed scientists' understanding of the fundamental phenomena of chemical processes and has led to the development of enhanced research methods and materials.

SEAS Welcomes Bird

The School of Engineering and Applied Sciences welcomes Professor Jonathan Bird, formerly of the University of Arizona, to the Department of Electrical Engineering. Bird's appointment was facilitated by the New York State Office of Science, Technology, and Academic Research (NYSTAR), which awarded him a Faculty Development Award totaling $750,000. The grant, prepared by the Department of Electrical Engineering, was one of four that NYSTAR awarded in 2004. The grants are designed to assist New York State institutions of higher education in recruiting or retaining scientists, helping to ensure the continued long-term growth of the state's high-technology industries.

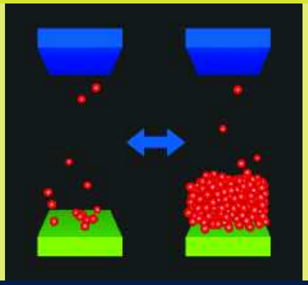
According to SEAS dean Mark Karwan, the successful recruitment of Bird strengthens UB's focus on nanotechnology. Bird's research ranges from fabrication of novel nanoelectronic structures and the characterization of their electrical qualities to quantum chaos in quantum dots and proof-of-principle demonstrations of spintronic devices that exploit unique properties of semiconductor nanostructures.

Phase Behavior of Fluids Confined in Nanoscopic Environments

Jeffrey Errington, assistant professor of chemical and biological engineering, is aiming to enhance the ability of scientists and engineers to predict surface phase behavior—a goal with far-reaching implications for applications ranging from carbon nanotubes used for gas storage to nanoparticles used in stain-repellent khakis.

Such nanoscale technologies are complicated because they involve contact between a fluid and one or more solid substrates. Knowledge of the fluid's phase behavior is required before a device or process in which a fluid-substrate combination is used. Unfortunately, quantitative prediction of the phase behavior of even the simplest of confined systems often proves difficult. In fact, in many cases, generating even a qualitative description of the system's behavior represents a significant challenge.

Errington's work may help other researchers overcome these challenges by providing a fundamental understanding of the phase behavior of fluids confined on nanoscopic length scales. The work is well under way: Errington and his colleagues are already using computer simulation to investigate the behavior of well-defined molecular models that closely approximate real fluids. This approach enables researchers to readily understand the behavior of a system in terms of its underlying microscopic interactions, ultimately allowing them to control the operation of nanodevices by tuning molecular-level details.



Working with three of his undergraduate students—Ravi Chopra, Michael Sellers, and David Wilbert—Errington has characterized the behavior of a model system under a range of conditions. The research has led to a quantitative determination of how pre-wetting transitions influence capillary condensation transitions. Errington and his colleagues have also determined how pre-wetting transitions evolve with wall strength and temperature, and they have performed calculations to determine the boundary tension along pre-wetting saturation lines.

SEAS News

Michael E. Ryan, professor of chemical and biological engineering, is now the University at Buffalo's vice provost and dean of undergraduate studies. For nine years Ryan served as associate dean for undergraduate studies in the School of Engineering and Applied Sciences. Among Ryan's many accomplishments as associate dean is the school's successful Student Excellence Initiative, established to increase undergraduate retention rates.

With Ryan's departure, John E. Van Benschoten, professor of civil, structural, and environmental engineering, has been appointed associate dean for undergraduate studies. A UB faculty member since 1988, Van Benschoten teaches courses and conducts research in wastewater treatment, physical and chemical treatment processes for water and hazardous waste, remediation of contaminated soils, and potable water treatment. Additionally, he has served as director of undergraduate studies in his department and has been involved in a number of undergraduate curricular initiatives at UB.