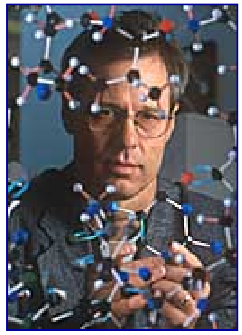
Research Horizons

Winter 2001

COVER STORY

Bioinformatics



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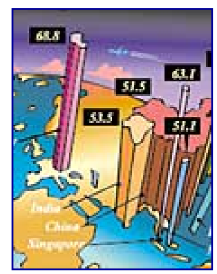

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Research Horizons

Bioinformatics: The Art & Science of Decoding Life

Georgia researchers are finding genes and breaking barriers with bioinformatics.

By Jane M. Sanders

CGCGTGAACTGCTTCCTGCAGGCTGGCCATGGCGCTTCACGTTCCCAAGGCTCCGGGCTTTGC
CCAGATGCTCAAGGAGGGAGCGAAACACTTTTCAGGATTAGAAGAGGCTGTGTATAGAAACAT
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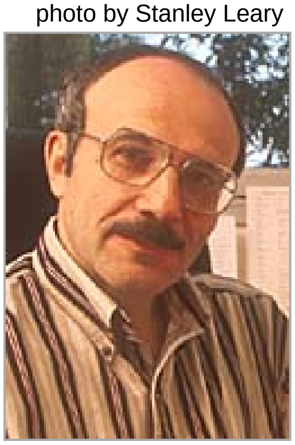
TAGAAGTACAGCATCCTGCTGCAAAAATGATTGTAATGGCTTCTCATATGCAAGAGCAAGAAGTT
GGAGATGGCACAAACTTTGTTCTGGTATTTGCTGGAGCTCT

No, this gibberish is not a misprint. This string of letters A, C, G and T – which represent the four chemical bases or building blocks of life – is a small portion of a human DNA sequence. Within this entire sequence of 1,821 characters are genes, some of which are chemically activated, and thus "turned on" or expressed. Expressed genes make RNA, which in turn makes proteins that are the building blocks of cells and control their function.

photo by Gary Meek

The Georgia Research Alliance, headed by Mike Cassidy, plans to devote a significant portion of its proposed budget for fiscal year 2002 to a bioinformatics initiative. The organization's ultimate goal is the growth of high-tech industry in Georgia. (300-dpi JPEG version - 489k)

photo by Stanley Leary



Bioinformatics is the future of life sciences, says Georgia Tech Prof. Mark Borodovsky. He created GeneMark, one of the most used and accurate software programs for finding genes in genomic DNA sequences.

Finding the genes and proteins they code for within this relatively small sequence is a large task in itself. But magnify the problem to three billion sequenced letters – the result of the Human Genome Project, a draft of which was completed last year. How can scientists possibly manage this amount of data – and more that is on the way – and then mine it for valuable genetic discoveries to aid in diagnosing, treating and even preventing disease, perhaps based on an individual's genetic makeup?

In a word, the answer is bioinformatics. Its definition varies, depending on the scope of one's interpretation. To bioinformatics pioneer Mark Borodovsky, a professor of biology and mathematics at the Georgia Institute of Technology, the term refers to the interdisciplinary science that combines mathematical, statistical and computer science methods to interpret biological data and answer biological questions.

"Bioinformatics is the future of life sciences," says Borodovsky, who created

GeneMark, one of the most used and most accurate software programs for finding genes in genomic DNA sequences. "A wealth of new genomic data conceals endless gems of biological knowledge and, with bioinformatics, researchers can generate new ideas and test new hypotheses much faster."

The definition of bioinformatics has broadened in the past several years from analysis of gene sequence data to the process of integrating many kinds of biological data to find new meaning, says Jim Prestegard, a professor of biochemistry and molecular biology at the University of Georgia.

"Now we're realizing that to have a full understanding of how biological systems work and how they relate to disease, you need more than analysis of genomic data," Prestegard says. "It is still necessary to deal with enormous amounts of data, so bioinformatics is the same today in that sense.... But now we need to integrate sequence information with information on gene expression and the character of protein products. Ultimately, we need to integrate our observations with physiological function of complete organisms and someday with clinical records."

Whatever the definition of bioinformatics, most scientists agree the field holds great promise not only for new discoveries, but also for increasing the speed at which those findings are delivered. "The interesting thing now is this paradigm shift in biology," says Scott Hemby, an assistant professor of pharmacology and psychiatry at Emory University. "We've gone from analyzing one gene at a time to tens of thousands in one fell swoop. This a leap of science."

This paradigm shift will make it possible to see major results from today's basic scientific research in one-half to one-third of the time, Hemby adds.

photo by Gary Meek

Scott Hemby, director of the DNA Microarry Facility at Emory University, is combining the power of bioinformatics with microarray technology to find genes that are critical in disease formation. Microarray technology allows researchers to analyze 10,000 to 20,000 genes simultaneously. (300-dpi JPEG version - 417k)

This shift has not gone unnoticed by economic developers and entrepreneurs, including those in Georgia. With the development of high-tech industry as its ultimate goal, the Georgia Research Alliance (GRA) plans to devote a significant portion of its proposed budget for fiscal year 2002 to a bioinformatics initiative. Over the next two years, the money would fund 10 to 12 new "GRA Eminent Scholars," equipment and facilities at six Georgia research universities – Georgia Tech, the University of Georgia, Emory University, the Medical College of Georgia, Georgia State University and Clark Atlanta University.

Already, the GRA has funded 12 Eminent Scholars and their labs to do research associated with bioinformatics and life sciences. Plans call for the creation of a Center for Bioinformatics Research, which will support life science studies in all GRA institutions. Meanwhile, Georgia Tech is preparing students for careers in bioinformatics with a master's degree program that began in 1999. Funded by the Alfred Sloan Foundation, it was the first such program in the nation.

"We're populating our universities with the best and brightest scientists who are doing cutting-edge work that will lead to the best scientific discoveries at our universities," says Mike Cassidy, president of the GRA. "In turn, that will become a magnet that will attract more companies in genomics and bioinformatics to the state."

To plan its bioinformatics initiative, the GRA staff talked at length with its current Eminent Scholars. "We want to know what drives them, what their passion is about, what their science is and what they think that science can be applied to," Cassidy explains. "That's how we're going to build a whole new industry in the state of Georgia. We don't have a lot of traditional biotechnology industry in the state, but we're convinced that this is going to be very big. Unless we do something very aggressive and very bold, we'll be left behind. So we're moving rapidly to make sure we're making the right investments in the state."

Their efforts seem to be paying off already with the development of biotechnology business incubators, the rise in start-up companies – some of which academic researchers have founded – and the recent moves of two established companies to Georgia. EmTech Bioscience is a commercial research and development center focussed on the life sciences. EmTech, a partnership between the GRA and Georgia Tech's Advanced Technology Development Center, is operated by both Emory and Georgia Tech. NuTec Science, an established bioinformatics and supercomputing company, moved to Georgia last summer and became the anchor corporation at EmTech.

Meanwhile, the Center for Applied Genetic Technologies (AGTEC) at the University of Georgia in Athens is an incubator for agriculture-related biotech companies, including start-ups ProLinia and AviGenics. Also, Merial Ltd., a major manufacturer of animal vaccines, recently relocated its headquarters to Atlanta. Its plans call for the construction of a pilot vaccine development plant in Athens. Both animal and human vaccines will be manufactured there, bringing new high-tech jobs to Georgia.

"Georgia's initiative in bioinformatics has a huge amount of potential," says Gary Schuster, dean of the College of Sciences at Georgia Tech. "It's interesting that five years ago, almost nobody knew what bioinformatics was. Now we are charting its course, and that can be difficult. But almost everyone agrees that bioinformatics is at the core of all the promises the 'Biological Revolution' has to offer. It is being able to manage huge data sets, being able to mine huge data sets and determine what's important and what's not, whether it's for drug discovery or fundamental knowledge."

Many researchers – from molecular biologists to bioengineers to animal scientists – are fascinated by the prospects of bioinformatics and dependent upon its analysis of biological data. Few are developing the tools of bioinformatics. Among those is Borodovsky with the creation of GeneMark software and the latest version GeneMark.hmm (for the Hidden Markov Model upon which its algorithms are based). The former has been used to completely decipher the genomes of dozens of bacterial species, including the infamous E. coli.

Both versions can analyze DNA sequences from higher organisms, including humans, but the latter more accurately predicts the boundaries between introns (non-coding regions) and exons (regions coding for proteins). In higher organisms, a gene starts in a sequence and then can be interrupted by an intron. Then the gene proceeds again with several more interruptions.

photo by Gary Meek

A Belgian researcher's study published in the November 1999 issue of the journal Bioinformatics found that GeneMark.hmm was the most accurate among several other state-of-the-art programs in predicting genes in plants.

GeneMark is licensed by about 150 companies and institutions worldwide, including Harvard, Stanford and Columbia universities, the National Center for Biotechnology Information, the Max Planck Institute and the European Bioinformatics Institute. Others use GeneMark via the software's Web site servers at Georgia Tech and in the United Kingdom. The U.S. server analyzes about 3,000 sequences a month.

Robert Nerem, director of Georgia Tech's Petit Institute for Bioengineering and Bioscience, believes the next generation of bioinformatics tools, available in five to 10 years, will be based more so than current ones on predictive mathematical models. (300-dpi JPEG version - 435k)

Borodovsky's research is funded by the National Institutes of Health through 2003. In the next several years, he plans to improve and diversify GeneMark, transforming it into a whole family of academically based software programs that are regularly updated and widely available. Borodovsky founded Gene Probe, a small spin-off company that provides technical support and distribution for GeneMark programs.

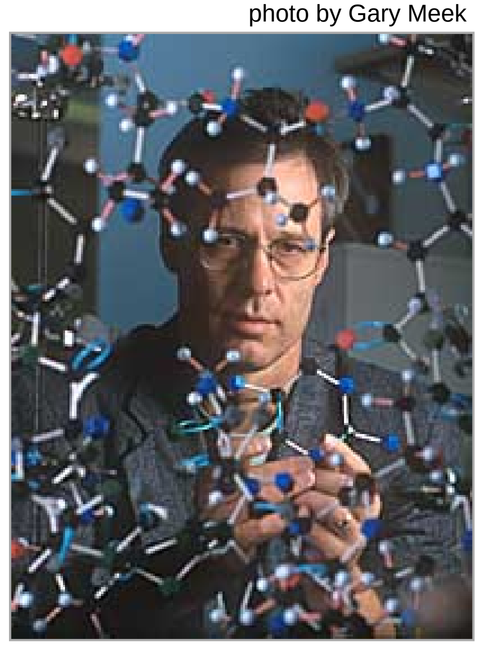
The next generation of bioinformatics tools, available in five to 10 years, will be based more so than current ones on predictive mathematical models, says Robert Nerem, director of both Georgia Tech's Petit Institute for Bioengineering and Bioscience (IBB) and the Georgia Tech/Emory Center for the Engineering of Living Tissues. Better tissue substitutes will depend upon these models, which should predict function of these materials both in the laboratory and the body.

IBB researchers are developing such models, as are a host of academic and corporate researchers across the nation. At Georgia Tech, involved faculty members are: Gang Bao, Robert Guldberg and Joe LeDoux in the Georgia Tech/Emory University Department of Biomedical Engineering; Ray Vito and Cheng Zhu in the School of Mechanical Engineering; Athanassios Sambanis in the School of Chemical Engineering; and, of course, Borodovsky.

Meanwhile, researchers at GRA institutions are using the current power of bioinformatics to make valuable leaps forward in basic science, biotechnology and medicine that could revolutionize diagnosis and treatment of disease. Much of this work is collaborative, particularly in biomedical engineering, because of degree program and research partnerships between Georgia Tech and Emory.

"Tech researchers need Emory scientists, who understand what the applications should be," says Don Giddens, chairman of the joint Department of Biomedical Engineering and a GRA Eminent Scholar. "Conversely, Emory researchers need the people who understand the technology and who can do the modeling."

photo by Gary Meek



The forces that control the structure of DNA – and ultimately chemical activation of some genes – are a hotly debated scientific question. Georgia Tech Professor Loren Williams is addressing these questions in his structural biology laboratory. (300-dpi JPEG version - 495k)

Moving the department's research beyond bioinformatics is Giddens' goal. "Engineering is a field that implements things," Giddens says. "So that's our connection. We want to plug into bioinformatics and be a part of it, but we are stressing how to move that information into the medical and clinical arenas."

Plans call for a GRA Eminent Scholar in the joint department; this researcher would focus on Giddens' vision of "bioinformatics and beyond." Giddens also cites two important ongoing projects. They are: (1) a basic scientific study by Gang Bao of the physical forces that change or disrupt DNA; (2) a technology under development by Joe LeDoux for delivering genes for gene therapy.

Researchers in the Georgia Tech School of Electrical and Computer Engineering also depend upon bioinformatics. Professor William Hunt is developing microelectronic biosensor devices for molecular detection of target molecules. Knowing the target molecules around which to design the biosensor is the product of biomedical research and bioinformatics.

One application of Hunt's research could be for rapid protein screening. For cancer screening, a biosensor would know the proteins to search for in a urine sample. The result might be an early detection of a specific cancer.

Hunt's current devices can detect as little as a 3-hertz shift in a 250-megahertz resonant frequency of a surface acoustic wave biosensor. The shift occurs when molecules bind to the surface of the device. That sensitivity level is equivalent to about 10 parts per billion, but Hunt does not know if it will be sufficient for detecting proteins for early cancer screening. To that end, he is evaluating the acoustic design of his devices, as well as the design of the chips on which the microelectronic system resides.

While he awaits more information on the appropriate target molecules, Hunt is focusing on the development of increasingly more sensitive devices. "What I am working on has to be part of a collaborative effort," Hunt says. "I can build sensitive devices, but unless I know what target molecule to look for, I am just an electrical engineer building neat stuff."

Just down the hall from Hunt, Assistant Professor Bruno Frazier has begun a five-year collaborative research project funded by the National Institutes of Health. He and his collaborators from Princeton University, the University of Virginia and Agilent Technologies are miniaturizing sample preparation for biological and biochemical analysis. Specifically, Frazier is developing ways to prepare blood for genetic analysis. The technology will allow scientists to take a blood sample and extract the important components, such as DNA, from it.

"This project is one component in a total analysis system that includes sample prep, an analysis component and a detection/bioinformatics component," Frazier explains. ".... Ultimately, this system could be used for minimally invasive diagnosis or treatment of certain types of cancers or other diseases."

Frazier's work occurs at the interface of electrical systems, such as an integrated circuit, with biological components, such as cells. Specifically, he approaches the sample prep system's task of cell sorting and selection through electrophysiology, the study of electrical properties of cells. In the case of blood, Frazier uses electrical components, such as a conductor, to measure its passive electrical properties (e.g., resistance and capacitance). He has found that certain types of cells have certain electrophysiological signatures. The micro system device can use those signatures to sort red and white blood cells and to sort and detect certain types of cancer cells.

Researchers will use the tools of bioinformatics to analyze data gathered by Frazier's micro system. Then they can visualize the data with a contour plot, for example. This process is what gives the data meaning, Frazier says. In the project's final phase, researchers plan to build a portable biochemical analysis device that will incorporate Frazier's system.

Researchers at Emory University are combining the power of bioinformatics with DNA microarray technology to find genes that are critical in disease formation. DNA microarray technology allows researchers to analyze 10,000 to 20,000 genes simultaneously. At the GRA-funded DNA Microarray Facility at Emory, researchers put about 10,000 spots of DNA on a microscope slide. Then through a process called reverse transcription, researchers label RNA and hybridize it with DNA on the slide.

"It's like putting a puzzle together," explains Hemby, director of the facility. "All the pieces are there. You just have to put them back together in the right places."

Scientists then bombard the slide with light under a microscope that is like a laser scanner. What is emitted is either green or red. Using the tools of bioinformatics, researchers then analyze the intensities of emitted light to determine the abundance of genes and possibly whether the genes are mutated, either of which could be indicators for disease. Many diseases have genetic components; these include certain types of cancers and psychiatric disorders, such as schizophrenia, autism and drug abuse. Hemby is studying psychiatric disorders.

The evaluation and results of microarray experiments are what Hemby and his colleagues call a gene expression profile. They have patented a technique for creating the profiles for schizophrenia and drug abuse.

"When we learn more about diseases, we will be able to diagnose based on what genes are expressed," says Mike Kuhar, a GRA Eminent Scholar and chief of the Neuroscience Division at Emory's Yerkes Primate Research Center. "So the genetic profile provides us with a bull's eye to shoot at with medications. What medication may be right for me might not be right for you."

For example, Hemby is collaborating with Emory Professor and GRA Eminent Scholar Rafi Ahmed to identify a subset of genes responsible for HIV patients' tolerance to medications called highly active antiretroviral therapies (HAART). After the researchers identify the subset, Hemby's lab will use a smaller candidate gene chip to expedite this approach of Ahmed's research. Eventually, it may be possible for patients to use a self-test device to see if they are developing drug tolerance.

This is an example of the individualization of medicine, Hemby says. Other Emory researchers are working to tailor medicines to best treat certain types of cancer. Hemby plans to use microarray and bioinformatics technologies to create a database of genetic profiles for a variety of psychiatric diseases, all of which scientists believe will yield a specific expression profile.

In other research at Emory, Kuhar and his colleagues used bioinformatics technology to study a new neurotransmitter in the brain; it is called the CART peptide for Cocaine and Amphetamine Regulated Transcript. CART helps control food intake and is partly responsible for the feeling of satiety. The finding may eventually lead to new medications for obesity.

"Imagine the power of bioinformatics," Kuhar says. ".... Without a single experiment in the laboratory, just by sitting at a computer, the uncovered information at the terminal drives the direction of subsequent research. Bioinformatics told us that CART was a neuropeptide, so our research went in a different direction than it would have if we found that CART was another kind of protein."

Animal scientists have also discovered the power of bioinformatics, as well as microarray analysis. At the University of Georgia, Associate Professor Steve Stice is cloning livestock to make more copies of the best animals. Eventually, he hopes to make genetic changes in the clones to produce animals that are more disease resistant, use fewer resources and are more environmentally friendly (e.g., manipulating the genes that control animal odors).

"Scientists are finding more genes all the time, so there are many possibilities for what we can do," says Stice, also a GRA Eminent Scholar. "I like to say the pigs are piggybacking on the mouse and human genome projects. We don't know as much about the genes of pigs and cattle, but we are learning a lot more."

In fact, the Human Genome Project has revealed that there is an 80 to 90 percent similarity in genetic makeup between humans and farm animals. The difference occurs in how those genes are expressed, and in what and how many proteins are produced, Stice explains.

"That's where bioinformatics comes in," he says. "It's not just the ability to know the genes, but to know how they interact in the body. That's the really important part."

photo by Rick O'Quinn

At the University of Georgia, Associate Professor Steve Stice is cloning livestock to make more copies of the best animals. He says bioinformatics helps his research team determine what genetic information is useful.

Stice is collaborating with Hemby at the DNA Microarray Facility to determine why some cloned cattle embryos develop better than others. Now, only one in 50 cloned embryos eventually produce offspring. Microarray technology will allow Stice to compare gene expression in embryos that succeed in development and those that don't. Then he can devise a genetic technique for dealing with that difference, he says.

"This work is still in a very early stage," Stice says. "We are still learning how to use this technology with cattle. But bioinformatics is so important. It will help us determine what genetic information is useful."

In the vitally important arena of basic scientific research, bioinformatics is also playing a role. At Georgia Tech, Loren Williams in the School of Chemistry and Biochemistry is focusing on structural biology. Genes are expressed in both the sequence of DNA bases and the three-dimensional shape of DNA. The forces that control the structure of DNA are a hotly debated scientific question – one that Williams is addressing. Scientists do not yet understand how a linear meter of DNA gets folded to fit into a tiny cell nucleus, or how a cell recognizes which part of the DNA to unfold and read.

Williams uses X-ray diffraction to help answer these questions. In X-ray diffraction, the researcher takes a sample protein or piece of DNA or RNA, purifies it and then crystallizes it – essentially dehydrating the sample in a chemical "soup." At that point, he exposes the sample to an X-ray beam and collects the diffraction pattern. Some of this work is done on the synchrotron beam lines at Argonne and Brookhaven national laboratories, which provide especially brilliant X-ray sources. Cameras equipped with light-sensitive integrated circuits called charge-coupled devices collect the X-ray diffraction patterns from the synchrotron, and high-speed computers process the data. It takes about three months for scientists to determine the three-dimensional structure of a macromolecule by X-ray diffraction. Within a couple years, the process will take only three days and eventually only three hours or so, Williams predicts.

photo by Gary Meek

The slow part of Williams' research is interpreting the three-dimensional structures, trying to understand molecular interactions. For example, he is interested in why a DNA macromolecule takes on a particular shape. "The structural information is starting to come in to us too fast," Williams says. "Now we have a bioinformatics problem. Bioinformatics gives us a way of asking the whole database these questions."

Learning why macromolecules take particular shapes is potentially useful in application-driven research such as drug design. But the information is also critical for understanding fundamental phenomena in DNA bending and protein folding. The applications of such basic research are never obvious, but neither were the applications of the Internet when it was first built, Williams says. Quoting from the movie "Field of Dreams," Williams hastens to add, "If you build it, they will come."

"Basic research leads to unexpected things," Williams says. "Bioinformatics has given scientists huge databases to which they can ask questions. We are only limited by our imaginations."

Georgia Tech Professor William Hunt is developing microelectronic biosensor devices for molecular detection of target molecules. One application of Hunt's research could be in rapid protein screening for early cancer detection. (300-dpi JPEG version - 990k)

At the University of Georgia, structural biologists use both X-ray diffraction, or crystallography, and nuclear magnetic resonance (NMR) technology to study proteins. They are collaborating with researchers from Georgia State University, the University of Alabama at Birmingham and Huntsville, and a Huntsville company called Research Genetics to form one of seven recently funded NIH pilot centers for structural genomics. Eminent Scholar and Professor B.C. Wang is the lead investigator, and GRA Eminent Scholar Prestegard is one of seven other co-investigators. The goal of the center is to provide structural information on proteins in a volume useful to bioinformaticists, Prestegard says.

"We're working with a very new paradigm in science," he explains. ".... Historically, structural biologists have worked from a recognized biological function back to fundamental information, such as the three-dimensional structure of proteins and gene sequences. Now, we are almost turning that approach upside down. The philosophy of structural genomics is to start from the genes.... Even if we don't know the function of the protein, we can crystallize it and use X-ray crystallography or NMR to get structural information on it."

X-ray crystallography delivers about 80 percent of structural protein information; NMR provides the remainder. Prestegard uses NMR, the same technology used in biomedical imaging, but on an atomic scale. Typically, determination of a complete protein structure (i.e., knowing where every atom is placed) using NMR would take three to four weeks of data acquisition and then a lot more time for data analysis. Instead of pursuing this course, Prestegard's research team developed an efficient technique for studying only the "backbone fold" of a protein. They believe the backbone fold's restrictions on placement of the various chemical side chains will help identify a protein's function. The research is helped, in part, by the highly sophisticated laboratory equipment purchased with funds from the GRA.

"We believe this technique will be a very useful stepping stone that, along with the tools of bioinformatics, will allow us to make functional predictions from a more fundamental level," Prestegard says. "This technique is increasing the rate of data acquisition from three to four weeks to just three to four days.

".... There's a lot of work to be done," Prestegard says. "It's not just getting the basic structure. We need to bring together information from a lot of sources like gene transcription profiles and mass spectrometry data on expressed proteins. In my view, that's where modern bioinformatics is going. We're not only focusing on analysis. The real payoff is in integrating the information. That's the frontier."

At the GRA, Cassidy wants Georgia on the bioinformatics frontier and fast.

"There will be a rapid explosion in bioinformatics in the next five years," Cassidy says, "particularly in the tools needed to decipher and interpret genomic data. Estimates indicate that bioinformatics will become a $49 billion industry in the next four to six years."

Long-term economic development prospects related to bioinformatics are in therapeutics and pharmaceuticals. Researchers in this arena are expected to increase their drug discovery targets from about 400 to 4,000 over the next 20 years as bioinformatics matures and individualized medicine becomes commonplace, Cassidy says. The pharmaceutical industry is expected to increase from $300 billion a year to $300 trillion during that timeframe.

photo by Rick O'Quinn

University of Georgia Professor Jim Prestegard and his colleagues have developed an efficient technique for studying only the "backbone fold" of a protein. They are using the technique and the tools of bioinformatics to help identify protein function.

Georgia's academic researchers are excited by the prospects, too, but they caution that many factors will affect the state's ultimate success in bioinformatics-related economic development.

"There is a long way between knowledge accumulation and a medical treatment revolution," Borodovsky says of the promises touted by the Human Genome Project. "There has been a fundamental, revolutionary change in biological science. The Human Genome Project has been a groundbreaking thing. Scientists are changing how they do experiments, how they collect information before doing experiments, how they interpret results. Everything is different from the way it was 10 years ago.

"But there is still a process of hard scientific work to go inch by inch with generating and testing ideas, and making sense out of data," Borodovsky says. "It's a process of trial and error. It's not just a jump into a gold mine."

Nerem believes Georgia could become one of several hubs for bioinformatics-related industry. He is particularly encouraged by the relocation of NuTec Science to Atlanta. More companies and more Eminent Scholars, particularly in molecular and cell biology, are needed to build a solid infrastructure, he says.

Others agree on the point of bringing more GRA Eminent Scholars to Georgia. "We need more investment," Prestegard says. "But all of this takes quite a while. Georgia is doing the right things. It has a tremendous advantage in the GRA. Not many states have such a mechanism."

Williams hopes to see a "perfect synergy" between the long-term basic scientific research of academia and the short-term applied research of industry. "We can push the envelope of science if companies and academia will share their resources," he says.

Giddens cites the complementary capabilities of the six GRA universities. There are those developing the tools of bioinformatics, those gathering the data, those analyzing and interpreting the data, and those who will integrate the data with new tools of bioinformatics.

"We don't yet know the potential of bioinformatics," Williams says. "The databases are getting bigger. We have new kinds of information. We are getting better algorithms. It's inconceivable what we can learn with these new tools."

For more information, contact Robert Nerem, Petit Institute of Bioengineering and Bioscience, Georgia Institute of Technology, Atlanta, GA 30332-0405. (Telephone: 404-894-2768) (E-mail: robert.nerem@ibb.gatech.edu); or Gary Schuster, College of Sciences, Georgia Institute of Technology, Atlanta, GA 30332-0365. (Telephone: 404-894-3300) (E-mail: gary.schuster@cos.gatech.edu); or Mike

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Research Horizons

Learning by Doing

Undergraduate research at Georgia Tech teaches students by involving them in faculty projects.

By Jane M. Sanders

In 1990, a Georgia Institute of Technology freshman was struggling in her classes when she signed up for a part-time laboratory research job that sounded like a fun way to make some money for school.

She reported to the lab of chemical engineering Professor Charles Eckert, who after talking with the student, believed she was intelligent, but bored in class. Eckert – whose self-proclaimed role is to open doors for undergraduates to see what they can accomplish – accepted the mission.

photo by Walt Ennis

An undergraduate research experience at Georgia Tech had a significant impact on the career direction pursued by Cindy Harrell Willis. She now holds a doctoral degree in chemical engineering and works as a researcher at W.L. Gore & Associates, the manufacturers of Gore-Tex™ fabric.

"I gave her work that would have been challenging for a Ph.D. student," Eckert recalls. "I was lucky. I guessed right. She was bored. Within a year she was getting A's in her classes. Research got her excited, and she was able to do things I didn't think an undergraduate could do."

Today, that former student, Cindy Harrell Willis, holds a doctorate in chemical engineering and is a researcher at W.L. Gore & Associates, makers of Gore-Tex™ fabric.

"My experience with undergraduate research convinced me to go on for five more years of graduate school," Willis says. "Doing research at Georgia Tech changed my career path. I knew a graduate degree would open up more doors for me, and it has."

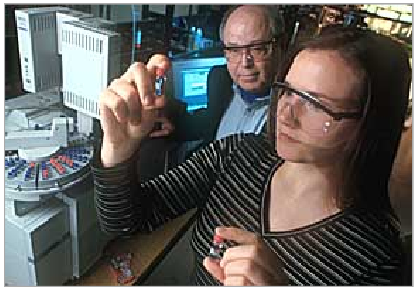
Eckert, the J. Erskine Love Jr. Institute Professor, and other Georgia Tech faculty members have involved undergraduates in their research – in one form or another – throughout their careers. They have found the experiences not only have a positive impact on students, but also give them personal fulfillment.

"A research experience adds something that we cannot do completely in class," Eckert explains. "It teaches students teamwork and leadership. It teaches them the applications of what they're learning in the classroom, and it makes their class work more meaningful."

For Eckert, the experience is fun. "I'm here because I'm a teacher," he says. "I get my satisfaction from seeing people become successful. If I didn't feel that way, I could work somewhere else, but I really enjoy working with students. It's more fun to me to see a student discover something than to discover it myself."

Recognizing the benefits to both students and faculty, Georgia Tech administrators have begun an initiative to increase participation in research programs for undergraduates. Meanwhile, administrators are also encouraging more senior faculty to teach an occasional freshman- or sophomore-level class, in hopes of getting students excited by a discipline and possibly interested in research.

photo by Gary Meek



Professor Charles Eckert has mentored many undergraduate students in his chemical engineering laboratory through the years. Now, sophomore Ashley Wallin works for him. She has already decided to pursue an advanced degree and a career in chemical or bioengineering research.

"Involving undergraduate students in research really goes to the heart of what we intend for the undergraduate education to be about," says Bob McMath, vice provost for undergraduate studies and academic affairs. "We're not simply opening up their heads and pouring stuff in. We are really equipping them to be lifelong learners. We're equipping them for discovery and success."

Georgia Tech's administration is committed to excellence in both research and teaching. "The question is how do we leverage the tremendous human resources we have on the research side to increase the quality of undergraduate education," McMath adds. "We simply have to take advantage of who we are."

That means convincing more senior faculty members to hire undergraduates as research assistants, or enrolling them in research, independent study and internship courses, McMath explains. The number of research assistants is unknown, but in the 1999-2000 school year, enrollment in research-oriented courses numbered 1,120. (This number represents some overlap of students.) So only about one-tenth of undergraduates are taking these courses. Meanwhile, 74 students are conducting research in the Georgia Tech Research Institute as co-op students, alternating semesters of working and attending classes.

To boost participation in undergraduate research, the administration is offering faculty some modest incentives, including lab equipment funds and travel money for students to present their research at conferences. Also, several faculty members with projects funded by the National Science Foundation (NSF) have gotten additional money by involving undergraduates. Others have operated NSF-funded, summer research programs for undergraduates.

Incentives are great, faculty members say. But perhaps more important to the administration's campaign is the power of persuasion by one's peers. Many faculty members concur with and practice McMath's educational philosophy.

In the College of Sciences, every student is given an opportunity to participate in some sort of research, and within some degree tracks, research is a requirement, says Gary Schuster, dean of the college.

"Often it is the research experience that motivates students to high-level achievement," Schuster says. "It is the process of investing yourself emotionally in the search for answers to questions. Nobody else in the world knows it before you do. It's a great thrill."

One student reports the exhilaration of his summer research experience last year in the chemistry lab of Professor Mostafa El-Sayed. Man Houn Han conducted an experiment on the interactions between gold nanorods and semiconductor particles when they are mixed.

"The experiment was not that successful because the expected phenomenon did not occur," Han says. "However, it was the best experiment that I have ever had in my college years.... I learned how a research experiment is conducted, and what it takes to be a researcher. I know I have lots to learn, but I am very confident that I am ready for the next step. Since my goal is to be a successful researcher and educator, this experiment will be the base of everything I do in the future."

In the College of Engineering, a variety of research programs are engaging undergraduates. For example, a team of 55 students worked on a research project called FutureTruck. The team had to transform a Chevy Suburban into a hybrid electric vehicle. While maintaining the vehicle's ability to carry cargo and pull heavy loads, they had to reduce its fuel consumption and air-polluting emissions. In a national competition, the team won two first-place awards.

In the College of Computing, Assistant Professor Amy Bruckman started the Undergraduate Research Opportunities in Computing in 1998 with support from Microsoft. Participants conduct research, publish technical papers and present their findings at conferences.

"Students learn better if they work on something they really care about," Bruckman says. "They use the knowledge they have gained from their classes. And they have an opportunity to build relationships with graduate students and faculty, who can become their role models."

In the Ivan Allen College – which includes economics, history of technology and public policy – students are involved in independent study research courses and internships. For example, in the School of Public Policy, Associate Professor Ann Bostrom and Professor Richard Barke hired an undergraduate for an NSF-sponsored project on the effects of privatization on risk perception and environmental policy in Eastern Europe. "We hired an undergraduate public policy major with excellent statistics skills – but as important, great enthusiasm – to help us with data analysis," Barke says. "He extended our capabilities and inspired us to apply statistical techniques that were not part of our original research plan."

The College of Architecture operates six research centers, all of which involve undergraduates. Some of the centers work on projects for industry, and students are regularly involved in this work, says Thomas Galloway, dean of the college. These centers relate to rehabilitative technology, geographic information systems, interactive multimedia for animation and rendering, advanced wood products, construction research and smart growth.

As an undergraduate, master's degree student Cory Benson worked with a team of undergraduate researchers in the multimedia lab, creating Web-based information systems, developing Web sites for the College and applying virtual reality technology to visualize buildings in 3D. Benson is continuing to conduct research, now in the Advanced Wood Products Laboratory.

Still another research opportunity is a cooperative program where students alternate semesters of taking classes and working as a "co-op." The Georgia Tech Research Institute (GTRI) hires many of these students. While helping develop software at GTRI, co-op student David Phillips says, "I experienced a larger project in the real world and got real, hands-on experience with the collaboration and teamwork required to combine the work of different people into a finished product."

Another GTRI co-op student, Jessica Shearer, worked with Professor Krishan Ahuja to develop "Quiet Curtains," which transform curtains that hang around a nursing home patient's bed into a product that not only provides visual privacy, but also acts as an acoustical shield. The curtains could also be used in offices and schools. Shearer is listed as a co-inventor on the product patent. And co-op student Danny Diaz is working on a Department of Defense project to allow communication between radar systems operating on different platforms to form a common tactical picture for operators.

photo by Gary Meek

"GTRI benefits from talented, bright students and their hard work on research projects," says director Edward Reedy. "They are an integral part of our project teams. We also have the added benefit of looking at students who might be potential researchers or scientists after graduation and want to come to work for us. Students also bring a fresh perspective to the research challenges of today's R&D environment."

Another opportunity is the learning community sponsored by the Women in Science and Technology Program, co-directed by Professor Mary Frank Fox and Associate Professor Carol Colatrella. In this pilot program,a group of female students voluntarily live together in one section of a residence hall. There, they have guest speakers and other interaction with

The Entertainers

Professors use creative approaches to teach difficult concepts.

In a freshman chemistry class, Professor Mostafa El-Sayed clarifies the difficult concept of entropy by comparing the driving forces behind it to analogous ones in marriage. His students perk up and listen.

When two chemicals react to form one final product, you cut each chemical's degree of freedom. This leads to a decrease in entropy, and nature does not like it. But if the product has stronger and more chemical bonds than the two reacting chemicals, the reaction will proceed. Similarly in marriage, each person gives up some freedom in hopes of experiencing stronger bonding and a better life.

Most students easily relate to this situation. Now they understand entropy plays a role in chemical reactions.

"Undergraduates are wonderful young people," says El-Sayed, one of the Georgia Institute of Technology's senior professors who regularly teaches at that level. "You can see it in their eyes whether you have reached them, more so than you can with graduate students. With undergrads, the feedback is spontaneous. Teaching them is more fun."

El-Sayed and others at Georgia Tech – including some full-time researchers at the Georgia Tech Research Institute – are setting an example the institution's administration is hoping many other senior professors will follow. In fact, the administration has appointed a committee to formulate a strategy for giving undergraduates more opportunities to benefit from the knowledge of senior faculty – both in the classroom and the laboratory.

"There is a tradition across the country of prominent people getting involved with undergraduates like this as sort of a responsibility of their stature," says Dr. Bob McMath, vice provost for undergraduate studies and academic affairs. "But for many of them, it's also an interesting intellectual challenge to take this incredibly complex knowledge and distill it in such a way that it is intelligible to undergraduates.... The ability to articulate what we know as scholars and researchers in a way that makes sense to non-specialists is one of the most important things we do. It makes our science very public."

El-Sayed thrives on this communication challenge. "Teaching undergraduates keeps you in touch," he says. "All the time you have to be recalibrating things to relate to what they are thinking.... Really, I benefit as much as they do."

Earth and Atmospheric Sciences Professor William Chameides says relating the concepts of his discipline to young undergraduates requires him "to do a bit of entertaining." For example, in his freshman earth systems class, he shines a flashlight around the room to explain the effects of sunlight on the Earth's surface, and Chameides employs a ball and string to explain light as an electromagnetic wave and a photon.

faculty and campus visitors. Each student has a faculty mentor, and all are engaged in research. This program could be a model for a more expanded effort, McMath says.

In the College of Computing, Assistant Professor Amy Bruckman regularly meets with undergraduate students who conduct research under her advisement.

No matter the discipline, undergraduates report that their research experiences are valuable in many ways. Shearer, an applied physics major, found that her experience put her ahead of her peers in class. For example, she had already helped write and publish a technical paper when she was given a report assignment in an advanced lab class. "I had a huge jump on my classmates because I already knew how to write a technical report," she says. "I knew where errors could occur and what kind of details to pay attention to and record."

Diaz also discovered a complementary relationship between his classes and research. "All of my coursework has played into my research," says Diaz, a computer engineering major. "The research has helped me apply general concepts I have learned in my coursework."

Undergraduate researchers also have the opportunity to mature and improve skills they will need in their careers. "Doing research has helped me with my presentation skills," Diaz says. "I have learned to convey my thoughts and ideas to a group. I've learned responsibility. Things have to be done at a certain time or else.... And working in a research environment makes you think for yourself a lot."

photo by Gary Meek

Professor Mostafa El-Sayed taught undergraduate student Man Houn Han during a summer chemistry research program last year. Han calls the experience the best so far in his college career.

Research experiences also help students make educational and career decisions. Both Eckert and El-Sayed have had students about to quit school when they began research and changed their minds. "Research is one important way to connect students to something meaningful at Georgia Tech," McMath says. "Connecting like this increases the likelihood of their graduating."

For other students, research has helped clarify their decision-making. Chemical engineering major Ashley Wallin has been working in Eckert's lab since the spring of 2000. "Doing research has shown me what I want to do and what I don't," she says.

Like many undergraduate researchers, Wallin, just a sophomore, has already decided to pursue an advanced degree and a career in chemical or bioengineering research.

"Exposure to research at the undergraduate level is essential to students who want to go to graduate school," says GTRI senior research engineer Rich Combes. "As an undergraduate, they will be in a less-demanding research role than graduate research assistants. But when we identify students with ability, we give them as much work as they can take on.... Having this research exposure gives students a better understanding of the value of a graduate degree.... They start to see their path on a personal level."

That path eventually leads many undergraduates to careers in research. "If you talk to most scientists and ask them what experience convinced them to become researchers, by and large they will say that research at the undergraduate level was the key factor," Schuster says. "It was being involved in the research culture, in prying out each of nature's secrets."

"The advantage I have in earth science is that the outdoors and the Earth are things all of us can relate to on various levels," Chameides says.

In addition to giving young undergraduates an exciting introduction to their disciplines, many of these senior professors also want students to learn critical thinking skills that will benefit them throughout their college years and into their careers.

"We get students here who have done well in high school and on the SAT (Scholastic Assessment Test) exam," says chemical engineering Professor Charles Eckert. "They have had 12 or more years' experience in learning how to avoid mistakes. Students who get good grades and do well on the SAT are very good at avoiding mistakes. But if students are going to be creative in research, they need to learn to make mistakes. They need to know that not only is it OK to make mistakes, they have to be willing to try new things. And they need to know that we consider it OK for them to try new things and make mistakes.

".... So what we're teaching them, even in the freshman year, is a different kind of thinking," Eckert adds. "They still need to be able to do integrals and derivatives correctly. But when it comes to broader ideas, I want them to have the right and the impetus to try new things."

McMath has interviewed many students, and they want the unique experience of having senior-level, distinguished faculty members teaching them, he says. They realize the benefits even before the opportunities arise.

"We are pleased by how many of our senior faculty are already engaged in undergraduate research and teaching opportunities," McMath says. "Now we need more of these senior-level people who are teaching undergraduates because they just want to do it. They want to bring what they know – their incredible research bases of knowledge – to the undergraduate level."

— Jane M. Sanders

When faculty reflect on their reasons for involving undergraduates in research, they reply with both practical and philosophical answers. In GTRI, Ahuja cites the cost and time advantages.

"It's hard to win large research contracts unless you are creative," Ahuja explains. "Quite a bit of our work is experimental research that doesn't require technicians with high-level knowledge – for example, taking routine measurements in a wind tunnel. But this work done by undergraduates is very valuable. It allows us to be creative and competitive in the research contract market."

Ahuja had to invest a lot of time to train co-ops when he first started hiring them. But eventually the trained researchers taught the new ones. Now, Ahuja only directs co-op students' research through regular meetings. "I see having five co-ops as like having 10 extra arms doing very productive work," he adds. Ahuja's students, meanwhile, get rewarded with co-authorship on at least one technical paper, travel to conferences, sometimes co-inventorship on patents and experience that makes them hot commodities in the job market.

El-Sayed echoes Ahuja's point on productivity. "Undergraduates know their time here is limited, so they want to accomplish something," he explains.

Faculty members also benefit from students' enthusiasm. "Our students bring fresh ideas and perspectives to research projects," says Barke from Public Policy. "And we all know that one of the best ways to learn is to teach others, so working with undergraduates often draws new ideas out of faculty researchers."

Eckert has experienced this fresh perspective. "One reason I like working with undergraduate researchers is their utter irreverence," he explains. "They simply don't know what can't be done, so they do it. All too often in industrial research, researchers are reluctant to undertake risky projects because they see them as potential career-enders. Students are fearless in this regard."

And then there's the reward of mentoring students. "Mentoring is why we're here," McMath says. ".... At the end of the day, this is simply who we are. In addition to being a great graduate research university, we are a public university that is educating close to 10,000 undergraduates at any given time. As members of the faculty, we need to be involved with them."

photo by Stanley Leary

Undergraduate student Jessica Shearer worked with Professor Krishan Ahuja to develop "Quiet Curtains." The concept transformed privacy curtains surrounding nursing home patients' beds into noise-reduction shields. The curtains may also be used in offices and schools.

With many faculty members and students sharing their success stories of undergraduate research and also agreeing on its multiple benefits, the Georgia Tech administration is hopeful about increasing participation.

Bruckman believes that is possible. "What I find is that a lot of faculty members have never thought about involving undergraduates in research," she says. "But when they think about it, they believe it will be mutually beneficial. So this is an opportunity to educate faculty about this."

Questions remain about organizing a more formal undergraduate research program. For example, Bruckman asks, "How many students can be meaningfully involved given faculty members' time limits?" And how do you ensure that students are given actual research to do, not "busy work"? A committee formed by the administration is addressing some of those questions, and Bruckman is a member.

"I believe Georgia Tech is moving in a great direction, and I'm there to help support it," Bruckman says.

McMath adds: "Georgia Tech is making the improvement of teaching and learning a major emphasis. Our niche for doing that is to take the strengths of a research university and apply them."

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Research Horizons

Flying Low-Drag Trucks

Aerodynamic concepts and controls for aircraft will cut fuel use and improve control in trucks.

By John Toon

Bob Englar would like to help tractor-trailer trucks fly ... not literally, of course. With support from the U.S. Department of Energy and American Trucking Associations, Englar is applying aerodynamic concepts and "Circulation Control" flight systems developed for aircraft to 18-wheelers. The goals include reducing fuel consumption and giving drivers better control of the big rigs under adverse conditions.

photo by Gary Meek

Researchers Bob Englar, left, and Graham Blaylock test an aerodynamic control system designed for aircraft on small-scale 18-wheel truck models in GTRI's low-speed wind tunnel. Researchers hope the system will reduce the trucks' fuel consumption and give drivers better control under adverse conditions. (300-dpi JPEG version - 500k)

"We are taking flight-proven aircraft technology that we've already shown works on streamlined cars and applying it to trucks," says Englar, principal research engineer at the Georgia Tech Research Institute (GTRI). "Current trucks, primarily the trailers, are anything but streamlined, so whatever can be done to reduce the drag will help fuel economy."

Englar expects the work – done under contract with the Oak Ridge National Laboratory – to reduce aerodynamic drag by at least 35 percent, and perhaps by 50 percent or more. A 35 percent drag reduction translates to about a 12 percent drop in fuel consumption for tractor-trailers. If applied to the entire U.S. fleet, that would save an estimated 1.2 billion gallons of fuel a year.

Beyond the fuel savings, however, the Circulation Control system being developed and evaluated in GTRI's wind tunnel could improve directional control for trailers, increase traction and augment braking. Also known as pneumatic control, this aerodynamic system could also create lift on the trailer, effectively reducing its weight. That would cut rolling resistance on tires, reduce wear and also increase fuel economy.

The pneumatic system works by blowing compressed air from slots located on different parts of the trailer. Air blown over curved surfaces on top of the trailer smooths airflow there, decreasing drag and making the entire trailer act like a wing to lift as much as 15 percent of the weight off the tires. Blowing air from slots on the bottom of the truck would have the opposite effect, multiplying downward force on the tires to improve traction and braking when needed. Combined blowing from all sides further reduces flow separation and drag.

Blowing slots on each side of the trailer could counter crosswinds, giving the driver a way to fight the effects of sway, as well as jackknifing. By selecting the right slot combination and blowing rates, the pneumatics could be used to increase drag to augment aerodynamic braking.

"We can augment force and/or moment, either increasing it or decreasing it, and produce it in whatever direction is needed, all without any moving external surfaces," Englar explains. "Producing aerodynamic drag and increasing resistance on the tires could really help truckers in difficult downhill areas or for emergency stopping. Beyond the fuel cost issue, there is a lot of interest in this from the standpoint of improving safety."

Controlled by internal fast-acting valves, the pneumatic system would respond quickly to driver actions. "It would only take a fraction of a second between when the driver initiated the pulse and when the system would cause the effect," Englar says. "Using an automated system, the driver wouldn't even have to think about how it works. Pressing the brakes or accelerator, or moving the steering wheel, would cause the proper blowing slots to come on and assist the conventional controls."

Compressed air for the system could come from exhaust gases, the turbocharger on the truck engine, storage tanks or an electrically powered compressor in the trailer.

Englar's research team at the GTRI Aerospace, Transportation & Advanced Systems Lab has begun testing small-scale truck models in GTRI's low-speed wind tunnel. With computational support from Assistant Professor Marilyn Smith and graduate students in Georgia Tech's School of Aerospace Engineering, this initial program will evaluate the effectiveness of the pneumatic system and pave the way for eventual testing on full-size vehicles. The work was described in a recent paper at a meeting of the Society of Automotive Engineers (SAE).

"There would be both fuel savings and a safety payoff, so the synergies are really quite interesting," says Victor Suski, a senior automotive engineer with the American Trucking Associations. "Everybody who has heard about this intuitively feels there is great potential here."

Rising fuel costs have boosted interest in fuel economy improvements, but most efforts so far have focused on the tractors that pull the large trailers. Suski believes future efforts should target reducing drag on the trailers.

"All of the benefits that are yet to be gained in fuel economy will probably come from refining the trailer aerodynamics," he says. "Until that is done, we will continue to see trucking companies going out of business because they cannot afford their fuel bills. Fuel is not going to get cheaper over the long term."

Suski sees the potential for improving the average fuel efficiency in heavy trucks to as much as 12 miles a gallon, up from an industry average of less than 6.8 miles a gallon today. If testing on full-sized vehicles demonstrates the savings expected, truck purchasers will demand the new technology, and manufacturers will incorporate it, he predicts.

Because fuel savings can be easily quantified, they will drive advancement of Circulation Control technology. But if the expected safety improvements ultimately result in lower accident rates, reduced insurance premiums could also add to the benefit, he notes.

Circulation Control systems were developed and tested on fixed-wing and rotary-wing aircraft by Englar and his associates in the 1970s and 1980s as a simplified means of greatly increasing lift, improving control and reducing take-off and landing distances. During the 1990s, GTRI engineers applied the technique to automobiles, demonstrating significant savings in drag and energy use.

Protected by two patents, the automotive application – known as "GTRI FutureCar" – produced measured drag reductions of up to 35 percent by altering the flow separation and vortex formation around the rear of the vehicle. Englar believes even larger reductions may be possible on trucks, which will gain substantial drag reductions above the basic streamlining already used in passenger cars.

"Clever design can already take perhaps 10 to 15 percent off the drag on a tractor-trailer just through good non-blown aerodynamics," he says. "The trucking industry is already making use of fairings and other devices to reduce drag, but much more can be done."

Rounding off corners on trailers, matching the fairing height on tractors to the height of trailers and reducing the gap between tractor and trailer are among the steps that GTRI tests have shown would reduce drag and improve fuel economy, he notes.

The Georgia Tech team has been working with major manufacturers of tractors and trailers to ensure that recommended changes would be practical. Englar expects much of the technology could be retrofitted onto the existing truck fleet as it becomes standard equipment on new vehicles.

Once the Circulation Control techniques have been demonstrated in the wind tunnel, the researchers will work with the Department of Energy and the American Trucking Associations to scale them up for testing on real vehicles. Trucks equipped with the new devices would be tested against standard vehicles across a wide range of conditions.

The research is sponsored by the U.S. Department of Energy, Assistant Secretary for Energy Efficiency and Renewable Energy, Office of Heavy Vehicle Technologies, under contract DE-AC05-00OR22725 with UT-Battelle, LLC.

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Research Horizons

Lowering the Cost of Ownership

Information technology pays dividends in maintenance and logistics for aircraft, transit buses and other high-value systems.

By John Toon

"We're finding ways to lower the total cost of ownership."

That statement wouldn't be unusual in the context of the latest corporate accounting software or a new heating and air conditioning system. But when Gisele Welch says it, she's discussing the P-3 Orion, a Navy antisubmarine aircraft built by Lockheed Martin Aeronautics Company starting in the 1960s.

courtesy Lockheed Martin Aeronautics Co.

A P-3 Orion military aircraft flies over Stone Mountain in metro Atlanta.

As director of the Logistics and Maintenance Applied Research Center (LandMARC) at the Georgia Tech Research Institute, Welch includes in that goal a wide range of complex systems that are costly to maintain, from transit buses and trains to industrial equipment and aircraft like the P-3.

The goal is to use the latest information technology – along with sensors, hand-held diagnostics, wearable computers, CD-ROMs, Web portals, radio frequency tags, airborne recording devices, computer-based training and whole range of other technologies – to improve a long-neglected aspect of these systems: maintenance and logistics. The center focuses on four major areas: integrated logistics, supply chain management, systems sustainment and predictive diagnostics.

"We intend to improve every aspect of logistics and maintenance using technology that has already been developed for other applications and integrating it into open-architecture systems," she explains.

A recent Department of Defense study found that maintenance accounts for more than 60 percent of the lifetime costs for complex military systems, notes Ron Wagner, a former Navy aviation maintenance officer and co-director of LandMARC. As these systems continue in active service much longer than their designers envisioned, maintenance becomes more difficult, costly and time-consuming. Yet until recently, cost containment efforts in federal agencies focused largely on initial acquisition costs.

Saving the Navy $1 Million a Year on One Repair

The LandMARC approach offers tremendous potential benefits. For instance, Georgia Tech, Lockheed Martin and a team of small businesses are working together on a project aimed at cutting $1 million a year from P-3 maintenance costs by improving diagnostic techniques on just one major repair item.

The demonstration project focuses on the engine-driven compressor, which supplies air for several key systems and is the aircraft's single most costly repair item. Because the equipment is difficult to diagnose, more than 40 percent of the compressors replaced on the aircraft are not really defective. The cost of these unnecessary "false repairs" amounts to $4 million a year.

photo by Gary Meek

Georgia Tech and Lockheed Martin are working together on a project to reduce maintenance costs for the P-3 Orion. In the foreground are, left to right, Tom Sprague of Lockheed Martin, Gary O'Neill and Gisele Welch of Georgia Tech, and Charlie Levinge of Lockheed Martin. In the background are, left to right, students Jennifer Sheridan, Ben MacDonald, Keesah Hall and Ethan Adler. (300-dpi JPEG version - 497k)

But by providing technicians with better information and new equipment to more accurately troubleshoot problems, the partners expect to reduce that false removal rate by 25 percent, saving the U.S. Navy $1 million per year on that part alone.

A key part of the P-3 project is an Electronic Performance Support System (EPSS) that will integrate hand-held diagnostic equipment, electronic links to supply system computers, wearable computers for displaying repair manuals, computer-based training and airborne data collection equipment originally developed for electronic warfare testing.

GTRI researchers, including Georgia Tech computer science undergraduate and graduate students, are also merging disparate databases into a single Web-based information portal for repair technicians. That system will replace thousands of pages of paper documentation, making the information more accessible and easier to update.

"We are attacking the cost of labor by giving technicians better tools to reduce the time it takes to troubleshoot, fill out paperwork, repair a malfunctioning component, test it and put the aircraft back into service," Welch adds. "If we can make better use of the technician's time, we can reduce the cost of maintaining these older aircraft."

Work at LandMARC benefits from 30 years of Georgia Tech experience with testing electronic warfare equipment, planning routes for military aircraft, making documentation available through portable learning systems, integrating different types of information systems and connecting wireless devices to computer networks. The center plans to put these proven systems to work in new ways.

One example is the Firefly Data Recorder, originally developed to collect data from radar warning receiver tests. In LandMARC's hands, the equipment will monitor performance of engines, compressors and other aircraft systems, giving maintenance technicians a comprehensive view of system performance at the conclusion of a flight.

"Maintenance staffs need to know at the end of a flight what systems may need inspections," Wagner explains. "They also need to collect predetermined data to apply to their long-term scheduled maintenance."

Georgia Tech and Lockheed Martin hope this initial 18-month project, launched last summer, will lead to other opportunities to help the company's customers.

"Lockheed Martin's motivation is to demonstrate our support for education and research in our community, and at the same time reduce maintenance costs and improve operational readiness for our customers," says Charlie Levinge, Lockheed Martin P3/S-3 logistics manager.

Making a Difference in Buses & Industrial Systems

Older aircraft are just one target for LandMARC researchers.

"Aircraft, buses, trains and industrial equipment have a lot in common from a maintenance standpoint," notes Gary O'Neill, a former aerospace engineering duty officer and also a co-director of LandMARC. "By using open-architecture existing tools, it's usually straightforward to adapt the data set and architecture to other applications."

A Two-Way Street for Students

Graduate and undergraduate students form the backbone of research activities at universities like Georgia Tech. The contributions students make to the projects are obvious, but the benefits they receive can be equally important.

For Ethan Adler, Georgia Tech's P-3 maintenance project has meant a chance to develop a real-

Like aircraft, transit buses and trains have long lives and significant maintenance costs. The researchers have worked with the Metropolitan Atlanta Rapid Transit Authority on a proposal to apply advanced technologies to reduce maintenance costs – and perhaps head off breakdowns before they occur.

"Every day they take the buses to be fueled, and they could easily hook up a device that draws down diagnostic information from the previous day," says O'Neill. "That would allow them to track important parameters and discover systems that might need inspection. They could also develop long-term trends that would allow identification of emerging issues."

From a telltale vibration, such a monitoring system could warn of a failing transmission in time to avoid a breakdown. Analysis of repairs could allow a transit agency to reduce its parts inventory, stocking only those components likely to be needed.

One study showed that technicians spend as much as 40 percent of their time walking back and forth between the vehicle they're maintaining and the manuals housed at the technical center. Putting repair manuals online and making them accessible through portable computers would eliminate that wasted time and motion. These systems could also give technicians access to parts inventory information, and allow real-time consultation with engineering personnel at equipment manufacturers.

Information systems could also house the collective knowledge of many skilled technicians, making that expertise available to all and helping new personnel get up to speed faster.

"We are using the new information and communications technology to fuse information into a usable form and make it available at the repair point," Welch explains. "Improving the efficiency of maintenance and logistics is really an information technology issue – how information is collected and distributed."

Even non-mobile equipment could benefit from the application of information technology. Just-in-time production systems have made the reliability of industrial process equipment crucial. Shutting down a production line because of a machine failure can be expensive, especially if it means missing customer deadlines. Predictive diagnostics would set maintenance schedules and warn of impending failures in time to avoid them.

Information Technology to Help People Stay Healthy

Less obvious, but with even more potential impact, are the parallels between maintaining machines and maintaining human health. With their sea of records, medical information systems offer similar opportunities for improvement, Welch says. Giving medical personnel better electronic access to patient information and diagnostic reference data could help hold down costs and improve the quality of care.

"The infrastructure and architectures that we are developing apply to the medical field," she notes. "Right now, we are focused on the maintainer and technician, trying to get them the information they need. But you could easily apply that to medical personnel, bringing together different information systems in a way that would be transparent to the users."

world Oracle information system and learn how it works together with a Web interface. The task, along with Java programming, complements the more theoretical understanding he's gained in class.

"This will definitely be useful to me," says the College of Computing undergraduate. "We're doing a real-world project, and we have the freedom to study the needs and recommend the best way to approach it. Having this experience is extremely important."

Interviewing technicians at the Metropolitan Atlanta Transit Authority gave Valerie Lafond-Favieres new insight into the human-computer interface issues she's studying in class.

"It makes all the difference in knowing what kinds of questions to ask users, and knowing what kinds of things to look for," she says. "In some cases, our assumptions were wrong, and the technicians told us that. Having a real client gave us a good experience."

– RH

Beyond diagnostics, the information system could reduce paperwork and speed reimbursement by using intelligent agents to sort through records that must now be reviewed by medical consultants.

Students, Other Groups Keys to Center's Work

When Lockheed engineers designed the P-3 during the 1950s, they could never have imagined what would happen on a chilly day in November 2000. On that day, four Georgia Tech students scaled a ladder at Lockheed Martin's Marietta plant to walk through a P-3 being analyzed as part of a program to extend the aircraft's service life.

The students, none of whom had been born when the aircraft was built, are providing creativity and energy to accomplish LandMARC's mission. But it is a two-way street.

"I want to make sure these students can function in a real-world environment and not just be book-smart," says Welch, who holds an academic appointment in Georgia Tech's School of Electrical and Computer Engineering. "We allow students to gain an understanding of why they're doing what they do. They see why open architecture is important, why they should document the code they write, and why they should have regular group meetings. They are the system designers of tomorrow."

Drawing on resources from throughout Georgia Tech, including students and other researchers, will be key to the new center's success, Welch says. The center's small core staff will apply basic research done elsewhere in such diverse areas as logistics, predictive diagnostics, component re-engineering, technology insertion and advanced sensors.

Among the Georgia Tech groups involved are The Logistics Institute, the Center for Integrated Predictive Diagnostics, and five of GTRI's laboratories.

"We want to be a product development team," O'Neill adds. "We find the needs in the marketplace, bring them into Georgia Tech, assemble a team from the labs and academic schools, then produce a total solution. We will reach out wherever necessary to get the talent for the team."

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Research Horizons

Chemistry without Chemicals

Supercomputer helps theoretical chemists understand complex processes.

By John Toon

There are no test tubes, reagent bottles, fume hoods or hazardous waste containers in the laboratories of theoretical chemists Rigoberto Hernandez and David Sherrill.

The work of these researchers takes place instead at the keyboard of a powerful supercomputer. Using models based on deep knowledge of chemical processes, the computer simulates the hopping of electrical charges and breaking of chemical bonds at a level of detail no other technique could provide.

photo by Gary Meek

Theoretical chemists Rigoberto Hernandez, left, and David Sherrill are using a powerful IBM supercomputer to ask more complex questions and get faster, more detailed answers without mixing the first chemical. The technique provides clues to chemical engineering mysteries that cannot be investigated any other way, and reduces trial and error in research. (300-dpi JPEG version - 747k)

Though the results must still be verified by old-fashioned experimentation, computational chemistry allows scientists to ask more complex questions and get faster, more detailed answers without mixing the first chemical. The technique provides clues to chemical engineering mysteries that cannot be investigated any other way, and reduces trial and error in research.

At the Georgia Institute of Technology, researchers use this technique to study protein folding, anti-cancer drugs, molecules key to the vision process and polymerization.

"If you can do the experiments on the computer and try all the 'what-ifs' that way, at the very end, the one reaction you really need can be done in chemistry," says Hernandez, an assistant professor in the School of Chemistry and Biochemistry. "By finding the very best solution on the computer, you can limit the waste products by eliminating trial and error. This doesn't do away with experimentation, but it gives the chemist another tool."

Chemistry in Changing Environments

In common chemical processes, the reactants make up a small part of the overall environment, which does not change substantially as the reaction proceeds. In such systems, the environment is considered to be at equilibrium.

Hernandez, however, studies non-equilibrium reactions in which the reacting chemicals form a large part of the overall environment. In such systems, the environment changes as the reaction proceeds, affecting the chemistry in ways that are difficult to model and study. This complex interaction between reaction and changing environment affects the outcome in important ways.

"In many cases, the final properties of the material are determined by their history," he explains. "I want to understand how things are formed, not just to characterize their properties once they are formed."

Protein folding provides an important example. After creation, proteins fold through a complex chemical process that involves as many as 200 different amino acid residues. Different folds give the proteins different properties. In some cases, such as amyloidogenic proteins associated with "Mad Cow Disease," a wrong fold creates a harmful protein: the scrapie form of prions.

"There is increasing evidence that the wrong folds are due to a kinetic or dynamic process," Hernandez adds. "We as dynamicists are asking how a sequence with a given structure goes to that folded structure. By understanding those dynamics, we would be able to say something about altering the sequence and preventing it from folding that way."

A supercomputer model accounting for complex changes in reactants and environment may provide answers that researchers could find in no other way.

Among industrial applications is the way in which thermosetting polymer materials form. Used in applications such as microchip packaging and automobile parts, the starting materials include long-chain polymers, cross-linking agents, fillers and dyes. In manufacturing, the mixture is heated to liquid form, allowing the polymers to react and chemically link into a final product whose properties depend on its thermal history – that is, how quickly it was heated and allowed to cool.

Like protein folding, the polymerization reaction does not occur in equilibrium because the process of cross-linking significantly affects the reaction environment. A clearer understanding of the processing dynamics, obtained through computer models, should give materials scientists better control in selecting the starting materials.

"You would be able not only to predict what a particular composition is going to do, but also determine what the initial conditions should be for a desired outcome," Hernandez says. "That would allow you to design thermosetting polymeric blends that would be optimal for your particular mold or system."

Computational Quantum Chemistry

Understanding complex reactions is also important to Sherrill, an assistant professor whose focus is electronic structure theory and its application to photochemistry and highly reactive systems. His work has implications for improving anti-cancer drugs, understanding the process of vision and tracing the role of copper in the body.

The enediyne family of anti-cancer drugs provides a vital weapon in the battle against the dreaded disease. The highly reactive chemicals contain two radicals that "steal" hydrogen atoms from the DNA of cancer cells, triggering destruction of the cells. Although experiments have shown the basic steps of the diradical reaction, detailed computer models could give new insights into how to tune the reactivity by adjusting the chemical structures of the drugs. Having that information would help scientists produce better anti-cancer drugs.

These computational studies will require the development of new theoretical techniques because current models can't accurately describe the highly reactive diradicals, or more generally, any bond-making or bond-breaking processes.

"To get a very detailed understanding of the whole process, going from reactants to products and watching it happen in between, you usually are breaking chemical bonds," Sherrill explains. "You would like to be able to describe that theoretically, including the entire reaction path, not just the beginning and the end."

Sherrill also works with Professor Mostafa El-Sayed and Clemens Burda, both of Georgia Tech's Laser Dynamics Lab, in better understanding a family of molecules essential to the vision process. These molecules twist when they absorb photons of light, a process that has been studied – but not fully explained – using high-speed laser dynamics.

"Apparently something happens during the course of the twisting that isn't completely understood," Sherrill explains. "It is hypothesized that some intermediate structure influences the twisting, but that structure has not been observed. If we can find it through our modeling, it may apply to the whole class of molecules."

Beyond its implications for vision research, the work could lead to improvements in color photography and the capture of solar energy.

In a third major project, Sherrill helps Professor Christoph Fahrni in designing a molecule that will bind to copper ions and emit light. Measuring the phosphorescence would then allow scientists to see where copper concentrates in cells, information important because of the role copper plays in biochemistry.

Fahrni has begun designing candidate molecules in the laboratory even as Sherrill models them on his computer. In this collaboration, theory suggests directions for the experiments to take, and experiments calibrate the theory.

"If the theory gives good predictions, we can go ahead and tweak some of the parameters theoretically and suggest better alternatives that can then be made in the lab," Sherrill says. "This could help keep Christoph from having to make dozens of structures that may not work."

Already, the work with collaborator Professor Alan Gabrielli of Southern Polytechnic State University in Marietta, Ga., has led to unexpected results that further the understanding of the phosphorescence of such probe materials.

New Supercomputer Accelerates Efforts

The computational chemistry work of Hernandez and Sherrill advanced in October 2000 with the installation of a 72-processor IBM SP supercomputer that forms the core of the new Center for Computational Molecular Science and Technology. The machine, shared with other researchers in the College of Sciences and elsewhere at Georgia Tech, is one of the most powerful academic supercomputers in the Southeast.

It promises a dramatic increase in the speed at which simulations run, doing in a few hours what would have taken a week of number crunching on smaller computer workstations. It also allows researchers to undertake more complex and accurate simulations that they could not even attempt before.

"This will allow us to do some very high accuracy calculations on some benchmark molecules that were inaccessible before," Sherrill says. "It will make a tremendous difference."

Because the reactions Hernandez and Sherrill study are so complex, limits on computing power have forced them to rely on approximations that do not take into account all the variables that could influence the outcome. The supercomputer will alter that trade-off, enabling simulations with fewer compromises.

By speeding up the simulations, the machine will also change the way in which the researchers work, allowing them to be more productive and creative in following up unexpected results.

"If you have a calculation that takes a week for you to complete, you've got to have a lot of different things going on at once while you're waiting for the calculations to be done," Sherrill explains. "But if you could get the results in a couple of hours, you could immediately see what didn't work and how to change it. You could be a lot more interactive and recover more quickly from mistakes."

Based on IBM's new copper chip technology, the machine boasts 47 gigabytes of memory and 764 gigabytes of disk storage. Despite its power, Hernandez isn't advising researchers to discard their test tubes just yet.

"In order to do everything on a computer, we would have to devise a theoretical model able to mimic nature completely," he says. "I believe that we are always going to have surprises from nature."

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Research Horizons

A New Kind of Information Highway

Urban transit systems would take advantage of state-of-the-art computing and communications technology.

By Jane M. Sanders

In the past, all an urban commuter needed to get to work was a car and a highway. But now, metropolitan area highways have become clogged with rush-hour traffic, and commuters need more than their ride and the road. What they need, according to a Georgia Institute of Technology professor, is the power of computing and wireless digital communication.

"Advances in communications, primarily wireless, and computing have made it feasible to make massive substitutions of information technologies for hardware – such as roads, cars and rails – and energy, such as gasoline," says Steve Dickerson, a professor emeritus of mechanical engineering.

photo by Gary Meek

Professor Steve Dickerson has proposed a plan for an Information Intensive Transit System that will take advantage of digital and wireless communication technology and possibly reduce traffic congestion. (300-dpi JPEG version - 225k)

Dickerson has devised a plan that calls for commuters to use digital wireless devices to communicate with a central computer system that automates, and thus improves the efficiency and convenience of, mass transit systems, such as Atlanta's MARTA, and carpooling.

The Information Intensive Transit System (IITS) aims to reduce the uncertainty of pick up and trip times (estimates would be within 60 seconds of the actual time), and also give commuters mobility once they arrive at work. The system is based on digital wireless communication, global positioning system (GPS) locating technology and high-powered computers to provide real-time service for passengers and vehicle drivers. Dickerson and Georgia Tech applied for a provisional patent on the system in the spring of 2000, although by agreement any use in Georgia would be royalty free.

"The fundamental premise is that the technology needed for real-time service has become very cheap, particularly in terms of additional investment," Dickerson says. "A lot of the infrastructure is already in place."

The IITS would: (1) work with existing systems, such as rail and bus transit, vanpooling and carpooling; (2) create additional ride sharing; (3) provide convenient, low-cost car rentals throughout the metro area; and (4) feature electronic automatic billing and user identification.

Though his mechanical engineering research is not related to transportation, Dickerson has experience in the field. He served a year with the office of the Secretary for the U.S. Department of Transportation and started two successful bus and vanpool services in metro Atlanta. Now retired from Tech, he wants to find a mechanism to fully implement the IITS. It will dramatically reduce congestion on roadways and reduce air pollution, Dickerson says.

"We just have to do this. It just makes so much sense," he adds.

The IITS would work this way. Participants would pre-register for standard trips – such as a ride to work – which would be associated with defined origins and destinations. Then, participants could request a standard trip by pressing a single-digit code on a cellular phone or two-way pager.

Using an off-the-shelf telecommunications technology, the scheduling computer would know from the sending unit's signal the participant's name and what trip was being requested. The scheduling computer would then use GPS data, vehicle schedules and other information to find one or more trip alternatives (which would vary daily for increased ride-time flexibility) and tell the user the pickup point, pick up time and arrival time at the destination. The computer would notify the passenger via cell phone or pager, and the passenger could accept a ride or ask for more choices. If the passenger accepted a carpool or vanpool trip, the system would notify the driver via a hands-free, in-vehicle display and/or audio system. The passenger's telecommunications device would identify the approaching ride vehicle by a tone on the cell phone, for example.

photo by Everett Hullum

Atlanta's traffic is among the worst in the nation. (300-dpi JPEG version - 1.04mb)

"This system would make a shared ride more attractive, particularly for commuting trips," Dickerson says. ". . . To make shared rides attractive, you must reduce the uncertainty of the trip time and provide flexibility, which this system would do."

Once at work, commuters still need mobility at times, Dickerson says. So commuters need automated, low-cost access to rental cars, which could also be carpool vehicles during commuting hours. Other vehicles would be available to commuters who would need to rent a vehicle overnight.

Participants needing a car rental would also be registered for standard originations for rental trips. When a participant requested a rental, the system would ask the user for an estimate of time for the rental and then tell the user which car to take from the pool. Rental cars would not require a key, but rather be authorized for a particular user through the IITS telecommunications system.

Under Dickerson's plan, every IITS participant would have to be a subscriber who undergoes screening for criminal history, credit worthiness and, in the case of drivers, both driving record and insurance coverage. Safety features of the system would: (1) give drivers a description of riders and vice versa prior to pick up; (2) track participants' actual pick up and arrival times; and (3) give all participants the ability to notify the system and authorities of an emergency via pager and/or cell phone.

Scheduling and billing for rides, including mass transit, and rentals would be totally automated, so there would be minimal costs for operating the IITS. Dickerson estimates the cost per participant transaction with the system would be less than one cent for computing and communications.

Because ride sharing adds little to no cost for a driver who is already making the trip anyway, drivers would not be paid for driving. They would, however, receive a stipend from the system for their vehicle's operating and capital costs, depending on the average number of passengers hauled and flexibility in their schedules.

Dickerson cautions, however, that the IITS likely would need a public subsidy. He justifies it this way: "When you use mass transit or a ride share system, you create a benefit for other drivers using the road. You decrease congestion. It's called an economic externality. The benefits did not all accrue to participants in the ride-sharing system, but rather to all users of the road."

Also, Dickerson points out that the IITS would not compete with existing bus and rail transit. Rather, the system would increase ridership at less cost per additional passenger than a conventional expansion in terms of miles of rail or expanded bus routes. "The cost of additional passenger trips, on rail particularly, is very small if all that is required are longer trains," he explains. "The trick is to make such trips attractive in terms of certainty of schedule, mobility without a car at the destination, safety and ease of payment."

As for getting the IITS plan off the ground, Dickerson believes a pilot implementation in a target area of metro Atlanta would prove its worth for car rental and pooling. MARTA schedules could be included metro-wide without much difficulty, he adds.

"Atlanta is a great place for a pilot study," Dickerson says. "It has the right traffic conditions, population density and strong expertise in telecommunications and wireless service."

It would cost about $1 million to implement an IITS pilot program. Most of that cost would be for software development. If funding becomes available by early 2001 – perhaps through a corporate and government partnership – software development could begin shortly thereafter, and a pilot study might get started by the end of 2001. Full implementation of the system could begin as early as 2002, Dickerson says.

Getting leaders to "buy in" to the IITS is more of a challenge than funding, Dickerson admits. He hopes several groups will form a non-profit corporation representing a partnership between Georgia Tech, regional transportation and planning authorities, mass transit providers, cellular providers, communication technology suppliers and vehicle suppliers.

As for getting commuters' support, Dickerson estimates that 10 percent of them would initially participate in the IITS. After the system proved itself beneficial, more commuters would participate, he predicts. He likens short-term and long-term participation in the system to drivers' response to increased gas prices. In the short term, there has been little change in people's driving patterns. However, in the long-term, people will buy fewer gas-guzzling sport utility vehicles and be more receptive to mass transit – particularly if it has good performance.

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Research Horizons

Research Notes

Anticipating Devices of the Future

Studies lay groundwork for nanojets and silicon nanowires.

• Silicon Nanowires for Future Electronic Devices

Large-scale simulations of silicon nanowires just several atoms in diameter have given device designers new clues about how these nanometer-scale devices will one day perform. The work provides a basis for anticipating how the quantum mechanical effects that dominate behavior of materials at this size scale will alter the operation of future generations of electronic devices.

Writing in the Aug. 28, 2000, issue of *Physical Review Letters*, Uzi Landman, Robert Barnett and Andrew Scherbakov from the Georgia Institute of Technology, and Phaedon Avouris from the IBM T.J. Watson Research Center, report on issues pertaining to the atomic structure, electronic properties and electrical transport in silicon nanowires. These issues will have to be considered by designers using devices this small.

photo by Gary Meek

Georgia Tech physicist Uzi Landman won the 2000 Feynman Prize in Nanotechnology for his pioneering work in computation materials science for nanostructures. (300-dpi JPEG version - 776k)

"It's a much-discussed expectation that devices of this size will be different, but in what ways and by how much, remain unknown," says Uzi Landman, Regents' Professor of Physics and director of the Georgia Tech Center for Computational Materials Science. "In this study, we have explored certain unique properties of systems this small through first-principles quantum mechanical simulations. Such simulations, which are to the best of our knowledge the largest ones to date, are essential for gaining reliable and predictive information about these systems."

To boost speed and reduce energy use, engineers are being pushed to make electronic devices smaller and to pack more of them onto a chip. This pressure eventually will drive them to use features as small as 1 nanometer (one-billionth of a meter, or a hundred-thousandth the width of a human hair). When that happens, he noted, device operation will be dominated by quantum mechanical effects – and the expectations that have long governed device design will no longer apply.

The researchers simulated silicon nanowires etched from bulk silicon, or self-assembled from clusters containing 24 atoms of silicon. In each case, the silicon was passivated by attaching hydrogen atoms to unused bonds, and the wires were connected to aluminum leads.

The theoretical simulations produced data on the nanowires' electrical conductance, the influence of the silicon-metal interface and the role that doping with aluminum atoms may play in changing materials properties. The work also suggests new ways of doping ultra-small transistor channels that could circumvent some current technological issues.

"This work attempts to fill in some of the gaps in our knowledge in this area," says Avouris, manager of Nanometer Scale Science & Technology at the Watson Research Center in Yorktown Heights, N.Y. "While the wires on which we report here are significantly smaller than those likely to be used in the near future, they are particularly useful because they tell us what to expect in the fully quantum mechanical limit – the ultimate miniaturization limit. The calculations have revealed a number of significant changes in important properties."

Carried out on an IBM SP-2 computer at Georgia Tech, the simulations revealed that:

• Electronic states formed from a combination of orbitals from the aluminum leads and the silicon wire atoms penetrate all the way through nanowires of less than about 1 nanometer in length, giving such silicon bridges a finite conductance. But in longer structures, these electronic states penetrate only partially into the nanowire, with the silicon retaining its semiconducting properties.

• The transfer of electrons from the aluminum to the silicon at the junction between the two materials creates a localized dipole that forms a barrier to the flow of electrons. Simulations show the height of such Schottky barriers at nanoscale metal-to-semiconductor contacts may not be too different from those found at more familiar-size scales.

• The simulations suggest a way that could overcome some of the anticipated problems involved in doping the silicon used in devices this small. Doping of semiconductors is used routinely to tune and optimize device characteristics. But in nanoscale devices one may expect detrimentally large device-to-device statistical variations of the dopant concentration. This variability could cause severe problems at this size scale because electronics designers may not consistently predict the performance of a collection of such devices. But the simulations suggest that building nanowires from silicon clusters could offer a solution. Because the clusters form hollow cages, much like carbon fullerenes, they could be fabricated around a dopant atom. With each cluster then containing a dopant atom, device consistency may be achieved.

• The wave-like nature of the electrons could cause interference effects in the electric conductance through the silicon nanowires used as current channels. When voltage is applied to open the channel, electrons penetrating the silicon nanowire from one of the aluminum leads may bounce off the contact to the other lead and flow back toward the source contact. Upon reaching that contact, they may bounce off again, and the process may repeat itself.

This behavior results, at certain electron wavelengths and wire configurations, in interference resonances that cause the channel to appear transparent, leading to the occurrence of spikes in the current flowing through the nanoscale channel.

"When building a device, engineers would have to take this into account and either find ways to use it or avoid it," Landman adds. "In macroscopic devices, this phenomenon is of no particular consequence, showing again that small devices are different in ways that go beyond simple scaling with size."

The research was sponsored by the U.S. Department of Energy.

– ***John Toon***

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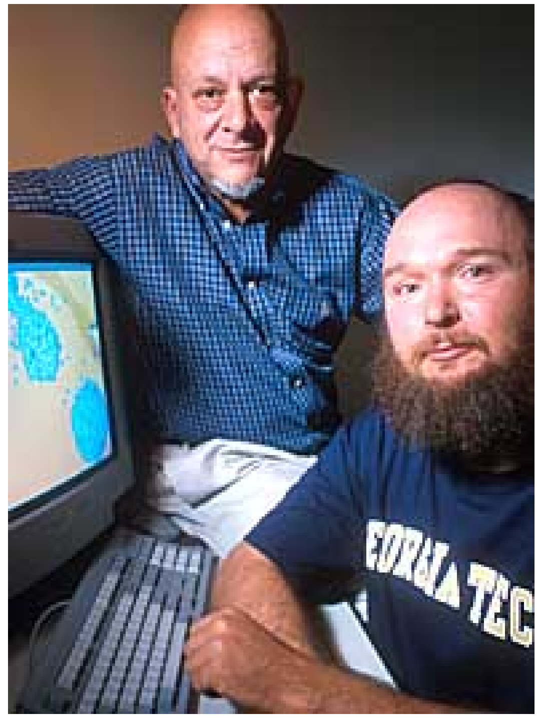
Anticipating Devices of the Future

• Nanojets for Smaller Circuitry, Gene Injection

Liquid jets a few nanometers in diameter could one day be used for producing ever-smaller electronic circuitry, injecting genes into cells, etching tiny features and even serving as fuel injectors for microscopic engines.

But on these smallest-of-size scales, physical processes are often different than at larger scales, forcing engineers to reconsider both their expectations of how such nanoscale devices would perform – and the established physical equations governing them.

photo by Gary Meek



Researchers Uzi Landman, left, and Michael Moseler display a sequence of simulations showing the exit of propane from a nozzle just six nanometers in diameter. Liquid jets a few nanometers in diameter could one day be used for producing ever-smaller electronic circuitry and injecting genes into cells.

Writing in the Aug. 18 issue of the journal *Science,* Georgia Tech researchers suggest that jets as small as 6 nanometers in diameter may be possible to produce. But these tiny devices would require special conditions to operate and be particularly sensitive to effects not of concern at more familiar-size scales.

"We are now being driven by fundamental, technological and economical considerations to explore and evaluate systems that are smaller and smaller," Landman says. "We need to understand these systems, because basic physics issues are especially important to them. There is no point in trying to make devices of this size scale without knowing what their physical behaviors and fundamental advantages or limitations are going to be."

To study jets just a few nanometers in diameter, Landman and collaborator Michael Moseler used molecular dynamics simulations to observe how some 200,000 propane (C_3H_8) molecules would behave when compressed within a tiny reservoir and then injected out of a narrow nozzle made of gold. Operating on an IBM SP2 parallel processing computer, the simulations recorded the dynamics of the fluid molecules on the femtosecond time scale over periods of several nanoseconds.

In a second phase of their work, the researchers attempted to model their observations through the use of the traditional fluid dynamics formulation – that is, the Navier-Stokes equations. They found, however, these equations did not account for the effect of thermally induced fluctuations that significantly influence the stability and dynamic evolution of nanojets. While these fluctuations are of much less importance at larger-size scales, they become dominant at the nanoscale regime. Consequently, the researchers derived a modified form of the equations that modeled their simulation results remarkably well – thus extending fluid hydrodynamics to the nanoscale domain.

As a next step, the researchers would like to create nanojets experimentally and use them to apply patterns that could replace current lithographic processes in the manufacture of nanoscale miniaturized circuits. They might also be used as "nano gene guns" to insert genetic materials into cells without causing damage.

The nanojet work is supported by the U.S. Department of Energy, the U.S. Air Force Office of Scientific Research and in part by the Deutsche Forshungsgemeinschaft.

– ***John Toon***

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Wrestling with Rendering's Malodors

Researchers develop model regulations, but still face the complicated task of assessing and controlling odors from rendering plants.

Developed in part by researchers at the Georgia Institute of Technology, Georgia's rules for controlling and assessing malodors from food waste rendering plants could become a model for other states facing the same problem.

photo by Gary Meek

Meanwhile malodor control and assessment remains a complicated task. So Georgia Tech and University of Georgia researchers are working to improve treatment of odors so they don't waft into communities surrounding rendering plants.

"The problem of malodors from rendering plants is a longstanding issue. In fact, the industry dates back to Roman times. Today, it is a nationwide issue," says Jim Walsh, a researcher at Georgia Tech's Economic Development Institute.

Every year in the United States, 43 billion pounds of food processing waste materials are sent to rendering plants, where they are converted into pet and animal feeds. Of that waste, 23 billion pounds is from poultry. "The bottom line is if we didn't render this material, it would be in landfills," Walsh says. "Instead, it's turned into usable byproducts."

Dealing with the unwanted byproduct – that is, malodors – is the difficult part of the equation. Though the problem is being addressed by the rendering industry, there is not a fix-all solution in sight, Walsh says. "It's just what we expected," he adds. "Odor is a complicated issue."

Researcher Jim Walsh examines packing material from a malodor control biofilter operation at a food processing waste rendering plant near Cumming, Ga. Biofilters take airborne emissions from the plant and push them through a box filled with packing material, such as wood shavings or ceramic balls. Bacteria grow on the packing material, and then they eat and remove most of the odorous chemicals. (300-dpi JPEG version - 1.48 megs)

In Georgia, the malodor issue reached a boiling point in 1999 when citizen complaints prompted the state's Department of Agriculture to develop rules to help manage the problem. Agriculture officials called on Georgia Tech for assistance, and Walsh helped them develop the state's Malodor Control and Assessment Program (MalodorCAP), which became mandatory for rendering plants in August 1999.

The MalodorCAP consists of a control program and a complaint response program. Rendering facilities determine their critical control points (points in the operation where odors are controlled), establish critical limits (operating conditions for control equipment) at each critical control point, and determine corrective actions to be taken if they exceed critical limits. The complaint response program requires a facility to respond to any complaint, record the response on a form approved by the Georgia Department of Agriculture and keep a log of the complaints. State officials, with Walsh's help, regularly review and help update facilities' MalodorCAPs.

Though Georgia is taking the lead nationally in monitoring malodors, there are no state or federal limitations on malodorous chemical compounds emitted unless these compounds are classified as volatile organic compounds (VOCs) or hazardous air pollutants (HAPs).

"Odor is a subjective and not a quantitative issue right now, so current regulations address odor as a nuisance issue," Walsh explains. "But Georgia's malodor control and assessment rules are unique. They could serve as a model program for other states."

Now the state-funded Traditional Industries Program for Food Processing (FoodPAC) and the Agricultural Technology Research Program are supporting Walsh's efforts as a liaison between industry, researchers and regulators. Walsh is tracking the latest technologies and research, including projects ongoing at Georgia Tech and the University of Georgia.

Recently, the two institutions began a collaborative project to enhance wet scrubber odor treatment technology and improve monitoring for odors and VOCs in the food processing industry. Wet scrubbers transfer odorous chemicals and VOCs in the air to the water and neutralize them using oxidizing chemicals. But wet scrubber operations are often process-specific, and there is limited data available to effectively improve their performance. University of Georgia Professors K.C. Das and Jim Kastner hope their ongoing work in developing methods for chemical characterization of air emissions from rendering operations will eventually advance wet scrubber design. Characterizing malodorous chemicals is difficult because they tend to vary and occur in trace amounts, Walsh explains.

In the current project, UGA researchers are focusing on the mass transfer of specific odorous compounds into water. Specifically, researchers are continuing their chemical characterization studies, and also evaluating the efficiency and appropriateness of water-based treatment technologies. Georgia Tech Research Institute engineer John Pierson is examining potential improvements to the gas-phase pre-treatment of total VOCs. Specifically, he is working with the developers of two different novel chemistries to improve wet scrubber efficiency, and Pierson is developing a predictive monitoring system to better manage rendering plant emissions. Both the U.S. Poultry and Egg Association's Protein and Fats Council and FoodPAC are funding this joint project.

Researchers elsewhere are working on improvements to biofilters, Walsh adds. Biofilters take airborne emissions from the plant and push them through a box filled with packing material, such as wood shavings or ceramic balls. Bacteria grow on the packing material, and then they eat and remove most of the odorous chemicals. In Georgia, rendering plants in Cumming and Cuthbert have installed customized biofilters.

Progress in controlling malodors seems slow sometimes, but Walsh says: "I am constantly hearing of people developing new chemical treatments. A lot of research and development is going on, not only new chemical treatments, but new ways of controlling processing operations to eliminate odors."

– By Jane M. Sanders

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Crossing the Digital Divide

Research generates new telecommunications services in rural Georgia.

A Georgia Institute of Technology research project examining community technology practices has led to the development of several approaches for building better telecommunications programs at the local level in Georgia.

Under the name of TechSmart, these services aim to increase information technology skills, attract technology jobs, encourage capital investment in information technology and make related products and services more available and less expensive across rural Georgia – in short, to help bridge "the digital divide."

The research, funded by Georgia Tech's Economic Development Research Program and the Georgia Department of Community Affairs, examined the feasibility of developing an assessment tool for evaluating community readiness in terms of information infrastructure. The tool measures economic development professionals' awareness of several components, including:

- types of support for technology professionals;

- hardware, software and Internet access available to businesses and residents;

- an understanding of needs of major telecommunications customers and providers;

- an awareness of major community Web sites;

- the role played by those with technical knowledge in economc development.

To obtain a benchmark, the analysis drew on experiences of communities recognized as early adopters of information technology. Those communities included Newnan, Ga., and Blacksburg, Va.

Researchers later tested the tool in three rural Georgia communities: Hawksinville/Pulaski County, Jesup/Wayne County and Reidsville/Tatnall County. Officials there supplied feedback to improve the tool.

"There are many information technology- and telecommunications-related initiatives under way in rural communities and much potential for more," says Jan Youtie, the Georgia Tech researcher who headed the study. "Interestingly, little knowledge of this exists at the local level because community leaders are not accustomed to paying attention to this area."

Essentially, such assessments determine the gap between the current and desired state of readiness for e-commerce and economic development. Assessment results include recommendations for community leadership development and projects to bridge those gaps.

TechSmart not only provides a mechanism to conduct assessments, it also offers technology leadership training, awareness-building workshops, and facilitation of information technology projects related to education, government and business. To place these services closer to rural communities, extension centers staffed by Georgia Tech specialists are planned for Albany and Dublin and proposed for north Georgia outside metro Atlanta.

– ***Lincoln Bates, EDI***

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Research Horizons

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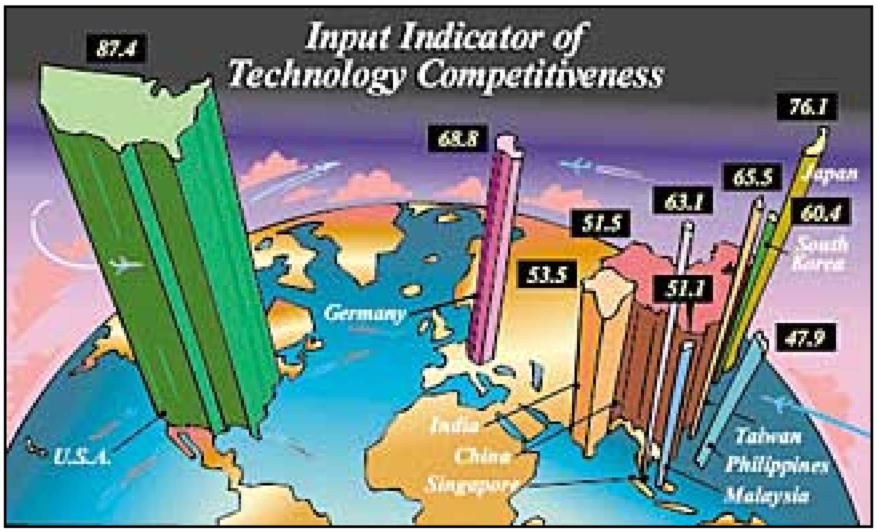
Competing for Technology Exports

Information-based economy is leveling the playing field, though U.S. retains lead.

A new study of international competitiveness may give U.S. producers of technology products another reason to be looking over their shoulders.

Illustration by Mac Evans



Composite competitiveness predictor (input) for selected countries, showing the leveling of the playing field for technology products. (higher resolution JPEG version - 130k)

Though the United States remains the undisputed world leader in exporting technology products, the Georgia Institute of Technology study of technological capabilities among 33 nations shows the industrializing countries of Asia quickly catching up, thanks to an information-based economy that facilitates rapid change. The National Science Foundation-sponsored study, "Indicators of Technology-Based Competitiveness," is the latest in a series of reports published every three years since 1987.

"Our study points to a much more competitive environment for the United States," says Alan Porter, director of the Technology Policy and Assessment Center at Georgia Tech. "The playing field is changing from a ski slope to a gentle plateau. No longer is the United States alone on the playing field with the Japanese."

Though the study evaluates nations as varied as Israel, Brazil and the Czech Republic, Porter sees the real action among the "Asian Cubs." These challengers – including China, India, Malaysia, Thailand, Indonesia and The Philippines – are moving up alongside traditional regional leaders, the "Asian Tigers" of South Korea, Taiwan and Singapore.

"There are eight or 10 countries in Asia that show dramatic changes," he says. "This includes countries like India and China that are going to be real technological powerhouses."

Over the past decade, these nations have developed the technological infrastructure to move from manufacturers of products to developers of products. The growth of indigenous engineering and management capabilities, development of research and development capabilities, and the rise of entrepreneurship signal this transition. Porter says, "When you put these together, you have a real productive capability."

An emphasis on information-based technology has facilitated the change.

"All of these industrialized and industrializing countries can now play in this technology arena," he explains. "The more information-based things become, the more quickly this happens because countries don't need as much heavy infrastructure. It's quicker to get up to speed on information-based technology than it was in heavy industry because of inertia."

The growing importance of new technologies such as genomics may step up that pace. Here, Porter warns, the cautious regulatory stance of the United States could prove a disadvantage in competition with nations that can easily adopt new information-based technology.

Porter and Professor David Roessner – also a faculty member with the Center – have jointly led the production of these "High Tech Indicators" every three years since 1987. Collaborators Nils Newman and Xiao-Yin Jin, respectively, led the compilation of statistical and expert opinion components (from an international panel of 300 experts).

The team derives four input indicators that influence a nation's long-term ability to produce technology products – national orientation (toward technology-based competition), socio-economic infrastructure to support this, technological infrastructure, and productive capacity. They likewise address three output indicators, including technological standing in world markets.

Among the output indicators, which measure the current state of technology export competition, the United States is the clear leader. In 1997, the United States exported $258 billion worth of high-tech products, compared to $152 billion for Japan, $140 billion for Germany, $105 billion for the United Kingdom, $90 billion for France and $70 billion for Singapore.

Of most interest are the input indicators that purport to predict future competitiveness of nations over roughly a 15-year horizon. A chart available online at gtresearchnews.gatech.edu/newsrelease/TECHCOMP.html presents a composite of the four indicators, each scaled to a maximum of 100 for the world's strongest country on that measure; they are then averaged. (The chart represents a composite for selected nations for 1999.) The tendency for toughening competition, particularly from the Asian nations, is apparent.

– John Toon

The full-text news release version of this article can be found at gtresearchnews.gatech.edu/newsrelease/TECHCOMP.html. **For more information,** contact Alan Porter, Technology Policy and Assessment Center, Georgia Tech, Atlanta, GA 30332-0205. (Telephone: 404-894-2330); (E-mail: alan.porter@isye.gatech.edu)

Coneheads at Work

70-Year-Old technology gets new life at Georgia Tech.

There are coneheads working in the Georgia Institute of Technology's School of Civil and Environmental Engineering. No, not the pointy-headed extraterrestrials of "Saturday Night Live" fame, but Georgia Tech engineers with more down-to-Earth interests.

courtesy of Paul Mayne

They take their nickname from a device called a cone penetrometer, which they use to ascertain the underlying stability and characteristics of a given parcel of land. The technique is actually some 70 years old, but it's getting a new look from these researchers.

Before the design of a major project such as a building, bridge or dam can begin, the ground underneath the proposed construction site must be tested to determine composition and other factors affecting its load-bearing capacity. The information helps engineers devise a foundation design to minimize settling and ensure the structure will stay in place.

In the United States, engineers prefer to gather this data by taking core samples. They use a drill to remove samples of earth at prescribed intervals and then bring them to the surface for study.

Below the James River Bridge in Virginia, Georgia Tech engineers use a cone penetrometer contained in a special GeoStar truck to probe up to 40 meters into the ground to determine soil composition and load-bearing capacity. Computers on the truck receive data directly from the penetrometer's four sensors. (300-dpi JPEG version - 1.9mb)

In the 1930s, Dutch engineers devised a system using a sensor probe with a pointed or cone-shaped end. Pushed into the ground, the probe's sensors electronically relay information about certain ground characteristics to technicians on the surface. Though still widely used in the Netherlands, where below-sea-level topography makes ground conditions an ongoing concern, the cone penetrometer attracted few followers in the United States. Then about 20 years ago with advances in computer technology, the benefits of cone penetrometers finally began attracting notice in this country.

Paul W. Mayne, a professor in the School of Civil and Environmental Engineering's Geosystems Division, has traveled across the Southeast collecting subsurface data in his research for the National Science Foundation and the U.S. Geological Survey.

His cone penetrometer is contained in a special GeoStar truck that also contains machinery for pushing the probe up to 40 meters into the ground and computers for receiving data directly from its four sensors.

"We can measure pore water pressure, resistivity, dielectric properties and shear wave as the probe is pushed into the ground," Mayne says. "It's much faster than boring out samples, plus you get four readings on a continuous basis. With the old-fashioned way, you have only one number for every 5 feet or whatever interval you're extracting samples."

In addition to accuracy, the penetrometer technique is cleaner because no large hole is excavated - the probe is a scant 36 millimeters in diameter. Also, measurements with a cone penetrometer cost about one-tenth of the price of the conventional method.

The basic penetrometer approach can be adapted to different applications, depending upon the properties the sensors are built to measure. Some devices provide information about ground chemistry, for instance, and are useful for environmental analysis of the subsurface. That particular use underscores the advantage of in-ground analysis because contaminated soil is not brought to the surface where it could cause further harm or, at the least, require costly containment steps.

While much of their work has been directed toward improved methods of evaluating cone penetrometer data, Mayne and his colleagues are inventing new types of "cones."

"We developed a device that measures the flow of water into the probe, and from that we're trying to determine the permeability of the soil material, also known as the hydraulic conductivity," he explains. Another design provides 10 independent readings of soil characteristics.

"We're trying to optimize and maximize the number of measurements we can make," Mayne says. "The more information that can be collected, the more applications we can find that will benefit from its use."

– Gary Goettling, *freelance writer*

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Faculty Awards and Honors

Professor **Phillip L. Ackerman** of the School of Psychology was appointed editor of the American Psychological Association's Journal of Experimental Psychology: Applied. Ackerman's research interests include adult learning, skill acquisition, selection, training, abilities and personality.

Assistant Professor **Dragomir Davidovic** of the School of Physics received a Packard Foundation Fellowship for his investigations of the physical properties of nanometer-scale conducting objects. Davidovic uses low temperatures and nanotechnology to test ideas that are vital to the quantum many-body theory. Packard Fellows receive research grants of $625,000 over five years.

Regents Professor **Mostafa A. El-Sayed** of the School of Chemistry and Biochemistry was elected a fellow of the American Association for the Advancement of Science (AAAS). He is recognized for his distinguished contributions to the field of ultrafast primary processes and for his service to physical chemistry as a journal editor.

Associate Professor **James Oliverio** of the College of Architecture was chosen by the American Society of Composers, Authors and Publishers (ASCAP) as the 2000 ASCAPlu $ Standard Award recipient. The cash grants are designed to help encourage the growth and development of future works by writers of serious music.

Jarek Rossignac, a professor in the College of Computing and director of Georgia Tech's Graphics, Visualization and Usability Center, was elected a fellow of the Eurographics

Association, the most prestigious computer graphics professional organization outside the United States.

Professor **Phillip B. Sparling** of the Department of Health & Performance Sciences was elected to membership in the American Academy of Kinesiology and Physical Education. Membership in the Academy honors individuals who have contributed significantly to the science of human movement and physical activity.

Laren M. Tolbert, professor and chair of the School of Chemistry and Biochemistry, was elected a fellow of the American Association for the Advancement of Science (AAAS). Each year AAAS presents several awards and elects fellows to recognize individuals who have made significant contributions to science or technology.

Professor **Z.L. Wang** of the School of Materials Science and Engineering received the 2001 S.T. Li Prize for Achievement in Science and Technology. The award was presented by the S.T. Li Foundation.

Professor Emeritus **Charles E. Weaver** has recently had his latest work of fiction published. His adventure novel "Global Bogeyman" touches on some of the same themes he taught during his years at Georgia Tech. Those include global warming and nuclear waste. Weaver founded and was director of the School of Earth and Atmospheric Sciences. He retired in 1992.

Research Professor **Juan Vitali** of the Georgia Tech Research Institute's Arlington Laboratory received the U.S. Environmental Protection Agency's 2000 Stratospheric Ozone Protection Award for his successful project to find an environmentally friendly alternative to Halon in U.S. military jets. Vitali and two Defense Department colleagues shared the award given to the U.S. Air Force Research Laboratory in the "Corporate and Military" category.

Professor **Z. John Zhang** of the School of Chemistry and Biochemistry won the American Chemical Society's 2000 ExxonMobil Solid State Chemistry Faculty Fellowship. He received a $10,000 award to support his research in using crystal field principles to advance the understanding, design and control of the magnetic properties of spinel ferrite nanoparticles. Work in this area may prove important for magnetics technologies, biomedical imaging and drug delivery.

Professor **Ben T. Zinn** of the School of Aerospace Engineering received the 2000 American Institute of Aeronautics and Astronautics' Pendray Aerospace Literature Award. He was recognized for "continuous, high-quality contributions to aerospace literature, especially for numerous pioneering papers in the field of oscillatory combustion and its control."

Also see *Research Notes* news stories.