What jumps out about Krish is his professionalism, courtesy and sincere interest in the development of our younger staff. And it’s contagious.

—Jim McMichael

Though he has been blessed, Ahuja’s life is not without stress, he says. Balancing various work responsibilities is difficult, and balancing work with home is even more difficult, Ahuja says. “It comes at a great sacrifice. I sometimes wonder if it’s worth it. I don’t write letters to my friends and relatives as much as I used to. I don’t have as much time with my family.

“But something always keeps you going. Sometimes it’s a question of survival. You have to keep going. I don’t want to become obsolete, and it’s very easy to become obsolete. Even now, I could become obsolete. So I try to read a lot.”

In addition to reading in his field, Ahuja has an appetite for learning about other disciplines. His favorite Web page is howthingswork.com, which helps him find explanations to things such as how microprocessors work, how GPS works and how quartz watches work. “I feel ... the time,” Ahuja says. “I tell my students that if they are not learning something new each day, there’s something wrong.”

Another example of Ahuja’s goal of learning is the book he’s reading. It’s E=MC$^2$ by David Bodanis about how Albert Einstein got the inspiration for the theory of relativity and its impact on humanity. His favorite bedtime reading, his wife says, are books with mathematical equations.

When he can make the time, Ahuja loves to sculpt. “I like to do things with my hands. What I have learned often becomes a building block for something else, like how to make things. First, I did pottery, then hand building with clay, then clay sculpture. I’ve been sculpting since 1987. Sculpting does something to me. For some people, it’s music or flowers. But wherever I go, I find sculpture to look at. Sometimes, I study a nose for half an hour. Sculpting takes a lot of concentration, but I find it relaxing.”

Though life has handed him a number of unexpected opportunities, Ahuja concedes that something more than luck has contributed to his success. He sums it up as his motto: “Whatever you do, do it with passion. That has lots of implications. To me, it’s just second nature now. If it’s not unique, I don’t consider doing it. So my motto, I guess, is to do everything that is unique. Use everything you know as a good building block.”

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Technology and Policy. He holds a Ph.D. from the California Institute of Technology. Goodman’s research interests include technology diffusion, information technology and national security, and the related public policy issues. His areas of geographic interest and research include the former Soviet Union and Eastern Europe, Latin America, the Middle East, South and Southeast Asia, and parts of Africa. Before joining the faculty of Georgia Tech in January 2000, Goodman was director of the Consortium for Research on Information Security and Policy at the Center for International Security and Cooperation and the School of Engineering at Stanford University. He has served as an advisor to the U.S. departments of Defense and Commerce and the President’s Commission on Critical Infrastructure Protection.

Technology can be a double-edged sword, Goodman says.

“Modern society has improved based on a wide variety of infrastructures that promote connectivity, efficiency and access,” Goodman says. “These infrastructures were not designed with security in mind. They are so widely available that they make easy targets.... For anti-American terrorists, it is the natural thing to do to bring fear to all of America. And frankly, we’re available for them to do this.”

Security is in conflict with the primary function of so many infrastructures, including transportation, emergency services, energy distribution and telecommunications, Goodman explains. And the Internet is another prime example. “A balance needs to be found,” he adds. “... New technologies to address the threats of terrorism must not seriously compromise values such as privacy or the primary functionality of the infrastructures.”

Though some infrastructures, such as civil aviation, are quickly addressing security issues, Goodman believes too little is being done to reduce our vulnerability to attack in cyberspace. The Internet was built without security in mind. In the Internet’s growth, access and efficiency, rather than security, have been the main focus of network technology.

“The costs to address Internet security will be substantial,” Goodman says, “not just in terms of money and people, but also in terms of some loss of privacy.”

The nature of the Internet makes it difficult to regulate in terms of security and privacy, Goodman says. For example, all telephone conversations in the United States are considered private, except those that are identified with just cause as likely to pertain to crime. But there is no equivalent to the phone tap for the Internet.

“The paradigm is the reverse for the Internet,” Goodman explains. “You capture all of the communication traffic and then decide what the bad stuff is. So there’s a lot of concern for privacy. This is a serious consideration as we go forward. We need a balance between security and other values.”

Goodman believes the information technology industry has the most wherewithal to improve security in cyberspace, but industry may not see the positive benefit to its bottom line unless customers start demanding better security and are willing to pay for it. Improvements also may come from legal and policy incentives and mandates that demand or value better-protected cyber infrastructures, he adds. Ultimately, governments will have to play an important role in this effort.

Because of global connectivity, international cooperation will have to occur to help prevent and respond to cyber-crime and terrorism, Goodman says. An extensive international convention with near-universal participation should be formed to:
we will have to learn to live with it. It will cost more in terms of security and lives and property. That’s not an entirely new thing to us. We live with the carnage of the automobile in terms of lives and property. We could develop technology to cut that loss dramatically, and we’ve had some success in getting it down. But there’s still a lot higher probability of getting killed in a traffic accident than a terrorist attack.”

The Ethical Dimensions of the War on Terrorism

Molly Cochran is director of undergraduate programs and an assistant professor in the Sam Nunn School of International Affairs. She earned a Ph.D. from the London School of Economics. Cochran’s research interests are ethics and international affairs; international relations theory; and international institutions and global governance. Her current research project focuses on democracy, global governance and international public spheres.

Determining an ethical response to terrorism presents some murky propositions in regard to the ethics of war — which has historically been governed by a code that makes moral distinctions regarding the conduct of war, Cochran says. “One moral distinction that is familiar to all of us is that concerning who is and is not a legitimate target of violence in war,” she explains.

“Terrorism breaks down this war convention because it does not recognize innocents or non-combatants and practices indiscriminate violence of an unconventional kind,” she explains. “The violence unleashed by terrorists is unconventional not only because it is indiscriminate, but also because it is not state-to-state, army-to-army conventional violence.”

Thus, terrorism challenges the norms of war defined in international law, Cochran says. So the United States is finding itself in the position of defining new norms in the war it is leading against terrorism.

“Terrorism is what it is because there is no recognition of the target as human,” she explains. “His or her individuality is not reciprocally respected. The relationship is one of thug to a victim. Does this mean that the victim can fight back in an unlimited manner? … I believe President Bush cannot assume limitlessness in his response to the terrorists, despite our victimization. He has a responsibility not only for Americans in his chosen response to the attack, but to: (1) the innocents of any country that may be the focus of a military attack on a state for its role in harboring terrorists. Moral action must mean that we maintain a stance that is above that of the terrorists; that is, we must make moral distinctions that they do not. In other words, we are clear in our policy that innocents are not to be killed; and (2) global civil
After finishing his Ph.D. in 1976, Ahuja was offered aeroacoustics research positions at Lockheed, Stanford University and NASA-Langley. It seemed that a career in the United States was almost inevitable.

“I had married a white South African woman, and because of apartheid, we could not move to South Africa,” Ahuja explains. “And it would have been awkward to return to India. So we decided to stay in the United States, and I chose the position at Lockheed because they were the first to offer to get permanent residency for me.”

So Ahuja began at Lockheed in Smyrna, northeast of Atlanta, as a full-time consultant to study new aspects of jet noise. Eventually, he became head of the aeroacoustics research program and acting manager of the Advanced Flight Sciences Department. Ahuja became an American citizen in the early 1980s after he was told that as a foreign national, he was not allowed to read some of the published research reports he had written at Lockheed for studies funded by NASA and the U.S. Air Force.

Ahuja worked at Lockheed until 1989, when the company moved its research operations to California. Atlanta was home to Ahuja, his freelance writer wife and two daughters, and none of them wanted to leave. Again, things worked out for him.

Though he left Lockheed, Ahuja was able to keep the same office and, most importantly, his laboratory. He suggested the administration of the Georgia Tech Research Institute (GTRI) ask Lockheed to donate its Smyrna facilities to GTRI. With Ahuja’s help, GTRI worked out a deal. Subsequently, GTRI hired Ahuja as a senior faculty research leader and Georgia Tech made him a professor in the School of Aerospace Engineering. Also, GTRI gave funds to Ahuja to start an aeroacoustics research program.

“I am one of the few who has luckily stayed in the same field for a long time,” Ahuja says. “I have been in aeroacoustics since I was in Derby at Rolls Royce.”

In aeroacoustics, Ahuja primarily deals with control and understanding of noise from anything that moves or has flow around it. Because of that, he researches flow control. His related interests are jet noise, design of quiet wind tunnels and engine test cells, thermoacoustics, advanced acoustic liners, community noise, automobile noise, the acoustic signatures of tornadoses (which could be used for improved weather forecasting) and the effects of noise on sleep. He has also developed an innovative noise-shielding prototype product called Quiet Curtains for use in nursing homes, schools and offices.

In his career, Ahuja has published more than 100 articles on noise in peer-reviewed journals. He also holds U.S. patents on three devices — one for a fluctuating pressure measuring apparatus, another for apparatuses and methods for sound absorption using hollow beads loosely contained in an enclosure, and a third for rapid charging of batteries using sound. The beads could be poured into existing structures — from the walls of homes, hotels and concert halls to the frameworks of aircraft and automobiles. In addition, Ahuja has six more patents pending award.

“Krish is the complete scientist,” says Edward Reedy, director of GTRI. “He is thorough, passionate, intelligent and, most important, always inquisitive. He is an example to all for his professionalism, interaction with students and contributions for the betterment of society.”

Through the years, Ahuja has received a number of offers to conduct research elsewhere, but he has stayed at GTRI. “I have a personal bond with these facilities,” he explains. “I took part in building them in 1976. They are very special, unique. I love uniqueness. That is my personal criteria. Everything has to be unique in some way. These facilities helped me develop my expertise, and they sharpened my saw in many ways. In my field, there are not many other places I could do this sort of research. GTRI is the only university in the United States that has an anechoic flight simulator with hot jet capability.”

“And GTRI management has always supported me. I have had good opportunities here. They worked very hard to make me a Regents Researcher, to get me the professorship. The confidence they have shown in me has kept me here,” he adds.

GTRI has also kept Ahuja busy. At one time, he had 15 research projects under way simultaneously. “That’s very tough,” he says. “I don’t have that many now. I couldn’t have done that anywhere else. I did it here because of my students. Students are great because they don’t have biases. They don’t have these attitudes. They are ready to learn and willing to take directions.

“If you are careful, you can use them effectively,” Ahuja explains. “I give credit to students. I publish with them and hold patents with them. They get so fired up... I constantly pat them on the back. I’m big on incentive-driven approaches... Most of my new students end up working on a special research project course for credit. They get the course credit, and I get students who are better prepared without my spending a penny. And their research results often yield data for proposals.”

Jeff Mendoza, a senior acoustics engineer at Honeywell Engines, Systems and Services, knows Ahuja’s mentoring style first hand. He was a doctoral student and graduate research assistant for Ahuja from 1992 to 1997.

“Krish placed a lot of responsibility on his doctoral candidates, allowing us to lead significant research.”

— Edward Reedy
Ahuja’s students — from undergraduates to doctoral degree candidates to post-doctoral fellows — actively participate in research projects in his lab. Ahuja says he is able to accomplish so much work with students because they are ready to learn and willing to take directions. Pictured (clockwise from upper left) are Richard Gaeta, Michael Parsons, Patrick McPherson, Professor Ahuja, Tomoyuki Minami and Scott Munro.

As a young student in India, Ahuja was a “bookworm,” and he loved to write science-related essays. He entered numerous essay competitions. Later, these experiences proved useful.

“I saw an ad asking for applications for the apprenticeship at Rolls Royce and I applied,” he recalls. “I had no idea what it was all about. I was invited to Delhi to take an entrance exam. The questions they asked, I knew the answers exactly. One of the questions was about wood joints, for example, and I was very interested in carpentry then and had read about it. They also asked me to write an essay on space research, and just a year before I had written an essay on space research for another contest.”

Soon thereafter, Rolls Royce awarded an apprenticeship to Ahuja. He arrived — with the requirement of bringing his own knife and fork for the cafeteria — and began extensive formal training in various departments, including the machine shop, the foundries, design drafting and a range of laboratories.

The training also included classroom instruction, though it was not intended to prepare apprentices for a university education. But Ahuja enrolled anyway and earned bachelor’s and master’s degrees in mechanical and aeronautical engineering from the University of London. Aeracoustics captured his interest when Rolls Royce assigned him to the noise department in the final year of his apprenticeship.

Meanwhile, he began conducting his master’s research at the National Gas Turbine Establishment (NGTE) outside London. “Again, I was very lucky,” Ahuja recalls. “There was great interest in jet exhaust noise research at the time. My experiments were among the first to get good, clean jet noise data. My data was used a lot in the United Kingdom, Europe and the United States. General Electric and Lockheed used it, in fact, so I was already known to the aeroacoustics community when I came to the United States in 1972.”

The move was another unplanned step. After completing his master’s degree, Ahuja spent a year conducting research at the prestigious Institute for Sound and Vibration Research in Southampton. There, he met a Syracuse University professor, Darshan S. Dosanjh, who had a U.S. Department of Transportation grant to develop a jet noise research facility. He invited Ahuja to join him and Ahuja, thinking the facility was ready, agreed to go.

“When we got there, Dr. Dosanjh showed me an open piece of land filled with snow,” Ahuja recalls. “It turned out to be a boon in disguise. He was a good mentor, had a large grant and gave me full freedom to help design the facility from scratch. It was painful, but I learned a lot.”

At Syracuse, Ahuja helped design an anechoic chamber, a reverberation chamber and a hot jet facility to study ways of controlling jet noise. Meanwhile, he worked on his Ph.D. in mechanical engineering.

Pennsylvania State University recently acquired the hot jet facility that Ahuja designed at Syracuse. Ahuja’s long-time colleague, Dennis McLaughlin, chairman of the aerospace engineering department at Penn State, says: “The more I looked over the facility, the more I was amazed at the quality of the engineering. Krish performed as a student. This development job was clearly an outstanding achievement, well beyond what might be expected even for an established researcher.”

At Syracuse, he met Philippa Maister, who became his wife; she was on a student visa from South Africa to earn a master’s degree in economics. “I hadn’t planned any of this,” Ahuja recalls. “One thing just led to another.”
society as a whole... because this was an attack on democracy and open society itself," Cochran adds.

"Across the world there is a loose confederation of those who share the values of democracy, establish civil societies, and contribute to a global civil society that upholds human rights and civil liberties. This community of global civil society is agast at the flagrant refusal on the part of the terrorists to recognize the humanity of those who were their targets."

So, Cochran believes an ethical response is one that is measured and sees its effects upon the international community, rather than America alone. Thus, it is vital that the United States continue to seek multilateral support in any action it takes.

"The legitimacy of our actions depends on two key factors — that we discriminate between legitimate and non-legitimate targets and that we are able to maintain the coalition. If it falters, it creates problems.... The moral basis for continuing this war is less strong without the coalition."

Beyond the war itself, an ethical controversy has arisen over trying those responsible for terrorist attacks. In mid-November, President Bush issued an executive order authorizing the use of military tribunals to try accused terrorists who are captured. Administration officials argue that trials by military tribunals would protect the identity of intelligence sources, among other things.

Cochran believes terrorists cannot get a fair trial on American soil and that military tribunals would eliminate even the possibility of a fair trial. Instead, she advocates the "Lockerbie model" — referring to the trial that followed the airliner bomb explosion over Lockerbie, Scotland, in 1988. Two defendants were tried under Scottish law, with judges instead of a jury, in the Netherlands, rather than Scotland.

"I am strongly opposed to military tribunals as they do not provide for the fairness in judicial proceedings that I think our ethical responsibilities to global civil society require in dealing with the terrorists," Cochran says. "Evidence deemed sensitive by the military would be presented in secret, and rules governing the conduct of the proceedings would be issued by the Pentagon. I believe that the U.S. government will not allow a trial off American soil along the lines of the Lockerbie model, but trials at home in federal courts would be much preferable to what is now being proposed if we are to live up to the ideals of justice that we in this country profess."

The European Response to the War on Terrorism

Katja Weber is an assistant professor in the Sam Nunn School of International Affairs. She earned a Ph.D. from the University of California at Los Angeles. Her research interests include international relations theory, the European Union; transatlantic security relations; and institutions and integration theory. Weber’s current research project focuses on normative visions of international order in post-war Germany.

Like the Bush Administration, European leaders want to avoid the portrayal of the war on terrorism as a war between Islamic countries and the West, Weber says. They are also stressing the importance of continuous coalition-building with Muslim nations. "This matters for geo-strategic reasons, ideology and for avoiding a coalition of the West against the rest," Weber explains.

Coalition-building must be continuous because there are so many vulnerabilities, she says. For example, the leadership of some Muslim countries is vulnerable as they support the coalition against the wishes of some of their citizens. The United States must provide financial support to these countries, as well as other types of aid, she adds.

Beyond the war in Afghanistan, Weber adds, "The Europeans have made it clear that they don’t want to get stuck in a Middle East conflict, once the United States withdraws, and be left alone to clean up the mess."

"The Europeans differentiate short- from long-
Responding to Terrorism

term horizon," she explains. "The short term means aiding the U.S., showing solidarity and promising to abide by their NATO commitment (as codified in Article V of the NATO Treaty), which allows for a broad range of support including mere rhetoric, provision of assets and military action (such as the troops sent by Great Britain, Germany and France). The long term means insisting on a division of labor between Europe and the United States. The Europeans try to deal with terrorist activities within their own borders — for example, freezing of terrorist assets in European banks and providing intelligence support to the U.S.

"It isn't surprising that Europeans want to deal with terrorism in their own way because any time one deals with security issues, countries are protective of their sovereignty," Weber adds. "They want to decide their own affairs."

Despite these concerns, many nations have recognized that multilateral solutions are essential in the war on terrorism because Sept. 11 was more than just an attack on the United States, but was really a crime against humanity, Weber says.

"At the same time, there can be no doubt that multilateral solutions are problematic," she adds. "First, there is no agreement on the nature of the problem. There are those who view the terrorist attacks as an act of war by evil people against western civilization. However, there are also those who view the attacks as the result of a larger evil, namely the failure of modern civilization to effectively address the horrendous suffering of millions of people in the world.... There are people who recognize that we can't hide behind the walls of peace and prosperity, who understand that globalization has not only brought global flows of capital, goods and information, but huge debt, unemployment, poverty and disease.... These people are calling for multilateralism and new forms of international cooperation because they recognize the interconnectedness of different forms of violence."

Where does this leave us? Weber asks. "We obviously don't have to agree with the terrorists' views and, in fact, should openly denounce their horrific methods. But, if we hope to achieve lasting peace, we need to understand where these views come from. Alternatively, we may have to do without many of the rights and freedoms we cherish and fought for for centuries." RH

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Regents Researcher Krishan Ahuja attributes his success to luck, but that’s just another word for his hard work and diligence ... in any of his endeavors, from his career in aeroacoustic engineering to his hobby of sculpting.

By Jane M. Sanders

A n essay in his high school magazine reveals that as a teenager in Calcutta, India, Krishan Ahuja already believed in luck. But to him it meant more than just being in the right place at the right time. It meant hard work and diligence. “Diligence is the best guarantee of success,” he wrote. Today, the internationally recognized Professor Krishan Ahuja still adheres to that philosophy. It has guided him through many doors of opportunity that have “luckily” opened for him.

Ahuja is a Regents Researcher and Georgia Institute of Technology professor of aerospace engineering, who studies aeroacoustics at the Georgia Tech Research Institute. His distinguished career began in 1965, just after high school, when the first of many doors to opportunity opened to him with an unexpected and prestigious five-year apprenticeship at aeroengine maker Rolls Royce in Derby, England. From there, one door after another opened, and life pleasantly greeted him as he entered.

“I didn’t know what to expect,” Ahuja recalls about his Rolls Royce apprenticeship. “Everything happened so fast.... I was from a middle-class family with hard-working parents. This was a dream come true for very rich people. But I believed then and now that if you enjoy what you’re doing and are sincere, everything will work out. And everything has led to something else just right for me. I consider myself one of the very lucky people in the world. It has been absolutely incredible how everything has just fallen into place for me.”
Researchers are making plans on how to handle crashes that may occur outside the metro area, Ogle adds. Fulton County 911 officials will open a cellular telephone line into the vehicle using the onboard speakerphone system to verify that a crash has occurred and determine its potential severity. Global positioning system signals transmitted to 911 officials from the vehicle will reveal the crash location.

Meanwhile, algorithms embedded in the MACBOX software will automatically analyze crash data, such as impact velocity and severity, and inform 911 personnel about the probability of injuries or casualties associated with the wreck. Then after quickly looking at these data and attempting to contact the driver, they will dispatch rescue workers and police to the scene.

The in-vehicle equipment will automatically notify the on-call Georgia Tech research team, which will deploy and investigate the crash in coordination with police departments. All six faculty members and six graduate students involved in the study underwent crash reconstruction and investigation training, including on-the-job practice with a metro area police department. Researchers will analyze the MACBOX data and crash scene information to determine the role of speed in the crash.

“Crash reconstruction is essentially more an art than a science,” says Safety Intelligence Systems’ Ricardo Martinez, a former NHTSA administrator and now an adjunct professor of civil engineering at Georgia Tech. “We look at the archaeology of the crash, witness reports and expert opinion to decide the ‘facts.’ With cars becoming more sophisticated like computers, we can actually measure what happens in a crash. So with the MACBOX, we can go from Flintstonian to Jetsonian.”

Based on a pilot study she did in 1997 in Texas, Ogle believes Drive Atlanta will be successful in terms of data collection technology and data analysis. Ogle will issue periodic reports to NHTSA throughout the study and a final report in the summer of 2004.

“There is a lack of comprehensive information on crashes,” Ogle says. “With ABS brakes, skid marks are not as detectable. But crash analysis is changing. The more information we have, the better off we are.”

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Technologists throughout our society are considering ways of addressing the recent acts of terrorism in the United States. In our profession, architects and engineers wonder how the recent events will change the way we design buildings and how the public will perceive our buildings.

What will our response be? Should we change the way buildings are designed and constructed in response to these new threats? If so, that discussion needs to begin now, so we make these changes in a rational manner — with a clear understanding of the tradeoffs we face as we begin to design and construct for greater security.

Many of us in building science research are puzzled that the response from our research community is barely noticeable. The public health community has responded vigorously to the recent bioterrorism attacks. The aviation industry is actively developing and implementing new technologies for ensuring the safety of airline travelers. The building design community seems more interested in discussing the plan for the redevelopment of lower Manhattan, instead of wondering whether all buildings need to be designed (or redesigned) in light of new threats and new modes of attack.

Three realities must be addressed as we push for a serious consideration of building security as part of the design process.

First, we must acknowledge that the building industry is fractured and diffuse, with no federal oversight or central source for building policy. There is no building science equivalent to the Federal Aviation Administration (FAA) or the Centers for Disease Control (CDC). Building “policy” is simply not set at a national level. Rather, buildings are shaped by codes and standards developed by consensus bodies that include building inspectors, architects, engineers and constructors. Code bodies like the National Fire Protection Association (NFPA) and the International Congress of Building Officials (ICBO) do not really involve themselves with building policy. Rather, they react to trends in the industry, to the development of new materials and to new modes of construction, and subsequently adapt their codes to include these new technologies where market forces or building research dictate.

A second problem is the level of and sources for funding building science research. The research community of which Georgia Tech is a part has organized itself to compete for federally funded research. There is no federal agency that funds research about “buildings.” Thus, there is little focus on building research. It is true that the National Science Foundation (NSF) funds research about specific building systems (e.g., structural, mechanical), and many of us have received grants from the NSF Civil and Mechanical Systems Division. NSF does not fund research in architecture because it is not a science, nor is it engineering. Nevertheless, the profession of architecture oversees the design and delivery of all of the commercial and many of the residential buildings in our country.

This leads to the third problem — the application of research knowledge in the building design community. Building designs are completed in teams led by
architects, and include engineering consultants who specialize in the design of building foundations, site works, structures and mechanical systems. Designs are bounded by building code requirements that dictate egress requirements, structural capacity, fire protection and energy efficiency. Do the codes therefore contain the "embodied knowledge" of the profession? In fact, codes do not contain the kernel of knowledge necessary to design buildings. Design knowledge comes from analysis of building precedent — a reflection on and critique of existing buildings, from the study of client needs and subsequent building programming, and from the professional training that architects receive as a condition for licensure. Knowledge on how to design for building security is missing — it is not contained in the embodied knowledge of our profession and is, subsequently, missing from codes as well.

And so, there are no building codes that focus on security. No provisions exist that say: "If anthrax is a credible threat, supply HEPA filtration at all building entries and mail sorting rooms, with a minimum air exchange rate of 25 room volumes per hour" or "if a package bomb is a credible threat, then the primary public entry of the building shall be hardened for blast resistance and bomb blast within this entry shall be vented externally to the building." It may appear easy to add such provisions to existing codes, but a number of key questions are raised by these two simple examples. What is a credible threat? Can HEPA filtration reliably remove anthrax spores? Can we detect the presence of anthrax on the HEPA filters using biosensors? What is the blast pressure profile from a package bomb? What is the best location for a bomb-screening device so it will injure the fewest people if a bomb explodes at the point of detection?

How do we answer these questions? The science of risk analysis can begin to explain the concept of "credible threat" to architects and building owners. It is they who will have to decide what is credible and what is not. Aerosol scientists can further our knowledge of filtration, and biologists can explore the creation of "sensors on a chip" to detect biological agents (see article on CERTIP, page 4).

Psychologists who study human movement through space can provide guidelines for the routing of people and material in buildings, so the introduction of an explosive into a building will inflict the least harm to its occupants.

A key problem in this scenario is that few research scientists focus on the application of their science to buildings. Once again we point to the lack of federal funding and the lack of a national policy, which emphasizes that architectural, engineering and science research should develop technologies that can be used to make buildings safer.

One approach to focusing the power of science and the problem solving of engineering to the question of building security is to develop a science of building vulnerability — a cross-disciplinary endeavor that relies on basic science, understands building operations and respects the design process. Basic research carried out under the umbrella of building vulnerability science would explore the transport of mists and particulates, the response of building materials to high impulse loading and the reaction of people within their environments in time of distress. Applied research in building vulnerability would develop better air filtration systems, new glazing materials to better withstand blast pressures and automated building systems to provide context-specific guidance to building occupants during an emergency.

Research carried out in the name of building vulnerability science must understand and be guided by the building design profession. Architects are already met with an immense range of technical challenges, client desires and cost constraints. Some client desires as voiced cannot be satisfied, and architects are required to confront and negotiate major design decisions that effect building security. For example, federal government guidelines suggest that buildings deemed to be at significant risk for terrorist attack should have 100-foot setbacks from any public street. The federal government has, at the same time, made a policy commitment to locating new courthouses and federal office buildings in city centers, where block sizes and existing buildings extend to within 10 feet of most sidewalks. How do we satisfy both desires? Does one take precedence? Is the 100-foot setback a prescriptive requirement that reflects on the lack of "science" in building design?

Fundamental questions about building vulnerability exist at the basic science and at the applied levels. Faculty in the College of Architecture at Georgia Tech are involved in research, sponsored by the U.S. General Services Administration (GSA), that characterizes the performance of building systems, provides tools for performance-based decision making about building design, and observes human reactions to buildings and their contents. We are proposing an initiative to create a national focus on building vulnerability science and look forward to helping create the knowledge base that will give the building design profession the tools necessary to design for building security.

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But researchers also want to learn more about travel patterns — how, when and where people drive. This information will be useful to both Ogle’s research team and to SMARTAQ (Strategies for Metropolitan Atlanta’s Regional Transportation and Air Quality), an ongoing Georgia Tech-led study to determine what types of land use and transportation investment policies have the best chance to reduce auto dependence.

“For years, we have collected information from the roadway and the vehicle,” Ogle says. “Now, we will also be able to gain information on driver behavior. This information will allow transportation officials to target their countermeasure programs. Countermeasures can come in the form of safety enhancements for the vehicle or the roadway environment, such as the roadside grading, signage, airbags, seatbelts or the setting of appropriate speed limits. This research may also lead to better driver training programs for younger and older drivers.”

Drive Atlanta is primarily funded by a $1.9 million contract with the National Highway Traffic Safety Administration (NHTSA) and a $1.2 million in-kind grant from Safety Intelligence Systems Inc. The private company is providing the development costs, prototyping and testing for the MACBOX™, an event data recorder, which will operate — transparently to the driver — in all the study vehicles for the next two years.

The MACBOX will record high-resolution data for each vehicle trip and download that information to the researchers’ secure server weekly. Data will include trip length, trip duration, route choice and second-by-second speed and acceleration.

Researchers will supplement MACBOX data with information on the freeway and major highway driving environments. The Atlanta Traffic Management Center will contribute data on prevailing traffic conditions, and researchers will gather weather data from the National Oceanic and Atmospheric Administration. They will combine all of these data within a geographic information system using the Georgia Department of Transportation roadway characteristics file and network as the basis for analyses.

Meanwhile, researchers will also be collecting data — both from the MACBOX and at the scene — when a study vehicle is involved in a crash. Based on statistical probabilities, they estimate that at least 100 crashes will occur during the study period.

When a crash occurs, the MACBOX will record all of the vehicle deceleration data and simultaneously transmit a Mayday message to the Fulton County Public Safety Access Point, or 911 center, the central emergency agency for all vehicles involved in the crash.

Fatal Crash Statistics for Georgia

These 2000 statistics from the National Highway Traffic Safety Administration’s Fatality Analysis Reporting System are the latest available.

- 1,541 people died in motor vehicle crashes.
- 63 percent of these deaths did not involve alcohol-related fatal crashes.
- 93 percent of these deaths did not involve drivers ages 16 or 17.
- The fatality rate was highest for the contributing factor of failure to keep in the proper lane or run off the road — 13.5 per 100,000 licensed drivers compared with 2.5 for failure to obey traffic stop sign or signal.

- Alcohol and illegal or unsafe speed were the next highest contributing factors at rates of 9.8 and 5.9 per 100,000 licensed drivers, respectively.
- 71 percent of drivers in fatal crashes were male.
- Almost one in 10 drivers in fatal crashes did not have a valid driver’s license.
- The fatality rate per 100 million vehicle miles traveled in rural Georgia was 1.8, compared with a fatality rate of 1.1 in the five primary metropolitan Atlanta counties. The rate in suburban Atlanta counties was 1.6.
- More than one in four fatalities occurred in crashes involving a pickup truck.
- More than one in seven fatalities occurred in crashes involving a sports utility vehicle.
- Proper child safety seat use by fatally injured motor vehicle occupants up to age 4 increased from 23.3 percent in 1999 to 25.0 percent in 2000.
- 18-year-old drivers had the highest fatality rate.
- Pedestrian fatalities accounted for 11 percent of all motor vehicle fatalities — the highest number of those occurring at night.
Conquering metro Atlanta's highways is like winning the Daytona 500 to many drivers. To cross the finish line, you've got to drive hard, drive fast and put in a lot of hours.

With so many drivers taking this approach, crashes are bound to happen, and some of them are deadly. More than 1,500 people a year die in crashes in Georgia, and more than 135,000 are injured. The concern is greatest perhaps in metro Atlanta counties, which exceed the national average crash rate of 5 percent a year among all registered vehicles. In fact, the crash rate is almost 10 percent in Fulton County, the heart of the metro area. Previous studies have shown that Atlantans drive harder, faster and longer than motorists in four other representative U.S. cities, including Los Angeles.

So Atlanta is the natural test bed for an unparalleled, comprehensive study of driver behavior and environment, and the role of speed in crashes. The Georgia Institute of Technology's Drive Atlanta study, which began in the spring of 2000, got into full swing recently when technicians began installation of data collection and telecommunications equipment in the cars of 1,100 metro drivers randomly recruited by researchers. Researchers expect that equipment installation in participating vehicles will be completed by this spring. In exchange for their participation, drivers have been assured of the privacy of data collected from their vehicles, and given the benefits of a vehicle theft-tracking system and automated 911 notification in the event of a crash.

"Ultimately, we hope the data we collect can help make the whole system — the driver, vehicle and the road — safer and more efficient," says Jennifer Ogle, lead investigator and a research scientist in the School of Civil and Environmental Engineering. "We don't know exactly what findings will result from this study, but we hope to learn about all three pieces of the system. The sheer size of the data set allows for nearly limitless analysis possibilities."

The role of speed in crashes is the primary focus of the study. Researchers led by Ogle and Associate Professors Karen Dixon and Randall Guensler, both of the Georgia Tech School of Civil and Environmental Engineering, and Simon Washington, an associate professor of civil engineering at the University of Arizona, hope to answer several questions. Does speeding lead to crashes? Are regular speeders more likely to crash? Do speeders have a higher risk of crashing only under certain conditions? "We know very little about pre-crash speeds," Ogle says. "Almost all of what we know relies on driver and witness reports or crash reconstruction activities. Each of these sources is subject to errors. Our equipment will actually measure and record speed for us."
While some investigators are still taking notes and filling out forms about the damage to buildings surrounding New York’s World Trade Center complex, a group of Georgia Institute of Technology researchers is taking a very different approach.

Researchers have digitally documented structure types, and qualitative and quantitative information on structural and non-structural damage. They correlated this data with digital photos and global positioning system (GPS) coordinates. The information will help them assess the condition of buildings in the area and rate how they performed.

Ultimately, researchers hope their findings will improve the design and structural integrity of
At the World Trade Center, the energy came from a relatively concentrated source and dissipated more rapidly as it moved outward," he explains. "Two or three blocks out, the impact was much diminished. It was a lot less energy than an earthquake. We found different damage on different sides of the buildings. So there was an orientation effect that required us to spend time modifying our software. We enabled it to let us describe in more detail how the damage varies from side to side and from upper levels to lower levels of buildings."

Researchers plan to investigate whether some non-structural elements could be improved to better withstand impact, Frost says. For example, the systems that connect glazing and granite fascia to buildings could be redesigned.

"We may find that different systems performed better than others under the same loading conditions," Frost says. "... So this information could result in a major engineering benefit."

It’s too early for researchers to make conclusions about structural damage, Frost adds. More research is needed. For example, forensic assessments might identify where pieces of debris came from in the building and correlate it with their condition. And simulation research might reveal how certain structural elements performed in such extreme conditions. Frost anticipates that some of his structural engineering colleagues at Georgia Tech will be involved in such longer-term studies.

Also, Frost believes his research in data collection the nation’s buildings, utilities and other infrastructure. The results may also improve emergency response to both natural and human-caused disasters.

Just a week after the terrorist attacks, the National Science Foundation awarded a $20,000 grant to David Frost, a professor of civil engineering, to assess the damaged area with an advanced digital data system he recently developed for earthquake reconnaissance missions. Frost’s research team actually began data collection in a 10-square-block area in and around the WTC complex in mid-October and have undertaken several field exercises since then.

Frost’s Palm Pilot software application called PQuake — which he beta tested following the devastating earthquake in Gujarat, India, last year — allows several research teams to simultaneously collect and input digital data, including photos and GPS coordinates. Because the information is already digitized, it is quickly integrated in a geographic information system (GIS) database, Frost explains. Rapid data analysis can then follow.

“Our application was developed for post-earthquake field reconnaissance, but we anticipated there would be other applications,” Frost says. "... We found some differences right away in the damage from earthquakes and the damage in New York. In an earthquake, energy is released over a very large area. You can look at a building from one direction, and its condition will be the same on all sides because the energy passes through the entire site."

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Also, Frost believes his research in data collection

Building Five of the WTC complex had extensive fire damage.

David Frost (inset), a professor of civil engineering, received a $20,000 grant from the National Science Foundation to assess the damaged area with an advanced digital data system he recently developed for earthquake reconnaissance missions.

Previous page: Debris from Tower One of the World Trade Center complex impaled the side of the World Financial Center Building 1 (Amex Building) 20 floors up.
intense laser beams to confine a few million atoms of rubidium while reducing their speed to a “crawl” (less than 10 centimeters per second).

“It’s kind of like slowing a car with a million ping-pong balls,” explains Sauer, a graduate student in Chapman’s team. “You just keep throwing the balls at the car until it slows down. The atoms are like moving cars, and we slow them by firing lasers that consist of photons.”

When the atoms in the trap reach the appropriate temperature — about 3 micro-Kelvin, a fraction of a degree above absolute zero — the magnetic fields and laser beams confining them are switched off. That allows the cold atoms to flow by gravity into a “funnel” made up of two current-carrying wires about a millimeter apart.

The funnel guides the atoms into the storage ring, where they are confined by magnetic fields created by parallel wires each carrying a few amps of electrical current.

“You can think of each atom as a tiny bar magnet,” Chapman explains, “and the magnetic fields from the wires are arranged to keep the atoms guided between the wires.”

A CCD camera records the passage of atom clouds by observing light scattered by the atoms from laser beams passing through tiny holes in the ring.

In the paper, Chapman’s team reported observing atom clouds making up to seven revolutions around the ring at velocities averaging one meter per second. The atoms ultimately stop moving due to “bumps” in the ring and encounters with stray atoms left in the vacuum chamber. In subsequent experiments, they have measured up to 10 revolutions, and Chapman believes an improved ring could increase the number of revolutions tenfold.

The team has also developed techniques for loading multiple batches of atoms into the ring, a first step toward a continuous atom flow. “If you get the timing right, you can get multiple atom clouds moving around in the ring,” Sauer says.

The research was partially supported by the National Security Agency and the Advanced Research and Development Activity of the Army Research Office.

For more information, you may contact Michael Chapman, School of Physics, Georgia Tech, Atlanta, GA 30332-0430. (Telephone: 404-894-5223); (E-mail: michael.chapman@physics.gatech.edu)
In a development that could lead to dramatic improvements in aircraft guidance systems and open new areas of study in basic physics, researchers at the Georgia Institute of Technology have demonstrated the first storage ring able to confine and guide the flow of ultra-cold neutral atoms in a circular path.

Dubbed the "Nevatron," the storage ring — a circular waveguide that uses magnetic fields from tiny electrical wires to direct low-energy atoms — marks a step toward "atom fiber optics" that could ultimately do for ordinary uncharged atoms what optical fiber has done for light. Details of the project were reported in the Dec. 31, 2001 issue of the journal Physical Review Letters.

"In contrast to high-energy particle storage rings in which the goal is to increase the energy of the confined particles up to and beyond the tera-electron (TeV) volt scale, we are interested in the opposite regime, using ultra-cold atoms with nano-electron (neV) volt energies," explains Michael Chapman, a Georgia Tech assistant professor of physics.

"In keeping with the theme of naming storage rings according to the energy scale, we call our device the Nevatron."

The 2-centimeter storage ring could serve as the foundation for a miniaturized atom interferometer that would improve the accuracy of inertial guidance systems used in commercial aircraft. Such systems now use optical interferometers in which a beam of light is split into two separate beams that travel in opposite directions through coils of optical fiber. By observing how changes in aircraft speed and direction differentially affect the two beams by recombining them with an interferometer, the instrument measures changes in aircraft motion.

Much heavier atoms traveling in rings would be affected more dramatically by aircraft directional changes, Chapman says. An atom interferometer would measure phase shifts in the deBroglie wave, a quantum effect associated with atoms.

"The sensitivity of these gyroscopes is proportional to the area enclosed by the interferometer and the mass of the particle," he explains. "The mass of an atom is about 10 orders of magnitude higher than the (relativistic) mass of an optical photon."

Atomic interferometers now exist, but they are too large for aircraft use. If Chapman's team can split an atom beam and make the beams travel in opposite directions around a circular ring, they could have the basis for an instrument small enough to fly.

"If our experiment were an interferometer, it would already have the potential to be a thousand times more sensitive than the best optical interferometer," Chapman says. "This is really going to be a major direction in the field of ultra-cold atoms. Making an atomic storage ring is the first step toward useful devices."

Developed with collaborators Jake Sauer and Murray Barrett, the Nevatron also provides new opportunities for creating continuous monochromatic atomic beams that could one day lead to the development of an atom laser with a continuous output. It also offers new opportunities for studying collisions between ultra-cold atoms.

Other researchers have produced straight-line waveguides for neutral atoms, but the Georgia Tech ring is the first to make neutral atoms move around a closed circle using magnetic confinement. Chapman believes the most significant accomplishment was a technique for loading atoms into the ring from a standard magneto-optical trap used to cool the atoms to micro-Kelvin temperatures.

The experiment takes place within a vacuum chamber. First, a standard magneto-optical trap (MOT) uses a combination of magnetic fields and
and software development will continue in more detail and result in collaboration with other researchers. NSF plans to fund some follow-up projects to the studies it funded just after the attacks.

“We want to take digital data collection technology to the next level,” Frost says. “We want to use a wireless communication network to upload the data we collect in the field in real time. Then we can make interpretations on the data as it’s being collected. Real-time analysis is an advantage, especially in earthquakes that have affected a large area. You want to cover as much area as you can without duplication or blanks in the data.

“Real-time analysis enhances the whole data collection process,” Frost adds. “Even with preliminary analysis, you may see some trends that will guide you and direct the data collection and perhaps even assist in the recovery of victims. If we’re able to assess a certain pattern of damage... it could help us understand where there is a more likely opportunity for a successful recovery.”

Frost believes P-Quake and his digital data collection system may also have applications in other disasters, such as building fires, a catastrophic rail accident or a ship hitting a bridge. In addition, it could help in the analysis of damage from tornados, hurricanes, and floods.

On a personal note, Frost says the experience of working at Ground Zero in New York was sobering. But he was not as surprised as some by the damage after having participated in four major earthquake reconnaissance studies.

“In New York, you almost had the feeling like you were working at a large construction site,” he recalls. “Everything was operating in such an organized manner, it fools you into thinking this. But then you are brought back to reality when the activity suddenly stops. You see vehicles coming down the street carrying flowers and people. Firefighters and family members conduct a little service right at the site when they find remains.

“The sense of being at a construction site is in stark contrast to some of the earthquake zones I have visited where buildings have collapsed and the damage is so widespread,” Frost says. “You find that little, if anything, is happening even several weeks later. People are just standing around. There’s no active recovery going on. They just don’t have the resources and the organization. The scale is so large. We take for granted here in the United States how organized we are and how quickly we can mobilize our resources.”

For more information, you may contact David Frost, School of Civil and Environmental Engineering, Georgia Tech, Atlanta, GA 30332-0360. (Telephone: 404-894-2280 or 912-652-3585) (E-mail: david.frost@ce.gatech.edu)
A trajectory of sodium counterions (purple) is shown superimposed on a short nucleobase sequence of DNA. The trajectory, taken from a 1.6-nanosecond molecular dynamics simulation, shows the high mobility of the counterions.

IMAGE COURTESY OF UZI LANDMAN
“To do this, we have to modify the unsteady flow equations with terms that account for the effect of the fish on the flow and solve them at the same time with the equations describing the fish motion,” Sotiropoulos explains. “So this model will be much more sophisticated. We will be using the massively parallel supercomputing facilities at Oak Ridge to do this work.”

This research is funded through ORNL by the U.S. Department of Energy’s Hydropower Program, which is focusing on the issue of what happens to fish as they pass through hydropower turbines. “The hydraulic stresses inside turbines are difficult to study because of their high velocities and chaotic structures,” says Michael Sale, head of ORNL’s Environmental Sciences Division. “Computer simulation is an important tool for understanding phenomena that we cannot observe directly.... (The enhanced version of) Virtual Fish will be an important method for predicting how real fish might respond to simulated velocity fields.”

Meanwhile, Sotiropoulos is also collaborating with ORNL and TVA researchers on an experimental project. Researchers are equipping several TVA dams to measure flow forces. They will compare data from this experiment with results from CFD modeling done by Sotiropoulos.

The other CFD model important to hydropower industry officials is Virtual Bubbles, which assesses auto-venting turbine (AVT) technology. With it, air is aspirated into the water as it flows through the turbine whenever the water’s dissolved oxygen level is below the minimum of 5 milligrams per liter. This level is recommended by the U.S. Environmental Protection Agency for supporting early-life stages of warm-water fisheries. AVTs rely on turbulent mixing and mass transfer to release as much dissolved oxygen as possible from the air bubbles into the water.

Hydropower operations reduce dissolved oxygen downstream, particularly in the summer. Daytime heating creates a warm layer of water at the top of a reservoir, while water at the bottom is colder. Minimal mixing of oxygen occurs in this situation, so the cold water below becomes depleted of dissolved oxygen. Power plants draw from the lower layers of the reservoir, so water that is released downstream is also depleted in dissolved oxygen. Such conditions create an unhealthy habitat for fish and other organisms and can create a smelly river not suitable for recreation.

TVA has installed several Voith Siemens Hydro AVTs to increase dissolved oxygen in its operations in the Southeast. The company is using Virtual Bubbles to evaluate and optimize the performance of this new turbine technology. The model uses CFD to calculate the flow environment downstream of the turbine and tracks the paths of individual air bubbles as they are carried by this simulated flow. The bubbles are allowed to exchange oxygen with the flow, collide and form bigger bubbles, and then break up into smaller bubbles.

Virtual Bubbles can help engineers determine: (1) whether AVTs are achieving maximum transfer of oxygen from the bubbles to the water; and (2) whether the new turbines are negatively affecting the energy efficiency of the power plant.

“Industry needed a tool to analyze possible scenarios and designs and to quantify the impact of air bubbles on efficiency and oxygen transfer,” Sotiropoulos explains. “Again, this model is based on a balance between having enough sophistication to be useful, but not being so complicated that it requires so many resources that it is beyond industry’s time scales.”

For more information, contact Fotis Sotiropoulos, School of Civil and Environmental Engineering, Georgia Tech, Atlanta, GA 30332-0355. (Telephone: 404-894-4432) (E-mail: fotis.sotiropoulos@ce.gatech.edu)

Virtual Fish, developed by Georgia Tech civil engineer Fotis Sotiropoulos, helps hydroturbine designers determine the water flow forces on fish drawn into the plant. In collaboration with fish biologists, engineers can then analyze this information to predict fish injury and mortality and identify specific design elements responsible for inducing harmful water forces.

Top: TVA’s Norris Hydropower Plant has an auto-venting turbine, which relies on turbulent mixing and mass transfer to release as much dissolved oxygen as possible from the air bubbles into the water downstream of dams.

PHOTO COURTESY OF TVA
A research group developed software called Virtual Fish and Virtual Bubbles.

Virtual Fish, developed with funding from and licensed by Voith Siemens Hydro Power Generation Inc., helps hydroturbine designers determine the water flow forces on fish drawn into the plant. In collaboration with fish biologists, engineers can then analyze this information to predict fish injury and mortality and identify specific design elements responsible for inducing harmful water forces.

Engineers are using Virtual Bubbles, developed with funding from and licensed by the Tennessee Valley Authority (TVA), to determine the effectiveness and efficiency of auto-venting turbines. These turbines introduce air bubbles into the water as it flows through the power plant — increasing dissolved oxygen, and thus improving water quality, downstream of dams.

Already, Voith Siemens Hydro has used findings from Virtual Fish to refine turbine design. New turbines, some of which have been installed on Columbia River dams in the Pacific Northwest, minimize turbulence and velocity shear. On the Columbia and its tributaries, migrating salmon have suffered population losses related to hydropower operations, but the new fish-friendlier designs are expected to help fish populations recover.

Using CFD, Virtual Fish calculates the impact of the complicated virtual flow environment on passing fish. It models fish as ellipsoid-type objects and assumes that fish have no free will — that is, they cannot react to the water forces that carry them through the plant. “That’s probably a good assumption for the most part because the fluid forces inside the plant are so strong,” Sotiropoulos says. “The fish may have little or no time to react.”

Sotiropoulos formulated a set of equations that describe how the ellipsoid object is transported and rotated by the flow from the upstream reservoir, through the turbines and in the downstream tailrace river reach. Virtual Fish allows the user to calculate the various water-induced forces that tend to shear, squeeze, stretch, bend, rotate or twist the fish at every point along its path through the power plant. With biological input, Virtual Fish users can then determine whether these forces are harmful to fish. For example, the user could find out how many times the fish was spun by the flow, revealing whether it is likely that the fish became disoriented, and thus more vulnerable to predators downstream.

“The Virtual Fish model is a significant advancement, but it is still a very approximate thing,” Sotiropoulos says. “It represents the turbulent and rapidly changing flow environment in the power plant with its statistical time average. Yet passing fish get injured by instantaneous water forces, whose magnitude could often be much higher than their statistical mean value. Also, the model doesn’t account for the effects fish have on the flow. And the fish (in the model) is not flexible. It is a stiff body right now....”

“But the model for Voith Siemens Hydro is a good one for the industry,” he adds. “You have to strike a balance between model sophistication and getting fast answers. But if you want to further enhance the understanding of specific flow mechanisms responsible for injury and mortality, you have to understand the instantaneous flow structures at the fish’s scale. To do this, we need to develop unsteady CFD models of the turbulent flow environment and account for the effect of the fish on the local flow field.”

Thus, Sotiropoulos began work last summer on a four-year project with Oak Ridge National Laboratory (ORNL) researchers to create the next generation of Virtual Fish. The enhanced model will feature a flexible fish, which can interact with and be distorted by instantaneous flow. It will allow engineers and biologists to study and understand the interaction of a much more realistic fish-like object with a flow environment much closer to that encountered by live fish passing through a power plant.
The environment surrounding DNA in living cells plays a surprisingly important role in regulating the movement of electronic charge through the life-coding molecule, suggests a paper published in the journal Science. The work could lead to a better understanding of how DNA is damaged by oxidative processes and offer clues to potential DNA applications in nanotechnology.

Based on experimental data, computer-based molecular dynamics simulations and complex electronic structure calculations, the Oct. 19, 2001 paper is the first to describe how sodium ions could control the migration of electron holes — also known as radical cations — through DNA. The electron holes, positively charged locations in the DNA structure, are created by normal cellular oxidation processes and everyday events such as exposure to sunlight.

Migrating through the DNA to distances up to 30 nanometers from their site of origin, the electron holes ultimately reach certain locations where they may initiate reactions that can damage the genetic coding.

“Our paper presents a new way of thinking about what controls electrical charge transport in DNA,” says Gary Schuster, a professor in the School of Chemistry and Biochemistry at the Georgia Institute of Technology and dean of its College of Sciences. “The motions of the water molecules, the sodium ions, the backbone of the DNA and the bases of the DNA together control the movement of charge in the DNA. It’s clear that we must consider both the DNA and its environment.”

Underlying the charge migration mechanism unveiled in this study are two physical principles:

(1) like electrical charges electrostatically repel one another, and

(2) thermal energy induces random motion — known as stochastic dynamic fluctuations — among the microscopic constituents of matter: ions, atoms and molecules.

In a 1999 paper published in Proceedings of the National Academy of Sciences, Schuster and his colleagues suggested that electrical charge moves through DNA in a “Slinky-like” process in which the molecule distorts itself in an effort to locally stabilize the charge. The new work seeks to explain why the charge moves at all, and to explain the dynamical mechanism of long-range transport in DNA.

In a nutshell, the paper’s authors argue that the positively charged electron holes — created by the removal of an electron — move when approached by positively charged sodium ions hydrated in the aqueous medium surrounding the DNA. Circulated by thermal energy in a random way, the diffusing sodium ions are attracted to specific locations in the DNA, such as the negatively charged phosphates that are part of the DNA backbone and certain atoms of the nucleo-bases.

“The electron holes in the DNA simply don’t like to be near the positively charged sodium ions, so the stochastic motion of the solvated ions initiates and gates the motion of the electron holes,” explains Uzi Landman, Regents’ professor of physics and director of the Georgia Tech Center for Computational Materials Science. “The motion of one charge repels the other, resulting in a correlated dance of the two.”

Using one of the largest electronic structure calculations ever done, Landman and colleagues Robert Barnett and Charles Cleveland predicted how the process would work theoretically. These computations were performed mainly on an IBM SP2 parallel computer at the Georgia Tech Center for Computational...
Materials Science, and on other supercomputers at national centers.

To provide experimental corroboration, Schuster and collaborator Abraham Joy modified a portion of DNA backbone by replacing the negatively charged phosphates with a methylphosphonates of the same size — but not carrying a formal electrical charge. They found that the modified backbone, no longer able to attract sodium ions, became an obstacle to the migration of electrical charge.

“In doing so we were motivated by intuitive arguments, supported by our molecular dynamics simulations, that the affinity for sodium ions to be around the DNA is greatly diminished by reducing the negative charge on the phosphates,” explains Landman. “Since the sodium ions show a reduced propensity to reside near the modified region of the DNA molecule, there is nothing there to effectively modulate and gate the motion of the positively charged electron holes. That reduces the probability of charges moving across the modified region.”

Beyond the implications for DNA damage in living organisms, the work has implications for proposed uses of DNA in nanotechnology. There, the self-recognition and self-assembly capabilities of the molecule make it potentially useful for sensors, tiny conductive structures and other applications.

But the work of Landman and Schuster suggests that the electronic transport properties may not be favorable outside of DNA’s native environment.

“Even when it conducts, DNA is not a good conductor in the sense of the speed at which charge flows through it,” says Landman. “Under the best of circumstances, it is a slow conductor. Under most other circumstances, especially in dry form, it is simply an insulator.”

Beyond the conclusions, Schuster believes the work demonstrates the value of close collaboration between experimental and theoretical scientists.

“For the past few years, we have been looking at charge transport in DNA from an experimental point of view, gathering data and making certain observations,” he says. “With Uzi Landman’s contribution, we were able to bring these observations together in a new and coherent way that allowed us to formulate a theory for charge transport in DNA that encompasses not only the data we have been able to gather, but also information gathered by other laboratories around the world.”

The ability to quickly test experimental results against theory and to refine theory based on new experiments offers a powerful tool. “We have achieved the ability to communicate between experiment and theory in real time,” Landman says. Adds Schuster: “Theory and experiment have formed a new partnership.”

For the future, Landman and Schuster hope to study the individual steps involved in charge migration and the complex reactions that cause damage to DNA. They also want to determine whether DNA strands contain “dumps,” non-coding sections designed to capture electrical charge and protect more critical components of genomic DNA.

The work was sponsored by the National Science Foundation, the U.S. Department of Energy, and the Air Force Office of Scientific Research.

For more information, you may contact Gary Schuster, College of Sciences, Georgia Tech, Atlanta, GA 30332-0365. (Telephone: 404-894-3300) (E-mail: gary.schuster@cos.gatech.edu), or Uzi Landman, School of Physics, Georgia Tech, Atlanta, GA 30332-0430. (Telephone: 404-894-3368) (E-mail: uzi.landman@physics.gatech.edu).
A Model Environment

Numerical models help hydropower industry reduce fish injury and improve water quality.

By Jane M. Sanders

The devil is in the details for engineers who are modeling the path of fish that get drawn into hydropower plants and, in some places, may be spit out into oxygen-poor water downstream.

With increased demand for environment-friendly energy sources, the power industry depends on detailed numerical models of the flow environment in hydroelectric power plants. The industry is using models developed at the Georgia Institute of Technology to better understand the water flow through the power plant to help design turbines that reduce the risk of injury to fish and increase the amount of dissolved oxygen downstream from dams.

“With numerical modeling, you can get a very detailed picture of what happens in various parts of the plant,” says lead researcher Fotis Sotiropoulos, an associate professor of civil engineering at Georgia Tech. “Of course, we always corroborate our computational results with field and laboratory measurements to validate our simulations. But the wealth of information and level of detail that we can extract by analyzing our numerical simulations cannot even compare with the limited insights you get from experiments, which are very difficult to do for flows as complex as those encountered in real-life power plants.”

Sotiropoulos models the flow of water through the power plant by numerically solving a set of non-linear mathematical equations — the Navier-Stokes equations — using state-of-the-art computational fluid dynamics (CFD) methods. With advanced CFD methods and fast computers, researchers can now simulate the details of flow in hydropower plants in terms of velocity components, pressure and intensities of turbulent fluctuations. To predict the impact of the flow environment on the aquatic habitat and water quality downstream of a dam, Sotiropoulos and his team can:

Engineers are using Virtual Bubbles, developed by Georgia Tech with funding from the Tennessee Valley Authority, to determine the effectiveness and efficiency of auto-venting turbines. These turbines introduce air bubbles into the water as it flows through the power plant — increasing dissolved oxygen, and thus improving water quality, downstream of dams. The Tennessee Valley Authority’s Norris Hydropower Plant, shown here, has an auto-venting turbine.

PHOTO COURTESY OF TVA