RAW POWER

School of Engineering and Applied Sciences

University at Buffalo *The State University of New York*

www.eng.buffalo.edu

Mark H. Karwan
Professor and Dean

In early 2002, I distributed our first issue of Igniting Ideas. This overview of UB's School of Engineering and Applied Sciences listed our research focus areas and articulated several of our strategic objectives, including a primary objective of performing high quality research that advances applied science or technology while preparing future researchers for industrial, academic, and government positions.

This first publication of a six-issue series highlighting each of our research focus areas focuses on bio research, specifically bioinformatics, bioengineering, and biotechnology, and also includes a few recent major awards won by faculty and a brief report on our fourth Industry University Day.

It is a pleasure to be dean of this exciting faculty. Their work is pushing the frontiers of knowledge in service to all. According to NSF 2001 figures, our school ranked sixth in the nation for NSF Engineering Directorate funding among engineering schools and the highest for major research equipment funding. Our total research expenditures for this past fiscal year exceeded $40 million, a substantial figure for a school of 112 faculty.

Please enjoy this sampling of our faculty and school's accomplishments.

Igniting Ideas Series available at: www.eng.buffalo.edu/IgnitingIdeas

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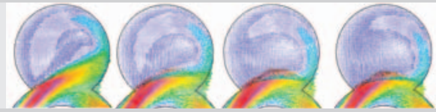
A "Fantastic Voyage"

Hui Meng, associate professor of mechanical and aerospace engineering, and Dale Taulbee, professor of mechanical and aerospace engineering, make Isaac Asimov's book Fantastic Voyage—the '60s Sci-Fi trip through the human body and brain—a reality as they advance research in hemodynamics and vascular biomechanics.



Their current focus is the treatment of stroke and cerebral aneurysms in collaboration with neurosurgeons and scientists at UB's Toshiba Stroke Research Center (TSRC). State-of-the-art computational fluid dynamics (CFD) and particle image velocimetry developed at their Laser Flow Diagnostics Lab, are linked to modern medical imaging modalities. Both in vitro and in vivo studies are conducted to understand how medical interventions affect blood flow patterns and subsequent biological responses.

Meng and Taulbee, working with a multidisciplinary TSRC team of physicians, neurosurgeons, neuroradiologists, bioengineers, and radiation physicists with diverse yet complementary expertise, are also developing anatomically realistic patient-specific models to help clinicians make scientifically sound decisions on diagnosis and treatment of vascular diseases. Sponsors of the work include the National Institutes of Health, National Science Foundation, Whitaker Foundation, Margaret L. Wendt Foundation, John R. Oishei Foundation, WNY Foundation, Boston Scientific Corporation, Diasonics Corporation of America, Cummings Fund, and Toshiba America Medical Systems.

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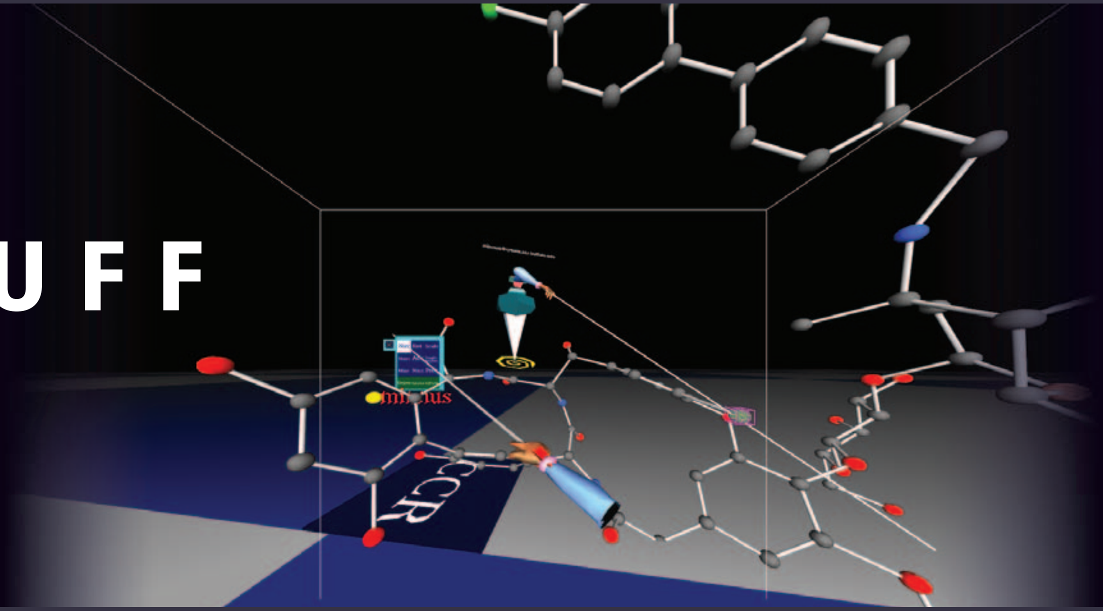
THE right STUFF

UB's CCR is fueling the bioinformatics boom with world-ranked power

Since its inception four years ago, UB's Center for Computational Research (CCR) has quickly become one of the largest and most powerful supercomputing facilities in the world.



A geographically distributed application that gives researchers located at distinct sites the ability to collaboratively manipulate molecules in real-time. Each user is represented by a unique avatar to give the sense of cooperative interaction.

CCR provides high-performance computing and high-end visualization capability. Directed by Russ Miller, University at Buffalo Distinguished Professor of Computer Science and Engineering, the center has garnered substantial funding since 1998, including $12.8 million for projects in which center staff have a lead scientific role, $95.5 million obtained by UB faculty for projects utilizing CCR resources, and $41.5 million of in-kind contributions from vendors supporting CCR's hardware and software.

Miller

In 2001, CCR's status as a top-ten academic supercomputing facility and Western New York's outstanding capability in biomedical research provided the impetus for New York State Governor Pataki to establish the Buffalo Center of Excellence in Bioinformatics, a partnership among the University at Buffalo, the Hauptman-Woodward Medical Research Institute and the Roswell Park Cancer Institute. New York State, the federal government, and corporate partners have contributed a combined total of more than $150 million in additional funding in support of the bioinformatics initiative.

CCR expanded significantly in 2002. The center acquired two large industry-standard clusters from Dell. The first machine is used to support research in protein folding and contains more processors than any cluster that Dell has ever delivered. This machine has a theoretical peak performance of 5.8 Teraflops (i.e., 5.8 trillion operations per second), 2 Terabytes of memory and 16 Terabytes of RAID storage. The second cluster is the most powerful system Dell has ever delivered for performing large-scale numerically intensive calculations. This system, which is listed as the twenty-second fastest supercomputer in the world (www.top500.com), achieved 2.004 Teraflops sustained performance on the Linpack Benchmark. After installing these two Dell Clusters in the third quarter of 2002, CCR was listed as the sixth largest supercomputing site in the world (www.gapcon.com) and first among U.S. universities.

CCR has also added a variety of high-end visualization and communication devices, including a tiled-display wall with roughly 20 times the resolution of a typical wall or monitor, and another new visualization system, the SGI Reality Center 3300W. Most recently, CCR installed an industry-standard Access Grid Node that enables large-scale remote collaborations using numerous audio and video signals. The interaction with multicast Internet sources occurs via three 100 Mbps Ethernet connections through a 1 Gbps uplink to NYSERNet and finally to the Internet2 Abilene backbone. The site can currently serve about a dozen participants and provides opportunities to comfortably interact with 50 sites simultaneously.

Today, CCR's modern infrastructure supports 40 research groups at UB and numerous companies and institutions in Western New York. Among the projects is Miller's collaborative research with Nobel Laureate Dr. Herbert Hauptman and Dr. Charles M. Weeks, both of the Hauptman-Woodward Medical Research Institute, that includes the design, analysis, and implementation of sequential and parallel algorithms to determine the precise structure of proteins from X-ray crystallographic data. This 15-year effort has led to a direct-methods procedure called "Shake-and-Bake," which is listed on the poster "The Top Ten Algorithms of the 20th Century" by *Computing in Science and Engineering* in 1999.

Engineering a new approach to biomedical transport problems

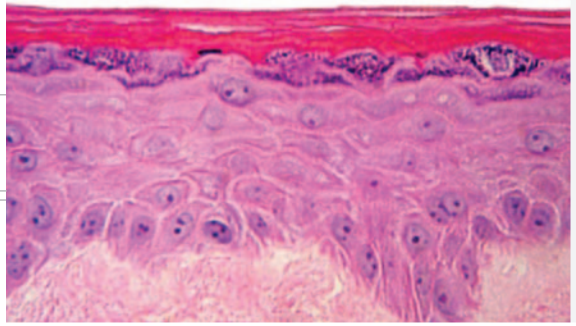
Biological systems present intricate structures and transport processes of which the unraveling and mechanistic understanding makes for truly fascinating interdisciplinary science.

Johannes Nitsche, professor of chemical engineering, looks at fundamental problems in transport phenomena, studying how molecules and particles get from one place to another within materials that have pores or other types of microscopic structure, and applying the understanding of diffusion processes to biological process modeling and biomedical applications.

One ongoing project, a mechanistic study of how drugs and chemicals pass through the skin, is directly applicable to transdermal drug delivery and risk assessment of chemical exposure. The skin is structured into layers, comprising an outermost "barrier layer" (the stratum corneum) that covers the epidermis, dermis and fat layers below. Although there is considerable understanding of molecular penetration through the stratum corneum at steady state, many questions exist regarding transient drug/chemical exposure, the role played by skin blood vessels in absorbing and redistributing molecules that diffuse in, and mechanisms by which hair follicles and other so-called skin appendages might bypass the barrier layer and furnish paths directly to the deeper tissue layers. Although many aspects of these processes are biological problems requiring experimentation, other aspects constitute physical problems where transport theory is having major impact since it allows predictive capability.

This long-term project represents a joint effort with Gerald B. Kasting, professor at the University of Cincinnati's College of Pharmacy. Past support came from NSF's GOALI program and a grant from Proctor & Gamble's International Program for Animal Alternatives. It is currently being funded by NIOSH.

Gene Therapy in Tissue Engineering



Engineered skin after 7 days of culture at the air-liquid interface. The tissue is well-stratified with multiple cell layers and a cornified cell layer at the top (orange ribbon-like structure). It is this layer that is mainly responsible for the barrier function of skin.

Tissue engineering holds promise for an entirely new approach to the repair and reconstruction of tissues and organs damaged by disease, injury, or genetic abnormalities. A promising therapeutic modality, gene therapy is broadly defined as the transfer of genes to cells or tissues for a therapeutic effect. Stelios Andreadis, assistant professor of chemical engineering and codirector of the Center for Biomedical Engineering, and his team are working to impart new functions to cells or enhance existing cellular activities in order to improve the therapeutic potential of skin substitutes, thus aiding burn victims or otherwise-injured individuals. Recent work in his laboratory has important implications for gene transfer to epidermal stem cells and they may also find wider applicability to stem cells of other tissues.

The team also prepares and uses three-dimensional skin equivalents as model systems to study tissue development and wound-healing. When engineered skin is transplanted onto mice that lack an active immune system, it integrates with the mouse skin. The transplanted tissues are then wounded to study wound-healing of human skin in vivo. Andreadis's group employs the technology of cDNA arrays to monitor the levels of gene expression during epidermopoiesis in vitro and in vivo. Specifically, cDNA arrays are used to study the response of engineered skin to barrier disruption and the protective effects of keratinocyte growth factor. This study revealed very interesting molecular information regarding the response of engineered tissue to injury and allowed the development of novel hypotheses to understand how complex molecular interactions lead to a certain tissue phenotype. Functional genomics is employed to obtain the molecular fingerprint of engineered tissues before application in the clinic or as cell biosensors.

Recently, Andreadis, James Russell, and Daniel Swartz have constructed engineered small-diameter blood vessels, with smooth muscle cells embedded in fibrin gels. The tissue-engineered vessels exhibit considerable mechanical strength and reactivity to multiple constrictors and dilators after only two weeks in culture. These tissues can be used as a biological model to address questions relating to vessel development, disease progression and as a toxicological model for drug testing, significantly impacting the treatment of cardiovascular disease.

More information is available at www.eng.buffalo.edu/~sandread/research.html.

Relating Evolutionary Trees

Xin He, professor of computer science and engineering, uses his expertise in algorithm design to solve problems in computational biology. His study of computing the "nearest neighbor interchange (nni)" distance and the related "subtree transfer" distance between phylogenetic trees, one that went unsolved for more than twenty-five years, resulted in showing the problem to be NP-complete. His approximation algorithms can be used to determine the similarities of evolutionary trees.

Fingerprint technology with a twist: rapid user customization

Venu Govindaraju, professor of computer science and engineering and associate director of the Center of Excellence for Document Analysis and Recognition (CEDAR), and his team are exploring identifying people through individual characteristics.

The team is working with Ultra-Scan Corp. to implement a new architecture for an automated fingerprint identification system (AFIS) using high-resolution ultrasonic imaging patented by Ultra-Scan. CEDAR is working on a scalable, networkable, three-tier architecture that will allow rapid customization and deployment. A developer library is also being designed to enable clients to incorporate the AFIS technology into their existing applications.

Machine recognition of faces and signatures is next to come.

Sigma Xi

Paschalis Alexandridis, associate professor of chemical engineering, has received the prestigious 2002 Sigma Xi Young Investigator Award. The national award, given every two years by the international science honors organization, recognizes an individual for scientific accomplishments, research, and ability to communicate the work to the general public.

Alexandridis

Alexandridis was recognized for work uncovering fundamental principles behind the ability of amphiphilic (dual-nature) molecules to self-assemble, work that is aimed at making intricate structures at scales ranging from nanometer (one billionth of a meter) to micrometer (one millionth of a meter).

Exploiting these copolymers will lead to new markets for products in a broad range of industries, from paints and coatings to pharmaceuticals and personal-care products.

Founder's Award

Eli Ruckenstein, SUNY Distinguished Professor in chemical engineering and winner of the National Medal of Science, received the 2002 Founder's Award, the highest award from the American Institute of Chemical Engineers (AIChE).

Ruckenstein

The Founder's Award is presented each year to an engineer who has had a profound impact on the way that chemical engineering is practiced, and whose achievements have advanced the profession in any of its aspects.

"There is virtually no aspect of modern chemical engineering that has not been profoundly influenced by Eli Ruckenstein," according to the text of the awards luncheon.

Excellence in Teaching

Alexander Cartwright, associate professor of electrical engineering, and Cyrus Madnia, associate professor of mechanical and aerospace engineering, received 2002 SUNY Chancellor's Awards for Excellence in Teaching, recognizing them for consistently demonstrating superb teaching at the undergraduate, graduate, or professional level.

Industry University Day

SEAS and UB held their fourth Industry University Day. In keeping with its theme—Vital Partners: Igniting Ideas—the event honored three major contributors to the Buffalo Center of Excellence in Bioinformatics: NYS Governor George E. Pataki; Michael D. Capellas, then chair and CEO of Compaq; and David H. Langstaff, president and CEO of Veridian Corporation.

Keynote speaker Pataki received his award for leadership in establishing the center, which he proposed early last year as the catalyst for creating thousands of high-tech jobs. A collaborative effort involving New York State, industry partners, and academic institutions, the center has attracted $50 million in state funding and more than $150 million in private-sector funding.

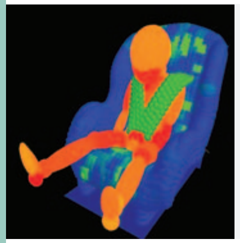
Speakers Capellas and Langstaff received awards for their companies' contributions to the center, which together totaled more than $95 million in intellectual property and funding.

"Each of these outstanding leaders truly exemplifies the spirit of the award, which is grounded in our belief that great things happen through collaboration," said UB president William R. Greiner.

"Building on the successful tradition of past Industry University Days, this one was our largest to date, with over 400 in attendance," related Dean Karwan. "We thank our colleague sectors for their continued generous support."

New technologies reinvent the tools of the trade for physicians

Led by Professor Christina L. Bloebaum, the New York State Center for Engineering Design and Industrial Innovation (NYSCEDII) is developing tools and techniques that apply state-of-the-art visualization technologies to biological applications. NYSCEDII staff and students, together with faculty and students from the UB Department of Mechanical and Aerospace Engineering and doctors from Children's Hospital, are developing a Surgical Teaching Suite. With partners Stryker Communications and SGI, concepts and applications are being developed that will enable enhanced simulation, visualization, and communication in the operating room, including 3D renderings from CT or MRI data, real-time video conferencing for surgeon-over-the-shoulder assistance, storage of all data for web-portals and pre-operative planning, and real-time training sessions for geographically separated participants. NYSCEDII is enabling researchers to use visualization to bring their ideas to life by using the center's state-of-the-art visualization technologies and the staff's expertise.



In addition to the Surgical Teaching Suite, NYSCEDII is collaborating with the Center for Transportation Injury Research, Calspan-UB Research Center, and UB mechanical engineering faculty (A. Patra, PI) to develop a prototype application that allows the 3-D stereo visualization of finite element method analysis results of a child's brain during a simulated brain trauma situation. NYSCEDII researchers, together with researchers from Toshiba Stroke Research Center (TSRC) have entered into an agreement with SGI to develop and market an application programmer's interface (API) to enable visualization of medical data.

Overcoming the challenges of global transcription profiling

Koffas

The progress of genomic research, with the availability of whole genome sequences, has allowed a more robust and global understanding of metabolic networks and their regulation, through the application of high-throughput tools such as DNA microarrays, a quantitative high-throughput method of screening using isolated genetic material as a target. As a result, there is a growing number of successful applications of this method for the generation of (mostly) prokaryotic recombinant or mutant strains with specific genetic traits. There are two major challenges related to global genome profiling being addressed by a research team led by Mattheos Koffas, assistant professor of chemical engineering.

The first relates to the growing need for global transcription data that rely on in vivo rather than in vitro measurements. The significant achievement is to examine cellular responses within living cells, that is, within the immensely complex environment that even the simplest bacterial species present. The second challenge relates to the need for genome-wide transcription data for species whose genome sequence is still not available.

Koffas' team is interested in addressing both these issues with the use of cellular arrays of reporter gene fusions. The group's long-term goals are: (i) identification of targets for the development of antibacterial agents and (ii) biotechnological processes optimization by identifying targets for metabolic pathway modification and eventually biocatalyst improvement.

Data mining and gene pattern analysis

Aidong Zhang, professor of computer science and engineering, addresses data mining with application in analysis of genomic data for diseases and treatment effects. With others, she has developed data mining and visualization algorithms for pattern analysis. Their approaches have been used to analyze patterns in the gene array data sets in the bioinformatics context. Current projects include:

- Data integration and data mining of clinical data and genomic data to advance clinical and epidemiological genetics, as well as drug effect studies
- Mapping the human genome and developments in array technology (these have provided considerable information for delineating the roles of genes in disease states)
- Gene pattern analysis for pharmacodynamic modeling
- Enhancing crystal structure determination through data mining, collaborative environments, and grid computing.

Zhang

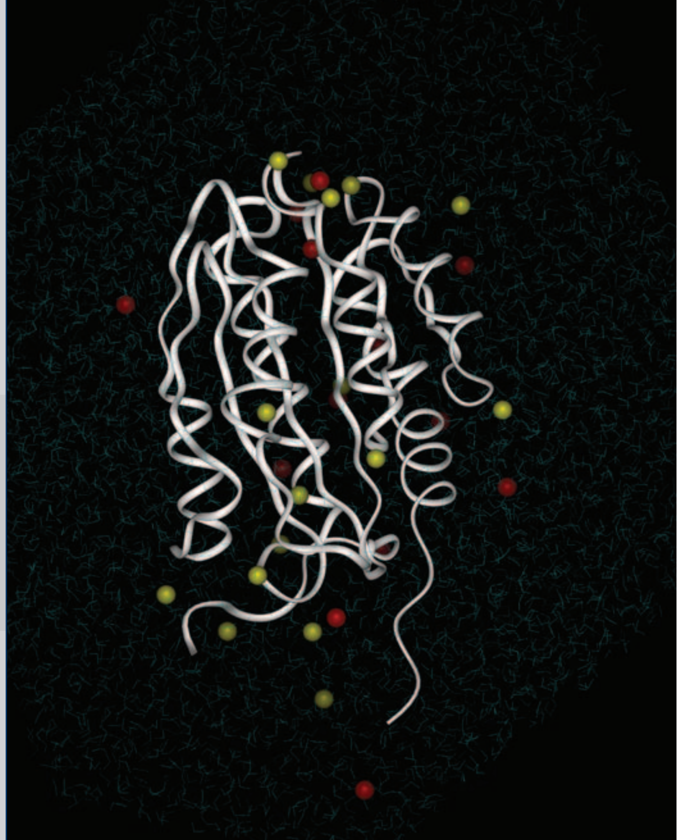
This project supports critical advances in the enabling technologies of automated tuning of software, learning via data mining, and geographically-distributed collaborative environments. These advances will be incorporated into the computationally intensive SnB program. Co-PI is Professor Russ Miller.

For her research success, the State University of New York Chancellor recognized Zhang in 2002 with the Research Recognition Award.

Biomedical Simulation & Visualization

Recent advances in modeling and simulation of biomechanical systems and virtual reality are being applied to improve medical procedures and physician training. An interdisciplinary UB team led by Thenkurussi Kesavadas, associate professor of mechanical and aerospace engineering, is addressing soft-tissue modeling, flow simulation, image-guided procedures, and 3-D imaging.

The team is developing virtual simulators as a first step toward "virtual humans." Recently, a virtual abdomen, a haptics atlas, and virtual intubation simulators have been developed. A hardware interface for medical diagnosis and simulation is also being designed. A new virtual data glove, invented at UB, helps physicians to collect soft-tissue properties during palpation procedures.



Getting to the bottom of select blood disorders

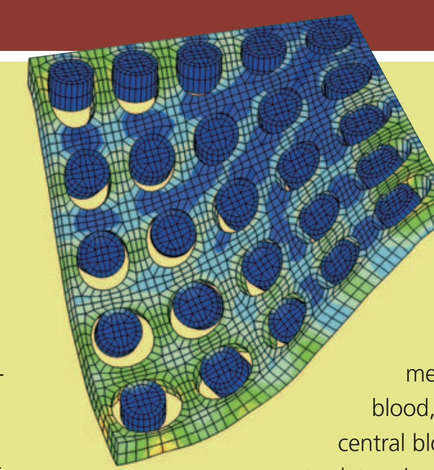
Sriram Neelamegham, assistant professor of chemical engineering and codirector of the Center for Biomedical Engineering, directs his research to understand the mechanisms regulating leukocyte, platelet, and endothelial cell function in the human circulatory system. Such studies are important because ailments of the blood involving these cell types account for a sizable fraction of inflammatory and cardiovascular disorders. Our ability to control blood cell function during these diseases may allow us to significantly alleviate morbidity and mortality caused by these ailments.

The Neelamegham laboratory is particularly known for the application of fluid mechanics in the fields of cellular and molecular bioengineering. Studies in the laboratory have led to the identification of novel molecules involved in the progress of inflammatory ailments, and they have provided a better understanding of how multiple molecules belonging to various classes of adhesion molecules function in a coordinated fashion to regulate cell adhesion under the fluid flow conditions found in human blood vessels. Aspects of this research are also leading to the development of novel therapeutic strategies, especially those directed against the selectin family of adhesion molecules.

Research work in this laboratory is conducted in close collaboration with investigators at the UB medical school and Roswell Park Cancer Institute. The work is presently supported by grants from the National Institutes of Health, the Whitaker Biomedical Engineering Foundation, and the American Heart Association.

ENGINEERING AT THE EDGE

Extreme conditions await diving super-suit



The challenge
Create an all-weather super-suit for U.S. Navy divers

The team
UB professors of engineering and physiology

The goal of Joseph Mollendorf, professor of mechanical and aerospace engineering, and David Pendergast, professor of physiology and biophysics, is to design and test a total body diver thermal protection garment. Sponsored by the Office of Naval Research, their aim is to develop a proof-of-concept suit that combines passive and active technologies to protect divers in both warm and cold water. The garment has seven principal components: super insulation, a zoned total body liquid cooling and heating suit, heat storage capacity, active heating and cooling, a heat exchanger to dump excessive heat, rechargeable power supply, and a physiological monitoring system.

The requirements for diver thermal insulation include not only a low value of the thermal conductivity, but also incompressibility, swim-flexibility, stretchability, mass manufacturability, stitchability (tailor-friendly) and durability. Even the engineering aspects of the design are highly interdisciplinary.

To understand the thermal interaction of the human body and the actively controlled zone heat transport garment, the mechanical engineers are creating a model of the human body and thermal regulation system. Each body component is composed of five compartmental layers in an "onion-like" fashion: local blood, core, muscle, fat, and skin connected to a central blood pool. The model enables the researchers to determine if the maintenance of skin temperature of the extremities can be accomplished through insulated active heating of the torso in extreme thermal conditions. The parameters of uniform liquid perfusion, which allow for diver comfort and maintain skin core temperatures under extreme thermal conditions, can now be quantified.

The team is on the threshold of constructing a prototype garment for swim and acoustic testing.

Next Issue: Infrastructure and Environment