The Computational Revolution

in Medicine, Engineering & Science

11th Annual Conference

January 16–17, 2014

THE ACADEMY OF
MEDICINE, ENGINEERING & SCIENCE
OF TEXAS

THE ACADEMY OF
MEDICINE, ENGINEERING & SCIENCE
OF TEXAS

January 16, 2014

Dear Participants:

Welcome to the 11th Annual Conference of The Academy of Medicine, Engineering & Science of Texas (TAMEST)! I am delighted that so many leaders from the fields of education, medicine, science, and business are attending this year's event in Austin.

In 2004, along with Nobel Laureates Michael Brown and the late Richard Smalley, I established TAMEST to strengthen the state's research community and to secure Texas' future as a leader in medicine, engineering and science. Membership in TAMEST consists of Texas' 263 members of the Institute of Medicine, National Academy of Engineering, and National Academy of Sciences, including our 10 Nobel Laureates.

As we celebrated our 10th year, we achieved a number of new milestones, including the highest number of members in the history of our organization. Since 2004 we have added 114 new TAMEST members, either through their election to one of the National Academies, or through the increasing numbers of leading researchers moving to Texas. Our Edith and Peter O'Donnell Awards program, established in 2006 to recognize the state's most promising young investigators, has honored a total of 36 individuals for their scientific achievements. This year's annual conference will be TAMEST's 19th major event, continuing our tradition of providing forums for interaction to foster collaboration and accelerate innovation across the state.

The program for this year's conference focuses on the emergence of computational science and engineering and its pervasive impact on virtually every aspect of scientific inquiry and technological innovation central to the progress, security, and welfare of modern civilization. The planning committee has assembled an outstanding group of speakers who will illustrate the transformative power of computational science and engineering across the disciplines.

Thank you for attending TAMEST's Annual Conference and for your continued support of the organization over the years.

Sincerely,

Kay Bailey Hutchison

Kay Bailey Hutchison

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AGENDA

THURSDAY, JANUARY 16

8:00AM – 5:00PM	**Registration**	**BARONS FOYER**
8:30 – 9:00AM	**TAMEST Membership Meeting** *(For TAMEST Members and Affiliate Members)*	**BARONS BALLROOM - ABCD**
9:00 – 9:15AM	**Break** *(Protégés and special guests are invited to join the meeting.)*	

MORNING SESSION **BARONS BALLROOM - ABCD**

9:15 – 10:00AM

Welcome and Remarks:
The Honorable Kay Bailey Hutchison, TAMEST Honorary Chair
The Honorable Joe Straus, Speaker of the Texas House of Representatives

Program Introduction: **J. Tinsley Oden, Ph.D. (NAE)**, 2014 Conference Program Chair
Associate Vice President for Research; Director, Institute for Computational Engineering and Sciences (ICES)
The University of Texas at Austin

10:00 – 10:45AM

Keynote Address:
The Curious Case of Making Clean: the Modeling & Simulation behind Improving Everyday Life
Thomas J. Lange, Director, R&D, Modeling & Simulation
Procter & Gamble Company

10:45 – 11:00AM **Break**

11:00 – 11:30AM

Monitored Destruction of the Mouse Genome by Random Germ Line Mutagenesis
Bruce A. Beutler, M.D. (Nobel Laureate, IOM, NAS), Director, Center for the Genetics of Host Defense
The University of Texas Southwestern Medical Center

11:30AM – 12:00PM

Integrating Big Data and Big Models via Bayesian Inference
Omar Ghattas, Ph.D., John A. and Katherine G. Jackson Endowed Chair in Computational Geosciences; Professor of Geological Sciences and Mechanical Engineering;
Director, Center for Computational Geosciences, Institute for Computational Engineering and Sciences (ICES)
The University of Texas at Austin

12:00 – 1:30PM **Networking Luncheon** **LOST PINES VI**

AFTERNOON SESSION **BARONS BALLROOM - ABCD**

1:45 – 2:30PM

Keynote Address:
Modeling Cardiac Function and Dysfunction
Natalia Trayanova, Ph.D., Murray B. Sachs Endowed Chair, Professor of Biomedical Engineering, Joint Appointment, Medicine, Institute for Computational Medicine
Johns Hopkins University

2:30 – 3:00PM

From Protein Folding to Molecular Machines in Biology
José N. Onuchic, Ph.D. (NAS), Professor of Physics and Astronomy, Chemistry, and Biochemistry and Cell Biology; Co-director, Center for Theoretical Biological Physics
Rice University

3:00 – 3:30PM

The Growing Scientific Importance and Competitive Advantage of Supercomputing to Science, Engineering, Medicine—and Texas
John (Jay) R. Boisseau, Ph.D., Director, Texas Advanced Computing Center
The University of Texas at Austin

3:30 – 3:45PM **Break**

AGENDA

AFTERNOON SESSION (continued) — **BARONS BALLROOM - ABCD**

3:45 – 4:00PM — **Special Address:**
A New Social Compact for Science
Harvey V. Fineberg, M.D., Ph.D. (IOM), President, Institute of Medicine

4:00 – 6:00PM — **Presentations by the Recipients of the 2014 Edith and Peter O'Donnell Awards**

6:15 – 7:00PM — **Reception** — **LOST PINES FOYER**

7:00 – 8:30PM — **O'Donnell Awards Dinner** — **LOST PINES BALLROOM**

8:30 – 10:00PM — **After-dinner Reception** — **SCRIBES CLUB**

FRIDAY, JANUARY 17

7:15 – 8:15AM — **Come-and-go Buffet Breakfast** — **BARONS BALLROOM - EFG**

8:30 – 9:15AM — **Keynote Address:**
Computational Science as a New Tool to Map the Human Brain
Henry Markram, Ph.D., Director, Blue Brain Project; Coordinator, Human Brain Project
École Polytechnique Fédérale de Lausanne

9:15 – 9:45AM — *Studying the Impacts and Mitigation of Hurricane Storm Surges and Oil Spills*
Clint N. Dawson, Ph.D., Professor and Edward S. Hyman Endowed Chair in Engineering, Department of Aerospace Engineering and Engineering Mechanics; Leader of the ICES Computational Hydraulics Group
The University of Texas at Austin

9:45 – 10:15AM — *Visualizing Viruses Inside and Outside the Cells*
Wah Chiu, Ph.D. (NAS), Alvin Romansky Professor of Biochemistry and Molecular Biology; Director, National Center for Macromolecular Imaging
Baylor College of Medicine

10:15 – 10:35AM — **Break**

10:35 – 11:05AM — *Digital Discovery and Design: toward the New Age of Materials on Demand*
Sharon C. Glotzer, Ph.D., Stuart W. Churchill Collegiate Professor of Chemical Engineering, Professor of Material Science & Engineering, Macromolecular Science and Engineering, and Physics
University of Michigan

11:05 – 11:35AM — *Computational Sciences in the Oil and Gas Industry*
Thomas C. Halsey, Ph.D., Chief Computational Scientist
ExxonMobil Upstream Research Company

11:45 AM – 2:00PM — **Closing Luncheon** — **LOST PINES VI-VIII**
Legislative Panel on Higher Education
Moderator: **Larry R. Faulkner, Ph.D.**, President Emeritus, The University of Texas at Austin
Panelists:
The Honorable Robert Duncan, Texas State Senator
The Honorable Donna Howard, Texas State Representative
The Honorable Diane Patrick, Texas State Representative
The Honorable Judith Zaffirini, Texas State Senator

2:00PM — **MEETING CONCLUDES**

FEATURED SPEAKERS

The Honorable Kay Bailey Hutchison

United States Senator, 1993–2012
TAMEST Honorary Chair

Kay Bailey Hutchison served in the U.S. Senate from 1993–2012. She served with distinction in the Senate leadership as vice chair of the Republican Conference and chair of the Republican Policy Committee, becoming the fourth-highest-ranking Republican senator. She was the ranking member on the Senate Committee on Commerce, Science, and Transportation and the Appropriations Subcommittee for Commerce, Justice, and Science. In addition, she was chair of the Military Construction Appropriations Subcommittee, served on the Defense Appropriations Subcommittee, and played an integral role in framing military policy.

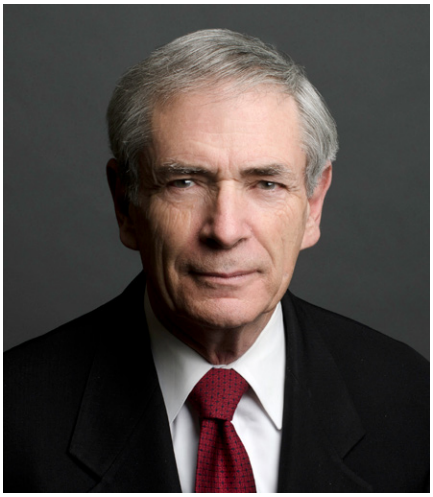
In 2004, Senator Hutchison was instrumental in establishing The Academy of Medicine, Engineering & Science of Texas (TAMEST) and continues to serve as its honorary chair. In just nine years, 114 members have joined TAMEST through induction into the National Academies or relocation to Texas, and Senator Hutchison has worked to move Texas from sixth to third in the nation in federal research funding.

The Honorable Joe Straus

Speaker of the Texas House of Representatives

Joe Straus was elected to his third term as Speaker of the Texas House by a unanimous vote in January 2013. Under Speaker Straus' leadership that year, the Texas House passed a balanced budget, improved public education, took historic action to address the state's water crisis, and passed reforms that will make state government more transparent and efficient. After the session, *Texas Monthly* named him one of the state's "Ten Best Legislators." In November, he led the effort to pass Proposition 6, securing a long-term water source that will allow the Texas economy to continue to grow. Texas voters approved Proposition 6 by a 3-to-1 margin. Speaker Straus is a small businessman and lifelong Republican who has represented Bexar County's House District 121 since 2005. He is a fifth-generation Texan and San Antonio native, and he and his wife Julie have two daughters.

FEATURED SPEAKERS



J. Tinsley Oden, Ph.D. (NAE)

Associate Vice President for Research; Director, the Institute for Computational Engineering and Sciences
The University of Texas at Austin
2014 Conference Program Chair

Dr. J. Tinsley Oden is the founding director of the Institute for Computational Engineering and Sciences (ICES), which supports broad interdisciplinary research and academic programs in computational engineering and sciences, involving five colleges and 18 academic departments within The University of Texas at Austin (UT Austin).

Dr. Oden is the author of over 500 scientific publications—books, book chapters, conference papers, and monographs. His treatise, *Finite Elements of Nonlinear Continua*, is cited as having not only demonstrated the great potential of computational methods for producing quantitative realizations of the most complex theories of physical behavior of materials and mechanical systems, but also established computational mechanics as a new, intellectually rich discipline that was built upon deep concepts in mathematics, computer sciences, physics, biology, and mechanics.

Dr. Oden has received numerous awards for his work, including the A. C. Eringen Medal, the Worcester Reed Warner Medal, the Lohmann Medal, the Theodore von Karman Medal, the John von Neumann Medal, the Newton/Gauss Congress Medal, and the Stephan P. Timoshenko Medal. He was also knighted as "Chevalier des Palmes Academiques" by the French government, and he holds six honorary doctorates, Honoris Causa, from universities in Portugal (Technical University of Lisbon), Belgium (Faculté Polytechnique de Mons), Poland (Cracow University of Technology), France (École Normale Supérieure Cachan), and the United States (Ohio State University and Presidential Citation, UT Austin). Most recently, he was awarded the 2013 Honda Prize for his role in establishing the field of computational mechanics, which enabled the development of computer simulation technology used broadly throughout industry and academia.

Harvey V. Fineberg, M.D., Ph.D. (IOM)

President, Institute of Medicine

A New Social Compact for Science

Harvey Fineberg is president of the Institute of Medicine. He previously served Harvard University as provost for four years and 13 years as dean of the School of Public Health. He helped found and served as president of the Society for Medical Decision Making and has been a consultant to the World Health Organization. His research has included assessment of medical technology, evaluation of vaccines, and dissemination of medical innovations. At the Institute of Medicine, he has chaired and served on a number of panels dealing with health policy issues, ranging from AIDS to new medical technology. He also served as a member of the Public Health Council of Massachusetts (1976–1979), as chairman of the Health Care Technology Study Section of the National Center for Health Services Research (1982–1985), and as president of the Association of Schools of Public Health (1995–1996). He is the author or co-author of numerous books and articles on subjects ranging from AIDS prevention to medical education. Dr. Fineberg holds four degrees from Harvard, including an M.D. and a Ph.D. in public policy.

The Computational Revolution

in Medicine, Engineering & Science

Henry Markram, Ph.D.
Director, Blue Brain Project
Coordinator, Human Brain Project
École Polytechnique Fédérale de Lausanne

Computational Science as a New Tool to Map the Human Brain

Modern neuroscience is producing exponentially growing volumes of experimental data, but our understanding of the brain is improving much more slowly—for two main reasons. The first is that we have no global plan for data integration and curation: most of the data we have comes from a vast array of small groups, each working within a specific discipline on a specific level of brain organization, and each using its own methods to answer its own scientific questions. The second is the sheer complexity of the brain: it has so many genes, proteins, cells, and synapses, and so many ways for them to organize and interact, that all our experiments together can only scratch the surface.

Today, we cannot completely map the brains of even the simplest of animals. Yet what we need are complete maps of different brains: male and female brains, from animals of different ages, belonging to different species, in different conditions of health and disease. To reach this goal, the Human Brain Project proposes a radically new, generic approach to mapping the brain. By applying computational engineering methods to partial data, the project will predict the biological design of the brain. Based on our current fragmentary knowledge, we will develop hypotheses about the basic principles governing the structural and functional organization of the brain within and across different levels of organization (genes, proteins, cells, microcircuits, brain regions, and the whole brain). By translating our principles into algorithms and applying them to minimal sets of experimental data, we will reconstruct complete maps of the brain in the form of computer models. We will then use the remaining available data to validate our models, thereby testing the accuracy of our initial data and our hypotheses. This approach will allow us to systematically refine our understanding of the brain's fundamental organizing principles, curate the existing literature, and identify priorities for future research. The ultimate goal is to lay the foundation for a unified theory of human brain function, opening the door to revolutionary applications in healthcare and computer technology.

KEYNOTE SPEAKERS

Thomas J. Lange

Director, R&D, Modeling & Simulation
Procter & Gamble Company

The Curious Case of Making Clean: the Modeling & Simulation behind Improving Everyday Life

We take them for granted, those products that help us start nearly every day. We shampoo and condition our hair, wash our skin, dry off with a fresh-smelling towel, shave, brush our teeth, and fix our hair.

What most people don't know is that behind each of those daily experiences lies an amazing amount of science, engineering, and high-performance computing. Procter & Gamble products like Pantene, Gillette, Crest, Covergirl, Hugo Boss, Pampers, Charmin, Cascade, and Tide must master engineering contradictions. Laundry treatments need to remove stains but protect fabrics—including cloth dyes—and be concentrated yet still easy to use. Containers should never leak but open easily. Containers, when dropped, should not break but use a bare minimum of plastic that is also recyclable. A shaving system should cut hair and leave a close shave but be comfortable and protect your skin.

We will get a rare behind the scenes glimpse of these experiences through the models and computer simulations that we use to explore thousands of innovations—before they ever exist in the real world.

Natalia Trayanova, Ph.D.

Murray B. Sachs Endowed Chair, Professor of Biomedical Engineering,
Joint Appointment, Medicine, Institute for Computational Medicine
Johns Hopkins University

Modeling Cardiac Function and Dysfunction

Simulating cardiac electrophysiological or electromechanical function is one of the most striking examples of a successful integrative multi-scale modeling approach applied to a living system directly relevant to human disease. Today, after nearly 50 years of research in the field and the rapid progress of high-performance computing, we stand at the threshold of a new era: anatomically-detailed, tomographically-reconstructed models that integrate from the ion channel or sarcomere to the electromechanical interactions in the intact heart are being developed. Such models hold high promise for interpretation of clinical and physiological measurements in terms of cellular mechanisms for improving the basic understanding of the mechanisms of dysfunction in disease conditions, such as reentrant arrhythmias, myocardial ischemia, and heart failure; and for the development and performance optimization of medical devices. Attempts are made to extend these models beyond electromechanics and include regulatory processes such as energy metabolism. This presentation will provide specific examples of the state-of-the-art in cardiac integrative modeling, including: 1) improving ventricular and atrial ablation procedures by using MRI reconstructed ventricular and atrial geometry and structure (including fibrotic scar) to investigate the reentrant circuits formed in the presence of an infarct scar; 2) employing an electromechanical model of the heart to determine the mechanisms for electromechanical delay in heart failure; 3) understanding the contributions of non-myocytes to cardiac function and dysfunction; and 4) understanding arrhythmogenesis in heart failure.

O'DONNELL AWARDS RECIPIENTS

MEDICINE

Richard K. Bruick, Ph.D.

Associate Professor and Michael L. Rosenberg Scholar in Biomedical Research, Department of Biochemistry
The University of Texas Southwestern Medical Center

Iron and Oxygen Sensors Governing Physiological Iron Homeostasis

Though iron and oxygen are required to sustain essential biological processes, an excess of either can damage cells. To govern iron and oxygen homeostasis, Hypoxia Inducible Factors regulate the transcription of genes facilitating low oxygen adaptation while Iron Regulatory Proteins (IRPs) mediate the translation or stability of mRNAs involved in iron metabolism. We have identified key regulatory factors for each pathway that sense both iron and oxygen availability. For example, an E3 ubiquitin ligase complex containing the FBXL5 protein targets IRP2 for proteasomal degradation in iron-replete cells. The stability of FBXL5 itself is regulated by a sensor of cellular iron and oxygen in the form of an internal hemerythrin-like domain. Targeted disruption of the FBXL5 gene alters both cellular and systemic iron homeostasis in mice. These observations reveal mechanistic links between metabolite status and physiological responses that may be exploited in therapeutic settings such as anemia and cancer.

ENGINEERING

Thomas M. Truskett, Ph.D.

Department Chair, Paul D. and Betty Robertson Meek Centennial Professor, Bill L. Stanley Endowed Leadership Chair
McKetta Department of Chemical Engineering
The University of Texas at Austin

Engineering via Targeted Self Assembly

Nanometer-scale particles suspended in a fluid can assemble into a wide variety of different structures depending on how they interact. These interactions are often tunable via physical or chemical modification of the particle surfaces or changes in the composition of the suspending solvent. For example, nanoparticle clusters can result from a balance between short-range co-solute mediated attractions and longer-range electrostatic repulsions. In contrast, low-coordinated superlattices with symmetries (e.g., diamond) interesting for technological applications can result from soft interparticle repulsions. In this talk, I explore how the ability to tune these interactions to reversibly assemble and dissociate such structures opens up possibilities for novel solutions to challenges in materials science, drug delivery, and other biomedical applications. Specifically, I discuss how basic principles of polymer physics and colloid science facilitate creation of materials with targeted crystal structures, liquid forms of therapeutic proteins for at-home treatment of disease, and biodegradable gold nanoclusters for biomedical imaging.

O'DONNELL AWARDS RECIPIENTS

SCIENCE

ZHIFENG REN, PH.D.

M.D. Anderson Chair Professor
Department of Physics and Texas Center for Superconductivity
University of Houston

The Beauty of Nanoscience and Nanotechnology

In this presentation, I will discuss my research in the fields of high temperature superconductivity, carbon nanotubes, zinc oxide nanostructures, nanostructured thermoelectric materials, drug delivery, and biosensing. A focus will be given to the thermoelectric materials with enhanced dimensionless thermoelectric figure-of-merit (ZT) by nanostructuring approach for their applications in efficient energy conversion systems. I will first introduce the nanostructure approach to enhance the ZT, then give a couple of examples to show the generality of the nanostructure approach, and finally focus on the development of half-Heuslers and waste heat recovery using these ZT enhanced materials. I will also show our very recent success with ZT enhancement on a couple of new materials. The application of nanostructures to biosystems to increase our capability for early stage diagnosis of illness to save lives will also be discussed at the end of the talk.

TECHNOLOGY INNOVATION

JAMES D. WALKER, PH.D.

Institute Scientist
Southwest Research Institute

Impact! and Technology for Its Assessment

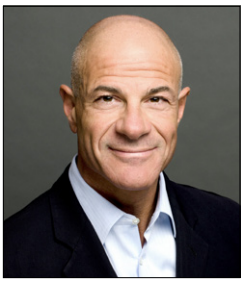
Complex mechanics occur when objects collide, especially when impact speeds are high. To accurately assess impact events and provide design and risk information, experiments, large-scale numerical simulations, and analytical models are employed. Determining materials' and structures' resistance to dynamic deformation is essential, and first-principles techniques have been developed to calculate this resistance based on material properties. One of the interesting aspects of designing protection systems is that a material is utilized all the way through failure since the protection equipment is used only once and there are weight constraints. My presentation describes various impacts and their analyses, including the foam strike on the wing of the space shuttle Columbia during ascent, aspects of vehicle and body armors to protect crews from impact and blast events, shielding for spacecraft and the International Space Station, and the potential use of hypervelocity impactors to deflect asteroids.

SPEAKERS

Bruce A. Beutler, M.D. (Nobel Laureate, IOM, NAS)
Director, Center for the Genetics of Host Defense
The University of Texas Southwestern Medical Center

Monitored Destruction of the Mouse Genome by Random Germ Line Mutagenesis

Using the chemical mutagen N-ethyl-N-nitrosourea, we randomly alter the coding sequences of an average of 134 genes in each spermatogonial cell of G0 male mice, leading to carrier status at an average of 67 loci in each of their G1 offspring. When G1 male mice are crossed to wild-type females and then bred with their own G2 daughters to produce G3 animals, a fraction of the mutations they carry are brought to homozygosity in each G3 mouse. Phenotypic effects are detected by screening, and cause and effect can be determined by genetic mapping. In principle, by creating mutations that affect all genes in the genome, the complete set of genes that have non-redundant function(s) in any measurable biological process can be determined. Our principal interest is focused on the immune system and the identification of genes needed for resistance to infection, but we have identified genes required for many other biological processes as well, ranging from metabolism to development to neurological function. To date, we have created and identified 82,936 mutations affecting 18,467 genes (81% of the total complement of protein-encoding genes in the mouse). More than 6,120 of the mutations are overtly destructive and these fall into 4,496 genes (20% of the total). Genetic mapping has become a real-time process in which only a few hours elapse between identification of a new phenotype and identification of the causative mutation. High speed saturation mutagenesis coupled with phenotypic screening and automated positional cloning depends upon strong computational resources capable of rapidly interpreting sequence data in many thousands of mice. I will describe the process in full, together with some of the discoveries we have made with it.



Omar Ghattas, Ph.D.
John A. and Katherine G. Jackson Endowed Chair in Computational Geosciences, Professor of Geological Sciences and Mechanical Engineering; Director, Center for Computational Geosciences
Institute for Computational Engineering and Sciences
The University of Texas at Austin

Integrating Big Data and Big Models via Bayesian Inference

We are in the midst of a sea change in science and engineering. Several centuries of advances in our understanding of complex natural and engineered systems have yielded mathematical models of these systems that are, in many cases, capable of sufficient fidelity to be used for prediction, design, control, and decision-making. Moreover, these models typically contain many uncertain parameters which can compromise their predictive value. Rapidly expanding volumes of observational data present opportunities to calibrate these models to reduce model uncertainties. At the same time, relentless advances in high-performance computing provide a powerful platform for executing the necessary computations. We now have the opportunity to realize the full potential of modeling and simulation by integrating large-data volumes with large-scale models on advanced computers, resulting in more predictive models and thus better tools for decision-making. I will argue that Bayesian inference provides the most systematic and rational approach to solving this so-called inverse problem. While enormous computational challenges are faced in prosecuting the Bayesian solution of inverse problems governed by complex models, the last several years have seen notable theoretical and computational advances. I will discuss these issues and provide illustrations in the context of a large-scale inverse problem for Antarctic ice sheet flow.

SPEAKERS

José N. Onuchic, Ph.D. (NAS)
Professor of Physics and
Astronomy, Chemistry, and
Biochemistry and Cell Biology;
Co-director, Center for Theoretical
Biological Physics
Rice University

From Protein Folding to Molecular Machines in Biology

It is amazing how cells have created a number of molecular machines specialized for undertaking tasks needed to control and maintain cellular functions with exquisite precision. Due to the fact that biomolecules fluctuate via thermal motion and their dynamics are diffusive, biological machines are fundamentally different from those experienced by conventional heat engines or machines in the macroscopic world. One of the key features of biological machines is the conformational changes triggered by the thermal noise under weak environmental perturbation. Therefore, we can explain how they behave using ideas borrowed from the energy landscape theory of protein folding and polymer dynamics. This new view allows us to envisage the dynamics of molecular motors from the structural perspective, and it provides the means to make several quantitative predictions that can be tested by experiments. For the kinesin motor, a prototype of the biological machines in the cell, molecular simulations of an explicit kinesin and microtubule structures show that fluctuations and flexibility inherent to the structure lead to versatile adaptation of the molecular structure, allosteric communication controlled by internal mechanics, and large amplitude stepping motion harnessing the thermal fluctuation.

John (Jay) R. Boisseau, Ph.D.
Director,
Texas Advanced Computing Center
The University of Texas at Austin

The Growing Scientific Importance and Competitive Advantage of Supercomputing to Science, Engineering, Medicine—and Texas

Advanced computing technologies are fundamental to enabling discoveries in science and engineering and are increasingly important in medical research and healthcare. Advanced computing, or supercomputing, enables high modeling and simulation of physical and biological processes, based on our best mathematical understanding, with ever-greater accuracy. Supercomputing is now also used to analyze the big data being generated and collected by the increasing scale, number, and type of digital instruments and sensors that provide high-resolution information about our environment, society, and bodies.

In Texas, we are now among the world leaders in designing, developing, and deploying the most powerful supercomputing technologies, and in using them for scientific, engineering, and medical research. Having this complementary spectrum of talent and expertise in Texas enables us to provide leadership that augments science and society for the world while providing us with competitive advantages to attract the talent and funding to Texas to sustain this leadership. The Texas Advanced Computing Center (TACC) at The University of Texas at Austin proudly supports the advancement of knowledge by open science researchers across the nation, and aims to continuously ensure that Texas leads the way to new discoveries that change the world.

SPEAKERS

Clint N. Dawson, Ph.D.
Professor and Edward S. Hyman Endowed Chair in Engineering, Department of Aerospace Engineering and Engineering Mechanics; Leader of the ICES Computational Hydraulics Group
The University of Texas at Austin

Studying the Impacts and Mitigation of Hurricane Storm Surges and Oil Spills

This talk will focus on how to develop an effective system to protect from inland flooding caused by hurricanes, a problem of critical importance to the future of Texas and many areas in the coastal United States. This effort involves collaboration between multiple disciplines—federal, state, and local agencies—and effective communication with the public. The presentation will focus on the scientific aspects of the problem, in particular the predictive simulation of storm surge and how numerical simulators may be used to study various proposed protection systems. There will be a specific focus on the Houston-Galveston region because stakeholders in this region are discussing different protection systems in the wake of Hurricane Ike. Protection systems under consideration include man-made structural options such as gates and levees, and natural options such as increasing wetland reserves and developing national seashores. The discussion will include recently proposed gate and levee systems and show how they might perform under hurricane scenarios similar to Hurricane Ike, and potential future hurricanes based on historical data. The presentation will also show how the same technology used to simulate hurricane storm surges has spin-offs to other natural disasters, such as the Deepwater Horizon Oil Spill.

Wah Chiu, Ph.D. (NAS)
Alvin Romansky Professor of Biochemistry and Molecular Biology; Director, National Center for Macromolecular Imaging
Baylor College of Medicine

Visualizing Viruses Inside and Outside the Cells

Double-stranded DNA viruses infecting both prokaryotes and eukaryotes share a common assembly pathway proceeding from a precursor (procapsid) to an infectious virion. In addition to the coat proteins forming an icosahedral cage, the procapsid requires scaffolding proteins, absent from the virion, for proper assembly and a portal machine for DNA packaging and subsequent DNA ejection. We have used single particle cryo-electron microscopy and a computationally intensive image analysis approach to determine the three-dimensional structures of several enteric and marine bacterial viruses at near atomic resolutions (Chen et al., PNAS 2011; Baker et al., PNAS 2013). Our structural analyses show a large conformation change of the virus particle before and after the viral genome encapsidation. Using cryo-electron tomography, we imaged Synechococcus cyanobacterium infected by Syn5 bacteriophage. Synechococcus is a marine photosynthetic bacterium distributed throughout the world's oceans and is a major organism responsible for fixing the carbon dioxide in the atmosphere. Extensive computational analysis of the subvolumes of virus-like particles in many tomograms of the virus infected bacteria led to the discovery of the structures of five types of virus particles representing distinct assembly intermediates inside the infected bacteria (Dai et al., Nature 2013). Such in situ structural studies provide a unique opportunity to determine not only the steps of the virus maturation process but also the effects on the structural organization of the molecular components in the infected host.

Acknowledgments: Our research has been supported by the National Institutes of Health (NIH) and the Robert Welch Foundation.

SPEAKERS

Sharon C. Glotzer, Ph.D.
Stuart W. Churchill Collegiate Professor of Chemical Engineering, Professor of Material Science & Engineering, Macromolecular Science and Engineering, and Physics
University of Michigan

Digital Discovery and Design: toward the New Age of Materials on Demand

From the Stone Age to the Bronze Age to the Iron Age to the Plastics Age to the Information (Silicon) Age, the materials available to humankind define the world we live in. Recently, unprecedented computer capabilities driven in part by the desire for better and faster video game graphics have found their way onto the computational scientist's workbench. These new capabilities are changing the course of materials research, making possible the discovery of new and complex materials designed and engineered with specific properties and functionalities in mind. In particular, they are enabling the birth of assembly engineering—a new design/optimization approach to materials fabrication that contributes to the new trend of additive manufacturing. In this talk, I will discuss breakthroughs from the field of nanotechnology, where nanoparticles are designed to assemble—like atoms, molecules, proteins, and viruses—into complex crystals when thermodynamic and kinetic conditions are optimized. These examples demonstrate how recent advances in computers are bringing us into a new age where materials are digitally discovered and designed on demand. In this new Age of Materials on Demand, the world will be shaped not by the discovery of a single material that enables a host of new technologies, but by the design of a host of materials demanded by the conception of new technologies.

Thomas C. Halsey, Ph.D.
Chief Computational Scientist
ExxonMobil Upstream Research Company

Computational Sciences in the Oil and Gas Industry

Computational science and high performance computing are revolutionizing science and technology development in the oil and gas sector. The paradigm shift in seismic technology to full wavefield inversion (FWI) and advances in modeling the flow of oil and gas through a subsurface reservoir are notable examples. In each of these cases, the application of high performance computing has enabled step changes in the accuracy and speed of these computations, improving the robustness of the corresponding business decisions. Most major oil and gas companies have established internal high performance computing facilities, many of which are competitive with those at leading national laboratories. Examples drawn from our experience at ExxonMobil of how advanced algorithms, combined with a world-class computing capability, are enabling innovation in the oil and gas industry will be included.

CLOSING LUNCHEON PROGRAM

The future of higher education in Texas will depend on many factors: identifying adequate revenue, attracting high quality faculty and graduate students, adapting to the state's rapidly changing demographics, and incorporating blended and online learning.

A panel of state senators and representatives will explore these and other issues during the closing luncheon program.

MODERATOR

LARRY R. FAULKNER, PH.D.
President Emeritus
The University of Texas at Austin
TAMEST Industry and Community Affiliates Committee Member

Over four decades, Dr. Larry Faulkner was a member of the chemistry faculties of Harvard University, the University of Illinois, and The University of Texas at Austin, where he served as the 27th President. He recently retired as president of the Houston Endowment, a position he held from 2006–2012.

Dr. Faulkner is a member of the American Academy of Arts and Sciences and serves on the board of Exxon Mobil Corporation. He was previously a member of the boards of Temple-Inland and Sandia National Laboratories and was chair of the board of trustees of Internet2. From 2006 into 2008, he chaired the National Mathematics Advisory Panel by designation of the president and the secretary of education.

LEGISLATIVE PANEL ON HIGHER EDUCATION

PANELISTS

The Honorable Robert Duncan
Texas State Senator, District 28

Robert Duncan was elected to District 84 in the Texas House in 1992, and in 1996 he won a special election to the Texas Senate. During his more than two decades in the Texas Legislature, Senator Duncan has crafted major legislation impacting water rights, healthcare transparency and affordability, the integrity of public investment funds, public and higher education, eminent domain, and the efficiency and effectiveness of our civil justice system. Since 2004, Senator Duncan has served as chairman of the State Affairs Committee. He was elected and served as president pro tempore of the Texas Senate during the 81st Legislative Session. Senator Duncan is also a member of the Natural Resources Committee, the Committee on Higher Education, and the Committee on Education.

The Honorable Donna Howard
Texas State Representative
District 48

First elected to the Texas House of Representatives in 2006, Donna Howard currently serves on the House Appropriations Committee and the House Higher Education Committee; additionally, she serves as vice-chair of the House Administration Committee. She serves on the Appropriations Subcommittee on Article III (Agencies of Education) and the Subcommittee on Budget Transparency and Reform. She previously served as vice-chair of the House Culture, Recreation, and Tourism Committee and as a member of the House Technology Committee.

The Honorable Diane Patrick
Texas State Representative
District 94

Dr. Diane Patrick was elected to the Texas House of Representatives in November of 2006. She is currently is the vice chair of the Higher Education Committee and also sits on the House Appropriations Committee and Rules and Regulations. During her four terms in office, she has successfully passed numerous pieces of significant legislation including the state's first comprehensive Anti-Bullying Legislation, developmental education reform, increased transparency in higher education, and the Texas Teacher Residency program.

The Honorable Judith Zaffirini
Texas State Senator
District 21

Senator Judith Zaffirini (D-Laredo) is the first Hispanic woman elected to the Texas Senate, the second highest-ranking senator and the highest-ranking woman and Hispanic senator. Senator Zaffirini is chair of the Government Organization Committee and served as chair of Higher Education (2006–2012) and as chair of Health and Human Services (1993–2000). She also is co-vice chair of the Joint Oversight Committee on Higher Education Governance, Excellence and Transparency and a member of the Legislative Budget Board and the Senate Finance, Higher Education, Health and Human Services, and Administration committees. The first Hispanic woman to serve as president pro tempore of the Texas Senate and as Governor for a Day, she also served seven terms on the Appropriations Conference Committee, 10 terms on the Senate Finance Committee, and 10 terms on the Senate Education Committee.

PROTÉGÉS

Protégés listed on these pages are invited to attend the conference as special guests of the TAMEST members listed below their organizations.

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WesternGeco/Schlumberger

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Associate Professor and The Beavers / William F. Urban '41 Fellow Zachry Department of Civil Engineering
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Roderick H. Dashwood, Ph.D.
Director, Center for Epigenetics & Disease Prevention
Institute of Biosciences & Technology
Texas A&M Health Science Center

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The University of Texas MD Anderson Cancer Center

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Baylor College of Medicine

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The University of Texas Southwestern Medical Center

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Pediatrician-in-Chief; Professor & Vice-Chair, Dept of Pediatrics
Children's Hospital of San Antonio; Baylor College of Medicine

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Texas A&M University

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Professor, Materials Science and Engineering
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Professor of Molecular Genetics
The University of Texas Southwestern Medical Center

Dr. Joseph Goldstein

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Vice Chancellor for Research and Innovation
The University of Texas System

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Rice University

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Associate Professor, Department of Civil & Environmental Engineering
Texas Tech University

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Professor and Chairman, Department of Cancer Biology
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Associate Professor, Aerospace Engineering and Engineering Mechanics
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Recipient of the 2013 O'Donnell Award in Technology Innovation

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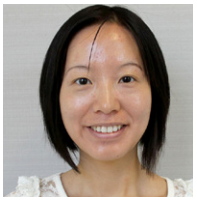

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University of Houston
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The University of Texas Health Science Center
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Texas Tech University
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William S. Saric, Ph.D.
University Distinguished Professor
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Department of Aerospace Engineering
NAE (2006)

Peter G. Wolynes, Ph.D.
Bullard-Welch Foundation Professor of Chemistry,
Department of Biochemistry and Cell Biology
Rice University
NAS (1991)

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Nobel Prize in Physiology or Medicine, 1985 | The University of Texas Southwestern Medical Center | TAMEST Founding Co-chair

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Nobel Prize in Chemistry, 1996 | Rice University

Johann Deisenhofer, Ph.D. (NAS)
Nobel Prize in Chemistry, 1988 | The University of Texas Southwestern Medical Center

Alfred G. Gilman, M.D., Ph.D. (IOM, NAS)
Nobel Prize in Physiology or Medicine, 1994 | The University of Texas Southwestern Medical Center

Joseph L. Goldstein, M.D. (IOM, NAS)
Nobel Prize in Physiology or Medicine, 1985 | The University of Texas Southwestern Medical Center

Dudley R. Herschbach, Ph.D. (NAS)
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Nobel Prize in Physics, 1996 | Texas A&M University

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Nobel Prize in Physics, 1979 | The University of Texas at Austin

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