

The Potential Impact of High-End Computing on Illustrative Fields of Science and Engineering

Committee

John W. Lyons

Chair

John W. Lyons retired Director of the Army Research Laboratory (ARL), is a physical chemist with degrees from Harvard College and Washington University in St. Louis, Missouri. He served in research and development positions with the Monsanto Company for eighteen years. In 1973 he joined the Commerce Department's National Bureau of Standards (NBS) at Gaithersburg, Maryland. At NBS Lyons was the first director of the Center for Fire Research and then in 1978 the first director of the National Engineering Laboratory, a unit that came to include about half of the NBS programs. In 1990 Lyons was appointed by President George Bush to be the ninth director of NBS, by that time renamed the National Institute of Standards and Technology or NIST. In September 1993, he was appointed the first permanent director of ARL. At ARL, Dr Lyons managed a broad array of science and technology programs; digitization/communications science, armor/armaments, soldier system, air & ground vehicle technology and survivability/lethality analysis. Dr. Lyons has published four books and over sixty papers. He holds a dozen patents. He has served on many boards and commissions, most recently the National Commission on Superconductivity, the National Critical Technologies Panel, the Federal Advisory Commission on Consolidation and Conversion of Defense Research and Development Laboratories, and in 1993, chaired the Blue Ribbon Committee on Research and Public Services for the Board of Regents, University of Maryland System. He currently serves on two boards of visitors at the University of Maryland and on the ARDEC Technology Base Peer Review Group at Picatinny Arsenal. Lyons was elected to the National Academy of Engineering in 1985. He is a Fellow of the American Association for the Advancement of Science and of the Washington Academy of Science, and a member of the American Chemical Society and of Sigma Xi.

David Arnett

Member

David Arnett is Professor of Astrophysics at the Steward Observatory of the University of Arizona. He is a theoretical astrophysicist who first demonstrated how explosive nucleosynthesis in supernovae produces the elements from carbon through iron and nickel. He constructed quantitative theoretical models of evolving massive stars and showed that the ejecta produce a good fit to the abundance of heavy elements in the galaxy. His research interests include nuclear astrophysics, formation of neutron stars and black holes, high-performance computers, theoretical physics, hydrodynamics, thermonuclear burning, stellar evolution, computer graphics, and computer modeling. Dr. Arnett is a member of the National Academy of Sciences.

Alok N. Choudhary

Member

Alok Choudhary is a Professor of Electrical and Computer Engineering at Northwestern University. He also holds an adjunct appointment with the Kellogg School of Management in the Marketing and Technology Innovation Departments. In 2000, he co-founded Accelchip, Inc., a developer of electronic design automation tools and services. Dr. Choudhary is the founder and director of the Center for Ultra-scale Computing and Information Security (CUCIS). His research interests are in high-performance computing and communication systems, power aware systems, computer architecture, high-performance I/O systems and software, and their applications in many domains including information processing and scientific computing. His interests include the design and evaluation of architectures and software systems, high-performance servers, high-performance databases, and input-output and software protection/security.

Phillip Colella

Member

Phillip Colella is a senior mathematician and group leader of the Applied Numerical Algorithms Group at Lawrence Berkeley National Laboratory. The mission of the Applied Numerical Algorithms Group (ANAG) is the development of advanced numerical algorithms and software for partial differential equations integrated with the application of the software to problems of independent scientific and engineering interest. The primary focus of our work is in the development of high-resolution and adaptive finite difference methods for partial differential equations in complex geometries, with applications to internal combustion engines and other industrial problems. In 1998, Dr. Colella was awarded the Sidney Fernbach Award from the IEEE Computer Society for his outstanding work in numerical algorithm development and parallel code design and implementation. The award is given annually to computational scientists who have achieved breakthroughs in high-performance computing. Colella's award cites his "fundamental contributions in the development of software methodologies used to solve numerical partial differential equations, and their application to substantially expand our understanding of shock physics and other fluid dynamics problems." Dr. Colella is a member of the National Academy of Sciences.

Joel L. Cracraft

Member

Joel L. Cracraft is Lamont Curator of Birds and Curator in Charge of the Division of Vertebrate Zoology and Ornithology at the American Museum of Natural History. He is also an Adjunct Professor in the Department of Earth and Environmental Sciences at Columbia University and in the Department of Biology at the City University of New York. His research interests include diversification in birds, diversification and evolution, and systematic and biogeographic theory and methods.

John A. Dutton

Member

John Dutton is Professor Emeritus in the College of Earth and Mineral Sciences at the Pennsylvania State University. His research interests involve dynamic meteorology, including dynamical systems, spectral models, predictability, climate theory, and global change. Dr. Dutton's interests span a number of topics in nonlinear atmospheric dynamics, with a current focus on the properties of attractors of hydrodynamical systems, on problems in predictability, and on global properties of atmospheric flow.

Scott V. Edwards

Member

Scott V. Edwards is a professor in the Department of Organismic and Evolutionary Biology at Harvard University. He studies the evolutionary biology of birds and relatives, combining field, museum, and genomics approaches to understand the basis of avian diversity, evolution, and behavior. His research involves population genetics, geographic variation and genome evolution; and systematics. He is current President of the Society of Systematic Biologists.

David J. Erickson, III

Member

David J. Erickson III is a Senior Research Staff member and Director of Climate and Carbon Research in the Center for Computational Sciences at Oak Ridge National Laboratory. He is also an Adjunct Professor in the Division of Earth and Ocean Sciences, Nicholas School of the Environment and Earth Sciences, Duke University. Dr. Erickson's research interests include global climate modeling, numerical modeling of atmospheric chemistry, and modeling the global air-sea exchange of energy, momentum, trace gases, and particles.

Teresa L. Head-Gordon

Member

Teresa Head-Gordon is an Associate Professor in the Department of Bioengineering at the University of California, Berkeley. Her research group combines experimental, theoretical, and computational approaches to the problems of protein folding, structure prediction, aqueous hydration, and structural biology. Her research is highly multidisciplinary and collaborative among the areas of structural biology, physical chemistry, physics, computer science, and mathematical optimization. She is studying hydration forces in the folding of proteins, a new protein folding model for annotating whole genomes, global optimization approaches to protein structure prediction, models of the condensed phase in ab initio molecular orbital theory, and modeling of chemical bonding effects for electron crystallography.

Lars E. Hernquist

Member

Lars Hernquist is Professor and Chair of the Harvard-Smithsonian Center for Astrophysics. His research interests include theoretical studies of dynamical processes in cosmology and galaxy formation and galaxy evolution, numerical simulations of stellar dynamical and hydrodynamical systems, and investigations of the physics of compact objects, particularly neutron stars and the interplay between thermal and magnetic processes in strongly magnetized neutron stars.

George E. Keller, II

Member

George E. Keller II is retired Senior Corporate Research Fellow at the Union Carbide Corporation and now Vice-Chairman of the Mid-Atlantic Technology, Research and Innovation Center (MATRIC), an independent, nonprofit, 501(c)(3) corporation headquartered in West Virginia. He is noted for invention and insightful analysis of novel separation processes. His expertise is in chemical and petroleum separation technologies, including distillation, membranes, adsorption, and extraction, and he is co-author of a recently published book, Separation Process Technology. Dr. Keller is a member of the National Academy of Engineering.

Nipam H. Patel

Member

Nipam Patel is Howard Hughes Investigator and Professor of Genetics and Development and of Integrative Biology in the Department of Molecular & Cell Biology of the University of California at Berkeley. His research program centers on the study of the evolution of development mechanisms with a focus on the genes that regulate segmentation and regionalization of the body plan. He is particularly interested in understanding how certain steps in patterns formation that require protein diffusion in *Drosophila* are accomplished in those insects and crustaceans in which cellularization of the growing embryos would seem to preclude formation of gradients by diffusion. His group also investigates the role of homeotic genes in generating body plan diversification in crustaceans. He is also investigating the function of the *Drosophila* segmentation genes during neuronal development and investigating how these genes may have contributed to the evolution of neural complexity.

Mary E. Rezac

Member

Mary Rezac is Professor and Head of the Department of Chemical Engineering at Kansas State University. Her fields of research include mass transport, polymer science, membrane separation processes, hybrid system (reactor-separator) designs, and applications to biological systems, environmental control, and novel materials.

Ronald B. Smith

Member

Ronald B. Smith is Professor of Geology and Geophysics and Mechanical Engineering at Yale University and Director of the Yale Center for Earth Observation. He leads Yale's program in mesoscale meteorology and regional climate, which includes atmospheric dynamics, observations of the atmosphere using aircraft and satellite, hydrometeorology using stable isotopes of water and theories of evaporation and rain, and satellite remote sensing of landscape changes and climate sensitivity.

James M. Stone

Member

James Stone is a Professor in the Department of Astrophysical Sciences at Princeton University, with a joint appointment in the Program in Applied and Computational Mathematics (PACM). His research group studies gas dynamics in a wide variety of astrophysical systems, from protostars to clusters of galaxies. As part of this effort, the group develops, tests, and applies numerical algorithms for astrophysical gas dynamics on high-performance computers.

John C. Wooley

Member

John Wooley is Associate Vice Chancellor for Research at the University of California at San Diego, where he is also an Adjunct Professor in the departments of Pharmacology and Chemistry & Biochemistry. He is also a Research Associate Professor of Biophysics at John Hopkins Medical School, a member of the NIH Resource for Macromolecular Modeling and Bioinformatics, Director of NSF's Biological Sciences Advisory Committee, and a member of the advisory committee for the National Biomedical Computation Resource. Prior to moving to UCSD, Dr. Wooley spent time in government service at NSF, NIH, and DOE. His research focuses on structure-function relationships in protein-nuclei acid complexes and the architecture of chromatin and ribonucleoproteins. He collaborated on the first stages of the genome project and established the first federal programs in bioinformatics and computational biology. As Associate Vice Chancellor, he is also taking the lead in a variety of biotechnology and computational biology projects, including centers for structural genomics, bioinformatics, cell signaling, biomimetic materials, and computation science/distributed computing. In general, he is creating and facilitating new interdisciplinary research and education efforts that cross traditional interdisciplinary boundaries and new scientific teams from the university and partner institutions.