



LECTURE SERIES

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1:30-2:30PM

STEW 314



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NCSA: Powering Cyber-research in the 21st Century

Since its creation by the National Science Foundation (NSF) and the state of Illinois in 1986, the National Center for Supercomputing Applications (NCSA) at the University of Illinois at Urbana-Champaign (UIUC) has been a leader in the development and deployment of new computing and software technologies for the scientific and engineering community. Many recent NSF reports have stressed the need for a national cyberinfrastructure for science and engineering with tools, services, and resources far beyond those currently available. To meet the needs of scientists and engineers in the 21st Century, NCSA will:

- **Create *cyberenvironments for science and engineering* to enable scientists and engineers to take full advantage of the resources available in the national cyberinfrastructure.**

- Provide *cyber-resources for science and engineering* to ensure that the most demanding scientific and engineering problems can be solved in a timely manner.
- Explore *innovative systems for science and engineering* to define the pathway to petascale computing and beyond.

In addition, NCSA staff intends to collaborate with faculty and staff at UIUC and other universities to move *cyberenvironments into the classroom*. This will bring the benefits of the national cyberinfrastructure are made available to educators and students throughout the country. In this overview, we will discuss all of these issues.



Bio: In December 2004 Thom H. Dunning, Jr. was appointed director of the National Center for Supercomputing Applications and Distinguished Chair for Research Excellence in the Department of Chemistry at the University of Illinois at Urbana-Champaign. He was formerly director of the Joint Institute for Computational Sciences, Distinguished Professor of Chemistry and Chemical Engineering at the University of Tennessee, and Distinguished Scientist in Computing and Computational Sciences at Oak Ridge National Laboratory. Before taking that position, Dr. Dunning was responsible for supercomputing and networking for the University of North Carolina System and a professor of chemistry at the University of North Carolina at Chapel Hill. Dr. Dunning was Assistant Director for Scientific Simulation in the Office of Science at the U.S. Department of Energy in 1999-2001, on leave from Pacific Northwest National Laboratory. In that position, he was instrumental in creating DOE's new scientific computing program, *Scientific Discovery through Advanced Computing*. Dr. Dunning joined PNNL as Associate Director for Theory, Modeling & Simulation in the Environmental Molecular Sciences Laboratory in August 1989. In EMSL, he established a world-class research program in theoretical and computational molecular science and founded the Molecular Science Computing Facility. In February 1994, Dr. Dunning was appointed Director of the Environmental Molecular Sciences Laboratory. As Director, he oversaw the construction of the EMSL as well as the development of its research instruments and scientific research programs—a \$230 million project—for DOE. In October 1997, Dr. Dunning was appointed the first Battelle Fellow at PNNL, establishing the highest scientific and engineering position in the Laboratory.

Dr. Dunning has authored nearly 150 scientific publications on topics ranging from advanced techniques for molecular calculations to computational studies of the spectroscopy of high power lasers and the chemical reactions involved in combustion. Five of his papers are "Citation Classics" with over 1,000 citations each (one has over 5,000 citations, another over 4,000). He has organized symposia and workshops for the National Research Council, the American Chemical Society, the U.S. Department of Energy, the National Science Foundation, and many other organizations. Dr. Dunning was the scientific leader of DOE's first "Grand Challenge" in computational chemistry,

which, along with the EMSL Project, led to the development of NWCHEM. NWCHEM is currently the only general computational chemistry code available for massively parallel computers, and has dramatically extended the range and accuracy of molecular calculations.

Dr. Dunning is a member of the American Chemical Society, and a Fellow of the American Physical Society and of the American Association for the Advancement of Science. He has served on numerous national advisory committees, including NRC's AFOSR Chemistry Review Committee (1987-1990), NSF's Advisory Committee for Chemistry (1991-3), and DOE's Council on Chemical Sciences (1996-9). He was the founding vice-chair of NRC's Chemical Sciences Roundtable (1996-1999) and organized its first two workshops. In April 1997, Dr. Dunning received DOE's E. O. Lawrence Award for "seminal contributions to the development and application of theoretical and computational chemistry" and, in February 2001, he was presented with DOE's Distinguished Associate Award for his research, management, and leadership in the chemical, molecular, and computational sciences for the Department.

Dr. Dunning received his B.S. in Chemistry in 1965 from the University of Missouri-Rolla and his Ph.D. in Chemical Physics from the California Institute of Technology in 1970. He was awarded a Woodrow Wilson Fellowship in 1965-66 and a National Science Foundation Fellowship in 1966-9. Previous positions include group leader of the Theoretical and Computational Chemistry Group at Argonne National Laboratory (1978-1989) and staff member and Associate Group Leader of the Laser Theory Group at Los Alamos National Laboratory (1973-78). These positions were preceded by postdoctoral appointments at the California Institute of Technology (1971-3) and Battelle Memorial Institute (1970-1).

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