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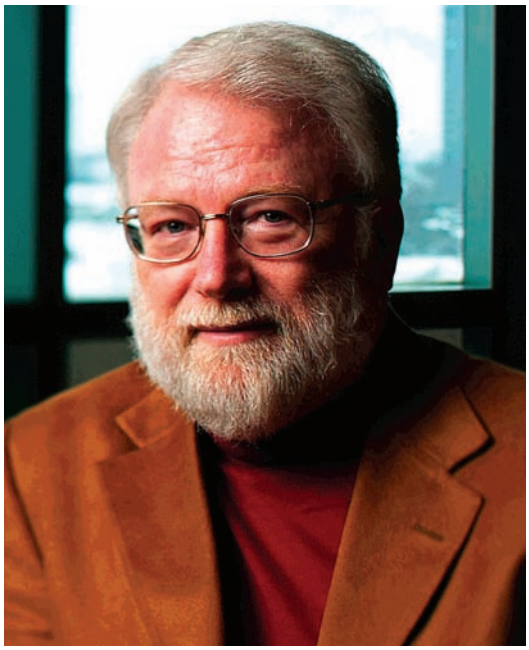

Tribute to Thom H. Dunning, Jr.

From the outset let us be clear, Thom is flourishing and moving to ever-greater success. This special issue and associated workshop merely recognize the many and diverse contributions of the first 60 years of his life.

Known to most as Thom rather than Doctor or, more recently, Professor Dunning, he provides a rather distinguished and even intimidating first impression. His white, previously more silver-gray, hair and beard coupled with a relaxed but steady stance and gaze contribute to his distinguished air. His natural, quiet reserve, even shyness, makes for a formidable first impression. Yet the man we know is warm, welcoming, and a loyal friend. While Thom was director of the Environmental and Molecular Sciences Laboratory at Pacific Northwest Laboratory, his responsibilities took him away from the daily practice of science and interaction with students and postdoctoral fellows, which he so greatly enjoyed. We regularly invited him for lunch with new postdoctoral fellows both to introduce them to him and to re-energize him by exposure to enthusiastic scientific discussions in the center that he was creating. And it is in that repeated act of creation—bringing a scientific research enterprise from concept to substance—that many of us understand Thom to find his greatest satisfaction and in which he is still engaged as director of the National Center for Supercomputing Applications (NCSA). His leadership alone (spanning Los Alamos National Laboratory, Argonne National Laboratory, the University of Tennessee and Oak Ridge National Laboratory, and the NCSA at the University of Illinois at Urbana Champaign) would be a tremendous legacy, but that would be ignoring Thom's substantial and highly cited scientific record.

All of us are familiar with his major contributions to the development of the basic mathematical approach used to solve the electronic Schrödinger equation in quantum chemical calculations—the basis set expansion technique using Gaussian functions. Three scientific publications in this series are "citation classics," that is, they have received (far) more than 1000 citations:

- "Gaussian Basis Sets for Use in Molecular Calculations. I. Contraction of (9s5p) Atomic Basis Sets for the First Row Atoms," J. Chem. Phys. *53*, 2823−2833 (1970);
- "Gaussian Basis Sets for Use in Correlated Molecular Calculations. I. The Atoms Boron through Neon and Hydrogen," J. Chem. Phys. *90*, 1007−1023 (1989); and
- "Electron Affinities

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of the First-Row Atoms Revisited. Systematic Basis Sets and Wave Functions," with R. A. Kendall and R. J. Harrison; J. Chem. Phys. *96*, 6796−6806 (1992).

While this work has garnered the most attention and has proven invaluable to a systematic approach for ab initio simulation in chemistry, his earlier research topics remain of current interest to both himself and the community. These include the development and assessment of methods for molecular electronic structure calculations, characterization of molecules important in the atmosphere and in chemical laser systems, the energetics of elementary chemical reactions, and the structure and energetics of aqueous clusters. His interest in the central and enabling role of high-performance computing in computational chemistry is a continuous thread unbroken from his days at LANL with the Cray 1-M (100 MFLOP/s and initially without error-correcting memory!) to the petascale era that he is now establishing at NCSA. His current goal is by 2011 to deploy for productive scientific research a computer capable of exceeding a sustained PFLOP/s.

The nearly 80 attendees at the workshop held in Santa Fe, NM, March 2006, were easily categorized by Thom as colleagues and friends from his days at Cal Tech, Battelle Memorial Institute, LANL, ANL, PNL, UNC, UT/ORNL, or UIUC/NCSA, but these labels are fluid, and one can see names such as Goddard, Wagner, and Schatz spanning multiple periods. The workshop provided us all with an even greater insight and appreciation for the extent of Thom's influence on so many of our careers, as well as upon our research and the fields of chemistry and scientific computing, as a whole.

Finally, no discussion of Thom would be complete without mention of his beautiful, personable, and energetic wife, Sylvia; this is truly a marriage of equals, and both are blessed, as well as their five children.

In closing, we express our collective gratitude to Thom for his intellectual contributions, community leadership and service, and personal friendship. We wish him all the best for the many years yet to come.

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