McCormick

Northwestern Engineering

The Civil and Environmental Engineering and Mechanical Engineering Departments present

The Ted Belytschko Lecture

October 14, 2014
4:00 p.m.
Ford Building ITW Room

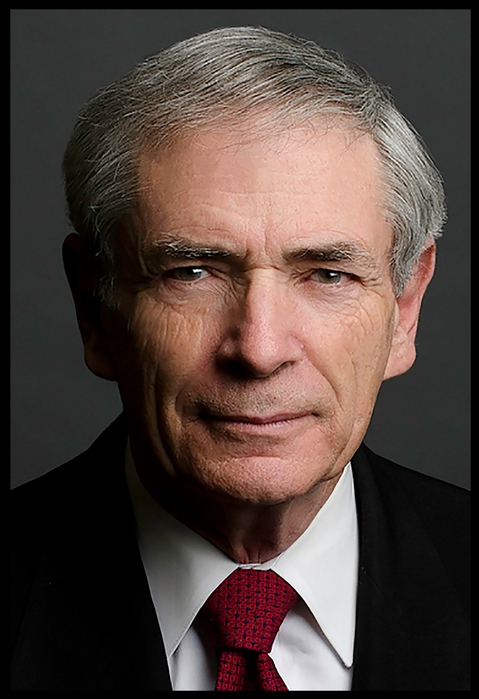
Ted Belytschko

A member of Northwestern's faculty since 1977, Belytschko's interests lie in the development of computational methods for engineering problems. Recently, he has worked on meshfree methods - techniques for representing arbitrary discontinuities in finite elements and multiscale coupling methods. He has developed explicit finite element methods that are widely used in crashworthiness analysis and virtual prototyping. The methods he developed have been instrumental in enabling the auto industry to replace physical prototype testing with computer simulation in crashworthiness design. These methods also have replaced prototype testing in many other industries, thus shortening the design cycle.

One of the most cited researchers in engineering science, Belytschko is the recipient of numerous honors, including membership in the U.S. National Academy of Engineering, the U. S. National Academy of Science, and the American Academy of Arts and Sciences. He was a founding director of the U.S. Association for Computational Mechanics, and in 2012, the association named a medal in his honor. The ASME Applied Mechanics Award was renamed the ASME Ted Belytschko Applied Mechanics Division Award in November 2007.

Professor Belytschko recently retired as editor-in-chief of the International Journal for Numerical Methods in Engineering and is co-author of the books *Nonlinear Finite Elements for Continua and Structures* and *A First Course in Finite Elements*.

The Ted Belytschko Lecture Endowment is made possible by the generosity of Professor Belytschko's friends, colleagues and former students, and by the McCormick School of Engineering and Applied Sciences, the Department of Civil and Environmental Engineering, and the Department of Mechanical Engineering.



John Tinsley Oden

Institute for Computational Engineering and Sciences
University of Texas at Austin

Predictability of Coarse-Grain Models of Atomistic Systems in the Presence of Uncertainty

It has been a common practice in molecular dynamics simulations of atomic systems, extending over many decades, to aggregate collections of atoms into molecular beads to reduce the number of degrees of freedom to sizes manageable on contemporary computer hardware. Such so-called coarse-grained models are used throughout computational chemistry, biology, and material science, and a very large literature exists on results of computer simulations obtained using such models. But, are such models always valid approximations of atomistic systems, especially in view of many uncertainties in model selection and data?

This exposition addresses the general questions of selection, calibration, validation, and uncertainty quantification in multiscale models of atomistic systems. A Bayesian framework is presented and new algorithms are described for coarse-grained model selection and validation. The concepts of model plausibility, model evidence, entropy-based priors, parameter sensitivities, and an adaptive algorithm designed around an interpretation of Occam's Razor are discussed, together with applications to typical atomistic systems in thermodynamic equilibrium.

Biography: Dr. John Tinsley Oden is Associate Vice President for Research and Director of the Institute for Computational Engineering and Sciences (ICES) at The University of Texas at Austin. He was the founding Director of that Institute, which supports broad interdisciplinary research and academic programs in computational engineering and sciences, involving five colleges and 18 academic departments within UT Austin. Oden holds the Cockrell Family Regents' Chair in Engineering and the Peter O'Donnell, Jr. Centennial Chair in Computer Systems at the University of Texas at Austin, where he is also a Professor of Aerospace Engineering and Engineering Mechanics, a Professor of Mathematics, and a Professor of Computer Science.

Dr. Oden is a member of the U.S. National Academy of Engineering. He is also a member of The American Academy of Arts and Sciences. He serves on numerous organizational, scientific, and advisory committees for international conferences and symposiums. He is an Editor of Computer Methods in Applied Mechanics and Engineering and serves on the editorial board of 29 scientific journals.

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