“Foundations of Predictive Computational Science: Selection and Validation of Models of Complex Systems in the Presence of Uncertainty”

Dr. J. Tinsley Oden
University of Texas, Austin

Abstract
Interest in a subject some call predictive computational science has emerged in recent years, mainly because of dramatic advances in computers and computational science. These advances have pushed computer modeling from a qualitative endeavor to a quantitative science in which specific predictions are sought as a basis for important, sometimes life and death, decisions: climate change, predictive medicine, design of new materials, drug design, manufacturing processes, and many other subjects. What has fueled concerns about computer predictions, and led to the study of predictive computational science, is their reliability? What factors determine the reliability of computer predictions, particularly in the presence of inevitable uncertainties? How can one quantify the uncertainty in computer predictions when every phase of the prediction process faces often confounding uncertainties: in observational data, in model selections, in modal parameters, and in targeted quantities of interest?

This lecture presents an introduction to mathematical, statistical, and philosophical issues underlying predictions in the presence of uncertainties – in model selection, in model parameters, in observational data, and in the epistemology underlying the quantification of uncertainty. It is argued that a Bayesian approach provides the most logical setting for addressing these issues, complimented with tools from information theory. We describe OPAL—the Occam Plausibility Algorithm, as an adaptive approach to model selection and validation. Applications to coarse-grained models of atomistic systems, phase-field models of tumor growth, and models of gamma wave radiation are discussed.

Bio
J. Tinsley Oden is Associate Vice President for Research and Director of the Institute for Computational Engineering and Sciences (ICES) at UT-Austin, where he holds the Cockrell Family Regents Chair in Engineering, and the Peter O’Donnell Jr. Centennial Chair in Computer Systems. He is a Professor of Aerospace Engineering and Engineering Mechanics, of Mathematics, and of Computer Science at UT-Austin. He is the founding Director of ICES and a member of the National Academy of Engineering and the American Academy of Arts and Sciences, an Honorary Member of the ASME, and a Life Member of ASCE. Oden serves on numerous organizational, scientific, and advisory boards. An editor of Computer Methods in Applied Mechanics and Engineering, Oden also serves on the editorial boards of 29 scientific journals. Dr. Oden is the author or editor of over 800 scientific works, including 57 books, monographs, and proceedings. His latest book, An Introduction to Mathematical Modeling: a Course in Mechanics, published in 2011 and reprinted in 2012. Numerous awards in recognition of his research accomplishments include being Knighted with the title of “Chevalier dans l’ordre des Palmes Académiques” from the French government, the Worcester Reed Warner Medal, the Stephen P. Timoshenko Medal, the O.C. Zienkiewicz Medal, and six honorary doctorates. Oden received the SIAM Distinguished Service Award in 2009, the SIAM Prize in Computational Science in 2011, and the USACM established the J. Tinsley Oden Medal in honor of his “outstanding and sustained contributions to computational science, engineering, and mathematics”, in 2012. He was named the 2013 Honda Foundation Prize Laureate for his role in establishing the field of computational mechanics. Dr. Oden is a Fellow of USACM, IACM, AAM, ASME, ASCE, SES, and SIAM.