11th World Congress on Computational Mechanics (WCCM XI)
5th European Conference on Computational Mechanics (ECCM V)
6th European Conference on Computational Fluid Dynamics (ECFD VI)
July 20 - 25, 2014, Barcelona, Spain

THE EMERGENCE OF PREDICTIVE COMPUTATIONAL MECHANICS

J. Tinsley Oden
Institute for Computational Engineering and Sciences (ICES)
The University of Texas at Austin

ABSTRACT

The Idea of predictive science has arisen in recent yeas in reference to the body of scientific knowledge that determines the predictability of mathematical and computational models of physical events. It embraces the processes of model selection, calibration, validation and verification and their use in forecasting specific features of physical events with quantified uncertainty.

In this presentation, we trace the foundations of scientific prediction from the classical notions of deductive and inductive logic, to the generalizations of probability in the writings of R.T. Cox, E.T. Jaynes, K.S. van Horn, and others, which argue that the natural extension of Aristotelian logic that accounts for uncertainty is Bayesian. We discuss general procedures for statistical model calibration and validation and demonstrate applications to the difficult problem of validating coarse-grained models of atomic and molecular systems. Beyond the Bayesian framework, maximum entropy methods and measures of information gain are presented as approaches for computing priors and designing validation experiments. We discuss, among several special topics, model inadequacy, divergence of miss-specified Bayesian sequences in non-parametric problems, model plausibilities and averaging as an approach to determine interaction potentials for molecular systems, and for quantifying uncertainty in quantities of interest.