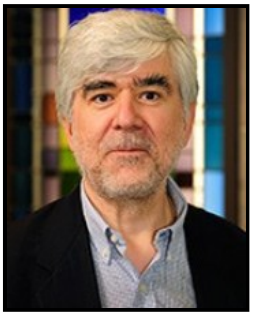

Frontiers of Scientific Computing Lecture Series

Bayesian Deep Learning for Predictive Scientific Computing

Nicholas Zabaras, University of Notre Dame

Viola D. Hank Professor of Computational Science and Engineering

Digital Media Center 1034
October 02, 2018 - 03:30 pm

Abstract:

We will briefly review recent advances in the solution of stochastic PDEs using Bayesian deep encoder-decoder networks. These models have been shown to work remarkably well for uncertainty quantification tasks in very-high dimensions. In this talk through examples in computational physics and chemistry, we will address their potential impact for modeling dynamic multiphase flow problems, accounting for model form uncertainty in coarse grained RANS simulations and providing the means to coarse graining in atomistic models. Emphasis will be given to the small data domain using Bayesian approaches. The training of the network is performed using Stein variational gradient descent. We will show both the predictive nature of these models as well as their ability to capture output uncertainties induced by the random input, limited data and model error. In closing, we will outline the integration of these surrogate models with generative adversarial networks for the solution of inverse problems.

Speaker's Bio:

Prof. Nicholas Zabaras joined Notre Dame in 2016 as the Viola D. Hank Professor of Computational Science and Engineering after serving as Uncertainty Quantification Chair and founding director of the “Warwick Centre for Predictive Modeling (WCPM)” at the University of Warwick. He is the Director of the interdisciplinary University of Notre Dame “Center for Informatics and Computational Science (CICS)” that aims to bridge the areas of data-sciences, scientific computing and uncertainty quantification for complex multiscale/multiphysics problems in science and engineering. He was also the Hans Fisher Senior Fellow with the Institute for Advanced Study at the Technical University of Munich where he is currently serving as "TUM Ambassador". He is also an Honorary Professor at the Dept. of Mathematics at the University of Hong Kong. Prior to this, he spent 23 years serving in all academic ranks of the faculty at Cornell University where he was the director of the “Materials Process Design and Control Laboratory (MPDC)”. He received his Ph.D. in Theoretical and Applied Mechanics from Cornell, after which he started his academic career at the faculty of the University of Minnesota. Professor Zabaras' research focuses on the integration of computational mathematics, statistics, and scientific computing for the predictive modeling of complex systems. He has been honored with the Wolfson Research Merit Award from the Royal Society, the Michael Tien '72 Excellence in Teaching Prize from Cornell University, and the Presidential Young Investigator Award from the National Science Foundation.

This lecture has refreshments @ 03:00 pm

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