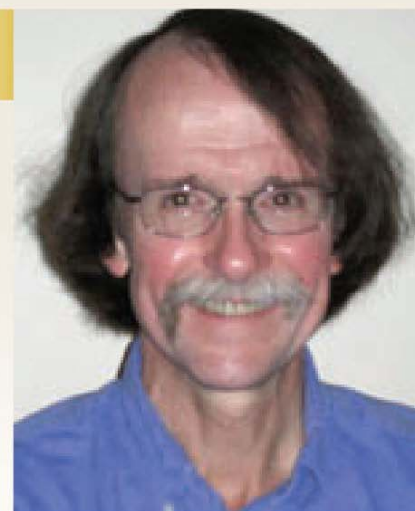


10th Anniversary

The AMSS-PolyU Joint Research Institute

Lecture Series

Professor C.T. Kelley
North Carolina State University
Sparse Grids, Quantum Chemistry,
and Solar Energy



Abstract

Photochemistry is the study of the effects of photons on molecules. The energy of a molecule depends on a large vector of molecular coordinates and is very expensive to compute. This means that reduced-order models are essential to simulate photochemical reactions and explore the energy hypersurfaces at the quantum states of interest. In this talk, we develop and analyze an reduced-order model of the energy functional, show how it can be integrated into a dynamic model which takes into account thermal fluctuations, and illustrate the ideas with some preliminary results for an application to solar energy. The model is based on sparse grids, which enable error estimation and control in an effective way.

Biography

C. T. Kelley is a Drexel Professor of Mathematics at North Carolina State University. His research interests are in numerical methods for nonlinear equations and optimization and applications of those methods. He is currently working on applications to neutron transport, subsurface hydrology, computation chemistry, and electronic structure computations. He is the author of four books and over 160 papers. He is a fellow of the Society for Industrial and Applied Mathematics (SIAM), editor-in-chief of SIAM Review, and chair of the SIAM Board of Trustees.

Date : 2 February 2015 (Monday)

Time : 3:00pm - 4:00pm

Venue : M1410, PolyU

ALL ARE WELCOME !

For enquiry, please contact Miss Eunice Hung at 3400 3908 or eunice.hung@polyu.edu.hk