CALIFORNIA STATE UNIVERSITY FULLERTON
NATURAL SCIENCES AND MATHEMATICS

CCAM
Center for Computational and Applied Mathematics

CCAM presents:

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Seminar Topic

Shake, Rattle, and Surface Hop: Using Clever Approximations to Tackle Complicated Problems in Chemistry

Nobel laureate Paul Dirac famously wrote in 1929 "The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much to complicated to be soluble. It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation."

Nearly a century later, the development of computational methods for tackling increasingly complex problems in chemistry remains an active area of research. In this talk, I will focus on one such method, Tully's fewest switches surface hopping (FSSH). Because of its remarkable simplicity and relatively low computational cost, FSSH has become a major method for modeling the dynamics associated with processes like photochemistry, electron transfer, and energy transfer. After describing the physical background of FSSH, I will briefly describe how I applied FSSH to problems involving spectroscopy (the interaction of molecules with light) in my post-doctoral research. I will end the talk with some examples of how my research group here at CSUF intends to use FSSH to study how our eyes are protected from harmful ultraviolet light as well as the dynamics that follow the attachment of low-energy electrons to molecules.

Friday, October 28, 2016
Location: MH – 476
Time: 3:00 p.m.
Refreshments will be served
For questions email: ccam@fullerton.edu