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Breakup of the H2 Molecule by Ultrashort XUV Laser Radiation: A Time-Dependent Treatment

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Digital Media Center Theatre
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Abstract:

As one of the most abundant molecules in the universe, the hydrogen molecule (H_2) has attracted interest from both theory and experiment not only for fundamental reasons, but also because it plays an essential role in many applications. In this talk, I will focus on breakup problems in H_2. Attosecond (10^{-18} s) physics provides a way of tracking the electronic motion of atoms and molecules in the time domain. Together with pioneering developments in femtosecond (10^{-15} s) physics/chemistry, it has paved a promising path to image and ultimately manipulate both the electronic and nuclear motion of molecules with photochemistry. Innovative progress in High Performance Computing (HPC) provides an opportunity to investigate the temporal response of electrons and nuclei in complex molecules irradiated by strong light sources at sub-femtosecond time scales.

Photo-induced few-body breakup is one of the fundamental processes in ultrafast laser-matter interaction, which offers a unique approach to understanding strongly correlated multi-particle system. Through a grid-based discretization method founded on first principles, I will discuss how we use supercomputers resources, provided through the network of eXtreme Science and Engineering Discovery Environment (XSEDE) of the National Science Foundation, to describe the response of this two-electron molecule to the driving laser field. I will present an effective parallel algorithm to cope with this six-dimensional time-dependent problem, which is governed by a two-center potential and the mutual electron-electron interaction. In particular, I will illustrate the excellent scaling of our code on massively parallel computing platforms such as Kraken at Oak Ridge National Laboratory and Stampede at the Texas Advanced Computing Center. Real-time observation of dynamics will be illustrated through movies. Our first attempts and the challenges faced in porting the MPI computer code to heterogeneous computing platforms, such as Intel's Many Integrated Core architecture, will be addressed as well. Unleashing the power of hybrid HPC will ultimately allow us to tackle even more complex large-scale problems, such as treating the entangled motion of electrons and nuclei in laser-molecule interaction.

Speaker's Bio:

Dr. Guan received his PhD from Jilin University (China) in 1998. He has been a research associate at the Chinese Academy of Sciences, the Queen's University of Belfast, the University of Kansas, and Drake University. His research interests and expertise include theoretical and computational laser-atom and laser-molecule interactions, as well as large-scale numerical solutions of time-dependent problems, in particular the development of effective parallel algorithms. The work of Dr. Guan's and his collaborators on superfast imaging of laser-molecule interactions has been selected as one of three case studies for the upcoming 2012-2013 XSEDE Science Highlight Magazine, to be presented at the SC13 supercomputing conference in Denver.