Matrix Computations & Scientific Computing Seminar

Organizer: James Demmel & Ming Gu

Wednesday, 11:00AM–12:00Noon, 380 Soda

Oct. 9 **Wibe de Jong**, LBNL

Advancing the performance and scalability of computational chemistry algorithms in NWChem

Computational chemistry is entering a new era of modeling. Large computing resources and improvements in algorithms are enabling researchers to tackle scientific problems that are larger and more realistic than ever before, and to include more of the complex dynamical behavior of nature. However, computational chemistry software needs to make significant advances so that researchers can make effective use of large numbers of processors and new complex architectures. Future architectures will be significantly different and require different programming paradigms. In this presentation we will discuss the performance, scalability, and some of the recent advances in NWChem. NWChem is DOEs premier open-source quantum chemistry software.