Matrix Computations & Scientific Computing Seminar

Organizer: James Demmel & Ming Gu

Wednesday, 11:00am–12:00pm, 380 Soda

Feb. 16 **Chao Yang**, Computational Research Division, LBL

Solving Large-scale Eigenvalue Problems in Nuclei Structure Calculation

One of the emerging computational approaches in nuclear physics is the configuration interaction (CI) method for solving the nuclear many-body problem. Like other quantum mechanics calculations, the basic computational problem is an eigenvalue problem. In many cases, one is interested in obtaining a few smallest eigenvalues and the corresponding eigenfunctions of a many-body Hamiltonian. In some applications, one may be interested in computing a relatively large number of small eigenvalues with a prescribed total angular momentum J or certain properties of a nucleus pertaining to a fixed J value. This type of calculation can be done by a simultaneous diagonalization of the Hamiltonian and the total angular momentum square operator. Although eigenvalue calculation is a well studied subject in numerical linear algebra, solving large-scale eigenvalue problems on high performance computers consisting of many thousands processing units is challenging. I will describe a number of techniques for achieving good performance in nuclear CI calculations.