

# Matrix Computations and Scientific Computing

Organizer: Jim Demmel and Ming Gu

Wednesday, 12:10–1:00 pm, 380 Soda Hall

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Oct 1      **Lin Lin**, UC Berkeley and LBNL

*Finding the sparse representation of a dense matrix*

Let  $\Psi$  be a unitary, dense matrix of size  $m \times n$  ( $m \gg n$ ). The  $\varepsilon$ -sparse representation of  $\Psi$  means that there is a matrix  $\Phi$  of size  $m \times n$  such that each column of  $\Phi$  is sparse,  $C$  is an  $n \times n$  invertible matrix, and  $\|\Psi - \Phi C\| < \varepsilon$ . In quantum physics, the existence of such sparse representation explains why many chemical systems exhibit local characters. In this talk we discuss some existing numerical techniques for finding such functions which originate from quantum physics literature. From a numerical linear algebra perspective, we introduce a new technique called the selected columns of the density matrix (SCDM), which finds such representation efficiently through a rank revealing QR procedure. Generalization for the case when  $\Psi$  is not unitary will also be discussed.