

# Matrix Computations & Scientific Computing Seminar

Organizer: James Demmel & Ming Gu

Wednesday, 11:00am–12:00pm, 380 Soda

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Dec. 8      **Yuji Nakatsukasa**, University of California at Davis  
*Solving Kohn-Sham nonlinear eigenproblems*

There has been considerable progress in recent years in understanding algorithms with inner-outer loop structure for solving extremely large linear eigenvalue problems. To solve nonlinear eigenvalue problems such as those arising from Kohn-Sham electronic structure calculations, a SCF (self-consistent field) eigensolver has a structure of three or more loops. Convergence analysis of such an SCF-eigensolver remains a largely open problem. In this talk, we focus on the convergence analysis of the innermost loop of the SCF-eigensolver. The innermost loop involves solving linear systems of equations and typically consumes most of the total runtime. We propose a scheme to detect the stagnation of the innermost iteration and apply it to improve the computational efficiency of the SCF-eigensolver.