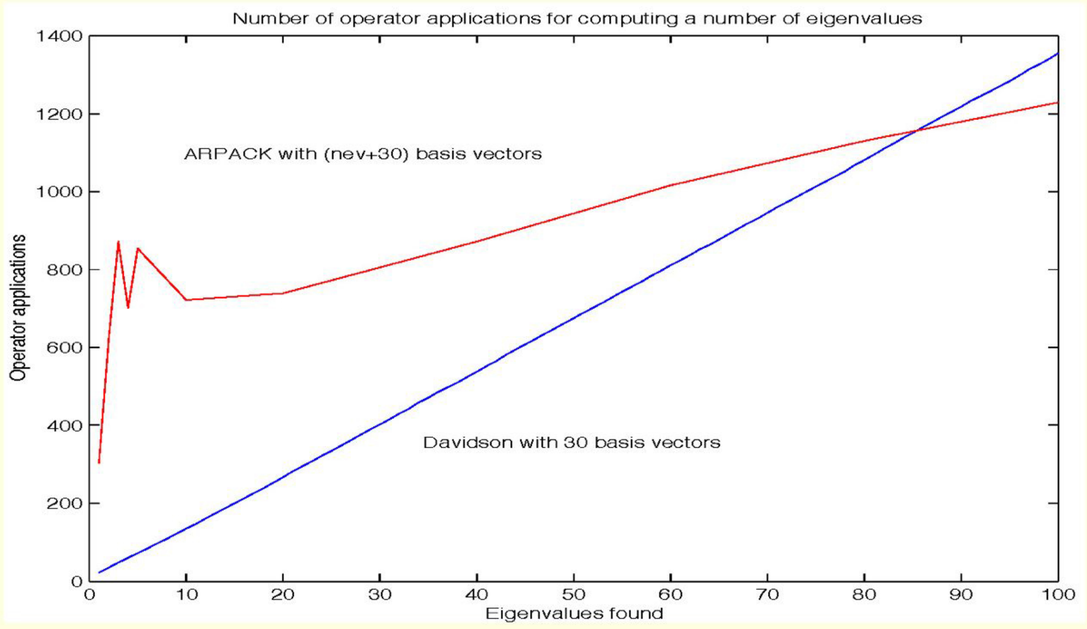
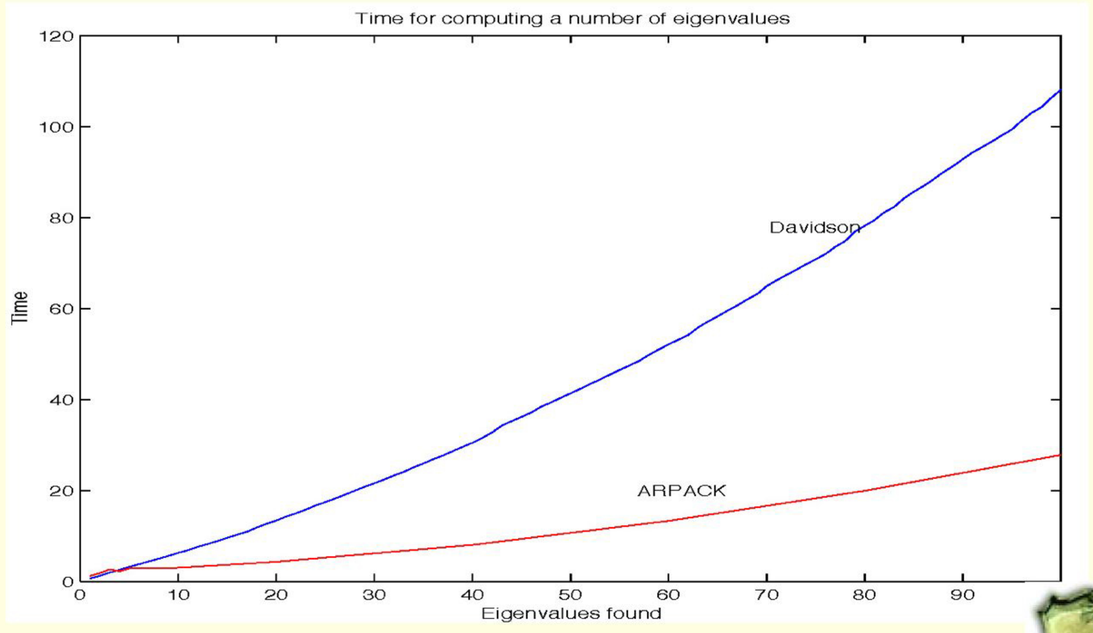
Institute for the Theory of Advanced Materials in Information Technology: James R. Chelikowsky, Yousef Saad and Renata Wentzcovitch (Minnesota), Steven G. Louie (UC Berkeley) and Efthimios Kaxiras (Harvard) (DMR-0325218): Role of Preconditioning

Electronic structure calculations often require the solution of an eigenvalue problem, sometimes involving hundres, if not thousands of eigenvalues. A commonly used method by our group is the generalized Davidson method. This method often uses powerful preconditioners to obtain the required solution. We have been investigating alternate methods such as ARPACK, which does not use preconditioners. We found for many cases that ARPACK is a faster method, although it requires more numerical operations.





From Andreas Stathopoulos