# On the computation of large-scale self-consistent-eld iterations

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The computation of the subspace spanned by the eigenvectors associated to the N lowest eigenvalues of a large symmetric matrix (or, equivalently, the projection matrix onto that subspace) is a di cult numerical linear algebra problem when the dimensions involved are very large. These problems appear when one employs the SCF (Self-Consistent-Field)

fixed-point algorithm or its variations for electronic structure calculations, which requires repeated solutions of the problem for different data, in an iterative context. The naive use of consolidated packages as Arpack does not lead to practical solutions in large-scale cases. In this paper we combine and enhance well-known purification iterative schemes with a specialized use of Arpack (or any other eigen-package) to address these large-scale challenging problems.