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A Constrained Minimization Algorithm for Solving Nonlinear Eigenvalue Problems in Electronic Structure Calculation

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One of the fundamental problems in electronic structure calculation is to determine electron orbitals associated with the minimum total energy of large atomistic systems. The total energy minimization problem is often formulated as a nonlinear eigenvalue problem and solved by an iterative scheme called Self Consistent Field (SCF) iteration. In this talk, a new direct constrained optimization algorithm for minimizing the Kohn-Sham (KS) total energy functional is presented. The key ingredients of this algorithm involve projecting the total energy functional into a sequences of subspaces of small dimensions and seeking the minimizer of total energy functional within each subspace. The minimizer of the projected energy functional not only provides a search direction along which the KS total energy functional decreases but also gives an optimal "step-length" to move along this search direction. Due to the small dimension of the projected problem, the minimizer of the projected energy functional can be computed by several different methods. These methwill be examined and compared in this talk. Numerical examples will be provided to demonstrate that this new direct constrained optimization algorithm can be more efficient and robust than the SCF iteration.