Analysis of SCF and minimization algorithms for electronic structure

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Nowadays, lots of different algorithms exist to solve the mathematical problems that arise in quantum chemistry and molecular simulation. Most of them are either based on the direct minimization of some energy under constraints or based on fixed point iterations to solve a self-consistent formulation of the problem. It is not clearly understood which class of algorithms is more convenient in which situation nor the cases where they are recommended to be used. We propose in this talk a first approach to the understanding of the intrinsic differences between two simple algorithms of each class: a damped SCF algorithm and a projected gradient descent. If their convergence is a classical result already known, we intend to provide some analysis of their behavior and some numerical results for illustration. We will also present ongoing works on the usage of these results for a posteriori error estimators.