1014-41-1519 **Reinhold Schneider*** (rs@numerik.uni-kiel.de), Lehrstuhl fr Numerische Mathematik, Christian-Albrechts-Platz 4, Christian-Albrechts-Universitt Kiel, 24098 Kiel, Germany. *Multiscale approximation in electronic structure calculation.*

Numerical simulations of electronic structures derived from the multi-particle stationary Schrödinger's equation, play a major role in molecular physics, chemistry, solid state physics, and material science. The electronic Schrödinger equation, including the Born Oppenheimer approximation, is a PDE in high dimensions. Moreover, the solution admits singularities (e.g. cusps) which hemper the efficiency of numerical methods. An approximation by one Slater determinant yields the Hartree-Fock model. This Hartree-Fock solution has only singularities at the center of the nucleons and cannot resolve electron-electron cusps. The same regularity can be assumed for effective one particle models, e.g. from *density functional theory* (DFT).

We give a detailed discussion of best N-Term approximation of these singularities of the orbitals as well as of the wave function and its influence on the accuracy of the calculated ground state energy. It turms out that this electron-nucleon cusp can be approximated by *best n-term approximation* with the rate n^{-s}, $s > 0$. However, the electron-electron cusp can only be approximated by a rate n^{-s} with $s < \frac{1}{2}$.

A short introduction into Hartree-Fock and post Hartree-Fock methods will be provided. (Received September 28, 2005)