

We present a new approach for performing all-electron density functional theory calculations based on integral equation methods. The Kohn-Sham equations are rearranged in such a way that they can be analytically inverted with Green's functions. The resulting integral equations are solved using Green's iteration, a fixed point iteration for the occupied Kohn-Sham orbitals and their corresponding energies. The motivation behind this approach is that gradient operators tend to magnify numerical errors, whereas integral operators tend to dampen them. By recasting the Kohn-Sham equations in integral form, we avoid computing any gradients throughout the calculation, however, this now requires computationally expensive convolution integrals. The novelty of our approach is that we accelerate the otherwise computationally intractable convolution integrals with the treecode, an algorithm designed for fast approximations of N-body force calculations. Furthermore, we developed a GPU version of the treecode using OpenACC, giving tremendous speedup over the CPU implementation. The treecode accelerated Kohn-Sham solver is demonstrated for a variety of atoms and small molecules, computing the ground state energies to within millihartree accuracy.