Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Multidomain decomposition approach to large scale electronic structure calculations[1] KALMAN VARGA, Vanderbilt University — A first-principles electronic structure calculation is presented using a domain decomposition technique. The domain decomposition leads to block tridiagonal Hamiltonian and overlap matrices. With the help of an LDL decomposition the block tridiagonal structure can be exploited and the Kohn-Sham states and/or the electron density can be calculated in an computationally efficient way. The electron density can be calculated from the Green's function or from the eigensolution obtained using subspace iteration. In both cases, the calculation of the density is divided into a series of independent computations that can be done in parallel. This approach allows us to determine tens of thousands of eigenstates with any desired accuracy. If the Kohn-Sham states are not required, the density can be calculated from the Green's function in a linearly scaling fashion. The linear scaling is achieved by using the special structure resulting from the domain decomposition and not by truncation or cutoff.

[1]ECCS0925422

Kalman Varga
Vanderbilt University

Date submitted: 16 Nov 2009 Electronic form version 1.4