Degree of freedom reduction of electronic structure problems of density functional theory
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Abstract
The model reduction technique presented here is based on direct minimization of the energy functional of a nanocrystalline electronic system with respect to the electron density. This solution of the minimization problem is aided by a two-level interpolation of the unknown functions using finite element (FEM) discretization of the physical space over which the solution is sought. Two grids are used. The first is a subatomic finite element grid which discretely describes the individual unit cells in the lattice. The spatial behavior of the electron density is represented at the nodes of the “electronic” FEM grid. The second grid is a macroscopic lattice grid in which unit cells are grouped into “lattice regions” which have been interpolated “unit cells” and “representative” unit cells. The profiles of the unknown functions of electronic density are interpolated across these lattice regions (in the interpolated unit cells) in terms of the electron density values at the representative unit cells of the lattice region in a unique way. Each lattice region may be thought of as akin to a linear finite element with nodal points at a specific cell-local position in the representative unit cell of the lattice region. In other words, the non-periodic part of the electron density and functions of the electron density are assumed to be smoothly varying macroscopic fields modified by an otherwise periodic density.

We use linear Finite Element shape functions of the electron density evaluated at the position r within the Cth representative unit cell to describe the interpolation of the unknown functions within the Cth representative unit cell using FEM shape functions that depend on the shape of the lattice region. The assumed near periodicity of the electron density allows for the applicability of DFT methods to systems with numbers of atoms far beyond current methods. The electron density is evaluated at the position r within the Cth representative unit cell (rC), the density value in the “representative unit cells” is interpolated using finite element (FEM) discretization.

Evaluation of Energy & Energy Gradients
The ground state electron density distribution minimizes the energy. To find this ground state, the energy and gradients must be calculated with respect to the vector of density values at the nodes of the two-level mesh. The energy terms in the electronic energy functional contain integrals over the entire computational domain with integrands that are functions of the electron density ρ(r) and functions of the local position zC. Using the integration scheme described, these integrals can be found as follows, where ξC is an element electronic density and “n” is used to mean that the element is contained in [and specified cell] C:

\[ E[\rho] = \int F(\rho(r)) G(r) dr \]

\[ \sum \int \int F(\rho(r)) G(r) d\rho d\psi \]

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Quasicontinuum-like interpolation of F(ρ(r)) using lattice level shape functions φC gives:

\[ \sum \int \int F(\rho(r)) G(r) d\rho d\psi \]

\[ F(\rho(r)) G(r) \]

The discretized energy and its gradient required for the optimization problem can now be written as

\[ E[\rho] = \int F(\rho(r)) G(r) dr \]

\[ \sum \int \int F(\rho(r)) G(r) d\rho d\psi \]

FEM interpolation of electronic elements using shape functions ψC which have compact support about the n-th electronic node, is performed as follows:

\[ F(\rho(r)) = \sum \int F(\rho(r)) G(r) d\rho d\psi \]

\[ \psi_{C}(\Delta t) = \psi(\Delta t) \]

\[ \sum \int F(\rho(r)) G(r) d\rho d\psi \]

The discretized energy and its gradient required for the optimization problem can now be written as

\[ E[\rho] = \int F(\rho(r)) G(r) dr \]

Future Work
- Implementation of energy and energy gradient calculation method described in progress.
- Integration with an optimization package to compute the representative electron density that minimizes the energy E[ρ].