ELSI: A unified software interface for Kohn–Sham electronic structure solvers

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ABSTRACT

Solving the electronic structure from a generalized or standard eigenproblem is often the bottleneck in large scale calculations based on Kohn–Sham density-functional theory. This problem must be addressed by essentially all current electronic structure codes, based on similar matrix expressions, and by high-performance computation. We here present a unified software interface, ELSI, to access different strategies that address the Kohn–Sham eigenvalue problem. Currently supported algorithms include the dense generalized eigensolver library ELPA, the orbital minimization method implemented in libOMM, and the pole expansion and selected inversion (PEXSI) approach with lower computational complexity for semilocal density functionals. The ELSI interface aims to simplify the implementation and optimal use of the different strategies, by offering (a) a unified software framework designed for the electronic structure solvers in Kohn–Sham density-functional theory; (b) reasonable default parameters for a chosen solver; (c) automatic conversion between input and internal working matrix formats, and in the future (d) recommendation of the optimal solver depending on the specific problem. Comparative benchmarks are shown for system sizes up to 11,520 atoms (172,800 basis functions) on distributed memory supercomputing architectures.

Program summary

Program title: ELSI Interface
Program Files doi: http://dx.doi.org/10.17632/y8vzhzdm62.1
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Programming language: Fortran 2003, with interface to C/C++
External routines/libraries: MPI, BLAS, LAPACK, ScLAPACK, ELPA, libOMM, PEXSI, ParMETIS, SuperLU_DIST
Nature of problem: Solving the electronic structure from a generalized or standard eigenvalue problem in calculations based on Kohn–Sham density functional theory (KS-DFT).
Solution method: To connect the KS-DFT codes and the KS electronic structure solvers, ELSI provides a unified software interface with reasonable default parameters, hierarchical control over the interface and the solvers, and automatic conversions between input and internal working matrix formats. Supported solvers are: ELPA (dense generalized eigensolver), libOMM (orbital minimization method), and PEXSI (pole expansion and selected inversion method).
Restrictions: The ELSI interface requires complete information of the Hamiltonian matrix.

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1. Introduction

Molecular and materials simulations based on Kohn–Sham (KS) [1] and generalized Kohn–Sham (gKS) [2,3] density-functional theory (DFT) are widely used to provide atomic-scale insights, understanding, and predictions across a wide range of disciplines in the sciences and in engineering. The number of DFT-related publications has grown rapidly over recent decades [4–6], exceeding 20,000 in 2016 [6]. In particular, simulations based on semilocal and hybrid density functionals serve as the production workhorses for a broad range of applications. Advances in both computational methods and high-performance computing hardware render it feasible to model large systems consisting of thousands of atoms, and linear scaling KS-DFT [7–9] can reach system sizes of millions of atoms [10,11]. Higher levels of density functional approximations, like the Random Phase Approximation (RPA), can be formulated to scale linearly with system size as well [12,13].

However, approaches for which the computational effort scales lower than \(O(N^3)\), where \(N\) is some measure of the system size, are, arguably, not yet fully established as mainstream methods of the field. There are several reasons for this status. Perhaps the simplest reason is that formally \(O(N^3)\) scaling approaches that solve an algebraic eigenvalue problem are generally applicable to any class of system, and the computational effort associated with them has a low prefactor, i.e., they are advantageous to use for systems comprised of up to roughly a few thousands of atoms, which account for the bulk of KS-DFT applications. In contrast, the transition to lower-scaling solution methods for larger systems is not necessarily simple. Such alternatives are typically restricted to certain classes of systems or problems. The transition is, therefore, not trivial to automate, requiring specific intervention and sometimes specialist knowledge by its users. This creates hurdles both from a user point of view (complexity of choice) and from a developer point of view (replication of often complex infrastructure to implement a particular method efficiently). The KS eigenvalue problem is thus in practice a bottleneck of KS-DFT simulations on current HPC architectures and for system sizes significantly exceeding several thousands of atoms.

We here present a software infrastructure, ELSI, that simplifies the approach to overcome the Kohn–Sham eigenproblem bottleneck as much as possible for electronic structure users and developers. ELSI provides an integrated and extendable interface to multiple strategies targeting the KS eigenproblem (referred to as Kohn–Sham electronic structure solvers throughout this paper). It presently (version: 2017.05) supports three solvers: ELPA (Eigenvalue solvers for Petaflop-Applications) [14,15], libO MM (Orbital Minimization Method) [16], and PEXSI (Pole Expansion and Selected Inversion) [17–19]. For the future, ELSI is expressly intended to integrate further solvers such as the linear-scaling solver CheSS (Chebyshev Sparse Solvers) [20], the iterative solver SIPS (Shift-and-Invert Parallel Spectral transformation eigen solver) [21], and others. By design, ELSI is an open infrastructure, intended to serve a community, and it can and should be flexibly adaptable to new solvers and new electronic structure codes’ needs in the future.

In this paper, we describe the outline and basic principles of ELSI, as well as a comparative assessment of the three solution strategies that are already supported in ELSI as of its 2017.05 release. The software presented here is a structural foundation that is already working in several electronic structure codes, and we expect it to become a focal point for new developments and solver cross-comparisons in the future.

2. Kohn–Sham density-functional theory

In KS-DFT [1], the many-electron problem for the Born–Oppenheimer electronic ground state is reduced to a system of single particle equations known as the Kohn–Sham equations

\[
\hat{H}^{\text{KS}} \psi_i = \epsilon_i \psi_i, \tag{1}
\]

where \(\psi_i\) and \(\epsilon_i\) are Kohn–Sham orbitals and their associated eigenenergies, and \(\hat{H}^{\text{KS}}\) denotes the Kohn–Sham Hamiltonian:

\[
\hat{H}^{\text{KS}} = \hat{t} + \hat{v}_{\text{ext}} + \hat{v}_{\text{xc}}, \tag{2}
\]

which includes the kinetic energy \(\hat{t}\), the average electrostatic potential of the electron density and of the nuclei \(\hat{v}_{\text{ext}}\) (i.e. the Hartree potential), the exchange–correlation potential \(\hat{v}_{\text{xc}}\), and possible additional potential terms \(\hat{v}_{\text{ext}}\) from external electromagnetic fields.

In almost all practical approaches, \(N_{\text{basis}}\) basis functions \(\phi_i(\mathbf{r})\) are employed to approximately expand the Kohn–Sham orbitals:

\[
\psi_i(\mathbf{r}) = \sum_{j=1}^{N_{\text{basis}}} c_{ij} \phi_j(\mathbf{r}). \tag{3}
\]

The choice of basis set is one of the critical decisions in the design of an electronic structure code [22]. Using non-orthogonal basis functions (e.g., Gaussian functions [22–28], Slater functions [29,30], numeric atom-centered orbitals [31–36], (linearized) augmented plane waves [37–41], finite elements [42]) in Eq. (3) converts Eq. (1) to a generalized eigenvalue problem

\[
\sum_j h_{ij} c_j = \epsilon_i \sum_j s_{ij} c_j, \tag{4}
\]

where \(h_{ij}\) and \(s_{ij}\) are the elements of the Hamiltonian matrix \(H\) and the overlap matrix \(S\), which can be computed through numerical integrations:

\[
h_{ij} = \int d^3r \phi_i^*(\mathbf{r}) \hat{H}^{\text{KS}} \phi_j(\mathbf{r}), \tag{5}
\]

\[
s_{ij} = \int d^3r \phi_i^*(\mathbf{r}) \phi_j(\mathbf{r}).
\]

Eq. (4) can thus be expressed in the following matrix form:

\[
H c = \epsilon S c. \tag{6}
\]

Here, the matrix \(c\) and diagonal matrix \(\epsilon\) contain the eigenvectors and eigenvalues, respectively, of the eigensystem of the matrices \(H\) and \(S\).

When using orthonormal basis sets (e.g., plane waves [9,43–47], multi-resolution wavelets [48–50], adaptive local basis set [51,52], grid-discretization based approaches [53,54]), the eigenproblem described in Eq. (6) reduces to a standard form where \(s_{ij} = \delta_{ij}\), or even can be circumvented completely by solving the KS equations in an integral formulation [22].

The explicit solution of Eq. (4) or (6) yields the Kohn–Sham orbitals \(\psi_i\), from which the electron density \(n(\mathbf{r})\) can be computed following an orbital-based method that scales as \(O(N^2)\):

\[
n(\mathbf{r}) = \sum_{j=1}^{N_{\text{basis}}} f_i \psi_i^*(\mathbf{r}) \psi_i(\mathbf{r}), \tag{7}
\]

where \(f_i\) denotes the occupation number of each orbital. In an actual computation, it is sufficient to perform the summation only for the occupied \((f_i > 0)\) orbitals. The ratio of occupied orbitals to the total number of basis functions can be below 1% for plane wave basis sets, whereas with some localized basis sets, fewer basis functions are required, leading to a larger fraction of occupied states typically between 10% and 40%.

An alternative method that scales as \(O(N)\) can be employed for localized basis functions:

\[
n(\mathbf{r}) = \sum_{i,j} \phi_i^*(\mathbf{r}) n_{ij} \phi_j(\mathbf{r}), \tag{8}
\]
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