ELSI Interface Development Version

User's Guide

The ELSI Team

http://elsi-interchange.org

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Contents

1 Introduction

1.1 The Cubic Wall of 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

$$\hat{h}^{\mathrm{KS}}\psi_l = \epsilon_l \psi_l, \tag{1.1}$$

where ψ_l and ϵ_l are Kohn-Sham orbitals and their associated eigenenergies, and $\hat{h}^{\mathrm{KS}}$ denotes the Kohn-Sham Hamiltonian, which includes the kinetic energy, the average electrostatic potential of the electron density and of the nuclei (i.e. the Hartree potential), the exchange-correlation potential, and possible additional potential terms from external electromagnetic fields. These terms depend on the electron density $\boldsymbol{n}$, which is determined by the Kohn-Sham orbitals ψ_l. These terms also enter the Hamiltonian $\hat{h}^{\mathrm{KS}}$, which determines the Kohn-Sham orbitals ψ_l.

Due to this circular dependency, the Kohn-Sham equations are in fact a non-linear optimization problem, and therefore must be solved iteratively. The most commonly used method is the self-consistent field (SCF) approach. It usually starts from an initial guess of the electron density, from which the kinetic energy, electrostatic potential, exchange-correlation potential, and external potential are computed, forming the Kohn-Sham Hamiltonian. Then, the Kohn-Sham orbitals (wavefunctions) are solved from the Hamiltonian, and new electron density is computed from the Kohn-Sham orbitals. To achieve self-consistency, the electron density is updated in every SCF iteration until converged to an acceptable level.

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

$$\psi_l(\boldsymbol{r}) = \sum_{j=1}^{N_{\mathrm{basis}}} c_{jl}\phi_j(\boldsymbol{r}). \tag{1.2}$$

The choice of basis set is one of the critical decisions in the design of an electronic structure code. Using non-orthogonal basis functions (e.g., Gaussian functions, Slater functions, numeric atom-centered orbitals) in 1.2 converts 1.1 to a generalized eigenvalue problem

$$\sum_j h_{ij}c_{jl} = \epsilon_l \sum_j s_{ij}c_{jl}, \tag{1.3}$$

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

$$\begin{aligned} h_{ij} &= \int d^3r[\phi_i^*(\boldsymbol{r})\hat{h}^{\mathrm{KS}}\phi_j(\boldsymbol{r})], \\ s_{ij} &= \int d^3r[\phi_i^*(\boldsymbol{r})\phi_j(\boldsymbol{r})]. \end{aligned} \tag{1.4}$$

1.3 can thus be expressed in the following matrix form:

$$\boldsymbol{Hc} = \boldsymbol{\epsilon Sc}. \tag{1.5}$$

Here, the matrix $\boldsymbol{c}$ and diagonal matrix $\boldsymbol{\epsilon}$ contain the eigenvectors and eigenvalues, respectively, of the eigensystem of the matrices $\boldsymbol{H}$ and $\boldsymbol{S}$.

When using orthonormal basis sets (e.g. plane waves, multi-resolution wavelets), the eigenproblem described in 1.5 reduces to a standard form where $s_{ij} = \delta_{ij}$.

The explicit solution of 1.3 or 1.5 yields the Kohn-Sham orbitals ψ_i, from which the electron density $n(\boldsymbol{r})$ can be computed following an orbital-based method:

$$n(\boldsymbol{r}) = \sum_{l=1}^{N_{\text{basis}}} f_l \psi_l^*(\boldsymbol{r}) \psi_l(\boldsymbol{r}), \tag{1.6}$$

where f_l denotes the occupation number of each orbital. In an actual computation, it is sufficient to perform the summation only for the occupied ($f_l > 0$) 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 50%.

An alternative method can be employed for localized basis functions:

$$n(\boldsymbol{r}) = \sum_{i,j}^{N_{\text{basis}}} \phi_i^*(\boldsymbol{r}) p_{ij} \phi_j(\boldsymbol{r}), \tag{1.7}$$

with p_{ij} being the elements of the density matrix $\boldsymbol{P}$ that need to be computed before the density update:

$$p_{ij} = \sum_{l=1}^{N_{\text{basis}}} f_l c_{il} c_{jl}. \tag{1.8}$$

From a viewpoint of computational complexity, with localized basis functions, almost all standard pieces of solving the Kohn-Sham equations can be formulated in a linear scaling fashion with respect to the system size. The only remaining bottleneck for semilocal functionals is the eigenproblem described in Eqs. 1.3 and 1.5. The density matrix is directly accessible through methods other than diagonalization, therefore it is not always necessary to explicitly solve the eigenproblem. Which algorithm to use depends on many factors such as the choice of basis set, and the system and characters of the physical systems. In an SCF calculation, the eigenproblem needs to be tackled repeatedly. If this step is treated with the most efficient algorithm, the whole SCF calculation can be greatly accelerated.

1.2 ELSI, the ELectronic Structure Infrastructure

ELSI unifies the community effort in overcoming the cubic-wall problem of KS-DFT by bridging the divide between developers of electronic structure solvers and KS-DFT codes. Via a unified interface, ELSI gives KS-DFT developers easy access to multiple solvers that solve or circumvent the Kohn-Sham eigenproblem efficiently. Solvers are treated on equal footing within ELSI, giving solver developers a unified platform for implementation and benchmarking across codes and physical systems. Solvers may be switched dynamically in an SCF cycle, allowing the KS-DFT developer to mix-and-match strengths of different solvers. Solvers can work cooperatively with one another within ELSI, allowing for acceleration greater than either solver can achieve individually. Most importantly, ELSI exists as a community for KS-DFT and solver developers to interact and work together to improve performance of solvers, with monthly web meetings to discuss progress on code development, yearly on-site "connector meetings", and planned webinars and workshops.

The current version of ELSI supports ELPA [2, 3], libOMM [4], NTPoly [5], PEXSI [6, 7], and SLEPc-SIPs [8, 9] solvers. Codes currently integrated with ELSI include DFTB+ [10], DGDFT [11], FHI-aims [12], and SIESTA [13].

Versatility: ELSI supports real-valued and complex-valued density matrix, eigenvalue, and eigenvector calculations. A unified software interface designed for rapid integration into a variety of electronic structure codes is provided. Fortran and C/C++ interfaces are provided.

Flexibility: ELSI supports both dense and sparse matrices as input/output. Supported matrix distribution layouts include 2D block-cyclic distribution, 1D block-cyclic distribution, and 1D block distribution. In situations where the input/output matrix format used by the electronic structure code and the format used internally by the requested solver are different, conversion and redistribution of matrices will be performed automatically.

Scalability: The solver libraries collected in ELSI are highly scalable. For instance, ELPA can scale to a hundred thousand CPU cores given a sufficiently large problem to solve, and PEXSI, with its efficient two-level parallelism, easily scales to tens of thousands of CPU cores.

Portability: ELSI and its redistributed library source packages have been confirmed to work on commonly-used HPC architectures (Cray, IBM, Intel, NVIDIA) using major compilers (Cray, GNU, IBM, Intel, PGI).

1.3 Kohn-Sham Solver Libraries Supported by ELSI

Solvers supported in the current version of ELSI are: ELPA [2, 3], libOMM [4], NTPoly [5], PEXSI [6, 7], and SLEPc-SIPc [8, 9]. The table below summarizes the supported data type, input/output matrix format, and possible output quantities of the solvers.

Solver	Data Type	Matrix format	Output
ELPA	Real/complex	Dense/sparse	Eigenvalues, eigenvectors, density matrix, energy-weighted density matrix, chemical potential, electronic entropy
libOMM	Real/complex	Dense/sparse	Density matrix, energy-weighted density matrix
NTPoly	Real	Dense/sparse	Density matrix, energy-weighted density matrix, chemical potential
PEXSI	Real/complex	Dense/sparse	Density matrix, energy-weighted density matrix, chemical potential
SLEPc-SIPs	Real	Dense/sparse	Eigenvalues, eigenvectors, density matrix, energy-weighted density matrix, chemical potential, electronic entropy

What follows is a brief introduction of the solvers currently supported in ELSI. For detailed technical descriptions of the solvers, the reader is referred to the original publications of the solvers, e.g., those in the reference list of this document.

1.3.1 ELPA

The explicit solution of a generalized or standard eigenproblem is a well-studied task. The generalized eigenproblem in 1.5 is first transformed to the standard form, e.g., by Cholesky decomposition of the overlap matrix $\boldsymbol{S}$:

$$\boldsymbol{S} = \boldsymbol{L}\boldsymbol{L}^*, \tag{1.9}$$

where $\boldsymbol{L}$ is a lower triangular matrix. Applying $\boldsymbol{L}$ to $\boldsymbol{H}$ and $\boldsymbol{c}$ in the following way

$$\begin{aligned} \tilde{\boldsymbol{H}} &= \boldsymbol{L}^{-1}\boldsymbol{H}(\boldsymbol{L}^*)^{-1}, \\ \tilde{\boldsymbol{c}} &= \boldsymbol{L}^*\boldsymbol{c}, \end{aligned} \tag{1.10}$$

transforms 1.5 to a standard eigenproblem

$$\tilde{\boldsymbol{H}}\tilde{\boldsymbol{c}} = \epsilon\tilde{\boldsymbol{c}}. \tag{1.11}$$

This standard eigenproblem is solved by further transforming it to a tridiagonal form

$$\boldsymbol{T} = \boldsymbol{Q}\tilde{\boldsymbol{H}}\boldsymbol{Q}^*, \tag{1.12}$$

where $\boldsymbol{Q}$ is a transformation matrix, and $\boldsymbol{T}$ is a tridiagonal matrix whose eigenvalues and eigenvectors are computed by, e.g., the divide-and-conquer approach or the MRRR method. This procedure is called "diagonalization", as the full matrix is reduced to a (tri)diagonal form.

The massively parallel direct eigensolver ELPA [2, 3] facilitates the direct solution of symmetric or Hermitian eigenproblems on high-performance computers by adopting a two-stage diagonalization algorithm, which first reduces the full matrix to a banded intermediate form, then to the tridiagonal form:

$$\begin{aligned} \boldsymbol{B} &= \boldsymbol{Q}_1\tilde{\boldsymbol{H}}\boldsymbol{Q}_1^*, \\ \boldsymbol{T} &= \boldsymbol{Q}_2\boldsymbol{B}\boldsymbol{Q}_2^*. \end{aligned} \tag{1.13}$$

where $\boldsymbol{Q}_1$ and $\boldsymbol{Q}_2$ are transformation matrices used in the two-stage diagonalization; $\boldsymbol{B}$ is a banded matrix; and $\boldsymbol{T}$ is a tridiagonal matrix. Compared to the one-stage diagonalization (1.12), the two-stage approach introduces two additional steps. Still, the two-stage approach has been shown to enable faster computation and better parallel scalability on present-day computers. Specifically, the matrix-vector operations (BLAS level-2 routines) in 1.12 can be mostly replaced by more efficient matrix-matrix operations (BLAS level-3 routines) in 1.13. The computational workload associated with the back-transformation of the eigenvectors is greatly alleviated if only a small fraction of the eigenvectors representing the lowest eigenstates is required, and by architecture-specific linear-algebra "kernels" provided with the ELPA library.

1.3.2 libOMM

Instead of diagonalizing the $N_{\text{basis}} \times N_{\text{basis}}$ eigenproblem, the orbital minimization method (OMM) minimizes an unconstrained energy functional using a set of auxiliary Wannier functions. At the minimum of the OMM energy functional, the Wannier functions can be used to construct the density matrix. Specifically, N_{W} non-orthogonal Wannier functions χ_k are employed to represent the occupied subspace of a system with N_{electron} electrons:

$$\chi_k = \sum_{j=1}^{N_{\text{basis}}} W_{kj}\phi_j. \tag{1.14}$$

For non-spin-polarized systems, the index k runs from 1 to $N_{\text{W}} = N_{\text{electron}}/2$. Then the matrices $\boldsymbol{H}$ and $\boldsymbol{S}$ are transformed into the occupied subspace

$$\begin{aligned} \boldsymbol{H}_{\text{omm}} &= \boldsymbol{W}^* \boldsymbol{H} \boldsymbol{W}, \\ \boldsymbol{S}_{\text{omm}} &= \boldsymbol{W}^* \boldsymbol{S} \boldsymbol{W}, \end{aligned} \tag{1.15}$$

where $\boldsymbol{W}$ is the coefficient matrix of the Wannier functions, whose dimension is $N_{\text{basis}} \times N_{\text{W}}$; $\boldsymbol{H}_{\text{omm}}$ and $\boldsymbol{S}_{\text{omm}}$ are $N_{\text{W}} \times N_{\text{W}}$ matrices. The OMM energy functional can then be evaluated from $\boldsymbol{H}_{\text{omm}}$ and $\boldsymbol{S}_{\text{omm}}$:

$$E[\boldsymbol{W}] = 4\text{Tr}[\boldsymbol{H}_{\text{omm}}] - 2\text{Tr}[\boldsymbol{S}_{\text{omm}}\boldsymbol{H}_{\text{omm}}]. \tag{1.16}$$

This energy functional, when minimized with respect to the coefficients of Wannier functions $\boldsymbol{W}$, is equal to the "band structure" energy

$$E_{\text{BS}} = \sum_{l=1}^{N_{\text{basis}}} f_l \epsilon_l, \tag{1.17}$$

i.e. the sum of the energies of all eigenstates, weighted with their respective occupation numbers. Furthermore, the Wannier functions are driven towards perfect orthonormality at this minimum. The density matrix is then constructed from the Wannier functions that minimize $E[\boldsymbol{W}]$. Although this density matrix is sufficient for the electron density update following 1.7, without knowledge of individual eigenstates, the orbital minimization method cannot handle systems with fractional occupation numbers.

Different from the originally proposed linear scaling OMM method, the OMM implementation in the libOMM library [4] is a cubic scaling density matrix solver. Theoretically, this implementation has a smaller prefactor than the direct diagonalization method. In libOMM, the minimization of the OMM energy functional is carried out with the conjugate-gradient (CG) method, whose performance mainly depends on the convergence rate of the minimization.

1.3.3 PEXSI

The pole expansion and selected inversion (PEXSI) method [6, 7] expands the density matrix $\boldsymbol{P}$ in 1.8 using a pole expansion:

$$\boldsymbol{P} = \sum \Im\left(\omega_l(\boldsymbol{H} - (z_l + \mu)\boldsymbol{S})^{-1}\right). \tag{1.18}$$

The shifts $\{z_l\}$ and weights $\{\omega_l^\rho\}$ of the poles are optimized to expand the Fermi operator. The number of terms needed by this expansion is proportional to $\log(\beta\Delta E)$, where $\beta = 1/(k_{\text{B}}T)$, k_{B} is the Boltzmann constant, T is the electronic temperature, and ΔE is the width of the eigenspectrum. This logarithmic scaling makes the pole expansion a highly

efficient approach. In most cases, ~ 20 poles are already sufficient for the result obtained from PEXSI to be fully comparable to that obtained from diagonalization.

In PEXSI, only selected elements of the object $(\boldsymbol{H} - (z_l + \mu)\boldsymbol{S})^{-1}$ (and thus the density matrix), which correspond to the non-zero elements of $\boldsymbol{H}$ and $\boldsymbol{S}$, are computed with the parallel selected inversion method. The computational cost scales at most as $O(N^2)$ for semilocal DFT. The actual complexity depends on the dimensionality of the system: $O(N)$, $O(N^{1.5})$, and $O(N^2)$ for 1D, 2D, and 3D systems, respectively. This favorable scaling hinges on the sparse character of the Hamiltonian and overlap matrices, but not on the existence of an energy gap. The PEXSI method is thus generally applicable to systems with and without a gap.

Designed in a multi-level parallelism structure, the PEXSI method is highly scalable, and can make efficient use of tens of thousands of processors on high performance computers.

1.3.4 SLEPc-SIPs

The shift-and-invert spectral transformation method, implemented in the SLEPc library [8], transforms the eigenproblem 1.5 by shifting the eigenspectrum:

$$(\boldsymbol{H} - \boldsymbol{\sigma}\boldsymbol{S}) = (\boldsymbol{\epsilon} - \boldsymbol{\sigma})\boldsymbol{S}\boldsymbol{c}, \tag{1.19}$$

where $\boldsymbol{\sigma}$ is a diagonal matrix with diagonal elements all equal to the shift σ. This shifted eigenproblem is converted to the standard form by inverting $(\boldsymbol{H} - \boldsymbol{\sigma}\boldsymbol{S})$ and $(\boldsymbol{\epsilon} - \boldsymbol{\sigma})$:

$$(\boldsymbol{H} - \boldsymbol{\sigma}\boldsymbol{S})^{-1}\boldsymbol{S}\boldsymbol{c} = (\boldsymbol{\epsilon} - \boldsymbol{\sigma})^{-1}\boldsymbol{c}, \tag{1.20}$$

which can be written in a form similar to 1.11:

$$\tilde{\boldsymbol{H}}\boldsymbol{c} = \tilde{\boldsymbol{\epsilon}}\boldsymbol{c}. \tag{1.21}$$

Here, the eigenvectors are not altered by the shift-and-invert transformation, and the eigenvalues of 1.21 relate to the original ones via

$$\tilde{\boldsymbol{\epsilon}} = (\boldsymbol{\epsilon} - \boldsymbol{\sigma})^{-1}. \tag{1.22}$$

If the shift can be chosen to be close to the target eigenvalue, 1.22 makes the magnitude of the transformed eigenvalues large, accelerating the convergence of the iterative Krylov-Schur eigensolver used in SLEPc.

On top of the basic shift-and-invert, the shift-and-invert parallel spectral transformation (SIPs) method [9] partitions the eigenspectrum of a given eigenproblem into N_{slice} slices. Accordingly, the processes involved in the calculation are split into N_{slice} groups, each of which solves one slice independently. Within the slices, carefully selected shifts are applied to the original problem. With this layer of parallelism across slices, the SLEPc-SIPs solver has the potential to exhibit enhanced scalability over direct diagonalization methods, especially when the load balance across slices can be guaranteed. Indeed, this has been reported to happen with very sparse Hamiltonian and overlap matrices out of density-functional tight-binding (DFTB) calculations [9].

1.4 Citing ELSI

Key concepts of ELSI and the first version of its implementation are described in the following paper [14]:

V. W-z. Yu, F. Corsetti, A. García, W. P. Huhn, M. Jacquelin, W. Jia, B. Lange, L. Lin, J. Lu, W. Mi, A. Seifitokaldani, Á. Vázquez-Mayagoitia, C. Yang, H. Yang, and V. Blum, ELSI: A Unified Software Interface for Kohn-Sham Electronic Structure Solvers, Computer Physics Communications, 222, 267-285 (2018).

In addition, an incomplete list of publications describing the solvers supported in ELSI may be found in the bibliography of this document. Please consider citing these articles when publishing results obtained with ELSI.

1.5 Acknowledgments

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2 Installation of ELSI

2.1 Overview

The ELSI package contains the ELSI Interface software as well as redistributed source code for the solver libraries ELPA (version 2016.11.001), libOMM, NTPoly, and PEXSI (version 1.0.2). We highly encourage all users to request access to our GitLab serverGitLab server, where we regularly update ELSI between releases while preserving stability.

Starting from the May 2018 (version 2.0.0) release, the installation of ELSI makes use of the CMake software.

2.2 Prerequisites

To build ELSI, the minimum requirements are:

```
CMake  [minimum version 3.0; newer version recommended]
Fortran compiler  [with Fortran 2003]
C compiler  [with C99]
MPI
```

Building the PEXSI solver (highly recommended) requires:

```
C++ compiler  [with C++ 11]
```

Additionally, building the SLEPc-SIPs solver requires:

```
SLEPc  [version 3.9.2 only]
PETSc  [version 3.9.3 only, with SuperLU_DIST, MUMPS, ParMETIS, and PT-SCOTCH enabled]
```

Linear algebra libraries should be provided for ELSI to link against:

```
BLAS, LAPACK, BLACS, ScaLAPACK
```

By default, the redistributed ELPA, libOMM, and NTPoly solvers will be built. If PEXSI is enabled during configuration, the redistributed PEXSI library and its dependencies, namely the SuperLU_DIST and PT-SCOTCH libraries, will be built as well. Optionally, the redistributed ELPA, libOMM, SuperLU_DIST and PT-SCOTCH libraries may be substituted by user's optimized versions. Please note that in the current version of ELSI, an external version of PEXSI or NTPoly is not officially supported.

2.3 CMake Basics

This section covers some basics of using CMake. Users who are familiar with CMake may safely skip this section.

The typical workflow of using CMake to build ELSI looks like:

```
$ ls

  CMakeLists.txt  external/  src/  test/  ...
```

```
$ mkdir build
$ cd build
$ cmake [options] ..

  ...
  ...
  -- Generating done
  -- Build files have been written to: /current/dir

$ make [-j np]
$ make install
```

Whenever CMake is invoked, one of the command line arguments must point to the path where the top level CMakeLists.txt file exists, hence the "`..`" in the above example.

By default, CMake generates standard UNIX makefiles including specific rules to build the project with GNU make. Other build systems may be chosen with the "`-G`" (G for generator) option of CMake. We recommend Ninja in particular, which is a small build system with a focus on speed. A version of Ninja with Fortran support is freely available here.

To build ELSI with Ninja:

```
$ ls

  CMakeLists.txt  external/  src/  test/  ...

$ mkdir build
$ cd build
$ cmake -G Ninja [options] ..

  ...
  ...
  -- Generating done
  -- Build files have been written to: /current/dir

$ ninja
$ ninja install
```

Ninja also accepts the `-j` flag. Without this flag, Ninja runs on the number of available threads plus two by default (e.g., 10 on a machine with 8 threads). Thus, `-j` is typically not necessary.

An option may be defined by adding "`-DKeyword=Value`" to the command line when invoking CMake. If "`Keyword`" is of type boolean, its "`Value`" may be "ON" or "OFF". If "`Keyword`" is a list of libraries or include directories, its items should be separated with ";" (semicolon) or " " (space).

For example,

```
-DCMAKE_INSTALL_PREFIX=/path/to/install/elsi
-DCMAKE_C_COMPILER=gcc
-DENABLE_TESTS=OFF
-DENABLE_PEXSI=ON
-DINC_PATHS="/path/to/include;/another/path/to/include"
-DLIBS="library1 library2 library3"
```

Available options for building ELSI with CMake are introduced in the next sections. Other options of CMake itself are available in its online documentation.

2.4 Configuration

2.4.1 Compilers

CMake automatically detects compilers. The choices made by CMake often work, but not necessarily lead to the optimal performance. In some cases, the compilers picked up by CMake may not be the ones desired by the user. To build ELSI, it is mandatory that the user explicitly sets the identification of the compilers:

```
-DCMAKE_Fortran_COMPILER=YOUR_MPI_FORTRAN_COMPILER
-DCMAKE_C_COMPILER=YOUR_MPI_C_COMPILER
-DCMAKE_CXX_COMPILER=YOUR_MPI_C++_COMPILER
```

Please note that the C++ compiler is not needed when building ELSI without PEXSI.

In addition, it is highly recommended to specify the compiler flags, in particular the optimization flags:

```
-DCMAKE_Fortran_FLAGS=YOUR_FORTRAN_COMPILE_FLAGS
-DCMAKE_C_FLAGS=YOUR_MPI_C_COMPILE_FLAGS
-DCMAKE_CXX_FLAGS=YOUR_MPI_C++_COMPILE_FLAGS
```

Note that with CMake versions older than 3.8.2, flags such as `-std=c99` and `-std=c++11` (or equivalents depending on the compilers) must be given in order to ensure compliance with the C99 and C++11 standards. Newer versions of CMake take care of this automatically.

2.4.2 Solvers

The ELPA, libOMM, NTPoly, and PEXSI solver libraries, as well as the SuperLU_DIST and PT-SCOTCH libraries (both required by PEXSI), are redistributed with the current ELSI package.

The redistributed version of ELPA comes with a few "kernels" specifically written to take advantage of processor architecture (e.g. vectorization instruction set extensions). A kernel may be chosen by the ELPA2_KERNEL keyword. Available options are:

```
-DELPA2_KERNEL=BGQ
-DELPA2_KERNEL=AVX
-DELPA2_KERNEL=AVX2
-DELPA2_KERNEL=AVX512
```

for the IBM Blue Gene Q, Intel AVX, Intel AVX2, and Intel AVX512 architectures, respectively. In ELPA, these kernels are employed to accelerate the calculation of eigenvectors, which is often a computational bottleneck when calculating a large percentage of eigenvectors. If this is the case in the user's application, it is highly recommended that the user selects the kernel most suited to their system architecture.

Experienced users are encouraged to link the ELSI interface against external, better optimized solver libraries. Relevant options for this purpose are:

```
-DUSE_EXTERNAL_ELPA=ON
-DUSE_EXTERNAL_OMM=ON
-DUSE_EXTERNAL_SUPERLU=ON
```

The external libraries and the include paths should be set via the following three keywords:

```
-DLIB_PATHS=DIRECTORIES_CONTAINING_YOUR_EXTERNAL_LIBRARIES
-DINC_PATHS=INCLUDE_DIRECTORIES_OF_YOUR_EXTERNAL_LIBRARIES
-DLIBS=NAMES_OF_YOUR_EXTERNAL_LIBRARIES
```

Each of the above keywords is a space-separated or semicolon-separated list. If an external library depends on additional libraries, LIBS should include all the relevant libraries. For instance, LIBS should include the ELPA library and CUDA libraries when using an external ELPA compiled with GPU (CUDA) support; LIBS should include the SuperLU_DIST library and the sparse matrix reordering library used to compile SuperLU_DIST when using an external SuperLU_DIST. Please note that in the current version of ELSI, an external version of PEXSI or NTPoly is not officially supported.

The PEXSI and SLEPc-SIPs solvers are not enabled by default. PEXSI may be activated by specifying:

```
-DENABLE_PEXSI=ON
```

if using redistributed SuperLU_DIST with PT-SCOTCH, or

```
-DENABLE_PEXSI=ON
-DUSE_EXTERNAL_SUPERLU=ON
-DINC_PATHS="/path/to/superlu_dist/include;/path/to/matrix/reordering/include"
-DLIB_PATHS="/path/to/superlu_dist/library;/path/to/matrix/reordering/include"
-DLIBS="superlu_dist;your_choice_of_matrix_reordering_library"
```

if using an externally compiled SuperLU_DIST. SuperLU_DIST 5.3.0 has been tested with this version of ELSI. Older/newer versions may or may not be compatible.

SLEPc-SIPs may be activated by specifying:

```
-DENABLE_SIPS=ON
-DUSE_EXTERNAL_SUPERLU=ON
-DINC_PATHS="/path/to/slepc/include;/path/to/slepc/${PETSC_ARCH}/include;
/path/to/petsc/include;/path/to/${PETSC_ARCH}/include"
-DLIB_PATHS="/path/to/slepc/${PETSC_ARCH}/library;/path/to/petsc/${PETSC_ARCH}/library"
-DLIBS="slepc;petsc;cmumps;dmumps;smumps;zmumps;mumps_common;pord;superlu_dist;parmetis;
metis;ptesmumps;ptscotchparmetis;ptscotch;ptscotcherr;esmumps;scotchmetis;scotch;scotcherr"
```

SLEPc 3.9.2 and PETSc 3.9.3 have been tested with this version of ELSI. Older/newer versions may or may not be compatible. The PETSc library must be compiled with MPI support, and (at least) with external packages SuperLU_DIST, MUMPS, ParMETIS, and PT-SCOTCH enabled. The SuperLU_DIST library redistributed through ELSI must be turned off by setting USE_EXTERNAL_SUPERLU to "ON", as SuperLU_DIST is already present in the PETSc installation.

2.4.3 Build Targets

By default, a static library (libelsi.a) will be created as the target of the compilation. Building ELSI as a shared library may be enabled by:

```
-DBUILD_SHARED_LIBS=ON
```

Building ELSI test programs may be enabled by:

```
-DENABLE_TESTS=ON
```

In either case, linear algebra libraries, BLAS, LAPACK, BLACS, and ScaLAPACK, should be valid in the LIB_PATHS and LIBS keywords.

If test programs are turned on, the compilation of ELSI may be verified by

```
$ make test
```

or

```
$ ninja test
```

depending on the generator option "`-G`" used when invoking CMake. Alternatively, issue

```
$ ctest
```

to invoke the CTest program which performs all tests automatically.

Note that the tests may not run if launching MPI jobs is prohibited on the user's working platform.

In order to install ELSI at the location specified by CMAKE_INSTALL_PREFIX, issue

```
$ make install
```

or

```
$ ninja install
```

depending on the CMake generator option "`-G`" used.

Among the files copied to the installation destinations is a CMake configuration file called `elsiConfig.cmake`. This file includes all the information about how the ELSI library and its dependencies should be included in an external CMake project. Please refer to 2.5 for information regarding linking a third-party package against ELSI.

2.4.4 List of All Configure Options

The options accepted by the ELSI CMake build system are listed here in alphabetical order. Some additional explanations are made below the table.

Option	Type	Default	Explanation
ADD_UNDERSCORE	boolean	ON	Suffix C functions with an underscore
BUILD_SHARED_LIBS	boolean	OFF	Build ELSI as a shared library
CMAKE_C_COMPILER	string	none	MPI C compiler
CMAKE_C_FLAGS	string	none	C flags
CMAKE_CXX_COMPILER	string	none	MPI C++ compiler
CMAKE_CXX_FLAGS	string	none	C++ flags
CMAKE_Fortran_COMPILER	string	none	MPI Fortran compiler
CMAKE_Fortran_FLAGS	string	none	Fortran flags
CMAKE_INSTALL_PREFIX	path	/usr/local	Path to install ELSI
ELPA2_KERNEL	string	none	ELPA2 kernel
ENABLE_C_TESTS	boolean	OFF	Build C test programs
ENABLE_PEXSI	boolean	OFF	Enable PEXSI support
ENABLE_SIPS	boolean	OFF	Enable SLEPc-SIPs support
ENABLE_TESTS	boolean	OFF	Build Fortran test programs
INC_PATHS	string	none	Include directories of external libraries
LIB_PATHS	string	none	Directories containing external libraries
LIBS	string	none	External libraries
MPIEXEC_NP	string	mpirun -n 4	Command to run tests in parallel with MPI
MPIEXEC_1P	string	mpirun -n 1	Command to run tests in serial with MPI
SCOTCH_LAST_RESORT	string	none	Command to invoke PT-SCOTCH header generator
USE_EXTERNAL_ELPA	boolean	OFF	Use external ELPA
USE_EXTERNAL_OMM	boolean	OFF	Use external libOMM and MatrixSwitch
USE_EXTERNAL_SUPERLU	boolean	OFF	Use external SuperLU_DIST

Remarks

1) ADD_UNDERSCORE: In the PEXSI and SuperLU_DIST code redistributed through ELSI, there are calls to functions of the linear algebra libraries, e.g. "dgemm". If ADD_UNDERSCORE is "ON", the code will call "dgemm_" instead of "dgemm". Turn this keyword on if routines are suffixed with "_" in external linear algebra libraries. Turn it off if routines are not suffixed with "_".

2) ELPA2_KERNEL: There are a number of computational kernels available with the ELPA solver. Choose from "BGQ" (IBM Blue Gene Q), "AVX" (Intel AVX), "AVX2" (Intel AVX2), and "AVX512" (Intel AVX512). See 2.4.2 for more information.

3) SCOTCH_LAST_RESORT: The compilation of the PT-SCOTCH library is a multi-step process. First, two auxiliary executables are created. Then, header files of the library are generated by running the two executables. Finally, the main source files of the library are compiled with the generated header files included. The header generation step may fail on platforms where directly running an executable is prohibited on a login/compile node. Often this can be circumvented by requesting an interactive session to a compute node and performing the compilation there, or by submitting the whole compilation as a job to the queuing system. However, this may still fail on platforms where an executable compiled with MPI must be launched by an MPI job launcher (aprun, mpirun, srun, etc). If the standard compilation of PT-SCOTCH fails due to this reason, the user may set SCOTCH_LAST_RESORT to the command that starts an MPI job with one

MPI task, e.g. "`mpirun -n 1`". This command will be used to launch the auxiliary executables to generate necessary header files for PT-SCOTCH.

4) External libraries: ELSI redistributes source code of ELPA, libOMM, PEXSI, SuperLU_DIST, and PT-SCOTCH libraries, which by default will be built together with the ELSI interface. Experienced users are encouraged to link the ELSI interface against external, better optimized solver libraries. See 2.4.2 for more information.

2.4.5 "Toolchain" Files

It is sometimes convenient to edit the settings in a "toolchain" file that can be read by CMake:

```
-DCMAKE_TOOLCHAIN_FILE=YOUR_TOOLCHAIN_FILE
```

Example "toolchains" are provided in the "./toolchains" directory of the ELSI package, which the user may use as templates to create new ones.

2.5 Importing ELSI into Third-Party Code Projects

2.5.1 Linking against ELSI: CMake

A CMake configuration file called `elsiConfig.cmake` should be generated after ELSI is successfully installed (see 2.4.3). This file contains all the information about how the ELSI library and its dependencies should be included in an external project. For a project using CMake, only two lines are required to find and link to ELSI:

```
find_package(elsi REQUIRED)
target_link_libraries(my_project PRIVATE elsi::elsi)
```

If a minimum version of ELSI is required, this information may be passed to "`find_package`" by:

```
find_package(elsi 2.0 REQUIRED)
```

If the installed ELSI version is older than the requested minimum version, CMake stops with an appropriate error message. Other options of "`find_package`" are available in the documentation of CMake.

2.5.2 Linking against ELSI: Makefile

For a project using makefiles, an example set of compiler flags to link against ELSI would be:

```
ELSI_INCLUDE = -I/PATH/TO/BUILD/ELSI/include
ELSI_LIB     = -L/PATH/TO/BUILD/ELSI/lib -lelsi \
               -lfortjson -lOMM -lMatrixSwitch -lelpa \
               -lNTPoly -lpexsi -lsuperlu_dist \
               -lptscotchparmetis -lptscotch -lptscotcherr \
               -lscotchmetis -lscotch -lscotcherr
```

Enabling/disabling PEXSI and SLEPc-SIPs or linking ELSI against preinstalled solver libraries will require the user modify these flags accordingly.

2.5.3 Using ELSI

ELSI may be used in an electronic structure code by importing the appropriate header file. For codes written in Fortran, this is done by using the ELSI module

```
USE ELSI
```

For codes written in C, the ELSI wrapper may be imported by including the header file

```
#include <elsi.h>
```

These import statements give the electronic structure code access to the ELSI interface. In the next chapter, we will describe the API for the ELSI interface.

3 The ELSI API

3.1 Overview of the ELSI API

In this chapter, we present the public-facing API for the ELSI Interface. We anticipate that fine details of this interface may change slightly in the future, but the fundamental structure of the interface layer is expected to remain consistent. While this chapter serves as a reference to the ELSI subroutines, the user is encouraged to explore the demonstration pseudo-codes of ELSI in 3.8.

To allow multiple instances of ELSI to co-exist within a single calling code, we define an `elsi_handle` data type to encapsulate the state of an ELSI instance, i.e., all runtime parameters associated with the ELSI instance. An `elsi_handle` instance is initialized with the elsi_init subroutine and is subsequently passed to all other ELSI subroutine calls.

ELSI provides a C interface in addition to the native Fortran interface. The vast majority of this chapter, while written from a Fortran-ic standpoint, applies equally to both interfaces. Information specifically about the C wrapper for ELSI may be found in 3.9.

3.2 Setting Up ELSI

3.2.1 Initializing ELSI

The ELSI interface must be initialized via the elsi_init subroutine before any other ELSI subroutine may be called.

elsi_init(handle, solver, parallel_mode, matrix_format, n_basis, n_electron, n_state)

Argument	Data Type	in/out	Explanation
handle	type(elsi_handle)	out	Handle to ELSI.
solver	integer	in	Desired KS solver. Accepted values are: 1 (ELPA), 2 (LIBOMM), 3 (PEXSI), 5 (SLEPc-SIPs), and 6 (NTPoly).
parallel_mode	integer	in	Parallelization mode. See remark 3. Accepted values are: 0 (SINGLE_PROC) and 1 (MULTI_PROC).
matrix_format	integer	in	Matrix format. See remark 1. Accepted values are: 0 (BLACS_DENSE), 1 (PEXSI_CSC), and 2 (SIESTA_CSC).
n_basis	integer	in	Number of basis functions, i.e. global size of Hamiltonian.
n_electron	real double	in	Number of electrons.
n_state	integer	in	Number of states. See remark 2.

Remarks

1) matrix_format: BLACS_DENSE(0) refers a dense matrix format in a 2-dimensional block-cyclic distribution, i.e. the BLACS standard. PEXSI_CSC(1) refers to a compressed sparse column (CSC) matrix format in a 1-dimensional block distribution. SIESTA_CSC(2) refers to a compressed sparse column (CSC) matrix format in a 1-dimensional block-cyclic distribution. As the Hamiltonian, overlap, and density matrices are symmetric (Hermitian), compressed sparse row (CSR) matrix format is effectively supported.

2) n_state: If ELPA or SLEPc-SIPs is the chosen solver, this parameter specifies the number of eigenstates to solve by the eigensolver. If libOMM is the chosen solver, n_state must be exactly the number of occupied states, as libOMM cannot handle fractional occupation numbers[4]. PEXSI and NTPoly do not make use of this parameter, thus a dummy value may be passed.

3) parallel_mode: The two allowed values of parallel_mode, 0 (SINGLE_PROC) and 1 (MULTI_PROC), allow for three parallelization strategies commonly employed by electronic structure codes. See below.

3a) SINGLE_PROC: Solves the KS eigenproblem following a LAPACK-like fashion. This option may only be selected when ELPA is chosen as the solver. This allows the following parallelization strategy:

SINGLE_PROC Example:

Every MPI task independently handles a group of $\boldsymbol{k}$-points uniquely assigned to it.

Example number of $\boldsymbol{k}$-points: 16
Example number of MPI tasks: 4

MPI task 0 handles $\boldsymbol{k}$-points 1, 2, 3, 4 sequentially;
MPI task 1 handles $\boldsymbol{k}$-points 5, 6, 7, 8 sequentially;
MPI task 2 handles $\boldsymbol{k}$-points 9, 10, 11, 12 sequentially;
MPI task 3 handles $\boldsymbol{k}$-points 13, 14, 15, 16 sequentially.

Pseudocode 1:

```
elsi_init(elsi_h, ..., parallel_mode=0, ...)
...
for i_kpt = 1, n_kpt_local, 1 do
    elsi_ev_{real|complex}(elsi_h, ham_this_kpt, ovlp_this_kpt, eval_this_kpt, evec_this_kpt)
end
```

3b) MULTI_PROC: Solves the KS eigenproblem following a ScaLAPACK-like fashion. This allows the usage of the following two parallelization strategies:

MULTI_PROC Example:

Groups of MPI tasks coordinate to handle the same $\boldsymbol{k}$-point, uniquely assigned to that group.

Example number of $\boldsymbol{k}$-points: 4
Example number of MPI tasks: 16

MPI tasks 0, 1, 2, 3 cooperatively handle $\boldsymbol{k}$-point 1;
MPI tasks 4, 5, 6, 7 cooperatively handle $\boldsymbol{k}$-point 2;
MPI tasks 8, 9, 10, 11 cooperatively handle $\boldsymbol{k}$-point 3;
MPI tasks 12, 13, 14, 15 cooperatively handle $\boldsymbol{k}$-point 4.

Pseudocode 2:

```
elsi_init(elsi_h, ..., parallel_mode=1, ...)
elsi_set_mpi(elsi_h, my_mpi_comm)
...
elsi_ev_{real|complex}(elsi_h, my_ham, my_ovlp, my_eval, my_evec)

or

elsi_init(elsi_h, ..., parallel_mode=1, ...)
elsi_set_mpi(elsi_h, my_mpi_comm)
elsi_set_kpoint(elsi_h, n_kpt, my_kpt, my_weight)
elsi_set_mpi_global(elsi_h, mpi_comm_global)
...
elsi_dm_complex(elsi_h, my_ham, my_ovlp, my_dm, global_energy)
```

Please note that when there is more than one $\boldsymbol{k}$-point, a global MPI communicator must be provided for inter-$\boldsymbol{k}$-point communications. See 3.2.4 for elsi_set_kpoint, elsi_set_spin, and elsi_set_mpi_global, which are used to set up a calculation with two spin channels and/or multiple $\boldsymbol{k}$-points.

3.2.2 Setting Up MPI

The MPI communicator used by ELSI is passed into ELSI by the calling code via the elsi_set_mpi subroutine. When there is more than one $\boldsymbol{k}$-point and/or spin channel, this communicator will be used only for solving one problem corresponding to one $\boldsymbol{k}$-point and one spin channel. See 3.2.4 for details.

elsi_set_mpi(handle, mpi_comm)

Argument	Data Type	in/out	Explanation
handle	type(elsi_handle)	inout	Handle to ELSI.
mpi_comm	integer	in	MPI communicator.

3.2.3 Setting Up Matrix Formats

When using the 2D block-cyclic distributed dense matrix format (BLACS_DENSE), BLACS parameters are passed into ELSI via the elsi_set_blacs subroutine. The matrix format used internally in the ELSI interface and the ELPA solver requires the block sizes of the 2-dimensional block-cyclic distribution are the same in the row and column directions. It is necessary to call this subroutine before calling any solver interface that makes use of the BLACS_DENSE matrix format.

elsi_set_blacs(handle, blacs_ctxt, block_size)

Argument	Data Type	in/out	Explanation
handle	type(elsi_handle)	inout	Handle to ELSI.
blacs_ctxt	integer	in	BLACS context.
block_size	integer	in	Block size of the 2D block-cyclic distribution, specifying both row and column directions.

When using the sparse matrix formats, namely 1D block distributed compressed sparse column (PEXSI_CSC) or 1D block-cyclic distributed compressed sparse column (SIESTA_CSC), the sparsity pattern should be passed into ELSI via the elsi_set_csc subroutine. It is necessary to call this subroutine before calling any solver interface that makes use of the sparse matrix formats.

elsi_set_csc(handle, global_nnz, local_nnz, local_col, row_idx, col_ptr)

Argument	Data Type	in/out	Explanation
handle	type(elsi_handle)	inout	Handle to ELSI.
global_nnz	integer	in	Global number of non-zeros.
local_nnz	integer	in	Local number of non-zeros.
local_col	integer	in	Local number of matrix columns.
row_idx	integer, rank-1 array	in	Local row index array. Dimension: local_nnz.
col_ptr	integer, rank-1 array	in	Local column pointer array. Dimension: local_col+1.

When using the 1D block distributed compressed sparse column (PEXSI_CSC) format, the block size of the distribution cannot be set by the user. This is because the PEXSI solver requires that the block size must be floor(N_basis/N_procs), where floor(x) is the greatest integer less than or equal to x, N_basis and N_procs are the number of basis functions and the number of MPI tasks, respectively. When using the 1D block-cyclic distributed compressed sparse column (SIESTA_CSC) format, the block size of the 1D distribution must be explicitly set by calling elsi_set_csc_blk.

elsi_set_csc_blk(handle, block_size)

Argument	Data Type	in/out	Explanation
handle	type(elsi_handle)	inout	Handle to ELSI.
global_nnz	integer	in	Block size of the 1D block-cyclic distribution.

In most cases, input and output matrices should be distributed across all MPI tasks. The only exception happens when using the PEXSI solver, one of the sparse density matrix interfaces (elsi_dm_real_sparse or elsi_dm_complex_sparse), and the PEXSI_CSC matrix format. In this case, an additional parameter, pexsi_np_per_pole, must be set by the user. Input and output matrices should be 1D-block-distributed among the first pexsi_np_per_pole MPI tasks (not all the MPI tasks). Please also read the 2$^{\text{nd}}$ remark in 3.5.4 for more information.

3.2.4 Setting Up Multiple $\boldsymbol{k}$-points and/or Spin Channels

When there is more than one $\boldsymbol{k}$-point and/or spin channel in the simulating system, the ELSI interface can be set up to support parallel calculation of the $\boldsymbol{k}$-points and/or spin channels. The base case is an isolated system, e.g. atoms, molecules, clusters, without spin-polarization. In this case, in each SCF iteration, there is one KS eigenproblem (1.5) to solve. If the isolated system is spin-polarized, there are two eigenproblems:

$$\begin{aligned} \boldsymbol{H}_\alpha \boldsymbol{c}_\alpha &= \boldsymbol{\epsilon}_\alpha \boldsymbol{S}_\alpha \boldsymbol{c}_\alpha, \\ \boldsymbol{H}_\beta \boldsymbol{c}_\beta &= \boldsymbol{\epsilon}_\beta \boldsymbol{S}_\beta \boldsymbol{c}_\beta, \end{aligned} \tag{3.1}$$

where α and β denote the two spin channels. The overlap matrices are generally the same for the two spin channels, but the Hamiltonian matrices are not. These two eigenproblems can be solved one after another using all available processes, or can be solved concurrently using half of the processes for each spin channel.

If the system is periodically repeated in space, according to the Bloch theorem, the KS eigenproblem has an additional index $\boldsymbol{k}$:

$$\boldsymbol{H}_{\boldsymbol{k}} \boldsymbol{c}_{\boldsymbol{k}} = \boldsymbol{\epsilon}_{\boldsymbol{k}} \boldsymbol{S}_{\boldsymbol{k}} \boldsymbol{c}_{\boldsymbol{k}}. \tag{3.2}$$

In practice, it is sufficient to study $\boldsymbol{k}$ within a single primitive unit cell in the reciprocal space, usually the first Brillouin zone. The physical quantities, e.g. the electron density, are represented by Brillouin zone integrals:

$$n(\boldsymbol{r}) = \sum_{l=1}^{N_{\text{basis}}} \int_{BZ} f_{l\boldsymbol{k}} \psi^*_{l\boldsymbol{k}}(\boldsymbol{r}) \psi_{l\boldsymbol{k}}(\boldsymbol{r}) d^3k, \tag{3.3}$$

which is approximated by using a finite mesh of $\boldsymbol{k}$-points in the first Brillouin zone:

$$n(\boldsymbol{r}) \approx \sum_{n=1}^{N_{\text{kpt}}} w_n \sum_{l=1}^{N_{\text{basis}}} f_{l\boldsymbol{k}_n} \psi^*_{l\boldsymbol{k}_n}(\boldsymbol{r}) \psi_{l\boldsymbol{k}_n}(\boldsymbol{r}). \tag{3.4}$$

Here, w_n is the weight of the n$^{\text{th}}$ $\boldsymbol{k}$-point; N_{kpt} is the number of $\boldsymbol{k}$-points. The weights of all $\boldsymbol{k}$-points add up to 1. Obviously, a denser grid of $\boldsymbol{k}$-points leads to a higher accuracy with higher computational cost. The Hamilton and overlap matrices for multiple $\boldsymbol{k}$-points are block-diagonal, such that each block on the diagonal corresponds to an eigenproblem of one $\boldsymbol{k}$-point. These eigenproblems can be solved separately.

The handling of spin-polarized case and periodic case in ELSI are more or less equivalent. The problems, either from two spin channels, or from multiple $\boldsymbol{k}$-points, are treated as equivalent "unit tasks". If the chosen solver is an eigensolver (e.g. ELPA), all the unit tasks are solved independently, returning separate eigensolutions to the electronic structure code. The electronic structure code can then assemble the pieces of the solutions and construct the electron density. When computing density matrices, the unit tasks are coupled together by the normalization condition of the number of electrons:

$$N_{\text{electron}} = \sum_{n=1}^{N_{\text{kpt}}} \sum_{m=1}^{N_{\text{spin}}} \sum_{l=1}^{N_{\text{basis}}} w_n f_{lmn}, \tag{3.5}$$

where N_{kpt}, N_{spin}, and N_{basis} are the number of $\boldsymbol{k}$-points, the number of spin channels, and the number of basis functions, respectively. w_n is again the weight of the n$^{\text{th}}$ $\boldsymbol{k}$-point. f_{lmn} is the occupation number of the l$^{\text{th}}$ state in the m$^{\text{th}}$ spin channel and the n$^{\text{th}}$ $\boldsymbol{k}$-point. To determine the occupation numbers, the eigenvalues at each unit task need to be collected across all the tasks. With the correct occupation numbers, density matrices can be computed by 1.8.

If the PEXSI solver is chosen, the pole expansion in 1.18 is performed for all the unit tasks in parallel, with the same trial chemical potential μ. The resulting number of electrons needs to be determined in order to refine the chemical potential. The chemical potential yielding the correct number of electrons is used to construct the density matrices on the unit tasks. If the OMM solver is chosen, the orbital minimization in 1.16 is performed for all the unit tasks to obtain density matrices. Again, OMM cannot handle systems with fractional occupation numbers.

At present, the SLEPc-SIPs and NTPoly solvers are not compatible with spin-polarized and/or periodic calculations.

To set up the ELSI interface for a calculation with more than one $\boldsymbol{k}$-point and/or more than one spin channel, the elsi_set_kpoint and/or elsi_set_spin subroutines are called to pass the required information into ELSI. The MPI communicator for each unit task is passed into ELSI by calling elsi_set_mpi. In addition, a global MPI communicator for all tasks is passed into ELSI by calling elsi_set_mpi_global. Note that the current ELSI interface only supports the case where the eigenproblems for all the $\boldsymbol{k}$-points and spin channels are fully parallelized, i.e., there is no MPI task handling more than one $\boldsymbol{k}$-point and/or more than one spin channel. Another limitation is that the two spin channels are always coupled by the normalization condition 3.5, with a uniform chemical potential for the two channels. The distribution of electrons among the two channels, and thus the net spin moment of the system, is solely determined by 3.5. Future work will enable calculations with a fixed, user-specified spin moment.

elsi_set_kpoint(handle, n_kpt, i_kpt, weight)

Argument	Data Type	in/out	Explanation
handle	type(elsi_handle)	inout	Handle to ELSI.
n_kpt	integer	in	Total number of $\boldsymbol{k}$-points.
i_kpt	integer	in	Index of the $\boldsymbol{k}$-point handled by this MPI task.
weight	integer	in	Weight of the $\boldsymbol{k}$-point handled by this MPI task.

elsi_set_spin(handle, n_spin, i_spin)

Argument	Data Type	in/out	Explanation
handle	type(elsi_handle)	inout	Handle to ELSI.
n_spin	integer	in	Total number of spin channels.
i_spin	integer	in	Index of the spin channel handled by this MPI task.

elsi_set_mpi_global(handle, mpi_comm_global)

Argument	Data Type	in/out	Explanation
handle	type(elsi_handle)	inout	Handle to ELSI.
mpi_comm_global	integer	in	Global MPI communicator used for communications among all $\boldsymbol{k}$-points and spin channels.

3.2.5 Finalizing ELSI

When an ELSI instance is no longer needed, its associated handle should be cleaned up by calling elsi_finalize.

elsi_finalize(handle)

Argument	Data Type	in/out	Explanation
handle	type(elsi_handle)	inout	Handle to ELSI.

3.3 Solving Eigenvalues and Eigenvectors

The following subroutines return all the eigenvalues and a subset of eigenvectors of the provided H and S matrices. Only eigensolvers may be selected as the desired solver when using these subroutines.

elsi_ev_real(handle, ham, ovlp, eval, evec)

Argument	Data Type	in/out	Explanation
handle	type(elsi_handle)	inout	Handle to ELSI.
ham	real double, rank-2 array	inout	Real Hamiltonian matrix in 2D block-cyclic dense format. See remark 1.
ovlp	real double, rank-2 array	inout	Real overlap matrix (or its Cholesky factor) in 2D block-cyclic dense format. See remark 1.
eval	real double, rank-1 array	inout	Eigenvalues. See remark 2.
evec	real double, rank-2 array	out	Real eigenvectors in 2D block-cyclic dense format. See remark 3.

elsi_ev_complex(handle, ham, ovlp, eval, evec)

Argument	Data Type	in/out	Explanation
handle	type(elsi_handle)	inout	Handle to ELSI.
ham	complex double, rank-2 array	inout	Complex Hamiltonian matrix in 2D block-cyclic dense format. See remark 1.
ovlp	complex double, rank-2 array	inout	Complex overlap matrix (or its Cholesky factor) in 2D block-cyclic dense format. See remark 1.
eval	real double, rank-1 array	inout	Eigenvalues. See remark 2.
evec	complex double, rank-2 array	out	Complex eigenvectors in 2D block-cyclic dense format. See remark 3.

elsi_ev_real_sparse(handle, ham, ovlp, eval, evec)

Argument	Data Type	in/out	Explanation
handle	type(elsi_handle)	inout	Handle to ELSI.
ham	real double, rank-1 array	inout	Real Hamiltonian matrix in 1D block or block-cyclic CSC sparse format.
ovlp	real double, rank-1 array	inout	Real overlap matrix in 1D block or block-cyclic CSC sparse format.
eval	real double, rank-1 array	inout	Eigenvalues. See remark 2.
evec	real double, rank-2 array	out	Real eigenvectors in 2D block-cyclic dense format. See remark 3.

elsi_ev_complex_sparse(handle, ham, ovlp, eval, evec)

Argument	Data Type	in/out	Explanation
handle	type(elsi_handle)	inout	Handle to ELSI.
ham	complex double, rank-1 array	inout	Complex Hamiltonian matrix in 1D block or block-cyclic CSC sparse format.
ovlp	complex double, rank-1 array	inout	Complex overlap matrix in 1D block or block-cyclic CSC sparse format.
eval	real double, rank-1 array	inout	Eigenvalues. See remark 2.
evec	complex double, rank-2 array	out	Complex eigenvectors in 2D block-cyclic dense format. See remark 3.

Remarks

1) The Hamiltonian matrix will be destroyed by ELPA during computation. ELPA will overwrite the overlap matrix in its initial execution with the Cholesky factor, which will be reused by subsequent subroutine calls to elsi_ev_real or elsi_ev_complex. When using elsi_ev_real_sparse, the Cholesky factor (which is not sparse) is stored internally in the BLACS_DENSE format. Starting from the second call to elsi_ev_real_sparse, the input sparse overlap matrix will not be referenced.

2) When using the ELPA solver, elsi_ev_real, elsi_ev_complex, elsi_ev_real_sparse, and elsi_ev_complex_sparse always compute all the eigenvalues, regardless of the choice of n_state specified in elsi_init. The dimension of eval thus should always be n_basis.

3) When using the ELPA solver, elsi_ev_real, elsi_ev_complex, elsi_ev_real_sparse, and elsi_ev_complex_sparse compute a subset of all eigenvectors. The number of eigenvectors to compute is specified by the keyword n_state in elsi_init. However, the local eigenvectors array should always be initialized to correspond to a global array of size n_basis × n_basis, whose extra part is used as working space in ELPA. Note that when using elsi_ev_real_sparse and elsi_ev_complex_sparse, the eigenvectors are returned in a dense format (BLACS_DENSE), as they are in general not sparse.

3.4 Computing Density Matrices

The following subroutines return the density matrix computed from the provided H and S matrices, as well as the energy corresponding to the occupied eigenstates. When the selected solver is ELPA, ELSI will internally construct the density matrix using the eigenvalues and eigenvectors returned by ELPA.

elsi_dm_real(handle, ham, ovlp, dm, bs_energy)

Argument	Data Type	in/out	Explanation
handle	type(elsi_handle)	inout	Handle to ELSI.
ham	real double, rank-2 array	inout	Real Hamiltonian matrix in 2D block-cyclic dense format.
ovlp	real double, rank-2 array	inout	Real overlap matrix (or Cholesky factor) in 2D block-cyclic dense format. See remark 1.
dm	real double, rank-2 array	out	Real density matrix in 2D block-cyclic dense format.
energy	real double	out	Energy corresponding to the occupied eigenstates ("band structure energy").

elsi_dm_complex(handle, ham, ovlp, dm, energy)

Argument	Data Type	in/out	Explanation
handle	type(elsi_handle)	inout	Handle to ELSI.
ham	complex double, rank-2 array	inout	Complex Hamiltonian matrix in 2D block-cyclic dense format.
ovlp	complex double, rank-2 array	inout	Complex overlap matrix (or its Cholesky factor) in 2D block-cyclic dense format. See remark 1.
dm	complex double, rank-2 array	out	Complex density matrix in 2D block-cyclic dense format.
energy	real double	out	Energy corresponding to the occupied eigenstates ("band structure energy").

elsi_dm_real_sparse(handle, ham, ovlp, dm, energy)

Argument	Data Type	in/out	Explanation
handle	type(elsi_handle)	inout	Handle to ELSI.
ham	real double, rank-1 array	inout	Non-zero values of the real Hamiltonian matrix in 1D block or block-cyclic CSC format.
ovlp	real double, rank-1 array	inout	Non-zero values of the real overlap matrix in 1D block or block-cyclic CSC format.
dm	real double, rank-1 array	out	Non-zero values of the real density matrix in 1D block or block-cyclic CSC format.
energy	real double	out	Energy corresponding to the occupied eigenstates ("band structure energy").

elsi_dm_complex_sparse(handle, ham, ovlp, dm, energy)

Argument	Data Type	in/out	Explanation
handle	type(elsi_handle)	inout	Handle to ELSI.
ham	complex double, rank-1 array	inout	Non-zero values of the complex Hamiltonian matrix in 1D block or block-cyclic CSC format.
ovlp	complex double, rank-1 array	inout	Non-zero values of the complex overlap matrix in 1D block or block-cyclic CSC format.
dm	complex double, rank-1 array	out	Non-zero values of the complex density matrix in 1D block or block-cyclic CSC format.
energy	real double	out	Energy corresponding to the occupied eigenstates ("band structure energy").

Remarks

1) If the chosen solver is ELPA or libOMM, the Hamiltonian matrix will be destroyed during the computation. ELPA will overwrite the overlap matrix in its initial execution with the Cholesky factor, which will be reused by subsequent calls to elsi_dm_real.

3.5 Customizing ELSI

In ELSI, reasonable default values have been provided for a number of parameters used in the ELSI interface the the supported solvers. However, no set of default parameters can adequately cover all use cases. Parameters that can be overridden are described in the following subsections.

3.5.1 Customizing the ELSI Interface

In all the subroutines listed below, the first argument (input and output) is an elsi_handle. The second argument (input) of each subroutine is the name of parameter to set.

Note that logical variables are not used in all ELSI API. Integers are used to represent logical, with 0 being false and any positive integer being true.

elsi_set_output(handle, out_level)

elsi_set_output_log(handle, out_log)

elsi_set_write_unit(handle, write_unit)

elsi_set_unit_ovlp(handle, unit_ovlp)

elsi_set_zero_def(handle, zero_def)

elsi_set_sing_check(handle, sing_check)

elsi_set_sing_tol(handle, sing_tol)

elsi_set_sing_stop(handle, sing_stop)

elsi_set_mu_broaden_scheme(handle, mu_broaden_scheme)

elsi_set_mu_mp_order(handle, mu_mp_order)

elsi_set_mu_broaden_width(handle, mu_broaden_width)

elsi_set_mu_tol(handle, mu_tol)

Argument	Data Type	Default	Explanation
out_level	integer	0	Output level of the ELSI interface. 0: no output. 1: standard ELSI output. 2: 1 + info from the solvers. 3: 2 + additional debug info.
out_log	integer	0	If not 0, a separate log file in JSON format will be written out.
write_unit	integer	6	The unit used in ELSI to write out information.
unit_ovlp	integer	0	If not 0, the overlap matrix will be treated as an identity (unit) matrix in ELSI and the solvers. See remark 1.
zero_def	real double	10^{-15}	When converting a matrix from dense to sparse format, values below this threshold will be discarded.
sing_check	integer	0	If not 0, the singularity check of the overlap matrix will be performed. See remark 2.
sing_tol	real double	10^{-5}	Eigenfunctions of the overlap matrix with eigenvalues smaller than this threshold will be removed to avoid ill-conditioning. See remark 1.
sing_stop	integer	0	If not 0, the code always stops if the overlap matrix is detected to be singular. See remark 1.
mu_broaden_scheme	integer	0	The broadening scheme employed to compute the occupation numbers and the Fermi level. 0: Gaussian. 1: Fermi-Dirac. 2: Methfessel-Paxton. 4: Marzari-Vanderbilt.
mu_mp_order	integer	0	The order of the Methfessel-Paxton broadening scheme. No effect if Methfessel-Paxton is not the chosen broadening scheme.
mu_broaden_width	real double	0.01	The broadening width employed to compute the occupation numbers and the Fermi level. See remark 3.
mu_tol	real double	10^{-13}	The convergence tolerance (in terms of the absolute error in electron count) of the bisection algorithm employed to compute the occupation numbers and the Fermi level.

Remarks

1) If the input overlap matrix is an identity matrix, all settings related to the singularity (ill-conditioning) check take no effect.

2) If the singularity check is not disabled, in the first iteration of each SCF cycle, possible singularity of the overlap matrix is checked by computing all its eigenvalues. If there is any eigenvalue smaller than sing_tol, the matrix is considered to be singular.

3) In all supported broadening schemes, there is a term $(\epsilon - E_{\mathrm{F}})/W$ in the distribution function, where ϵ is the energy of an eigenstate, and E_{F} is the Fermi level. The broadening_width parameter should be set to W, in the unit of ϵ and E_{F}.

3.5.2 Customizing the ELPA Solver

elsi_set_elpa_solver(handle, elpa_solver)

elsi_set_elpa_n_single(handle, elpa_n_single)

elsi_set_elpa_gpu(handle, elpa_gpu)

elsi_set_elpa_gpu_kernels(handle, elpa_gpu_kernels)

elsi_set_elpa_autotune(handle, elpa_autotune)

Argument	Data Type	Default	Explanation
elpa_solver	integer	2	1: ELPA 1-stage solver. 2: ELPA 2-stage solver. The latter is usually faster and more scalable.
elpa_n_single	integer	0	Number of SCF steps using single precision ELPA to solve standard eigenproblems. See remark 1.
elpa_gpu	integer	0	If not 0, try to enable GPU-acceleration in ELPA. See remark 2.
elpa_gpu_kernels	integer	0	If not 0, try to enable GPU-acceleration and GPU kernels in ELPA. See remark 2.
elpa_autotune	integer	1	If not 0, try to enable auto-tuning of runtime parameters in ELPA. See remark 3.

Remarks

1) elpa_n_single: If single precision arithmetic is available in an externally complied ELPA library, it may be enabled by setting elpa_n_single to a positive integer, then the standard eigenprolems in the first elpa_n_single SCF steps will be solved with single precision. The transformations between generalized eigenproblem and the standard form are always performed with double precision. Although this keyword accelerates the solution of standard eigenproblems, the overall SCF convergence may be slower, depending on the physical system and the SCF settings used in the electronic structure code. This keyword is ignored if single precision calculations are not available, which is the case if the internal version of ELPA is used, or if an external ELPA has not been complied with single precision support.

2) elpa_gpu and elpa_gpu_kernels: If GPU-acceleration is available in an externally compiled ELPA library, it may be enabled by setting elpa_gpu to a non-zero integer. Note that by setting elpa_gpu, the GPU kernels for eigenvector back-transformation will not be used. To enable the GPU kernels, elpa_gpu_kernels should be set to a non-zero value. These two keywords are ignored if GPU-acceleration is not available, which is the case if the internal version of ELPA is used, or if an external ELPA has not been complied with GPU support.

3) elpa_autotune: If auto-tuning of runtime parameters is available in an externally complied ELPA library, it may be enabled by setting elpa_autotune to a nonzero integer. This keyword is ignored if auto-tuning is not available, which is the case if the internal version of ELPA is used.

3.5.3 Customizing the libOMM Solver

elsi_set_omm_flavor(handle, omm_flavor)

elsi_set_omm_n_elpa(handle, omm_n_elpa)

elsi_set_omm_tol(handle, omm_tol)

Argument	Data Type	Default	Explanation
omm_flavor	integer	0	Method to perform OMM minimization. See remark 1.
omm_n_elpa	integer	6	Number of SCF steps using ELPA. See remark 2.
omm_tol	real double	10^{-12}	Convergence tolerance of orbital minimization. See remark 3.

Remarks

1) omm_flavor: Allowed choices are 0 for a basic minimization of a generalized eigenproblem and 2 for a Cholesky factorization of the overlap matrix transforming the generalized eigenproblem to the standard form. Usually 2 (Cholesky) leads to a faster convergence of the OMM energy functional minimization, at the price of transforming the eigenproblem. When using sufficiently many steps of ELPA to stabilize the SCF cycle, 0 (basic) is probably a better choice to finish the remaining SCF cycle. See also remark 2 below.

2) omm_n_elpa: It has been demonstrated that OMM is optimal at later stages of an SCF cycle where the electronic structure is closer to its expected local minimum, requiring only one CG iteration to converge the minimization of the OMM energy functional. Accordingly, it is recommended to use ELPA initially, then switching to libOMM after omm_n_elpa SCF steps.

3) omm_tol: A large minimization tolerance of course leads to a faster convergence, however unavoidably with a lower accuracy. omm_tol should be tested and chosen to balance the desired accuracy and computation time of the calling code.

3.5.4 Customizing the PEXSI Solver

elsi_set_pexsi_n_pole(handle, pexsi_n_pole)

elsi_set_pexsi_n_mu(handle, pexsi_n_mu)

elsi_set_pexsi_np_per_pole(handle, pexsi_np_per_pole)

elsi_set_pexsi_np_symbo(handle, pexsi_np_symbo)

elsi_set_pexsi_temp(handle, pexsi_temp)

elsi_set_pexsi_gap(handle, pexsi_gap)

elsi_set_pexsi_delta_e(handle, pexsi_delta_e)

elsi_set_pexsi_mu_min(handle, pexsi_mu_min)

elsi_set_pexsi_mu_max(handle, pexsi_mu_max)

elsi_set_pexsi_inertia_tol(handle, pexsi_inertia_tol)

Argument	Data Type	Default	Explanation
pexsi_n_pole	integer	20	Number of poles used by PEXSI. See remark 1.
pexsi_n_mu	integer	2	Number of mu points used by PEXSI. See remark 1.
pexsi_np_per_pole	integer	-	Number of MPI tasks assigned to each mu point. See remark 2.
pexsi_np_symbo	integer	1	Number of MPI tasks for symbolic factorization. See remark 3.
pexsi_temp	real double	0.002	Temperature. See remark 4.
pexsi_gap	real double	0.0	Spectral gap. See remark 5.
pexsi_delta_e	real double	10.0	Spectral radius. See remark 6.
pexsi_mu_min	real double	-10.0	Minimum value of mu. See remark 7.
pexsi_mu_max	real double	10.0	Maximum value of mu. See remark 7.
pexsi_inertia_tol	real double	0.05	Stopping criterion of inertia counting. See remark 7.

Remarks

1) In PEXSI, 20 poles are usually sufficient to get an accuracy that is comparable with the result obtained from diagonalization. The chemical potential is determined by performing Fermi operator expansion at several chemical potential values (referred to as "points" by PEXSI developers) in an SCF step, then interpolating the results at all points to the final answer. The pexsi_n_mu parameter controls the number of chemical potential "points" to be evaluated. 2 points followed by a simple linear interpolation often yield reasonable results.

In short, we recommend pexsi_n_pole = 20 and pexsi_n_mu = 2.

2) pexsi_np_per_pole: PEXSI has, by construction, a 3-level parallelism: the 1st level independently handles all the poles in parallel; within each pole, the 2nd level evaluates the Fermi operator at all the chemical potential points in parallel; finally, within each point, parallel selected inversion is performed as the 3rd level. The value of pexsi_np_per_pole is the number of MPI tasks assigned to a single chemical potential point, for the parallel selected inversion at that point. Ideally, the total number of MPI tasks should be pexsi_np_per_pole × pexsi_n_mu × pexsi_n_pole, i.e., all the three levels of parallelism are fully exploited. In case that this is not feasible, PEXSI can also process the poles in serial, whereas all the chemical potential points must be evaluated simultaneously. The user should make sure that the total number of MPI tasks is divisible by the product of the number of MPI tasks per pole and the number of points. The code will stop if this requirement is not fulfilled.

When using the BLACS_DENSE or SIESTA_CSC matrix formats, pexsi_np_per_pole is automatically determined to balance the three levels of parallelism in PEXSI. Input and output matrices should be distributed across all MPI tasks in either a 2D block-cyclic distribution (BLACS_DENSE) or a 1D block-cyclic distribution (SIESTA_CSC).

Note that when using the PEXSI_CSC matrix format together with the PEXSI solver, input and output matrices should be distributed among the first pexsi_np_per_pole MPI tasks (not all the MPI tasks) in a 1D block distribution. The block size of the distribution must be floor(N_basis/N_procs), where floor(x) is the greatest integer less than or equal to x, N_basis and N_procs are the number of basis functions and the number of MPI tasks, respectively.

when using the PEXSI_CSC matrix format with the ELPA, libOMM, or SLEPc-SIPs solver, input and output matrices should be distributed across all the MPI tasks in a 1D block distribution. Again, the block size of the distribution must be floor(N_basis/N_procs).

3) pexsi_np_symbo: Unless there is a memory bottleneck, using 1 MPI task for matrix reordering and symbolic factorization is favorable. When running in serial, the matrix reordering in PT-SCOTCH or ParMETIS introduces a minimal number of "fill-ins" to the factorized matrices. Using more MPI tasks introduces more fill-ins. As the matrix reordering and symbolic factorization are performed only once per SCF cycle (with a fixed overlap matrix), using 1 MPI task should not affect the overall timing too much. On the other hand, more fill-ins lead to slower numerical factorization in every SCF step. In addition, the number of MPI tasks used for matrix reordering and symbolic factorization cannot be too large. Otherwise, the symbolic factorization may fail. Therefore, the default number of MPI tasks for symbolic factorization is 1. It is worth testing and increasing this number for large-scale calculations.

4) pexsi_temp: This value corresponds to the $1/k_{\mathrm{B}}T$ term (not T) in the Fermi-Dirac distribution function.

5) pexsi_gap: The PEXSI method does not require a gap. If an estimate of the gap is unavailable, the default value usually works.

6) pexsi_delta_e: This is the spectral width of the eigensystem, i.e., the difference between the largest and smallest eigenvalues. Use the default value if no access to a better estimate.

7) The chemical potential determination in PEXSI relies on inertia counting to narrow down the chemical potential searching interval in the first few SCF steps. The pexsi_inertia_tol parameter controls the stopping criterion of the inertia counting procedure. With a small interval obtained from the inertia counting step, PEXSI then selects a number of points in this interval to perform Fermi operator calculations, based on which a final chemical potential will be determined. The trick of this algorithm is that the chemical potential interval of the current SCF step can be used as a descent guess in the next SCF step. Therefore, the mechanism to choose input values for pexsi_mu_min and pexsi_mu_max is two-fold. For the first SCF iteration, they should be set to safe values that guarantee the true chemical potential lies

in this interval. Then, for the nth SCF step, pexsi_mu_min should be set to ($mu_{\text{min}}^{\text{n-1}} + \Delta V_{\text{min}}$), pexsi_mu_max should be set to ($mu_{\text{max}}^{\text{n-1}} + \Delta V_{\text{max}}$). Here, $mu_{\text{min}}^{\text{n-1}}$ and $mu_{\text{max}}^{\text{n-1}}$ are the lower bound and the upper bound of the chemical potential that are determined by PEXSI in the (n-1)th SCF step. They can be retrieved by calling elsi_get_pexsi_mu_min and elsi_get_pexsi_mu_max, respectively (see 3.6.2. Suppose the effective potential (Hartree potential, exchange-correlation potential, and external potential) is stored in an array V, whose dimension is the number of grid points. From one SCF iteration to the next, ΔV denotes the potential change, and ΔV_{min} and ΔV_{max} are the minimum and maximum values in the array ΔV, respectively. The whole process is summarized in the following pseudo-code.

```
mu_min = -10.0
mu_max = 10.0
ΔV_min = 0.0
ΔV_max = 0.0

while SCF not converged do
    Update Hamiltonian

    elsi_set_pexsi_mu_min(elsi_h, mu_min + ΔV_min)
    elsi_set_pexsi_mu_max(elsi_h, mu_max + ΔV_max)

    elsi_dm_{real|complex}(elsi_h, ham, ovlp, dm, bs_energy)

    elsi_get_pexsi_mu_min(elsi_h, mu_min)
    elsi_get_pexsi_mu_max(elsi_h, mu_max)

    Update electron density
    Update potential

    ΔV_min = minval(V_new - V_old)
    ΔV_max = maxval(V_new - V_old)

    Check SCF convergence
end
```

3.5.5 Customizing the SLEPc-SIPs Solver

elsi_set_sips_interval(handle, sips_lower, sips_upper)

elsi_set_sips_n_elpa(handle, sips_n_elpa)

elsi_set_sips_n_slice(handle, sips_n_slice)

Argument	Data Type	Default	Explanation
sips_lower	real double	-2.0	Lower bound of eigenspectrum. See remark 1.
sips_upper	real double	2.0	Upper bound of eigenspectrum. See remark 1.
sips_n_elpa	integer	0	Number of SCF steps using ELPA. See remark 2.
sips_n_slice	integer	1	Number of slices. See remark 3.

Remarks

1) sips_lower and sips_upper: SLEPc-SIPs relies on some inertia counting steps to estimate the lower and upper bounds of the spectrum. Only eigenvalues within this interval, and their associated eigenvectors, will be solved. The inertia-counting-based eigenvalue searching starts from the interval determined by sips_lower and sips_upper. Depending on the results of inertia counting, this interval may expand or shrink to make sure that the 1st to the n_stateth eigenvalues are all within this interval. If a good estimate of the lower and upper bounds of the eigenspectrum is available, it should be set by elsi_set_sips_interval.

2) sips_n_elpa: The performance of SLEPc-SIPs mainly depends on the load balance across slices. Optimal performance is expected if the desired eigenvalues are evenly distributed across slices. In an SCF calculation, eigenvalues obtained in the current SCF step can be used as an approximated distribution of eigenvalues in the next SCF step. This approximation should become better as the SCF cycle approaches its convergence. On the other hand, at the beginning of an SCF cycle, the load balance is only coarsely checked by inertia calculations. Using the direct eigensolver ELPA in the first sips_n_elpa SCF steps can circumvent the load imbalance of spectrum slicing in the initial SCF steps.

3) sips_n_slice: SLEPc-SIPs partitions the eigenspectrum into slices and solves the slices in parallel. The sips_n_slice parameter controls the number of slices to use in SLEPc-SIPs. The default value, 1, should always work, but by no means leads to the optimal performance of the solver. There are some general rules to set this parameter. Firstly, as a requirement of the SLEPc library, the total number of MPI tasks must by divisible by sips_n_slice. Secondly, setting sips_n_slice to be equal to the number of computing nodes (not MPI tasks) usually yields better performance, as the communication between nodes is minimized in this case. The optimal value of sips_n_slice depends on the actual problem as well as the computing hardware.

3.5.6 Customizing the NTPoly Solver

elsi_set_ntpoly_method(handle, ntpoly_method)

elsi_set_ntpoly_filter(handle, ntpoly_filter)

elsi_set_ntpoly_tol(handle, ntpoly_tol)

Argument	Data Type	Default	Explanation
ntpoly_method	integer	0	Method to perform density matrix purification. See remark 1.
ntpoly_filter	real double	10^{-15}	When performing sparse matrix multiplications, values below this filter will be discarded. See remark 2.
ntpoly_tol	real double	10^{-8}	Convergence tolerance of purification. See remark 2.

Remarks

1) ntpoly_method: Allowed choices are 0 for the canonical purification, 1 for the trace correcting purification, 2 for the 4th order trace resetting purification, and 3 for the generalized hole-particle canonical purification.

2) ntpoly_filter and ntpoly_tol control the accuracy and computational cost of the density matrix purification methods. Small values of ntpoly_filter and ntpoly_tol, e.g. the default choices here, lead to highly accurate results that are comparable to the results obtained from diagonalization. However, linear scaling can only be achieved with a relatively large ntpoly_filter such as 10^{-6}. Correspondingly, ntpoly_tol may be set to 10^{-3}.

3.6 Getting Additional Results from ELSI

In 3.3 and 3.4, the interfaces to compute and return the eigensolutions and the density matrices have been introduced. Internally, ELSI and the solvers perform additional calculations whose results may only be useful at a certain stage of an SCF calculation. One example is the energy-weighted density matrix that is employed to evaluate the Pulay forces during a geometry optimization calculation. The subroutines introduced in the following subsections are used to retrieve such additional results from ELSI.

3.6.1 Getting Results from the ELSI Interface

In all the subroutines listed below, the first argument (input and output) is an `elsi_handle`. The second argument (output) of each subroutine is the name of parameter to get.

elsi_get_initialized(handle, handle_init)

elsi_get_n_sing(handle, n_sing)

elsi_get_mu(handle, mu)

elsi_get_entropy(handle, ts)

elsi_get_edm_real(handle, edm_real)

elsi_get_edm_complex(handle, edm_complex)

elsi_get_edm_real_sparse(handle, edm_real_sparse)

elsi_get_edm_complex_sparse(handle, edm_complex_sparse)

Argument	Data Type	Explanation
handle_init	integer	0 if the ELSI handle has not been initialized; 1 if initialized.
n_sing	integer	Number of eigenvalues of the overlap matrix that are smaller than the singularity tolerance. See 3.5.1.
mu	real double	Chemical potential. See remark 1.
ts	real double	Entropy. See remark 1.
edm_real	real double, rank-2 array	Real energy-weighted density matrix in 2D block-cyclic dense format. See remark 2.
edm_complex	complex double, rank-2 array	Complex energy-weighted density matrix in 2D block-cyclic dense format. See remark 2.
edm_real_sparse	real double, rank-1 array	Non-zero values of the real density matrix in 1D block CSC format. See remark 2.
edm_complex_sparse	complex double, rank-1 array	Non-zero values of the complex density matrix in 1D block CSC format. See remark 2.

Remarks

1) In ELSI, the chemical potential will only be available if one of the density matrix solver interfaces has been called, with ELPA, NTPoly, or PEXSI being the chosen solver. The chemical potential can be retrieved by calling elsi_get_mu. The entropy will only be available if one of the density matrix solver interfaces has been called with ELPA being the chosen solver. The user should avoid calling the subroutine when the chemical potential or the entropy is not ready.

2) In general, the energy-weighted density matrix is only needed in a late stage of an SCF cycle to evaluate forces. It is, therefore, not calculated when any of the density matrix solver interface is called. When the energy-weighted density matrix is actually needed, it can be requested by calling the elsi_get_edm subroutines. Note that these subroutines all have the requirement that the corresponding elsi_dm subroutine must have been invoked. For instance, elsi_get_edm_real_sparse only makes sense if elsi_dm_real_sparse has been successfully executed.

3.6.2 Getting Results from the PEXSI Solver

elsi_get_pexsi_mu_min(handle, pexsi_mu_min)

elsi_get_pexsi_mu_max(handle, pexsi_mu_max)

Argument	Data Type	Explanation
pexsi_mu_min	real double	Minimum value of mu. See remark 1.
pexsi_mu_max	real double	Maximum value of mu. See remark 1.

Remarks

1) Please refer to the 7^{th} remark in 3.5.4 for the chemical potential determination algorithm in PEXSI and ELSI.

3.7 Parallel Matrix I/O

To test the solvers in ELSI, it is convenient to use matrices generated from actual electronic structure calculations. There exist a number of libraries invented for high-performance parallel I/O that are particularly capable of reading and writing a large amount of data with hierarchical structures and complex metadata. However, the I/O task in ELSI is very simple in terms of the complexity of the data to manipulate. The data structure is simply arrays that represent matrices, with a few integers to define the dimension of the matrices. In order to circumvent the unavoidable development and performance overhead associated with a high level I/O library, the parallel I/O functionality defined in the MPI standard is directly used to read and write matrices in ELSI.

When ELSI runs in parallel with multiple MPI tasks, the matrices are distributed across tasks. The choice of writing the distributed matrices into N_{procs} separate files, where N_{procs} is the number of MPI tasks, is not promising due to the difficulty of managing and post-processing a large number of files, especially with a different number of MPI tasks. The implementation of matrix I/O in ELSI adopts collective MPI I/O routines to write data to (read data from) a single binary file, as if the data was gathered onto a single MPI task then written to one file (read from one file by one MPI task then scattered to all tasks). The optimal I/O performance, both with MPI I/O and in general, is often obtained by making large and contiguous requests to access the file system, rather than small, non-contiguous, or random requests. Therefore, before being written to file, matrices are always redistributed to a 1D block distribution. This guarantees that each MPI task writes a contiguous trunk of data to a contiguous piece of file. Similarly, matrices read from file are in a 1D block distribution, and can be redistributed automatically if needed.

A matrix is always stored in the CSC format in an ELSI matrix file. A dense matrix is automatically converted to the CSC format before writing to file, and can be converted back after reading from file.

Next, we present the API for parallel matrix I/O.

3.7.1 Setting Up Matrix I/O

An `elsi_rw_handle` must be initialized via the elsi_init_rw subroutine before any other matrix I/O subroutine may be called. This `elsi_rw_handle` is subsequently passed to all other matrix I/O subroutine calls.

elsi_init_rw(handle, task, parallel_mode, n_basis, n_electron)

Argument	Data Type	in/out	Explanation
handle	type(elsi_rw_handle)	out	Handle to matrix I/O instance.
task	integer	in	Matrix I/O task to perform. Accepted values are: 0 (READ_MATRIX) and 1(WRITE_MATRIX).
parallel_mode	integer	in	Parallelization mode. The only accepted value is 1 (MULTI_PROC) for now.
n_electron	real double	in	Number of electrons. See remark 1.
n_basis	integer	in	Number of basis functions, i.e. global size of matrix.

Remarks

1) n_electron: Many matrices written out with ELSI matrix I/O are from real electronic structure calculations. Having the information of the number of electrons available makes the matrix file useful for testing density matrix solvers such as PEXSI. Therefore, it is recommended to set the correct number of electrons when initializing an matrix I/O handle, although setting it to an arbitrary number will not affect the matrix I/O operation.

2) n_basis: This can be set to an arbitrary value if task is 0 (READ_MATRIX). Its value will be read from file when calling elsi_read_mat_dim or elsi_read_mat_dim_sparse.

The MPI communicator which encloses the MPI tasks to perform the matrix I/O operation needs to be passed into ELSI via the elsi_set_rw_mpi subroutine.

elsi_set_rw_mpi(handle, mpi_comm)

Argument	Data Type	in/out	Explanation
handle	type(elsi_rw_handle)	inout	Handle to matrix I/O instance.
mpi_comm	integer	in	MPI communicator.

When reading or writing a dense matrix, BLACS parameters are passed into ELSI via the elsi_set_rw_blacs subroutine.

elsi_set_rw_blacs(handle, blacs_ctxt, block_size)

Argument	Data Type	in/out	Explanation
handle	type(elsi_rw_handle)	inout	Handle to matrix I/O instance.
blacs_ctxt	integer	in	BLACS context.
block_size	integer	in	Block size of the 2D block-cyclic distribution, specifying both row and column directions.

When writing a sparse matrix, its dimensions are passed into ELSI via the elsi_set_rw_csc subroutine. The only sparse matrix format currently supported by ELSI matrix I/O is the PEXSI_CSC format. When reading a sparse matrix, there is no need to call this subroutine. The relevant parameters will be read from file when calling elsi_read_mat_dim or elsi_read_mat_dim_sparse.

elsi_set_rw_csc(handle, global_nnz, local_nnz, local_col)

Argument	Data Type	in/out	Explanation
handle	type(elsi_rw_handle)	inout	Handle to matrix I/O instance.
global_nnz	integer	in	Global number of non-zeros.
local_nnz	integer	in	Local number of non-zeros.
local_col	integer	in	Local number of matrix columns.

When a matrix I/O instance is no longer needed, its associated handle should be cleaned up by calling elsi_finalize_rw.

elsi_finalize_rw(handle)

Argument	Data Type	in/out	Explanation
handle	type(elsi_rw_handle)	inout	Handle to matrix I/O instance.

3.7.2 Writing Matrices

The following two subroutines write a dense matrix to file. Before writing a dense matrix, MPI and BLACS should be set up properly using elsi_set_rw_mpi and elsi_set_rw_blacs.

elsi_write_mat_real(handle, filename, mat)

Argument	Data Type	in/out	Explanation
handle	type(elsi_rw_handle)	in	Handle to matrix I/O instance.
filename	string	in	Name of file to write.
mat	real double, rank-2 array	in	Local matrix in 2D block-cyclic dense format.

elsi_write_mat_complex(handle, filename, mat)

Argument	Data Type	in/out	Explanation
handle	type(elsi_rw_handle)	in	Handle to matrix I/O instance.
filename	string	in	Name of file to write.
mat	complex double, rank-2 array	in	Local matrix in 2D block-cyclic dense format.

The following two subroutines write a sparse matrix to file. Before writing a sparse matrix, MPI and CSC matrix format should be set up properly using elsi_set_rw_mpi and elsi_set_rw_csc.

elsi_write_mat_real_sparse(handle, filename, row_idx, col_ptr, mat)

Argument	Data Type	in/out	Explanation
handle	type(elsi_rw_handle)	in	Handle to matrix I/O instance.
filename	string	in	Name of file to write.
row_idx	integer, rank-1 array	in	Local row index array.
col_ptr	integer, rank-1 array	in	Local column pointer array.
mat	real double, rank-1 array	in	Local non-zero values in 1D block CSC format.

elsi_write_mat_complex_sparse(handle, filename, row_idx, col_ptr, mat)

Argument	Data Type	in/out	Explanation
handle	type(elsi_rw_handle)	in	Handle to matrix I/O instance.
filename	string	in	Name of file to write.
row_idx	integer, rank-1 array	in	Local row index array.
col_ptr	integer, rank-1 array	in	Local column pointer array.
mat	complex double, rank-1 array	in	Local non-zero values in 1D block CSC format.

When writing a dense matrix to file, values smaller than a predefined threshold will be discarded. The default value of this threshold is 10^{-15}. It can be overridden via elsi_set_rw_zero_def.

elsi_set_rw_zero_def(handle, zero_def)

Argument	Data Type	in/out	Explanation
handle	type(elsi_rw_handle)	inout	Handle to matrix I/O instance.
zero_def	real double	in	When writing a dense matrix to file, values below this threshold will be discarded.

An array of eight user-defined integers can be optionally set up via elsi_set_rw_header. This array will be attached to the matrix file written out by the above subroutines. When reading a matrix file, this array may be retrieved via elsi_get_rw_header.

elsi_set_rw_header(handle, header)

Argument	Data Type	in/out	Explanation
handle	type(elsi_rw_handle)	inout	Handle to matrix I/O instance.
header	integer, rank-1 array	in	An array of eight integers.

3.7.3 Reading Matrices

The following subroutines read a dense or sparse matrix from file. While writing a matrix to file can be done in one step, it is easier to read a matrix from file in two steps, i.e., first read the dimension of the matrix and allocate memory accordingly, then read the actual data of the matrix.

The following three subroutines read a dense matrix from file. Before reading a dense matrix, MPI and BLACS should be set up properly using elsi_set_rw_mpi and elsi_set_rw_blacs. elsi_read_mat_dim is used to read the dimension of a matrix, including the number of electrons in the physical system (for testing purpose), the global size of the matrix, and the local size of the matrix. Memory needs to be allocated according to the return values of local_row and local_col. Then elsi_read_mat_real or elsi_read_mat_complex may be called to read a real or complex matrix, respectively.

elsi_read_mat_dim(handle, filename, n_electron, n_basis, local_row, local_col)

Argument	Data Type	in/out	Explanation
handle	type(elsi_rw_handle)	inout	Handle to matrix I/O instance.
filename	string	in	Name of file to read.
n_electron	real double	out	Number of electrons.
n_basis	integer	out	Number of basis functions, i.e. global size of matrix.
local_row	integer	out	Local number of matrix rows.
local_col	integer	out	Local number of matrix columns.

elsi_read_mat_real(handle, filename, mat)

Argument	Data Type	in/out	Explanation
handle	type(elsi_rw_handle)	inout	Handle to matrix I/O instance.
filename	string	in	Name of file to read.
mat	real double, rank-2 array	out	Local matrix in 2D block-cyclic distribution.

elsi_read_mat_complex(handle, filename, mat)

Argument	Data Type	in/out	Explanation
handle	type(elsi_rw_handle)	inout	Handle to matrix I/O instance.
filename	string	in	Name of file to read.
mat	complex double, rank-2 array	out	Local matrix in 2D block-cyclic distribution.

The following three subroutines read a sparse matrix from file. Before reading a sparse matrix, MPI should be set up properly using elsi_set_rw_mpi. elsi_read_mat_dim_sparse is used to read the dimension of a matrix, including the number of electrons in the physical system (for testing purpose), the global size of the matrix, and the local size of the matrix. Memory needs to be allocated according to the return values of local_nnz and local_col. Then elsi_read_mat_real_sparse or elsi_read_mat_complex_sparse may be called to read a real or complex matrix, respectively.

elsi_read_mat_dim_sparse(handle, filename, n_electron, n_basis, global_nnz, local_nnz, local_col)

Argument	Data Type	in/out	Explanation
handle	type(elsi_rw_handle)	inout	Handle to matrix I/O instance.
filename	string	in	Name of file to read.
n_electron	real double	out	Number of electrons.
n_basis	integer	out	Number of basis functions, i.e. global size of matrix.
global_nnz	integer	out	Global number of non-zeros.
local_nnz	integer	out	Local number of non-zeros.
local_col	integer	out	Local number of matrix columns.

elsi_read_mat_real_sparse(handle, filename, row_idx, col_ptr, mat)

Argument	Data Type	in/out	Explanation
handle	type(elsi_rw_handle)	inout	Handle to matrix I/O instance.
filename	string	in	Name of file to read.
row_idx	integer, rank-1 array	out	Local row index array.
col_ptr	integer, rank-1 array	out	Local column pointer array.
mat	real double, rank-1 array	out	Local non-zero values in 1D block CSC format.

elsi_read_mat_complex_sparse(handle, filename, row_idx, col_ptr, mat)

Argument	Data Type	in/out	Explanation
handle	type(elsi_rw_handle)	inout	Handle to matrix I/O instance.
filename	string	in	Name of file to read.
row_idx	integer, rank-1 array	out	Local row index array.
col_ptr	integer, rank-1 array	out	Local column pointer array.
mat	complex double, rank-1 array	out	Local non-zero values in 1D block CSC format.

An array of eight user-defined integers can be optionally set up via elsi_set_rw_header. This array will be attached to the matrix file written out by the above subroutines. When reading a matrix file, this array may be retrieved via elsi_get_rw_header.

elsi_get_rw_header(handle, header)

Argument	Data Type	in/out	Explanation
handle	type(elsi_rw_handle)	inout	Handle to matrix I/O instance.
header	integer, rank-1 array	out	An array of eight integers.

3.8 Demonstration Pseudo-Code

The typical workflow of ELSI within an electronic structure code is demonstrated by the following pseudo-code.

3.8.1 2D Block-Cyclic Distributed Dense Matrix + ELSI Eigensolver Interface

```
SCF initialize

elsi_init(elsi_h, ELPA, MULTI_PROC, BLACS_DENSE, n_basis, n_electron, n_state)
elsi_set_mpi(elsi_h, mpi_comm)
elsi_set_blacs(elsi_h, blacs_ctxt, block_size)

while SCF not converged do
    Update Hamiltonian

    elsi_ev_{real|complex}(elsi_h, ham, ovlp, eval, evec)

    Update electron density
    Check SCF convergence
end

elsi_finalize(elsi_h)
```

3.8.2 1D Block Distributed CSC Sparse Matrix + ELSI Eigensolver Interface

```
SCF initialization

elsi_init(elsi_h, ELPA, MULTI_PROC, PEXSI_CSC, n_basis, n_electron, n_state)
elsi_set_mpi(elsi_h, mpi_comm)
elsi_set_blacs(elsi_h, blacs_ctxt, block_size)
elsi_set_csc(elsi_h, global_nnz, local_nnz, local_col, row_idx, col_ptr)

while SCF not converged do
    Update Hamiltonian

    elsi_ev_{real|complex}_sparse(elsi_h, ham, ovlp, eval, evec)

    Update electron density
    Check SCF convergence
end

elsi_finalize(elsi_h)
```

Remarks

1) The calculated eigenvectors are returned in the BLACS_DENSE format, which is required to be properly set up.

3.8.3 1D Block-Cyclic Distributed CSC Sparse Matrix + ELSI Eigensolver Interface

```
SCF initialization

elsi_init(elsi_h, ELPA, MULTI_PROC, SIESTA_CSC, n_basis, n_electron, n_state)
elsi_set_mpi(elsi_h, mpi_comm)
elsi_set_blacs(elsi_h, blacs_ctxt, block_size)
elsi_set_csc(elsi_h, global_nnz, local_nnz, local_col, row_idx, col_ptr)
elsi_set_csc_blk(elsi_h, block_size)

while SCF not converged do
    Update Hamiltonian

    elsi_ev_{real|complex}_sparse(elsi_h, ham, ovlp, eval, evec)

    Update electron density
    Check SCF convergence
end

elsi_finalize(elsi_h)
```

Remarks

1) The calculated eigenvectors are returned in the BLACS_DENSE format, which is required to be properly set up.

3.8.4 2D Block-Cyclic Distributed Dense Matrix + ELSI Density Matrix Interface

---

SCF initialization

elsi_init(elsi_h, LIBOMM, MULTI_PROC, BLACS_DENSE, n_basis, n_electron, n_state)
elsi_set_mpi(elsi_h, mpi_comm)
elsi_set_blacs(elsi_h, blacs_ctxt, block_size)

while *SCF not converged* **do**
  Update Hamiltonian

  elsi_dm_{real|complex}(elsi_h, ham, ovlp, dm, bs_energy)
  elsi_get_edm_{real|complex}(elsi_h, edm)

  Update electron density
  Check SCF convergence
end

elsi_finalize(elsi_h)

3.8.5 1D Block Distributed CSC Sparse Matrix + ELSI Density Matrix Interface

---

SCF initialization

elsi_init(elsi_h, PEXSI, parallel_mode, PEXSI_CSC, n_basis, n_electron, n_state)
elsi_set_mpi(elsi_h, mpi_comm)
elsi_set_csc(elsi_h, global_nnz, local_nnz, local_col, row_idx, col_ptr)

while *SCF not converged* **do**
  Update Hamiltonian

  elsi_dm_{real|complex}_sparse(elsi_h, ham, ovlp, dm, bs_energy)
  elsi_get_edm_{real|complex}_sparse(elsi_h, edm)

  Update electron density
  Check SCF convergence
end

elsi_finalize(elsi_h)

Remarks

1) Refer to the 7$^{\text{th}}$ remark in 3.5.4 for the chemical potential determination algorithm in PEXSI.

3.8.6 1D Block-Cyclic Distributed CSC Sparse Matrix + ELSI Density Matrix Interface

```
SCF initialization

elsi_init(elsi_h, PEXSI, parallel_mode, SIESTA_CSC, n_basis, n_electron, n_state)
elsi_set_mpi(elsi_h, mpi_comm)
elsi_set_csc(elsi_h, global_nnz, local_nnz, local_col, row_idx, col_ptr)
elsi_set_csc_blk(elsi_h, block_size)

while SCF not converged do
    Update Hamiltonian

    elsi_dm_{real|complex}_sparse(elsi_h, ham, ovlp, dm, bs_energy)
    elsi_get_edm_{real|complex}_sparse(elsi_h, edm)

    Update electron density
    Check SCF convergence
end

elsi_finalize(elsi_h)
```

Remarks

1) Refer to the 7$^{\text{th}}$ remark in 3.5.4 for the chemical potential determination algorithm in PEXSI.

3.8.7 Multiple k-points Calculations

```
SCF initialization

elsi_init(elsi_h, ELPA, parallel_mode, BLACS_DENSE, n_basis, n_electron, n_state)
elsi_set_mpi(elsi_h, mpi_comm)
elsi_set_blacs(elsi_h, blacs_ctxt, block_size)

elsi_set_kpoint(elsi_h, n_kpt, i_kpt, weight)
elsi_set_mpi_global(elsi_h, mpi_comm_global)

while SCF not converged do
    Update Hamiltonian

    elsi_dm_{real|complex}(elsi_h, ham, ovlp, dm, bs_energy)
    elsi_get_edm_{real|complex}(elsi_h, edm)

    Update electron density
    Check SCF convergence
end

elsi_finalize(elsi_h)
```

Remarks

1) When there are multiple $\boldsymbol{k}$-points, other than setting up the $\boldsymbol{k}$-points and a global MPI communicator, there is no change in the way ELSI solver interfaces are called.

2) The electronic structure code needs to assemble the real-space density from the density matrices returned for the $\boldsymbol{k}$-points. The returned band structure energy, however, is already summed over all $\boldsymbol{k}$-points with respect to the weight of each $\boldsymbol{k}$-point. Refer to 3.2.4 for more information.

3) Calculations with two spin channels can be set up similarly.

3.9 C/C++ Interface

ELSI is written in Fortran. A C interface around the core Fortran code is provided, which can be called from a C or C++ program. Each C wrapper function corresponds to a Fortran subroutine, where we have prefixed the original Fortran subroutine name with c_ for clarity and consistency. Argument lists are identical to the associated native Fortran subroutine. For the complete definition of the C interface, the user is encouraged to look at the `elsi.h` header file directly.

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