



# **ELSI Interface Development Version**

## **User's Guide**

The ELSI Team

<http://elsi-interchange.org>

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# 1 Introduction

## 1.1 The Cubic Wall of Kohn-Sham Density-Functional Theory

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

$$\hat{h}^{\text{KS}}\psi_l = \epsilon_l\psi_l, \quad (1.1)$$

where  $\psi_l$  and  $\epsilon_l$  are Kohn-Sham orbitals and their associated eigenenergies, and  $\hat{h}^{\text{KS}}$  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  $\mathbf{n}$ , which is determined by the Kohn-Sham orbitals  $\psi_l$ . These terms also enter the Hamiltonian  $\hat{h}^{\text{KS}}$ , which determines the Kohn-Sham orbitals  $\psi_l$ .

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,  $N_{\text{basis}}$  basis functions  $\phi_i(\mathbf{r})$  are employed to approximately expand the Kohn-Sham orbitals:

$$\psi_l(\mathbf{r}) = \sum_{j=1}^{N_{\text{basis}}} c_{jl}\phi_j(\mathbf{r}). \quad (1.2)$$

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

$$\sum_j h_{ij}c_{jl} = \epsilon_l \sum_j s_{ij}c_{jl}, \quad (1.3)$$

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

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

1.3 can thus be expressed in the following matrix form

$$\mathbf{H}\mathbf{C} = \mathbf{S}\mathbf{C}\boldsymbol{\epsilon}. \quad (1.5)$$

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

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  $\psi_i$ , from which the electron density  $n(\mathbf{r})$  can be computed following an orbital-based method:

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

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.

An alternative method can be employed for localized basis functions:

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

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

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

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], PEXSI [5, 6], SLEPc-SIPs [7, 8], and NTPoly [9] solvers. Codes currently integrated with ELSI include DFTB+ [10], DGDFE [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 Solver Libraries Supported by ELSI

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

Solver	Data type	Matrix format	Spin/ $k$ -point	Output
ELPA	real/complex	dense/sparse	yes/yes	eigenvalues, eigenvectors, density matrix, energy-weighted density matrix, chemical potential, electronic entropy
libOMM	real/complex	dense/sparse	yes/yes	density matrix, energy-weighted density matrix
PEXSI	real/complex	dense/sparse	yes/yes	density matrix, energy-weighted density matrix, chemical potential
SLEPc-SIPs	real	dense/sparse	no/no	eigenvalues, eigenvectors, density matrix, energy-weighted density matrix, chemical potential, electronic entropy
NTPoly	real/complex	dense/sparse	yes/yes	density matrix, energy-weighted density matrix, chemical potential

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  $\mathbf{S}$ :

$$\mathbf{S} = \mathbf{L}\mathbf{L}^*, \quad (1.9)$$

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

$$\begin{aligned} \tilde{\mathbf{H}} &= \mathbf{L}^{-1}\mathbf{H}(\mathbf{L}^*)^{-1}, \\ \tilde{\mathbf{C}} &= \mathbf{L}^*\mathbf{C}, \end{aligned} \quad (1.10)$$

transforms 1.5 to a standard eigenproblem

$$\tilde{\mathbf{H}}\tilde{\mathbf{C}} = \tilde{\mathbf{C}}\epsilon. \quad (1.11)$$

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

$$\mathbf{T} = \mathbf{Q}\tilde{\mathbf{H}}\mathbf{Q}^*, \quad (1.12)$$

where  $\mathbf{Q}$  is a transformation matrix, and  $\mathbf{T}$  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:

$$\begin{aligned} \mathbf{B} &= \mathbf{Q}_1\tilde{\mathbf{H}}\mathbf{Q}_1^*, \\ \mathbf{T} &= \mathbf{Q}_2\mathbf{B}\mathbf{Q}_2^*. \end{aligned} \quad (1.13)$$

where  $\mathbf{Q}_1$  and  $\mathbf{Q}_2$  are transformation matrices used in the two-stage diagonalization;  $\mathbf{B}$  is a banded matrix; and  $\mathbf{T}$  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,  $N_{\text{W}}$  non-orthogonal Wannier functions  $\chi_k$  are employed to represent the occupied subspace of a system with  $N_{\text{electron}}$  electrons:

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

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

$$\begin{aligned} \mathbf{H}_{\text{omm}} &= \mathbf{W}^* \mathbf{H} \mathbf{W}, \\ \mathbf{S}_{\text{omm}} &= \mathbf{W}^* \mathbf{S} \mathbf{W}, \end{aligned} \quad (1.15)$$

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

$$E[\mathbf{W}] = 4\text{Tr}[\mathbf{H}_{\text{omm}}] - 2\text{Tr}[\mathbf{S}_{\text{omm}} \mathbf{H}_{\text{omm}}]. \quad (1.16)$$

This energy functional, when minimized with respect to the coefficients of Wannier functions  $\mathbf{W}$ , is equal to the band structure energy, i.e. the sum of the energies of all eigenstates, weighted with their respective occupation numbers. Furthermore, the Wannier functions are driven towards orthonormality at this minimum. The density matrix is then constructed from the Wannier functions that minimize  $E[\mathbf{W}]$ .

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 [5, 6] expands the density matrix  $\mathbf{P}$  with rational functions:

$$\mathbf{P} = \sum_l \text{Im} \left( \frac{\omega_l}{\mathbf{H} - (z_l + \mu)\mathbf{S}} \right), \quad (1.17)$$

where  $\mu$  is the chemical potential of the system;  $\{z_l\}$  and  $\{\omega_l\}$  are complex shifts and weights of the expansion terms. About 20 poles are usually sufficient for the result obtained from PEXSI to be fully comparable to that obtained from diagonalization. These poles can be processed in parallel, making PEXSI a highly scalable method on high performance computers.

Only selected elements of the object  $(\mathbf{H} - (z_l + \mu)\mathbf{S})^{-1}$  corresponding to non-zero elements of  $\mathbf{H}$  and  $\mathbf{S}$  are computed with the parallel selected inversion method. The computational complexity of Eq. 1.17 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 does not rely on the existence of an energy gap. The PEXSI method is thus generally applicable to insulating as well as metallic systems, which differentiates PEXSI from traditional linear scaling algorithms.

### 1.3.4 SLEPc-SIPs

The shift-and-invert spectral transformation method, implemented in the SLEPc library [7], transforms the eigenproblem 1.5 by shifting the eigenspectrum:

$$(\mathbf{H} - \sigma \mathbf{S}) \mathbf{C} = \mathbf{S} \mathbf{C} (\epsilon - \sigma), \quad (1.18)$$

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

$$(\mathbf{H} - \sigma \mathbf{S})^{-1} \mathbf{S} \mathbf{C} = (\epsilon - \sigma)^{-1} \mathbf{C}, \quad (1.19)$$

If the shift can be chosen to be close to the target eigenvalue, 1.19 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 [8] partitions the eigenspectrum of a given eigenproblem into  $N_{\text{slice}}$  slices. Accordingly, the processes involved in the calculation are split into  $N_{\text{slice}}$  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 [8].

### 1.3.5 NTPoly

Density matrix purification is an established way to achieve linear scaling KS-DFT. Assuming an orthogonal basis set, the density matrix  $\mathbf{P}$  should satisfy the following conditions:

$$\begin{aligned}\mathbf{P} &= \mathbf{P}^*, \\ \text{Tr}(\mathbf{P}) &= N_{\text{electron}}, \\ \mathbf{P} &= \mathbf{P}^2.\end{aligned}\tag{1.20}$$

An initial guess of such a matrix can be obtained by scaling the Hamiltonian matrix to make sure its eigenvalues lie in between 0 and 1. Then, the “purification” method iteratively updates the density matrix until it converges to a certain criterion. The converged density matrix satisfies the three conditions in 1.20.

The process of density matrix purification can be written in the general form

$$\mathbf{P}_{n+1} = f(\mathbf{P}_n),\tag{1.21}$$

where  $\mathbf{P}_n$  is the density matrix in the  $n^{\text{th}}$  purification iteration,  $\mathbf{P}_{n+1}$  is the density matrix in the  $(n+1)^{\text{th}}$  iteration, and  $f(\mathbf{P})$  is usually a matrix polynomial, which can be calculated by matrix-matrix multiplications.

Various algorithms have been developed to carry out the density matrix purification efficiently, such as the canonical purification [14], the trace resetting purification methods [15], and the generalized canonical purification [16]. These methods are implemented in the NTPoly library [9] using its distributed-memory sparse matrix-matrix multiplication kernel. Given sufficiently sparse matrices, the computational complexity of density matrix purification with NTPoly is  $O(N)$  for insulating systems.

## 1.4 Citing ELSI

Key concepts of ELSI and the first version of its implementation are described in the following paper [17]:

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 Prerequisites

The ELSI package contains the ELSI interface software as well as redistributed source code for the solver libraries ELPA (version 2016.11.001), libOMM, PEXSI (version 1.2.0), and NTPoly (version 2.3.1). The installation of ELSI makes use of the CMake software. Minimum requirements include:

`CMake` [minimum version 3.0; newer version recommended]  
`Fortran compiler` [Fortran 2003 compliant]  
`C compiler` [C99 compliant]  
`MPI` [MPI-3 recommended]

Building the PEXSI solver (highly recommended) requires:

`C++ compiler` [C++ 11 compliant]

Additionally, building the SLEPc-SIPs solver requires:

`SLEPc` [version 3.9 or newer]  
`PETSc` [version 3.9 or newer, 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, PEXSI, SuperLU\_DIST, PT-SCOTCH, and NTPoly libraries may be substituted by user's optimized versions.

### 2.2 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 should 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](#).

## 2.3 Configuration

### 2.3.1 Compilers

CMake automatically detects compilers. The choices made by CMake often work, but they do 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_CXX_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_CXX_COMPILE_FLAGS
```

With CMake versions older than 3.8.2, flags such as `-std=c99` and `-std=c++11` (or equivalents depending on the compilers) should be given in order to ensure compliance with the C99 and C++11 standards.

### 2.3.2 Solvers

The ELPA, libOMM, PEXSI, and NTPoly 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 bottleneck when calculating a large portion of the eigenspectrum. 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.

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

```
-DENABLE_PEXSI=ON
```

PEXSI 1.2.0 has been tested with this version of ELSI. Older/newer versions may or may not be compatible. The PEXSI library must be compiled with Fortran support.

SLEPc-SIPs may be activated by specifying:

```
-DENABLE_SIPS=ON
```

SLEPc and PETSc versions 3.9, 3.10, and 3.11 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 packages SuperLU\_DIST, MUMPS, ParMETIS, and PT-SCOTCH enabled.

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

```
-DUSE_EXTERNAL_ELPA=ON  
-DUSE_EXTERNAL_OMM=ON  
-DUSE_EXTERNAL_PEXSI=ON  
-DUSE_EXTERNAL_NTPOLY=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. Similarly, [LIBS](#) should include the PEXSI library and all its dependencies when using an external PEXSI.

### 2.3.3 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
```

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 2.4 for information regarding linking a third-party package against ELSI.

### 2.3.4 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
<a href="#">ADD_UNDERSCORE</a>	boolean	ON	Suffix C functions with an underscore
<a href="#">BUILD_SHARED_LIBS</a>	boolean	OFF	Build ELSI as a shared library
<a href="#">CMAKE_C_COMPILER</a>	string	none	MPI C compiler
<a href="#">CMAKE_C_FLAGS</a>	string	none	C flags
<a href="#">CMAKE_CXX_COMPILER</a>	string	none	MPI C++ compiler
<a href="#">CMAKE_CXX_FLAGS</a>	string	none	C++ flags
<a href="#">CMAKE_Fortran_COMPILER</a>	string	none	MPI Fortran compiler
<a href="#">CMAKE_Fortran_FLAGS</a>	string	none	Fortran flags
<a href="#">CMAKE_INSTALL_PREFIX</a>	path	/usr/local	Path to install ELSI
<a href="#">ELPA2_KERNEL</a>	string	none	ELPA2 kernel
<a href="#">ENABLE_C_TESTS</a>	boolean	OFF	Build C test programs
<a href="#">ENABLE_PEXSI</a>	boolean	OFF	Enable PEXSI support
<a href="#">ENABLE_SIPS</a>	boolean	OFF	Enable SLEPc-SIPs support
<a href="#">ENABLE_TESTS</a>	boolean	OFF	Build Fortran test programs
<a href="#">INC_PATHS</a>	string	none	Include directories of external libraries
<a href="#">LIB_PATHS</a>	string	none	Directories containing external libraries
<a href="#">LIBS</a>	string	none	External libraries
<a href="#">MPIEXEC_NP</a>	string	mpirun -n 4	Command to run tests in parallel with MPI
<a href="#">MPIEXEC_1P</a>	string	mpirun -n 1	Command to run tests in serial with MPI
<a href="#">SCOTCH_LAST_RESORT</a>	string	none	Command to invoke PT-SCOTCH header generator
<a href="#">USE_EXTERNAL_ELPA</a>	boolean	OFF	Use external ELPA
<a href="#">USE_EXTERNAL_NTPOLY</a>	boolean	OFF	Use external NTPoly
<a href="#">USE_EXTERNAL_OMM</a>	boolean	OFF	Use external libOMM and MatrixSwitch
<a href="#">USE_EXTERNAL_PEXSI</a>	boolean	OFF	Use external PEXSI (if PEXSI enabled)
<a href="#">USE_MPIALLGATHER</a>	boolean	ON	Use non-blocking collective MPI functions

#### 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 2.3.2 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, NTPoly, 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 2.3.2 for more information.

5) [USE\\_MPI\\_IALLGATHER](#): NTPoly makes use of non-blocking collective MPI functions such as `MPI_Iallgatherv` to overlap its computation and communication. If these MPI functions are not available in the user's MPI version, set [USE\\_MPI\\_IALLGATHER](#) to 'OFF'. Using this flag may lead to reduced performance. Upgrade MPI if possible.

### 2.3.5 “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.

## 2.4 Importing ELSI into Third-Party Code Projects

### 2.4.1 Linking against ELSI: CMake

A CMake configuration file called `elsiConfig.cmake` should be generated after ELSI is successfully installed (see 2.3.3). 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.

### 2.4.2 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.

### 2.4.3 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 standpoint, applies equally to both interfaces. Information specifically about the C wrapper for ELSI may be found in 3.9.

In the source code of ELSI, there may exist subroutines that are not documented as public API here. Usage of those undocumented subroutines is not recommended, as they are usually experimental and subject to modification or removal without notice.

### 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
<code>handle</code>	<code>type(elsi_handle)</code>	out	Handle to ELSI.
<code>solver</code>	integer	in	Desired solver. Accepted values are: 0 (AUTO), 1 (ELPA), 2 (libOMM), 3 (PEXSI), 5 (SLEPc-SIPs), and 6 (NTPoly). See remark 1.
<code>parallel_mode</code>	integer	in	Parallelization mode. Accepted values are: 0 (SINGLE_PROC) and 1 (MULTI_PROC). See remark 4.
<code>matrix_format</code>	integer	in	Matrix format. Accepted values are: 0 (BLACS_DENSE), 1 (PEXSI_CSC), 2 (SIESTA_CSC), and 3 (GENERIC_COO). See remark 2.
<code>n_basis</code>	integer	in	Number of basis functions, i.e. global size of Hamiltonian.
<code>n_electron</code>	real double	in	Number of electrons.
<code>n_state</code>	integer	in	Number of states. See remark 3.

#### Remarks

1) `solver`: Refer to 1.3 for supported features of each solver. The `AUTO(0)` option attempts to automate the solver selection procedure based on benchmarks performed and experiences gained in the ELSI project. User-supplied information



may assist in finding the optimal solver. In particular, see [elsi\\_set\\_dimensionality](#) and [elsi\\_set\\_energy\\_gap](#) in 3.5. Simply put, the solver selection favors ELPA for small-and-medium-sized problems, PEXSI for large, sparse, low-dimensional problems, and NTPoly for extra-large, sparse systems with a decent energy gap.

**2) matrix.format:** [BLACS\\_DENSE](#)(0) refers to 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. [GENERIC\\_COO](#)(3) refers to a coordinate (COO) sparse matrix format in an arbitrary distribution. Please refer to 3.2.3 for specifications of these matrix formats.

**3) n.state:** If ELPA or SLEPc-SIPs is the chosen solver, this parameter specifies the number of eigenstates to solve. libOMM, PEXSI and NTPoly do not make use of this parameter, thus a dummy value may be passed.

**4) 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. Every MPI task independently handles a group of  $k$ -points uniquely assigned to it.

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

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

**3b) MULTI\_PROC:** Solves the KS eigenproblem following a ScaLAPACK-like fashion. This allows the usage of the following parallelization strategy:

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

- Example: 4  $k$ -points, 16 MPI tasks.
- MPI tasks 0, 1, 2, 3 cooperatively handle  $k$ -point 1;
- MPI tasks 4, 5, 6, 7 cooperatively handle  $k$ -point 2;
- MPI tasks 8, 9, 10, 11 cooperatively handle  $k$ -point 3;
- MPI tasks 12, 13, 14, 15 cooperatively handle  $k$ -point 4.

```
call elsi_init (eh, ..., parallel_mode=1, ...)
call elsi_set_mpi (eh, my_mpi_comm)
call elsi_set_kpoint (eh, n_kpt, my_kpt, my_weight)
call elsi_set_mpi_global (eh, mpi_comm_global)
...
call elsi_{ev|dm}_{real|complex} (eh, my_ham, my_ovlp, ...)
```

Please note that when there is more than one  $k$ -point, a global MPI communicator must be provided for inter- $k$ -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  $k$ -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  $k$ -point and/or spin channel, this communicator will be used only for solving one problem corresponding to one  $k$ -point and one spin channel. See 3.2.4 for details.

[elsi\\_set\\_mpi](#)(handle, mpi\_comm)

Argument	Data Type	in/out	Explanation
<a href="#">handle</a>	type(elsi_handle)	inout	Handle to ELSI.
<a href="#">mpi_comm</a>	integer	in	MPI communicator.

### 3.2.3 Setting Up Matrix Formats

Four matrix formats are currently supported by ELSI, namely 2D block-cyclic distributed dense matrix format ([BLACS\\_DENSE](#)), 1D block distributed compressed sparse column format ([PEXSL\\_CSC](#)), 1D block-cyclic distributed compressed sparse column format, ([SIESTA\\_CSC](#)), arbitrarily distributed coordinate sparse format ([GENERIC\\_COO](#)).

When using the [BLACS\\_DENSE](#) format, 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](#) format.

[elsi\\_set\\_blacs](#)(handle, blacs\_ctxt, block\_size)

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

When using the [PEXSL\\_CSC](#) or [SIESTA\\_CSC](#) format, 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 CSC sparse matrix formats.

[elsi\\_set\\_csc](#)(handle, global\_nnz, local\_nnz, local\_col, row\_idx, col\_ptr)

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

The block size of the [PEXSL\\_CSC](#) format cannot be set by the user. This is because the PEXSI solver requires that the block size must be  $\text{floor}(\text{N\_basis}/\text{N\_procs})$ , where  $\text{floor}(x)$  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. The block size of the [SIESTA\\_CSC](#) must be explicitly set by calling [elsi\\_set\\_csc\\_blk](#).

[elsi\\_set\\_csc\\_blk](#)(handle, block\_size)

Argument	Data Type	in/out	Explanation
<a href="#">handle</a>	type(elsi_handle)	inout	Handle to ELSI.
<a href="#">global_nnz</a>	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 is when using the PEXSI solver, one of the sparse density matrix interfaces ([elsi\\_dm\\_real\\_sparse](#) or [elsi\\_dm\\_complex\\_sparse](#)), and the

PEXSL\_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<sup>nd</sup> remark in 3.5.4 for more information.

When using the `GENERIC_COO` format, the sparsity pattern should be passed into ELSI via the `elsi_set_coo` subroutine. It is necessary to call this subroutine before calling any solver interface that makes use of the COO sparse matrix format.

`elsi_set_coo`(handle, global\_nnz, local\_nnz, row\_idx, col\_idx)

Argument	Data Type	in/out	Explanation
<code>handle</code>	type(elsi_handle)	inout	Handle to ELSI.
<code>global_nnz</code>	integer	in	Global number of non-zeros.
<code>local_nnz</code>	integer	in	Local number of non-zeros.
<code>row_idx</code>	integer, rank-1 array	in	Local row index array. Dimension: local_nnz.
<code>col_idx</code>	integer, rank-1 array	in	Local column index array. Dimension: local_nnz.

The distribution of matrix elements in the `GENERIC_COO` format is arbitrary. Both sorted and unsorted inputs are supported.

### 3.2.4 Setting Up Multiple $k$ -points and/or Spin Channels

When there is more than one  $k$ -point and/or spin channel in the simulating system, the ELSI interface can be set up to support parallel calculation of the  $k$ -points and/or spin channels. The base case is a system isolated in space, e.g. free atoms, molecules, clusters, without spin-polarization. In this case, there is one eigenproblem in each iteration of an SCF cycle. When a spin-polarized periodic system is considered, 1.3 should have an index  $\alpha$  denoting the spin channel, and an index  $k$  denoting points in reciprocal space:

$$H_k^\alpha C_k^\alpha = S_k C_k^\alpha \epsilon_k^\alpha. \quad (3.1)$$

In total, there are  $N_{\text{kpt}} \times N_{\text{spin}}$  eigenproblems to solve. They can be solved in an embarrassingly parallel fashion. In ELSI, eigenproblems in 3.1 are considered as equivalent “unit tasks”. The available computer processes are divided into  $N_{\text{kpt}} \times N_{\text{spin}}$  groups, each of which is responsible for one unit task.

To set up the ELSI interface for a calculation with more than one  $k$ -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  $k$ -points and spin channels are fully parallelized, i.e., there is no MPI task handling more than one  $k$ -point and/or more than one spin channel. In ELSI, the two spin channels are always coupled by a uniform chemical potential. The distribution of electrons among the two channels, and thus the net spin moment of the system, cannot be specified. Calculations with a fixed, user-specified spin moment can be performed by initializing two independent ELSI instances for the two spin channels.

In this version of ELSI, the SLEPc-SIPs eigensolver is not supported in spin-polarized and/or periodic calculations.

`elsi_set_kpoint`(handle, n\_kpt, i\_kpt, weight)

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

`elsi_set_spin`(handle, n\_spin, i\_spin)

Argument	Data Type	in/out	Explanation
<code>handle</code>	type(elsi_handle)	inout	Handle to ELSI.
<code>n_spin</code>	integer	in	Total number of spin channels.
<code>i_spin</code>	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
<a href="#">handle</a>	type(elsi_handle)	inout	Handle to ELSI.
<a href="#">mpi_comm_global</a>	integer	in	Global MPI communicator used for communications among all $k$ -points and spin channels.

### 3.2.5 Reinitializaing ELSI

When a geometry update takes place in geometry optimization or molecular dynamics calculations, the overlap matrix changes due to the movement of localized basis functions. Calling [elsi\\_reinit](#) instructs ELSI to flush geometry-related variables and arrays that cannot be used in the new geometry step, e.g., the overlap matrix and its sparsity pattern. Other runtime parameters are kept within the ELSI instance and reused throughout multiple geometry steps. Note that the chemical potential determination in PEXSI must be restarted for every new geometry. See the 5<sup>th</sup> remark in 3.5.4 for details.

[elsi\\_reinit](#)(handle)

### 3.2.6 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
<a href="#">handle</a>	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 generalized eigenproblem defined by H and S matrices. For standard eigenproblems, please see [elsi\\_set\\_unit\\_ovlp](#) in 3.5.1. Only ELPA and SLEPc-SIPs may be selected as the solver when using these subroutines.

[elsi\\_ev\\_real](#)(handle, ham, ovlp, eval, evvec)

Argument	Data Type	in/out	Explanation
<a href="#">handle</a>	type(elsi_handle)	inout	Handle to ELSI.
<a href="#">ham</a>	real double, rank-2 array	inout	Real Hamiltonian matrix in 2D block-cyclic dense format. See remark 1.
<a href="#">ovlp</a>	real double, rank-2 array	inout	Real overlap matrix (or its Cholesky factorization) in 2D block-cyclic dense format. See remark 1.
<a href="#">eval</a>	real double, rank-1 array	inout	Eigenvalues. See remark 2.
<a href="#">evvec</a>	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
<a href="#">handle</a>	type( <a href="#">elsi_handle</a> )	inout	Handle to ELSI.
<a href="#">ham</a>	complex double, rank-2 array	inout	Complex Hamiltonian matrix in 2D block-cyclic dense format. See remark 1.
<a href="#">ovlp</a>	complex double, rank-2 array	inout	Complex overlap matrix (or its Cholesky factorization) in 2D block-cyclic dense format. See remark 1.
<a href="#">eval</a>	real double, rank-1 array	inout	Eigenvalues. See remark 2.
<a href="#">evec</a>	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
<a href="#">handle</a>	type( <a href="#">elsi_handle</a> )	inout	Handle to ELSI.
<a href="#">ham</a>	real double, rank-1 array	inout	Real Hamiltonian matrix in 1D block CSC, 1D block-cyclic CSC, or generic COO sparse format.
<a href="#">ovlp</a>	real double, rank-1 array	inout	Real overlap matrix in 1D block CSC, 1D block-cyclic CSC, or generic COO sparse format.
<a href="#">eval</a>	real double, rank-1 array	inout	Eigenvalues. See remark 2.
<a href="#">evec</a>	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
<a href="#">handle</a>	type( <a href="#">elsi_handle</a> )	inout	Handle to ELSI.
<a href="#">ham</a>	complex double, rank-1 array	inout	Complex Hamiltonian matrix in 1D block CSC, 1D block-cyclic CSC, or generic COO sparse format.
<a href="#">ovlp</a>	complex double, rank-1 array	inout	Complex overlap matrix in 1D block CSC, 1D block-cyclic CSC, or generic COO sparse format.
<a href="#">eval</a>	real double, rank-1 array	inout	Eigenvalues. See remark 2.
<a href="#">evec</a>	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 with its Cholesky factorization, which will be reused by subsequent subroutine calls to [elsi\\_ev\\_real](#) or [elsi\\_ev\\_complex](#). When using [elsi\\_ev\\_real\\_sparse](#), the Cholesky factorization (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. 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 band structure energy.

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

Argument	Data Type	in/out	Explanation
<code>handle</code>	<code>type(elsi_handle)</code>	inout	Handle to ELSI.
<code>ham</code>	real double, rank-2 array	inout	Real Hamiltonian matrix in 2D block-cyclic dense format.
<code>ovlp</code>	real double, rank-2 array	inout	Real overlap matrix (or Cholesky factorization) in 2D block-cyclic dense format. See remark 1.
<code>dm</code>	real double, rank-2 array	out	Real density matrix in 2D block-cyclic dense format.
<code>energy</code>	real double	out	Band structure energy.

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

Argument	Data Type	in/out	Explanation
<code>handle</code>	<code>type(elsi_handle)</code>	inout	Handle to ELSI.
<code>ham</code>	complex double, rank-2 array	inout	Complex Hamiltonian matrix in 2D block-cyclic dense format.
<code>ovlp</code>	complex double, rank-2 array	inout	Complex overlap matrix (or its Cholesky factorization) in 2D block-cyclic dense format. See remark 1.
<code>dm</code>	complex double, rank-2 array	out	Complex density matrix in 2D block-cyclic dense format.
<code>energy</code>	real double	out	Band structure energy.

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

Argument	Data Type	in/out	Explanation
<code>handle</code>	<code>type(elsi_handle)</code>	inout	Handle to ELSI.
<code>ham</code>	real double, rank-1 array	inout	Non-zero values of the real Hamiltonian matrix in 1D block CSC, 1D block-cyclic CSC, or generic COO sparse format.
<code>ovlp</code>	real double, rank-1 array	inout	Non-zero values of the real overlap matrix in 1D block CSC, 1D block-cyclic CSC, or generic COO sparse format.
<code>dm</code>	real double, rank-1 array	out	Non-zero values of the real density matrix in 1D block CSC, 1D block-cyclic CSC, or generic COO sparse format.
<code>energy</code>	real double	out	Band structure energy.

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

Argument	Data Type	in/out	Explanation
<code>handle</code>	<code>type(elsi_handle)</code>	inout	Handle to ELSI.
<code>ham</code>	complex double, rank-1 array	inout	Non-zero values of the complex Hamiltonian matrix in 1D block CSC, 1D block-cyclic CSC, or generic COO sparse format.
<code>ovlp</code>	complex double, rank-1 array	inout	Non-zero values of the complex overlap matrix in 1D block CSC, 1D block-cyclic CSC, or generic COO sparse format.
<code>dm</code>	complex double, rank-1 array	out	Non-zero values of the complex density matrix in 1D block CSC, 1D block-cyclic CSC, or generic COO sparse format.
<code>energy</code>	real double	out	Band structure energy.

## Remarks

1) When using `elsi_dm_real` or `elsi_dm_complex` with ELPA or libOMM, the Hamiltonian matrix will be destroyed during the computation. The overlap matrix will be used to store its Cholesky factorization, which will be reused until the overlap matrix changes.

## 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 ELSI API. Integers are used to represent logical, with 0 being false and any positive integer being true.

`elsi_set_output(handle, output_level)`

`elsi_set_output_unit(handle, output_unit)`

`elsi_set_output_log(handle, output_log)`

`elsi_set_save_ovlp(handle, save_ovlp)`

`elsi_set_unit_ovlp(handle, unit_ovlp)`

`elsi_set_zero_def(handle, zero_def)`

`elsi_set_illcond_check(handle, illcond_check)`

`elsi_set_illcond_tol(handle, illcond_tol)`

`elsi_set_spin_degeneracy(handle, spin_degeneracy)`

`elsi_set_energy_gap(handle, energy_gap)`

`elsi_set_spectrum_width(handle, spectrum_width)`

`elsi_set_dimensionality(handle, dimensionality)`

`elsi_set_mu_broaden_scheme(handle, mu_broaden_scheme)`

`elsi_set_mu_broaden_width(handle, mu_broaden_width)`

`elsi_set_mu_tol(handle, mu_tol)`

`elsi_set_mu_mp_order(handle, mu_mp_order)`

`elsi_set_write_unit(handle, write_unit)`

`elsi_set_sing_check(handle, sing_check)`

`elsi_set_sing_tol(handle, sing_tol)`

Argument	Data Type	Default	Explanation
<code>output_level</code>	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.
<code>output_unit</code>	integer	6	Unit used in ELSI to write out information.
<code>output_log</code>	integer	0	If not 0, a separate log file in JSON format will be written out.
<code>save_ovlp</code>	integer	0	If not 0, the overlap matrix will be saved for extrapolation of density matrix or eigenvectors to a new geometry.
<code>unit_ovlp</code>	integer	0	If not 0, the overlap matrix will be treated as an identity (unit) matrix in ELSI and the solvers. See remark 1.
<code>zero_def</code>	real double	$10^{-15}$	When converting a matrix from dense to sparse format, values below this threshold will be discarded.
<code>illcond_check</code>	integer	0	If not 0, the eigenvalues of the overlap matrix will be calculated in order to check if it is ill-conditioned. See remark 2.
<code>illcond_tol</code>	real double	$10^{-5}$	Eigenfunctions of the overlap matrix with eigenvalues smaller than this threshold will be removed to avoid ill-conditioning. See remark 2.
<code>spin_degeneracy</code>	real double	$2.0/n_{\text{spin}}$	Spin degeneracy that controls the maximum number of electrons on a state.
<code>energy_gap</code>	real double	0	Energy gap. See remark 3.
<code>spectrum_width</code>	real double	$10^3$	Width of the eigenspectrum. See remark 3.
<code>dimensionality</code>	integer	3	Dimensionality (1, 2, or 3) of the simulating system. Only used for automatic solver selection.
<code>mu_broaden_scheme</code>	integer	0	Broadening scheme employed to compute the occupation numbers and the Fermi level. 0: Gaussian. 1: Fermi-Dirac. 2: Methfessel-Paxton. 4: Marzari-Vanderbilt.
<code>mu_broaden_width</code>	real double	0.01	Broadening width employed to compute the occupation numbers and the Fermi level. See remark 4.
<code>mu_tol</code>	real double	$10^{-13}$	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.
<code>mu_mp_order</code>	integer	0	Order of the Methfessel-Paxton broadening scheme. No effect if Methfessel-Paxton is not the chosen broadening scheme.
<code>write_unit</code>	integer	6	Deprecated. Use <code>elsi_set_output_unit</code> instead.
<code>sing_check</code>	integer	0	Deprecated. Use <code>elsi_set_illcond_check</code> instead.
<code>sing_tol</code>	real double	$10^{-5}$	Deprecated. Use <code>elsi_set_illcond_tol</code> instead.

## Remarks

- 1) If the overlap matrix is set to be an identity matrix, all settings related to the singularity (ill-conditioning) check take no effect. The `ovlp` argument passed into `elsi_ev_real`, `elsi_ev_complex`, `elsi_ev_real_sparse`, `elsi_ev_complex_sparse`, `elsi_dm_real`, `elsi_dm_complex`, `elsi_dm_real_sparse`, and `elsi_dm_complex_sparse` will not be referenced.
- 2) If the ill-conditioning check is not disabled, in the first iteration of each SCF cycle, all eigenvalues of the overlap matrix is computed. If there is any eigenvalue smaller than `illcond_tol`, the matrix is considered to be ill-conditioned.
- 3) `spectrum_width` and `energy_gap` refer to the width and the gap of the eigenspectrum. Simply use the default values if there is no better estimate.
- 4) In all supported broadening schemes, there is a term  $(\epsilon - E_F)/W$  in the distribution function, where  $\epsilon$  is the energy of an eigenstate, and  $E_F$  is the Fermi level. The `broadening_width` parameter should be  $W$  in the same unit of  $\epsilon$  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
<code>elpa_solver</code>	integer	2	1: ELPA 1-stage solver. 2: ELPA 2-stage solver. The latter is usually faster and more scalable.
<code>elpa_n_single</code>	integer	0	Number of SCF steps using single precision ELPA to solve standard eigenproblems. See remark 1.
<code>elpa_gpu</code>	integer	0	If not 0, try to enable GPU-acceleration in ELPA. See remark 2.
<code>elpa_gpu_kernels</code>	integer	0	If not 0, try to enable GPU-acceleration and GPU kernels in ELPA. See remark 2.
<code>elpa_autotune</code>	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 compiled ELPA library, it may be enabled by setting `elpa_n_single` to a positive integer, then the standard eigenproblems 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 compiled 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. Setting `elpa_gpu` itself does not enable the GPU kernels for eigenvector back-transformation. To enable the GPU kernels, use `elpa_gpu_kernels`. 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 compiled with GPU support.

3) `elpa_autotune`: If auto-tuning of runtime parameters is available in an externally compiled 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
<code>omm_flavor</code>	integer	0	Method to perform OMM minimization. See remark 1.
<code>omm_n_elpa</code>	integer	6	Number of SCF steps using ELPA. See remark 2.
<code>omm_tol</code>	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_mu_min(handle, pexsi_mu_min)
elsi_set_pexsi_mu_max(handle, pexsi_mu_max)
elsi_set_pexsi_inertia_tol(handle, pexsi_inertia_tol)
elsi_set_pexsi_gap(handle, pexsi_gap)
elsi_set_pexsi_delta_e(handle, pexsi_delta_e)
```

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

#### 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`).

Please 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  $\text{floor}(\text{N\_basis}/\text{N\_procs})$ , where  $\text{floor}(x)$  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  $\text{floor}(\text{N\_basis}/\text{N\_procs})$ .

3) `pexsi_np_symbolo`: 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  $1/k_B T$  term (not  $T$ ) in the Fermi-Dirac distribution function.

```
do geometry update
  mu_min = -10.0
  mu_max = 10.0
  delta_V_min = 0.0
  delta_V_max = 0.0

  do SCF cycle
    Update Hamiltonian

    call elsi_set_pexsi_mu_min (eh, mu_min + delta_V_min)
    call elsi_set_pexsi_mu_max (eh, mu_max + delta_V_max)

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

    call elsi_get_pexsi_mu_min (eh, mu_min)
    call elsi_get_pexsi_mu_max (eh, mu_max)

    Update electron density
    Update potential

    delta_V_min = minval (V_new - V_old)
    delta_V_max = maxval (V_new - V_old)

    Check SCF convergence
  end do
end do
```

5) 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 of each geometry step, they should be set to safe values that guarantee the true chemical potential lies in this interval. Then, for the  $n^{\text{th}}$  SCF step, `pexsi_mu_min` should be set to  $(\mu_{\text{min}}^{n-1} + \Delta V_{\text{min}})$ , `pexsi_mu_max` should be set to  $(\mu_{\text{max}}^{n-1} + \Delta V_{\text{max}})$ . Here,  $\mu_{\text{min}}^{n-1}$  and  $\mu_{\text{max}}^{n-1}$  are the lower bound and the upper bound of the chemical potential that are determined by PEXSI in the  $(n-1)^{\text{th}}$  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,  $\Delta V$  denotes the potential change, and  $\Delta V_{\text{min}}$  and  $\Delta V_{\text{max}}$  are the minimum and maximum values in the array  $\Delta V$ , respectively. The whole process is summarized in the pseudo-code above. The (re-)initialization and finalization of ELSI are omitted.

6) `pexsi_gap`: The PEXSI method does not require an energy gap. If no knowledge is available, the default value usually works.

### 3.5.5 Customizing the SLEPc-SIPs Solver

```
elsi_set_sips_ev_min(handle, ev_min)

elsi_set_sips_ev_max(handle, ev_max)

elsi_set_sips_n_elpa(handle, sips_n_elpa)

elsi_set_sips_n_slice(handle, sips_n_slice)

elsi_set_sips_interval(handle, sips_lower, sips_upper)
```

Argument	Data Type	Default	Explanation
<code>ev_min</code>	real double	-2.0	Lower bound of eigenspectrum. See remark 1.
<code>ev_max</code>	real double	2.0	Upper bound of eigenspectrum. See remark 1.
<code>sips_n_elpa</code>	integer	0	Number of SCF steps using ELPA. See remark 2.
<code>sips_n_slice</code>	integer	1	Number of slices. See remark 3.
<code>sips_lower</code>	real double	-2.0	Deprecated. Use <code>elsi_set_sips_ev_min</code> instead.
<code>sips_upper</code>	real double	2.0	Deprecated. Use <code>elsi_set_sips_ev_max</code> instead.

#### Remarks

1) `ev_min` and `ev_max`: 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 `ev_min` and `ev_max`. Depending on the results of inertia counting, this interval may expand or shrink to make sure that the 1<sup>st</sup> to the `n_state`<sup>th</sup> eigenvalues are all within this interval. If a good estimate of the lower or upper bounds of the eigenspectrum is available, it should be set by `elsi_set_sips_ev_min` or `elsi_set_sips_ev_max`.

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 be 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
<code>ntpoly_method</code>	integer	2	Method to perform density matrix purification. See remark 1.
<code>ntpoly_filter</code>	real double	$10^{-15}$	When performing sparse matrix multiplications, values below this filter will be discarded. See remark 2.
<code>ntpoly_tol</code>	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. Tight choices of `ntpoly_filter` and `ntpoly_tol`, e.g. the default values 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  $10^{-3}$ . Note that the purification may not converge if `ntpoly_filter` is too large relative to `ntpoly_tol`. Setting `ntpoly_filter` to be  $\leq 10^{-3} \times \text{ntpoly\_tol}$  is safe in most cases.

## 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_version(handle, major, minor, patch)`

`elsi_get_datestamp(handle, date_stamp)`

`elsi_get_n_illcond(handle, n_illcond)`

`elsi_get_ovlp_ev_min(handle, ev_min)`

`elsi_get_ovlp_ev_max(handle, ev_max)`

`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)

[elsi\\_get\\_n\\_sing](#)(handle, n\_sing)

Argument	Data Type	Explanation
<a href="#">handle_init</a>	integer	0 if the ELSI handle has not been initialized; 1 if initialized.
<a href="#">major</a>	integer	Major version number.
<a href="#">minor</a>	integer	Minor version number.
<a href="#">patch</a>	integer	Patch level.
<a href="#">date_stamp</a>	integer	Date stamp of ELSI (yyyymmdd).
<a href="#">n_illcond</a>	integer	Number of eigenvalues of the overlap matrix that are smaller than the ill-conditioning tolerance. See 3.5.1.
<a href="#">ev_min</a>	real double	Lowest eigenvalue of the overlap matrix. See remark 1.
<a href="#">ev_max</a>	real double	Highest eigenvalue of the overlap matrix. See remark 1.
<a href="#">mu</a>	real double	Chemical potential. See remark 2.
<a href="#">ts</a>	real double	Entropy. See remark 2.
<a href="#">edm_real</a>	real double, rank-2 array	Real energy-weighted density matrix in 2D block-cyclic dense format. See remark 3.
<a href="#">edm_complex</a>	complex double, rank-2 array	Complex energy-weighted density matrix in 2D block-cyclic dense format. See remark 3.
<a href="#">edm_real_sparse</a>	real double, rank-1 array	Non-zero values of the real density matrix in 1D block CSC format. See remark 3.
<a href="#">edm_complex_sparse</a>	complex double, rank-1 array	Non-zero values of the complex density matrix in 1D block CSC format. See remark 3.
<a href="#">n_sing</a>	integer	Deprecated. Use <a href="#">elsi_get_n_illcond</a> instead.

## Remarks

1) In ELSI, ill-conditioning check of the overlap matrix is enabled by default when ELPA is the chosen solver. It may be disabled by calling [elsi\\_set\\_illcond\\_check](#), and is automatically disabled when the chosen solver is not ELPA. [ev\\_min](#) and [ev\\_max](#) are computed only if ill-conditioning check is enabled. Otherwise the return value may be zero.

2) In ELSI, the chemical potential will only be available if one of the density matrix solver interfaces has been called, with ELPA, PEXSI, or NTPoly 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.

3) 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. These subroutines 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
<a href="#">pexsi_mu_min</a>	real double	Minimum value of mu. See remark 1.
<a href="#">pexsi_mu_max</a>	real double	Maximum value of mu. See remark 1.

## Remarks

1) Please refer to the 5<sup>th</sup> remark in 3.5.4 for the chemical potential determination algorithm in PEXSI and ELSI.

### 3.6.3 Extrapolation of Wavefunctions and Density Matrices

In a single point total energy calculation, a simple way to construct an initial guess of the electron density is using the superposition of free atom densities. In geometry calculations, the initial guess in the  $(n+1)^{\text{th}}$  geometry step can be made better than free atom superposition, by reusing the wavefunctions or density matrix calculated in the  $n^{\text{th}}$  geometry step. However, due to the movement of atoms and localized basis functions around them, wavefunctions obtained in the  $n^{\text{th}}$  geometry step are no longer orthonormalized in the  $(n+1)^{\text{th}}$  geometry step. Similarly, density matrix from the  $n^{\text{th}}$  geometry step does not satisfy the conditions in Eq. 1.20 with respect to the new overlap matrix.

The following subroutines orthonormalize eigenvectors (coefficients of wavefunctions) in the  $n^{\text{th}}$  geometry step with respect to the overlap matrix in the  $(n+1)^{\text{th}}$  geometry step with a Gram-Schmidt algorithm.

`elsi_orthonormalize_ev_real(handle, ovlp, evvec)`

Argument	Data Type	in/out	Explanation
<code>handle</code>	<code>type(elsi_handle)</code>	inout	Handle to ELSI.
<code>ovlp</code>	real double, rank-2 array	in	Real overlap matrix in 2D block-cyclic dense format.
<code>evvec</code>	real double, rank-2 array	inout	Real eigenvectors in 2D block-cyclic dense format.

`elsi_orthonormalize_ev_complex(handle, ovlp, evvec)`

Argument	Data Type	in/out	Explanation
<code>handle</code>	<code>type(elsi_handle)</code>	inout	Handle to ELSI.
<code>ovlp</code>	complex double, rank-2 array	in	Complex overlap matrix in 2D block-cyclic dense format.
<code>evvec</code>	complex double, rank-2 array	inout	Complex eigenvectors in 2D block-cyclic dense format.

`elsi_orthonormalize_ev_real_sparse(handle, ovlp, evvec)`

Argument	Data Type	in/out	Explanation
<code>handle</code>	<code>type(elsi_handle)</code>	inout	Handle to ELSI.
<code>ovlp</code>	real double, rank-1 array	in	Real overlap matrix in 1D block CSC, 1D block-cyclic CSC, or generic COO sparse format.
<code>evvec</code>	real double, rank-2 array	inout	Real eigenvectors in 2D block-cyclic dense format. See remark 1.

`elsi_orthonormalize_ev_complex_sparse(handle, ovlp, evvec)`

Argument	Data Type	in/out	Explanation
<code>handle</code>	<code>type(elsi_handle)</code>	inout	Handle to ELSI.
<code>ovlp</code>	complex double, rank-1 array	in	Complex overlap matrix in 1D block CSC, 1D block-cyclic CSC, or generic COO sparse format.
<code>evvec</code>	complex double, rank-2 array	inout	Complex eigenvectors in 2D block-cyclic dense format. See remark 1.

#### Remarks

1) When using `elsi_orthonormalize_ev_real_sparse` and `elsi_orthonormalize_ev_complex_sparse`, the eigenvectors are stored in a dense format (`BLACS_DENSE`), as they are in general not sparse.

The following subroutines extrapolate density matrix in the  $n^{\text{th}}$  geometry step to satisfy conditions 1.20 with respect to the overlap matrix in the  $(n+1)^{\text{th}}$  geometry step.



`elsi_extrapolate_dm_real(handle, ovlp, dm)`

Argument	Data Type	in/out	Explanation
<a href="#">handle</a>	<code>type(elsi_handle)</code>	inout	Handle to ELSI.
<a href="#">ovlp</a>	real double, rank-2 array	inout	Real overlap matrix in 2D block-cyclic dense format. See remark 1.
<a href="#">dm</a>	real double, rank-2 array	inout	Real density matrix in 2D block-cyclic dense format. See remark 2.

`elsi_extrapolate_dm_complex(handle, ovlp, dm)`

Argument	Data Type	in/out	Explanation
<a href="#">handle</a>	<code>type(elsi_handle)</code>	inout	Handle to ELSI.
<a href="#">ovlp</a>	complex double, rank-2 array	inout	Complex overlap matrix in 2D block-cyclic dense format. See remark 1.
<a href="#">dm</a>	complex double, rank-2 array	inout	Complex density matrix in 2D block-cyclic dense format. See remark 2.

`elsi_extrapolate_dm_real_sparse(handle, ovlp, dm)`

Argument	Data Type	in/out	Explanation
<a href="#">handle</a>	<code>type(elsi_handle)</code>	inout	Handle to ELSI.
<a href="#">ovlp</a>	real double, rank-1 array	inout	Real overlap matrix in 1D block CSC, 1D block-cyclic CSC, or generic COO sparse format. See remark 1.
<a href="#">dm</a>	real double, rank-1 array	out	Real density matrix in 1D block CSC, 1D block-cyclic CSC, or generic COO sparse format. See remark 3.

`elsi_extrapolate_dm_complex_sparse(handle, ovlp, dm)`

Argument	Data Type	in/out	Explanation
<a href="#">handle</a>	<code>type(elsi_handle)</code>	inout	Handle to ELSI.
<a href="#">ovlp</a>	complex double, rank-1 array	inout	Complex overlap matrix in 1D block CSC, 1D block-cyclic CSC, or generic COO sparse format. See remark 1.
<a href="#">dm</a>	complex double, rank-1 array	out	Complex density matrix in 1D block CSC, 1D block-cyclic CSC, or generic COO sparse format. See remark 3.

## Remarks

- 1) [ovlp](#): This should be the overlap matrix in the  $(n+1)^{\text{th}}$  geometry step. [elsi\\_set\\_save\\_ovlp](#) must have been called to store the overlap matrix in the  $n^{\text{th}}$  geometry step internally. If ELPA is the chosen solver, [ovlp](#) will be overridden with its Cholesky factorization, which will be reused by subsequent calls to the solver interfaces.
- 2) [dm](#): Input should be the density matrix in the  $n^{\text{th}}$  geometry step. Output is the extrapolated density matrix.
- 3) [dm](#): With the sparse density matrix extrapolation interface, the density matrix in the  $n^{\text{th}}$  geometry step is stored internally. Output is the extrapolated density matrix.

## 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 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 data structure in ELSI is simply arrays that represent matrices, with a few integers to define the dimension of the matrices. In order to circumvent the



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  $N_{\text{procs}}$  separate files, where  $N_{\text{procs}}$  is the number of MPI tasks, is not promising due to the difficulty of managing and post-processing a large number of files. 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 being read 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
<code>handle</code>	<code>type(elsi_rw_handle)</code>	out	Handle to matrix I/O instance.
<code>task</code>	integer	in	Matrix I/O task to perform. Accepted values are: 0 (READ_MATRIX) and 1(WRITE_MATRIX).
<code>parallel_mode</code>	integer	in	Parallelization mode. The only accepted value is 1 (MULTIPROC) for now.
<code>n_electron</code>	real double	in	Number of electrons. See remark 1.
<code>n_basis</code>	integer	in	Number of basis functions, i.e. global size of matrix.

#### Remarks

1) `n_electron`: Matrices written out with ELSI matrix I/O are usually from actual electronic structure calculations. Having 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
<code>handle</code>	<code>type(elsi_rw_handle)</code>	inout	Handle to matrix I/O instance.
<code>mpi_comm</code>	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
<a href="#">handle</a>	type(elsi_rw_handle)	inout	Handle to matrix I/O instance.
<a href="#">blacs_ctxt</a>	integer	in	BLACS context.
<a href="#">block_size</a>	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
<a href="#">handle</a>	type(elsi_rw_handle)	inout	Handle to matrix I/O instance.
<a href="#">global_nnz</a>	integer	in	Global number of non-zeros.
<a href="#">local_nnz</a>	integer	in	Local number of non-zeros.
<a href="#">local_col</a>	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
<a href="#">handle</a>	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
<a href="#">handle</a>	type(elsi_rw_handle)	in	Handle to matrix I/O instance.
<a href="#">filename</a>	string	in	Name of file to write.
<a href="#">mat</a>	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
<a href="#">handle</a>	type(elsi_rw_handle)	in	Handle to matrix I/O instance.
<a href="#">filename</a>	string	in	Name of file to write.
<a href="#">mat</a>	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
<a href="#">handle</a>	type(elsi_rw_handle)	in	Handle to matrix I/O instance.
<a href="#">filename</a>	string	in	Name of file to write.
<a href="#">row_idx</a>	integer, rank-1 array	in	Local row index array.
<a href="#">col_ptr</a>	integer, rank-1 array	in	Local column pointer array.
<a href="#">mat</a>	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
<a href="#">handle</a>	type(elsi_rw_handle)	in	Handle to matrix I/O instance.
<a href="#">filename</a>	string	in	Name of file to write.
<a href="#">row_idx</a>	integer, rank-1 array	in	Local row index array.
<a href="#">col_ptr</a>	integer, rank-1 array	in	Local column pointer array.
<a href="#">mat</a>	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
<a href="#">handle</a>	type(elsi_rw_handle)	inout	Handle to matrix I/O instance.
<a href="#">zero_def</a>	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
<a href="#">handle</a>	type(elsi_rw_handle)	inout	Handle to matrix I/O instance.
<a href="#">header</a>	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
<a href="#">handle</a>	type(elsi_rw_handle)	inout	Handle to matrix I/O instance.
<a href="#">filename</a>	string	in	Name of file to read.
<a href="#">n_electron</a>	real double	out	Number of electrons.
<a href="#">n_basis</a>	integer	out	Number of basis functions, i.e. global size of matrix.
<a href="#">local_row</a>	integer	out	Local number of matrix rows.
<a href="#">local_col</a>	integer	out	Local number of matrix columns.

[elsi\\_read\\_mat\\_real](#)(handle, filename, mat)

Argument	Data Type	in/out	Explanation
<a href="#">handle</a>	type(elsi_rw_handle)	inout	Handle to matrix I/O instance.
<a href="#">filename</a>	string	in	Name of file to read.
<a href="#">mat</a>	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
<a href="#">handle</a>	type(elsi_rw_handle)	inout	Handle to matrix I/O instance.
<a href="#">filename</a>	string	in	Name of file to read.
<a href="#">mat</a>	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
<a href="#">handle</a>	type(elsi_rw_handle)	inout	Handle to matrix I/O instance.
<a href="#">filename</a>	string	in	Name of file to read.
<a href="#">n_electron</a>	real double	out	Number of electrons.
<a href="#">n_basis</a>	integer	out	Number of basis functions, i.e. global size of matrix.
<a href="#">global_nnz</a>	integer	out	Global number of non-zeros.
<a href="#">local_nnz</a>	integer	out	Local number of non-zeros.
<a href="#">local_col</a>	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
<a href="#">handle</a>	type(elsi_rw_handle)	inout	Handle to matrix I/O instance.
<a href="#">filename</a>	string	in	Name of file to read.
<a href="#">row_idx</a>	integer, rank-1 array	out	Local row index array.
<a href="#">col_ptr</a>	integer, rank-1 array	out	Local column pointer array.
<a href="#">mat</a>	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
<a href="#">handle</a>	type(elsi_rw_handle)	inout	Handle to matrix I/O instance.
<a href="#">filename</a>	string	in	Name of file to read.
<a href="#">row_idx</a>	integer, rank-1 array	out	Local row index array.
<a href="#">col_ptr</a>	integer, rank-1 array	out	Local column pointer array.
<a href="#">mat</a>	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
<a href="#">handle</a>	type(elsi_rw_handle)	inout	Handle to matrix I/O instance.
<a href="#">header</a>	integer, rank-1 array	out	An array of eight integers.

## 3.8 Example Pseudo-Code

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

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

```
SCF initialize

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

do SCF cycle
  Update Hamiltonian

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

  Update electron density
  Check SCF convergence
end do

call elsi_finalize(eh)
```

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

```
SCF initialize

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

do SCF cycle
  Update Hamiltonian

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

  Update electron density
  Check SCF convergence
end do

call elsi_finalize(eh)
```

#### Remarks

- 1) Eigenvectors are returned in the `BLACS_DENSE` format, which is required to be properly set up.

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

### SCF initialize

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

do SCF cycle
  Update Hamiltonian

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

  Update electron density
  Check SCF convergence
end do

call elsi_finalize(eh)
```

### Remarks

- 1) Eigenvectors are returned in the [BLACS\\_DENSE](#) format, which is required to be properly set up.

## Arbitrarily Distributed COO Sparse Matrix + ELSI Eigensolver Interface

### SCF initialize

```
call elsi_init (eh, ELPA, MULTI_PROC, GENERIC_COO, n_basis, n_electron, n_state)
call elsi_set_mpi (eh, mpi_comm)
call elsi_set_blacs (eh, blacs_ctxt, block_size)
call elsi_set_coo (eh, global_nnz, local_nnz, row_idx, col_idx)

do SCF cycle
  Update Hamiltonian

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

  Update electron density
  Check SCF convergence
end do

call elsi_finalize(eh)
```

### Remarks

- 1) Eigenvectors are returned in the [BLACS\\_DENSE](#) format, which is required to be properly set up.

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

```
SCF initialize

call elsi_init (eh, OMM, MULTI_PROC, BLACS_DENSE, n_basis, n_electron, n_state)
call elsi_set_mpi (eh, mpi_comm)
call elsi_set_blacs (eh, blacs_ctxt, block_size)

do SCF cycle
  Update Hamiltonian

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

  Update electron density
  Check SCF convergence
end do

call elsi_finalize(eh)
```

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

```
SCF initialize

call elsi_init (eh, PEXSI, MULTI_PROC, PEXSI_CSC, n_basis, n_electron, n_state)
call elsi_set_mpi (eh, mpi_comm)
call elsi_set_csc (eh, global_nnz, local_nnz, local_col, row_idx, col_ptr)

do SCF cycle
  Update Hamiltonian

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

  Update electron density
  Check SCF convergence
end do

call elsi_finalize(eh)
```

### Remarks

- 1) Refer to the 5<sup>th</sup> remark in 3.5.4 for the chemical potential determination algorithm in PEXSI.

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

### SCF initialize

```
call elsi_init (eh, PEXSI, MULTI_PROC, SIESTA_CSC, n_basis, n_electron, n_state)
call elsi_set_mpi (eh, mpi_comm)
call elsi_set_csc (eh, global_nnz, local_nnz, local_col, row_idx, col_ptr)
call elsi_set_csc_blk (eh, block_size)

do SCF cycle
  Update Hamiltonian

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

  Update electron density
  Check SCF convergence
end do

call elsi_finalize(eh)
```

### Remarks

- 1) Refer to the 5<sup>th</sup> remark in 3.5.4 for the chemical potential determination algorithm in PEXSI.

## Arbitrarily Distributed COO Sparse Matrix + ELSI Density Matrix Interface

### SCF initialize

```
call elsi_init (eh, PEXSI, MULTI_PROC, GENERIC_COO, n_basis, n_electron, n_state)
call elsi_set_mpi (eh, mpi_comm)
call elsi_set_coo (eh, global_nnz, local_nnz, row_idx, col_idx)

do SCF cycle
  Update Hamiltonian

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

  Update electron density
  Check SCF convergence
end do

call elsi_finalize(eh)
```

### Remarks

- 1) Refer to the 5<sup>th</sup> remark in 3.5.4 for the chemical potential determination algorithm in PEXSI.



## Multiple $k$ -points Calculations

### SCF initialize

```
call elsi_init (eh, NTPOLY, MULTI_PROC, BLACS_DENSE, n_basis, n_electron, n_state)
call elsi_set_mpi (eh, mpi_comm)
call elsi_set_blacs (eh, blacs_ctxt, block_size)
call elsi_set_kpoint (eh, n_kpt, i_kpt, i_wt)
call elsi_set_mpi_global (eh, mpi_comm_global)

do SCF cycle
  Update Hamiltonian

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

  Update electron density
  Check SCF convergence
end do

call elsi_finalize(eh)
```

### Remarks

- 1) When there are multiple  $k$ -points, 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  $k$ -points. The returned band structure energy, however, is already summed over all  $k$ -points with respect to the weight of each  $k$ -point. Refer to 3.2.4 for more information.
- 3) Spin-polarized calculations may be set up similarly.

## Geometry Relaxation Calculations

### SCF initialize

```
call elsi_init (eh, ...)
call elsi_set_* (eh, ...)

do geometry
  do SCF cycle
    Update Hamiltonian

    call elsi_{ev|dm}_{real|complex} (eh, ham, ovlp, ...)

    Update electron density
    Check SCF convergence
  end do

  Update geometry (overlap)

  call elsi_reinit (eh)
end do

call elsi_finalize(eh)
```

## 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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