

Lis 1.2.5 User's Manual

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0 Additions and changes from Lis 1.1

0.1 Additions

1. Added support of eigensolvers for real matrices

0.2 Changes

1. Changed some specifications
 - (a) Changed the names of `lis_output_residual_history()` and `lis_get_residual_history()` to `lis_solver_output_rhistory()` and `lis_solver_get_rhistory()`, respectively.

1 Introduction

Library of Iterative Solvers for Linear Systems (Lis) is a numerical library written in C and Fortran for solving the linear equation

$$Ax = b$$

or the eigenvalue problem

$$Ax = \lambda x$$

using iterative methods. Installation of Lis requires a computing environment in which a C compiler can be used. Fortran interface requires a compiler that supports FORTRAN 77. AMG preconditioner requires a compiler that supports Fortran 90. For parallel computing environments, OpenMP or MPI-1 is used.

Lis has the following features:

- 22 linear equation solvers, 7 eigensolvers, and 10 preconditioners can be combined
- 11 sparse matrix storage formats are supported
- Both the sequential and the parallel codes are supported by a common interface
- Both the double precision and the quadruple precision operations are supported by a common interface

The solvers supported here are listed in Table 1 and 2, respectively, and the preconditioners are listed in Table 3. Eleven types of data storage formats, including CRS, are used, as shown in Table 4.

Table 1: Linear Equation Solvers

| | |
|--------------|--------------|
| CG | CR |
| BiCG | BiCR[2] |
| CGS | CRS[3] |
| BiCGSTAB | BiCRSTAB[3] |
| GPBiCG | GPBiCR[3] |
| BiCGSafe[1] | BiCRSafe[4] |
| BiCGSTAB(1) | TFQMR |
| Jacobi | Orthomin(m) |
| Gauss-Seidel | GMRES(m) |
| SOR | FGMRES(m)[5] |
| IDR(s)[13] | MINRES[14] |

Table 2: Eigensolvers

| |
|-------------------------------|
| Power Iteration |
| Inverse Iteration |
| Approximate Inverse Iteration |
| Conjugate Gradient[19, 20] |
| Lanczos Iteration |
| Subspace Iteration |
| Conjugate Residual [21] |

Table 3: Preconditioners

| |
|------------------|
| Jacobi |
| SSOR |
| ILU(k) |
| ILUT[6, 7] |
| Crout ILU[8, 7] |
| I+S[9] |
| SA-AMG[10] |
| hybrid[11] |
| SAINV[12] |
| additive Schwarz |
| User defined |

Table 4: Matrix Storage Formats

| | |
|-------------------------------------|-------|
| Compressed Row Storage | (CRS) |
| Compressed Column Storage | (CCS) |
| Modified Compressed Sparse Row | (MSR) |
| Diagonal | (DIA) |
| Ellpack-Itpack generalized diagonal | (ELL) |
| Jagged Diagonal | (JDS) |
| Block Sparse Row | (BSR) |
| Block Sparse Column | (BSC) |
| Variable Block Row | (VBR) |
| Dense | (DNS) |
| Coordinate | (COO) |

2 Installation

This section describes the instructions for installing and testing Lis. We assume Lis being installed on a Linux cluster.

2.1 Required Systems

Installation of Lis requires a computing environment in which a C compiler can be used. The AMG preconditioner requires a compiler that supports Fortran 90. In parallel computing environments, OpenMP or MPI-1 is used. Lis has been verified to run in the environments shown in Table 5.

Table 5: Major Tested Platforms

| C Compiler (Required) | OS |
|---|------------------|
| Intel C/C++ Compiler 7.0, 8.0, 9.0, 9.1, 10.1 | Linux |
| IBM XL C/C++ V7.0 | Linux AIX 5.3 |
| Sun WorkShop 6 update 2, Sun ONE Studio 7 | Solaris 9 |
| Sun Studio 11, Sun Studio 12 | Solaris 10 |
| PGI 6.0, 7.1 | Linux |
| GCC 3.3, 4.1 | Linux |
| Fortran Compiler (Option) | OS |
| Intel Fortran Compiler 8.1, 9.0, 9.1, 10.1 | Linux |
| IBM XL Fortran V9.1 | Linux AIX 5.3 |
| Sun WorkShop 6 update 2, Sun ONE Studio 7 | Solaris 9 |
| Sun Studio 11, Sun Studio 12 | Solaris 10 |
| PGI 6.0, 7.1 | Linux |
| g77 3.3 | Linux |
| gfortran 4.3 | |
| g95 0.91 | |

2.2 Decompressing the Files

Enter the following command to decompress the files: (`$VERSION`) represents the version.

```
>gunzip -c lis-($VERSION).tar.gz | tar xvf -
```

This command creates the `lis-($VERSION)` directory along with its subfolders, as shown in Figure 1.

```
lis-($VERSION)
+ config
|  Configure files
+ include
|  Include files
+ src
|  Source files
+ test
  Test programs
```

Figure 1: Files contained in `lis-($VERSION).tar.gz`

2.3 Running configure script

Enter the following command to run the script:

- default settings: `>./configure`
- specifying the installation destination: `>./configure --prefix=<install-dir>`

Table 6 shows the option that can be specified for configuration. Table 7 shows the computer environment that can be specified by `TARGET`.

Table 6: Configuration Options

| | |
|--|---|
| <code>--enable-omp</code> | Use OpenMP |
| <code>--enable-mpi</code> | Use MPI |
| <code>--enable-fortran</code> | Use Fortran API |
| <code>--enable-saamg</code> | Use SA-AMG preconditioner |
| <code>--enable-quad</code> | Use quadruple precision operation |
| <code>--prefix=<install-dir></code> | Name of the installation target directory |
| <code>TARGET=<target></code> | Computing environments |
| <code>CC=<c_compiler></code> | C compiler |
| <code>CFLAGS=<c_flags></code> | Compilation options for C compilers |
| <code>FC=<fortran90_compiler></code> | Fortran 90 compiler |
| <code>FCFLAGS=<fc_flags></code> | Compilation options for the Fortran 90 compiler |
| <code>LDFLAGS=<ld_flags></code> | Link options |

2.4 Running make

In the `lis-($VERSION)` directory, run `make` by entering

```
>make
```

compilation is then performed.

2.5 Testing

Here, ensure that `make` (library compilation) has been successfully run.

To do so, in the `lis-($VERSION)` directory, enter the following:

```
>make check
```

This command performs a test using the executable files created in the `lis-($VERSION)/test` directory. The test reads matrix and vector data from the MatrixMarket file `lis-($VERSION)/test/testmat.mtx` and writes the approximate solution of the linear equation $Ax = b$ obtained with the BiCG method into `lis-($VERSION)/test/sol.txt`, and the residual history into `lis-($VERSION)/test/res.txt`. If all approximate solutions are 1, then the result is correct. The result on SGI Altix 3700 is shown below. The last two digits shown vary depending on the environment.

Table 7: Major TARGET options

| <target> | Configure scripts |
|---------------|---|
| cray_xt3 | ./configure CC=cc FC=ftn CFLAGS="-O3 -B -fastsse -tp k8-64" FCFLAGS="-O3 -fastsse -tp k8-64 -Mpreprocess" FCLDFLAGS="-Mnomain" ac_cv_sizeof_void_p=8 cross_compiling=yes --enable-mpi ax_f77_mangling="lower case, no underscore, extra underscore" |
| fujitsu_pq | ./configure CC=fcc FC=f90 ac_cv_sizeof_void_p=8 CFLAGS="-O3 -Kfast,ocl,preex" FFLAGS="-O3 -Kfast,ocl,preex -Cpp" FCFLAGS="-O3 -Kfast,ocl,preex -Cpp -Am" ax_f77_mangling="lower case, underscore, no extra underscore" |
| hitachi | ./configure CC=cc FC=f90 FCLDFLAGS="-lf90s" ac_cv_sizeof_void_p=8 CFLAGS="-Os -noprogram" FCFLAGS="-Oss -noprogram" ax_f77_mangling="lower case, underscore, no extra underscore" |
| ibm_bg1 | ./configure CC=blrts_xlc FC=blrts_xlf90 CFLAGS="-O3 -qarch=440d -qtune=440 -qstrict -I/bg1/BlueLight/ppcfloor/bglsys/include" FFLAGS="-O3 -qarch=440d -qtune=440 -qsuffix=cpp=F -qfixed=72 -w -I/bg1/BlueLight/ppcfloor/bglsys/include" FCFLAGS="-O3 -qarch=440d -qtune=440 -qsuffix=cpp=F90 -w -I/bg1/BlueLight/ppcfloor/bglsys/include" ac_cv_sizeof_void_p=4 cross_compiling=yes --enable-mpi ax_f77_mangling="lower case, no underscore, no extra underscore" |
| nec_es | ./configure CC=esmpic++ FC=esmpif90 AR=esar RANLIB=true ac_cv_sizeof_void_p=8 ax_vector_machine=yes cross_compiling=yes --enable-mpi --enable-omp ax_f77_mangling="lower case, no underscore, extra underscore" |
| nec_sx9_cross | ./configure CC=sxmpic++ FC=sxmpif90 AR=sxar RANLIB=true ac_cv_sizeof_void_p=8 ax_vector_machine=yes cross_compiling=yes ax_f77_mangling="lower case, no underscore, extra underscore" |

```

default
100 x 100 matrix  460 entries
Initial vector x = 0
PRECISION : DOUBLE
SOLVER    : BiCG 2
PRECON    : None
STORAGE   : CRS
lis_solve is normal end

BiCG: iter      = 15 iter_double = 15 iter_quad = 0
BiCG: times     = 5.178690e-03
BiCG: p_times   = 1.277685e-03 (p_c = 1.254797e-03 p_i = 2.288818e-05 )
BiCG: i_times   = 3.901005e-03
BiCG: Residual  = 6.327297e-15

```

```

--enable-omp
Max Procs   = 32
Max Threads = 2
100 x 100 matrix  460 entries
Initial vector x = 0
PRECISION : DOUBLE
SOLVER    : BiCG 2
PRECON    : None
STORAGE   : CRS
lis_solve is normal end

BiCG: iter      = 15 iter_double = 15 iter_quad = 0
BiCG: times     = 8.960009e-03
BiCG: p_times   = 2.297878e-03 (p_c = 2.072096e-03 p_i = 2.257824e-04 )
BiCG: i_times   = 6.662130e-03
BiCG: Residual  = 6.221213e-15

```

```

--enable-mpi
100 x 100 matrix  460 entries
Initial vector x = 0
PRECISION : DOUBLE
SOLVER    : BiCG 2
PRECON    : None
STORAGE   : CRS
lis_solve is normal end

BiCG: iter      = 15 iter_double = 15 iter_quad = 0
BiCG: times     = 2.911400e-03
BiCG: p_times   = 1.560780e-04 (p_c = 1.459997e-04 p_i = 1.007831e-05 )
BiCG: i_times   = 2.755322e-03
BiCG: Residual  = 6.221213e-15

```

2.6 Installation

In the `lis-($VERSION)` directory, enter the following:

```
>make install
```

This copies files as follows:

```
$(INSTALLDIR)
+include
|   +lis.h lisf.h
+lib
    +liblis.a
```

lis.h and lisf.h are the header files required when the library is used for C and Fortran, respectively.
liblis.a is a library file.

2.7 Test Programs

2.7.1 test1

In the `lis-($VERSION)/test` directory, enter the following:

```
>test1 matrix_filename rhs_setting solution_filename residual_filename [options]
```

This command reads matrix data from the matrix data file shown by `matrix_filename` and solves the linear equation $Ax = b$ with the solver specified by `options`. In addition, this command writes the approximate solution into `matrix_filename` and the residual history into `residual_filename`. The allowable matrix data format is MatrixMarket. The following value can be used for `rhs_setting`:

| | |
|---------------------------|--|
| 0 | use the right-hand side vector b , including the matrix file |
| 1 | use $b = (1, \dots, 1)^T$ |
| 2 | use $b = A \times (1, \dots, 1)^T$ |
| <code>rhs_filename</code> | right-hand side vector filename |

The supported file formats of `rhs_filename` are PLAIN format or MM format.

`test1f.f` is Fortran version of `test1.c`.

2.7.2 test2

In the `lis-($VERSION)/test` directory, enter the following:

```
>test2 m n matrix_type solution_filename residual_filename [options]
```

This command solves the linear equation $Ax = b$, which has a matrix, as the coefficient matrix, into which the Poisson equation has been dispersed at the five-point central difference using the matrix storage format specified by `matrix_type` and the solver specified by `options`. In addition, this command writes the approximate solution into `solution_filename` and the residual history into `residual_filename`. Note that the right-hand side vector is set such that all values for the solution vectors of the linear equation $Ax = b$ will be 1. The values `m` and `n` represent the numbers of lattice points in the vertical and horizontal directions, respectively.

2.7.3 test3

This is a program for solving the linear equation $Ax = b$ with a specified solver and a preconditioner to provide an approximate solution, where matrix A is a tridiagonal matrix of 12×12 .

$$A = \begin{pmatrix} 2 & 1 & & & \\ 1 & 2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & 2 & 1 \\ & & & 1 & 2 \end{pmatrix}$$

The right-hand side vector b is solved so that approximate solution x will be always 1.

`test3f.f` is Fortran version of `test3.c`.

2.7.4 test4

In the `lis-($VERSION)/test` directory, enter the following:

```
>test4 n gamma [options]
```

This command solves the linear equation $Ax = b$, where

$$A = \begin{pmatrix} 2 & 1 & & & \\ 0 & 2 & 1 & & \\ \gamma & 0 & 2 & 1 & \\ & \ddots & \ddots & \ddots & \ddots \\ & & \gamma & 0 & 2 & 1 \\ & & & \gamma & 0 & 2 \end{pmatrix}$$

and the solver specified by `options`. Note that the right-hand vector is set such that all values for the solution vectors of the linear equation $Ax = b$ will be 1. The value `n` is the dimension of matrix A . The value `gamma` is γ .

2.7.5 etest1

In the `lis-($VERSION)/test` directory, enter the following:

```
>etest1 matrix_filename solution_filename residual_filename [options]
```

This command reads matrix data from the matrix data file shown by `matrix_filename` and solves the eigenvalue problem $Ax = \lambda x$ with the solver specified by `options`. In addition, this command writes the extreme eigenvector into `solution_filename` and the residual history into `residual_filename`. The allowable matrix data format is MatrixMarket.

`etest1f.f` is Fortran version of `etest1.c`.

2.7.6 etest2

In the `lis-($VERSION)/test` directory, enter the following:

```
>etest2 m n matrix_type solution_filename residual_filename [options]
```

This command solves the eigenvalue problem $Ax = \lambda x$, which has a matrix, into which the Poisson equation has been dispersed at the five-point central difference using the matrix storage format specified by `matrix_type` and the solver specified by `options`. In addition, this command writes the extreme eigenvector into `solution_filename` and the residual history into `residual_filename`. The values `m` and `n` represent the numbers of lattice points in the vertical and horizontal directions, respectively.

2.7.7 etest3

This is a program for solving the eigenvalue problem $Ax = \lambda x$ with a specified solver to provide an approximate solution, where matrix A is a tridiagonal matrix of 12×12 .

$$A = \begin{pmatrix} 2 & 1 & & & \\ 1 & 2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & 2 & 1 \\ & & & 1 & 2 \end{pmatrix}$$

`etest3f.f` is Fortran version of `etest3.c`.

2.7.8 etest4

In the `lis-($VERSION)/test` directory, enter the following:

```
>etest4 matrix_filename tol [options]
```

This command reads matrix data from the matrix data file shown by `matrix_filename` and compute condition number with convergence criterion `tol`.

2.8 Restrictions

The current version has the following restrictions:

- Restrictions for the preconditioners
 - When a preconditioner other than the Jacobi or SSOR preconditioner is selected and matrix A is not in the CRS format, it is created in the CRS format at the time of preconditioning.
- Restrictions for quadruple precision operations
 - Jacobi, Gauss-Seidel, SOR, and IDR(s) methods are unsupported,
 - Eigensolvers are unsupported.
 - Jacobi, Gauss-Seidel and SOR are unsupported in hybrid preconditioner,
 - I+S and SA-AMG preconditioners are unsupported.
- Restrictions for the matrix storage formats
 - In the MPI environment, when the user prepares a necessary array for a target storage format, only CRS is accepted.

3 Basic Operations

This section describes how to use the library. Writing programs to solve the linear equation

$$Ax = b$$

or the eigenvalue problem

$$Ax = \lambda x$$

requires the following:

- Initialization
- Matrix creation
- Vector creation
- Solver creation
- Value assignment for matrix and vector
- Solver assignment for linear equation or eigenvalue problem
- Solve
- Finalization

In addition, each program must include the following `include` statement:

- C `#include "lis.h"`
- Fortran `#include "lisf.h"`

When Lis is installed in `$(INSTALLDIR)`, `lis.h` and `lisf.h` are located in `$(INSTALLDIR)/include`.

3.1 Initialization and Finalization

The initialization and finalization must be written as follows: The initialization must be executed at the beginning of the program, and the finalization must be executed at the end of the program.

```
C
1: #include "lis.h"
2: int main(int argc, char* argv[])
3: {
4:     lis_initialize(&argc, &argv);
5:     ...
6:     lis_finalize();
7: }
```

```
Fortran
1: #include "lisf.h"
2:     call lis_initialize(ierr)
3:     ...
4:     call lis_finalize(ierr)
```

Initialization

To perform initialization, the following functions are used:

- C `lis_initialize(int* argc, char** argv())`
- Fortran subroutine `lis_initialize(integer ierr)`

This function performs initialization of MPI, and specifies options through the command line.

Finalization

To perform finalization, the following functions are used:

- C `int lis_finalize()`
- Fortran subroutine `lis_finalize(integer ierr)`

3.2 Vector

Assume that the order of vector v is `global_n` and that the number of rows of each partial vector when the row block of vector v has been divided with `nprocs` units of the processor is `local_n`. If `global_n` can be divided into an integer answer, then `local_n = global_n / nprocs`. For example, when the row block of vector v is divided with two processors, as shown by Equation (3.1), `global_n` and `local_n` are 4 and 2, respectively.

$$v = \begin{pmatrix} 0 \\ 1 \\ 2 \\ 3 \end{pmatrix} \begin{matrix} \text{PE0} \\ \text{PE1} \end{matrix} \quad (3.1)$$

In the case of creating vector v in Equation (3.1), Sequential and OpenMP versions create vector v itself, while MPI version creates, at each processor, a partial vector into which the row block is divided with a given number of processors.

Programs to create vector v are as follows, where the number of processors for MPI version is assumed to be two:

C(Sequential, OpenMP)

```
1: int          i,n;
2: LIS_VECTOR    v;
3: n = 4;
4: lis_vector_create(0,&v);
5: lis_vector_set_size(v,0,n); /* or lis_vector_set_size(v,n,0); */
6:
7: for(i=0;i<n;i++)
8: {
9:     lis_vector_set_value(LIS_INS_VALUE,i,(double)i,v);
10: }
```

C(MPI)

```
1: int          i,n,is,ie;                /*or int  i,ln,is,ie;                */
2: LIS_VECTOR    v;
3: n = 4;                                  /*  ln = 2;                */
4: lis_vector_create(MPI_COMM_WORLD,&v);
5: lis_vector_set_size(v,0,n);             /*  lis_vector_set_size(v,ln,0); */
6: lis_vector_get_range(v,&is,&ie);
7: for(i=is;i<ie;i++)
8: {
9:     lis_vector_set_value(LIS_INS_VALUE,i,(double)i,v);
10: }
```

Fortran(Sequential, OpenMP)

```
1: integer      i,n
2: LIS_VECTOR    v
3: n = 4
4: call lis_vector_create(0,v,ierr)
5: call lis_vector_set_size(v,0,n,ierr)
6:
7: do i=1,n
9:     call lis_vector_set_value(LIS_INS_VALUE,i,DBLE(i),v,ierr)
10: enddo
```

Fortran(MPI)

```
1: integer      i,n,is,ie
2: LIS_VECTOR    v
3: n = 4
4: call lis_vector_create(MPI_COMM_WORLD,v,ierr)
5: call lis_vector_set_size(v,0,n,ierr)
6: call lis_vector_get_range(v,is,ie,ierr)
7: do i=is,ie-1
8:     call lis_vector_set_value(LIS_INS_VALUE,i,DBLE(i),v,ierr);
9: enddo
```

Declaring variables

As the second line shows, the declaration is stated as follows:

```
LIS_VECTOR    v;
```

Creating vectors

To create a vector *v*, the following functions are used:

- C `int lis_vector_create(LIS_Comm comm, LIS_VECTOR *vec)`
- Fortran subroutine `lis_vector_create(LIS_Comm comm, LIS_VECTOR vec, integer ierr)`

For the example program above, `comm` must be replaced with the MPI communicator. For Sequential and OpenMP versions, the value for `comm` is ignored.

Assigning vector size

To assign the size of a vector *v*, the following functions are used:

- C `int lis_vector_set_size(LIS_VECTOR vec, int local_n, int global_n)`
- Fortran subroutine `lis_vector_create(integer local_n, integer global_n, LIS_Comm comm, LIS_VECTOR vec, integer ierr)`

Either `local_n` or `global_n` must be provided. This function can create a vector in one of the following ways: Creating partial vectors of order `local_n` from `local_n`, or creating from `global_n` partial vectors into which the row block of the vector of order `global_n` has been divided with a given number of processors.

In the case of Sequential and OpenMP versions, `local_n = global_n`. This means that both `lis_vector_set_size(v,n,0)` and `lis_vector_set_size(v,0,n)` create a vector of order *n*.

For MPI version, `lis_vector_set_size(v,n,0)` creates a partial vector of order n_p at each processor *p*. On the other hand, `lis_vector_set_size(v,0,n)` creates a partial vector of order m_p at each processor *p*. The value for m_p is determined by the library.

Assigning elements

To assign an element to the *i*-th row of vector *v*, the following functions are used:

- C `int lis_vector_set(int flag, int i, LIS_SCALAR value, LIS_VECTOR v)`
- Fortran subroutine `lis_vector_set_value(int flag, int i, LIS_SCALAR value, LIS_VECTOR v, integer ierr)`

For MPI, the *i*-th row of the whole vector must be specified, rather than the *i*-th row of the partial vector. Either

LIS_INS.VALUE Assignment :`v[i] = value`, or

LIS_ADD.VALUE Assignment add:`v[i] = v[i] + value`

must be provided for `flag`.

Duplicating vectors

To create a vector that has the same information as for an existing vector, the following functions are used:

- C `int lis_vector_duplicate(LIS_VECTOR vin, LIS_VECTOR *vout)`
- Fortran subroutine `lis_vector_duplicate(LIS_VECTOR vin, LIS_VECTOR vout, integer ierr)`

This function does not copy the elements of the vector. To copy the elements as well, the following functions must be added after the above functions:

- C `int lis_vector_copy(LIS_VECTOR vsrc, LIS_VECTOR vdst)`
- Fortran subroutine `lis_vector_copy(LIS_VECTOR vsrc, LIS_VECTOR vdst, integer ierr)`

Removing a vector

To remove an unwanted vector from memory, the following functions are used:

- C `int lis_vector_destroy(LIS_VECTOR v)`
- Fortran subroutine `lis_vector_destroy(LIS_VECTOR vec, integer ierr)`

3.3 Matrix

Assume that the order of matrix A is `global_n` \times `global_n` and that the number of rows of each block into which the row block of matrix A has been divided with `nprocs` units of processors is `local_n`. If `global_n` can be divided into an integer solution, then `local_n` = `global_n` / `nprocs`. For example, when the row block of matrix A is divided with two processors, as shown by Equation (3.2), `global_n` and `local_n` are 4 and 2, respectively.

$$A = \left(\begin{array}{ccc} 2 & 1 & \\ 1 & 2 & 1 \\ & 1 & 2 & 1 \\ & & 1 & 2 \end{array} \right) \begin{array}{l} \text{PE0} \\ \text{PE1} \end{array} \quad (3.2)$$

A matrix for a desired storage method can be created in one of the following three ways:

1. The library prepares the arrays required by the desired storage type,
2. The user prepares the arrays required by the desired storage type,
3. Matrix data is read from a file.

Approach 1: The library prepares the arrays required by the desired storage type

In the case of creating matrix A in Equation (3.2) in the CRS format, Sequential and OpenMP versions create matrix A itself, and MPI version creates at each processor a partial matrix into which the row block is divided with a given number of processors.

Programs to create matrix A in the CRS format are as follows, where the number of processors for MPI version is assumed to be two:

C(Sequential, OpenMP)

```
1: int          i,n;
2: LIS_MATRIX   A;
3: n = 4;
4: lis_matrix_create(0,&A);
5: lis_matrix_set_size(A,0,n); /* or lis_matrix_set_size(A,n,0); */
6: for(i=0;i<n;i++) {
7:     if( i>0 ) lis_matrix_set_value(LIS_INS_VALUE,i,i-1,1.0,A);
8:     if( i<n-1 ) lis_matrix_set_value(LIS_INS_VALUE,i,i+1,1.0,A);
9:     lis_matrix_set_value(LIS_INS_VALUE,i,i,2.0,A);
10: }
11: lis_matrix_set_type(A,LIS_MATRIX_CRs);
12: lis_matrix_assemble(A);
```

C(MPI)

```
1: int          i,n,gn,is,ie;
2: LIS_MATRIX   A;
3: gn = 4;                      /* or n=2 */
4: lis_matrix_create(MPI_COMM_WORLD,&A);
5: lis_matrix_set_size(A,0,gn);  /* lis_matrix_set_size(A,n,0); */
6: lis_matrix_get_size(A,&n,&gn);
7: lis_matrix_get_range(A,&is,&ie);
8: for(i=is;i<ie;i++) {
9:     if( i>0 ) lis_matrix_set_value(LIS_INS_VALUE,i,i-1,1.0,A);
10:    if( i<gn-1 ) lis_matrix_set_value(LIS_INS_VALUE,i,i+1,1.0,A);
11:    lis_matrix_set_value(LIS_INS_VALUE,i,i,2.0,A);
12: }
13: lis_matrix_set_type(A,LIS_MATRIX_CRS);
14: lis_matrix_assemble(A);
```

Fortran(Sequential, OpenMP)

```
1: integer      i,n
2: LIS_MATRIX   A
3: n = 4
4: call lis_matrix_create(0,A,ierr)
5: call lis_matrix_set_size(A,0,n,ierr)
6: do i=1,n
7:     if( i>1 ) call lis_matrix_set_value(LIS_INS_VALUE,i,i-1,1.0d0,A,ierr)
8:     if( i<n ) call lis_matrix_set_value(LIS_INS_VALUE,i,i+1,1.0d0,A,ierr)
9:     call lis_matrix_set_value(LIS_INS_VALUE,i,i,2.0d0,A,ierr)
10: enddo
11: call lis_matrix_set_type(A,LIS_MATRIX_CRS,ierr)
12: call lis_matrix_assemble(A,ierr)
```

Fortran(MPI)

```
1: integer      i,n,gn,is,ie
2: LIS_MATRIX   A
3: gn = 4
4: call lis_matrix_create(MPI_COMM_WORLD,A,ierr)
5: call lis_matrix_set_size(A,0,gn,ierr)
6: call lis_matrix_get_size(A,n,gn,ierr)
7: call lis_matrix_get_range(A,is,ie,ierr)
8: do i=is,ie-1
9:     if( i>1 ) call lis_matrix_set_value(LIS_INS_VALUE,i,i-1,1.0d0,A,ierr)
10:    if( i<gn ) call lis_matrix_set_value(LIS_INS_VALUE,i,i+1,1.0d0,A,ierr)
11:    call lis_matrix_set_value(LIS_INS_VALUE,i,i,2.0d0,A,ierr)
12: enddo
13: call lis_matrix_set_type(A,LIS_MATRIX_CRS,ierr)
14: call lis_matrix_assemble(A,ierr)
```

Declaring variables

As the second line shows, the declaration is stated as the following:

```
LIS_MATRIX   A;
```

Creating a matrix

To create matrix A, the following functions are used:

- C `int lis_matrix_create(LIS_Comm comm, LIS_MATRIX *A)`
- Fortran subroutine `lis_matrix_create(LIS_Comm comm, LIS_MATRIX A, integer ierr)`

`comm` must be replaced with the MPI communicator. For sequential and OpenMP versions, the value for `comm` is ignored.

Assigning a matrix size

To assign a size to matrix A, the following functions are used:

- C `int lis_matrix_set_size(LIS_MATRIX A, int local_n, int global_n)`
- Fortran subroutine `lis_matrix_set_size(LIS_MATRIX A, integer local_n, integer global_n, integer ierr)`

Either `local_n` or `global_n` must be provided. This function can create matrices in one of the following two ways: Creating partial matrices of order `local_n` x `N` from `local_n`, or creating partial matrices into which the row block of order `global_n` x `global_n` from `global_n` with a given number of processors. `N` represents the total sum of `local_n` of each processor.

In the case of Sequential and OpenMP versions, `local_n = global_n`. This means that both `lis_matrix_set_size(A,n,0)` and `lis_matrix_set_size(A,0,n)` create a matrix of `n` x `n`.

For MPI version, `lis_matrix_set_size(A,n,0)` creates at each processor p a partial matrix of $n_p \times N$, where N is the total sum of n_p of each processor. On the other hand, `lis_matrix_set_size(A,0,n)` creates at each processor p a partial matrix of $m_p \times n$, where m_p is the number of the partial matrix, which is determined by the library.

Assigning elements

To assign an element to the cell at the i -th row and j -th column of matrix A, the following functions are used:

- C `int lis_matrix_set_value(int flag, int i, int j, LIS_SCALAR value, LIS_MATRIX A)`
- Fortran subroutine `lis_matrix_set_value(integer flag, integer i, integer j, LIS_SCALAR value, LIS_MATRIX A, integer ierr)`

For MPI, the i -th row and j -th column of the whole matrix must be specified, rather than the i -th row and j -th column of the partial matrix. Either

LIS_INS_VALUE Assignment : $A(i,j) = \text{value}$, or

LIS_ADD_VALUE Assignment add: $A(i,j) = A(i,j) + \text{value}$

must be provided for `flag`.

Assigning a storage format

To assign a storage format to matrix A, the following functions are used:

- C `int lis_matrix_set_type(LIS_MATRIX A, int matrix_type)`
- Fortran subroutine `lis_matrix_set_type(LIS_MATRIX A, int matrix_type, integer ierr)`

`matrix_type` of A is LIS_MATRIX_CRS when the matrix is created. The following storage formats are accepted:

| Storage formats | | matrix_type |
|-------------------------------------|-------|---------------------|
| Compressed Row Storage | (CRS) | {LIS_MATRIX_CRS 1} |
| Compressed Column Storage | (CCS) | {LIS_MATRIX_CCS 2} |
| Modified Compressed Sparse Row | (MSR) | {LIS_MATRIX_MSR 3} |
| Diagonal | (DIA) | {LIS_MATRIX_DIA 4} |
| Ellpack-Itpack generalized diagonal | (ELL) | {LIS_MATRIX_ELL 5} |
| Jagged Diagonal | (JDS) | {LIS_MATRIX_JDS 6} |
| Block Sparse Row | (BSR) | {LIS_MATRIX_BSR 7} |
| Block Sparse Column | (BSC) | {LIS_MATRIX_BSC 8} |
| Variable Block Row | (VBR) | {LIS_MATRIX_VBR 9} |
| Dense | (DNS) | {LIS_MATRIX_DNS 10} |
| Coordinate | (COO) | {LIS_MATRIX_COO 11} |

Assembling a matrix

After assigning elements, the following function must be used:

- C `int lis_matrix_assemble(LIS_MATRIX A)`
- Fortran subroutine `lis_matrix_assemble(LIS_MATRIX A, integer ierr)`

`lis_matrix_assemble` is assembled to the storage format specified with `lis_matrix_set_type`.

Removing a matrix

To remove an unwanted matrix, the following functions are used:

- C `int lis_matrix_destroy(LIS_MATRIX A)`
- Fortran subroutine `lis_matrix_destroy(LIS_MATRIX A, integer ierr)`

Approach 2: The user prepares the arrays required by the desired storage type

In the case of creating matrix A in Equation (3.2) in the CRS format, Sequential and OpenMP versions creates matrix A itself, and MPI version creates at each processor a partial matrix into which the row block is divided with a given number of processors.

Programs to create matrix A in the CRS format are as follows, where the number of processors for MPI version is assumed to be two:

C(Sequential, OpenMP)

```

1: int          i,k,n,nnz;
2: int          *ptr,*index;
3: LIS_SCALAR   *value;
4: LIS_MATRIX   A;
5: n = 4; nnz = 10; k = 0;
6: lis_matrix_malloc_crs(n,nnz,&ptr,&index,&value);
7: lis_matrix_create(0,&A);
8: lis_matrix_set_size(A,0,n); /* or lis_matrix_set_size(A,n,0); */
9:
10: for(i=0;i<n;i++)
11: {
12:     if( i>0 ) {index[k] = i-1; value[k] = 1; k++;}
13:     index[k] = i; value[k] = 2; k++;
14:     if( i<n-1 ) {index[k] = i+1; value[k] = 1; k++;}
15:     ptr[i+1] = k;
16: }
17: ptr[0] = 0;
18: lis_matrix_set_crs(nnz,ptr,index,value,A);
19: lis_matrix_assemble(A);

```

C(MPI)

```

1: int          i,k,n,nnz,is,ie;
2: int          *ptr,*index;
3: LIS_SCALAR   *value;
4: LIS_MATRIX   A;
5: n = 2; nnz = 5; k = 0;
6: lis_matrix_malloc_crs(n,nnz,&ptr,&index,&value);
7: lis_matrix_create(MPI_COMM_WORLD,&A);
8: lis_matrix_set_size(A,n,0);
9: lis_matrix_get_range(A,&is,&ie);
10: for(i=is;i<ie;i++)
11: {
12:     if( i>0 ) {index[k] = i-1; value[k] = 1; k++;}
13:     index[k] = i; value[k] = 2; k++;
14:     if( i<n-1 ) {index[k] = i+1; value[k] = 1; k++;}
15:     ptr[i-is+1] = k;
16: }
17: ptr[0] = 0;
18: lis_matrix_set_crs(nnz,ptr,index,value,A);
19: lis_matrix_assemble(A);

```

Associating arrays

To associate the arrays required by the CRS format created by the user with matrix A, the following functions are used:

- C `int lis_matrix_set_crs(int nnz, int row[], int index[], LIS_SCALAR value[], LIS_MATRIX A)`
- Fortran subroutine `lis_matrix_set_crs(integer nnz, integer row(), integer index(), LIS_SCALAR value(), LIS_MATRIX A, integer ierr)`

Approach 3: Reading matrix and vector data from a file

Programs to read matrix A in Equation (3.2) in CRS format and vector b in Equation (3.1) from a file are as follows:

C(Sequential, OpenMP, MPI)

```
1: LIS_MATRIX    A;
2: LIS_VECTOR    b,x;
3: lis_matrix_create(LIS_COMM_WORLD,&A);
4: lis_vector_create(LIS_COMM_WORLD,&b);
5: lis_vector_create(LIS_COMM_WORLD,&x);
6: lis_matrix_set_type(A,LIS_MATRIX_CRS);
7: lis_input(A,b,x,"matvec.mtx");
```

Fortran(Sequential, OpenMP, MPI)

```
1: LIS_MATRIX    A
2: LIS_VECTOR    b,x
3: call lis_matrix_create(LIS_COMM_WORLD,A,ierr)
4: call lis_vector_create(LIS_COMM_WORLD,b,ierr)
5: call lis_vector_create(LIS_COMM_WORLD,x,ierr)
6: call lis_matrix_set_type(A,LIS_MATRIX_CRS,ierr)
7: call lis_input(A,b,x,'matvec.mtx',ierr)
```

The content of the target file `matvec.mtx` resembles the following:

```
%%MatrixMarket matrix coordinate real general
4 4 10 1 0
1 2 1.0e+00
1 1 2.0e+00
2 3 1.0e+00
2 1 1.0e+00
2 2 2.0e+00
3 4 1.0e+00
3 2 1.0e+00
3 3 2.0e+00
4 4 2.0e+00
4 3 1.0e+00
1 0.0e+00
2 1.0e+00
3 2.0e+00
4 3.0e+00
```

Reading data from a file

To read the data for matrix A from a file, the following functions are used:

- C `int lis_input_matrix(LIS_MATRIX A, char *filename)`
- Fortran subroutine `lis_input(LIS_MATRIX A, character filename, integer ierr)`

`filename` must be replaced with the path to the target file. The following file formats are supported:

- MatrixMarket format
- Harwell-Boeing format
- LIS format (original format)

To read the data for matrix A and vectors b and x from a file, the following functions are used:

- C `int lis_input(LIS_MATRIX A, LIS_VECTOR b, LIS_VECTOR x, char *filename)`
- Fortran subroutine `lis_input(LIS_MATRIX A, LIS_VECTOR b, LIS_VECTOR x, character filename, integer ierr)`

filename must be replaced with the path to the target file. The following file formats are supported:

- MatrixMarket format (extended to allow vector data to be read)
- Harwell-Boeing format
- LIS format (original format)

3.4 Solving Linear Equation

The program to solve the linear equation $Ax = b$ with a specified solver resembles the following:

C(Sequential, OpenMP, MPI) —

```
1: LIS_MATRIX A;
2: LIS_VECTOR b,x;
3: LIS_SOLVER solver;
4:
5: /* Create matrix and vector */
6:
7: lis_solver_create(&solver);
8: lis_solver_set_option("-i bicg -p none",solver);
9: lis_solver_set_option("-tol 1.0e-12",solver);
10: lis_solver(A,b,x,solver);
```

Fortran(Sequential, OpenMP, MPI) —

```
1: LIS_MATRIX A
2: LIS_VECTOR b,x
3: LIS_SOLVER solver
4:
5: /* Create matrix and vector */
6:
7: call lis_solver_create(solver,ierr)
8: call lis_solver_set_option('-i bicg -p none',solver,ierr)
9: call lis_solver_set_option('-tol 1.0e-12',solver,ierr)
10: call lis_solver(A,b,x,solver,ierr)
```

Creating a SOLVER

To create a SOLVER, the following functions are used:

- C `int lis_solver_create(LIS_SOLVER *solver)`
- Fortran subroutine `lis_solver_create(LIS_SOLVER solver, integer ierr)`

Specifying options

To specify options such as a solver, the following functions are used:

- C `int lis_solver_set_option(char *text, LIS_SOLVER solver)`
- Fortran subroutine `lis_solver_set_option(character text, LIS_SOLVER solver, integer ierr)`

or,

- C `int lis_solver_set_optionC(LIS_SOLVER solver)`
- Fortran subroutine `lis_solver_set_optionC(LIS_SOLVER solver, integer ierr)`

ine opt `lis_solver_set_optionC` is a function that sets the option specified in the command line to SOLVER, when the user's program is run. When text is replaced with a desired command line option, the information will be stored in options and parameters.

The table below shows the allowable command line options, where `-i {cg|1}` means `-i cg` or `-i 1` and `-maxiter [1000]` indicates that `-maxiter` defaults to 1,000.

Specifying an Linear Equation Solver Default: `-i bicg`

| Method | Option | Auxiliary Option | |
|--------------|-------------------------------|----------------------------|--|
| CG | <code>-i {cg 1}</code> | | |
| BiCG | <code>-i {bicg 2}</code> | | |
| CGS | <code>-i {cgs 3}</code> | | |
| BiCGSTAB | <code>-i {bicgstab 4}</code> | | |
| BiCGSTAB(l) | <code>-i {bicgstabl 5}</code> | <code>-ell [2]</code> | Value for l |
| GPBiCG | <code>-i {gpbicg 6}</code> | | |
| TFQMR | <code>-i {tfqmr 7}</code> | | |
| Orthomin(m) | <code>-i {orthomin 8}</code> | <code>-restart [40]</code> | Value for Restart m |
| GMRES(m) | <code>-i {gmres 9}</code> | <code>-restart [40]</code> | Value for Restart m |
| Jacobi | <code>-i {jacobi 10}</code> | | |
| Gauss-Seidel | <code>-i {gs 11}</code> | | |
| SOR | <code>-i {sor 12}</code> | <code>-omega [1.9]</code> | Value for Relaxation Coefficient ω ($0 < \omega < 2$) |
| BiCGSafe | <code>-i {bicgsafe 13}</code> | | |
| CR | <code>-i {cr 14}</code> | | |
| BiCR | <code>-i {bicr 15}</code> | | |
| CRS | <code>-i {crs 16}</code> | | |
| BiCRSTAB | <code>-i {bicrstab 17}</code> | | |
| GPBiCR | <code>-i {gpbicr 18}</code> | | |
| BiCRSafe | <code>-i {bicrsafe 19}</code> | | |
| FGMRES(m) | <code>-i {fgmres 20}</code> | <code>-restart [40]</code> | Value for Restart m |
| IDR(s) | <code>-i {idrs 21}</code> | <code>-restart [40]</code> | Value for Restart s |
| MINRES | <code>-i {minres 22}</code> | | |

Specifying a Preconditioner Default: -p none

| Preconditioner | Option | Auxiliary Option | |
|------------------|---------------|----------------------|---|
| None | -p {none 0} | | |
| Jacobi | -p {jacobi 1} | | |
| ILU(k) | -p {ilu 2} | -ilu_fill [0] | Fill level k |
| SSOR | -p {ssor 3} | -ssor_w [1.0] | Relaxation Coefficient ω ($0 < \omega < 2$) |
| hybrid | -p {hybrid 4} | -hybrid_i [sor] | Linear Equation Solver |
| | | -hybrid_maxiter [25] | Maximum number of iterations |
| | | -hybrid_tol [1.0e-3] | Convergence criteria |
| | | -hybrid_w [1.5] | Relaxation Coefficient ω for the SOR method ($0 < \omega < 2$) |
| | | -hybrid_ell [2] | Value for l of the BiCGSTAB(l) method |
| | | -hybrid_restart [40] | Restart values for GMRES and Orthomin |
| I+S | -p {is 5} | -is_alpha [1.0] | Parameter α for preconditioner of a $I + \alpha S^{(m)}$ type |
| | | -is_m [3] | Parameter m for preconditioner of a $I + \alpha S^{(m)}$ type |
| SAINV | -p {sainv 6} | -sainv_drop [0.05] | Drop criteria |
| SA-AMG | -p {saamg 7} | -saamg_unsym [false] | Selection of asymmetric version (Matrix structure must be symmetric) |
| Crout ILU | -p {iluc 8} | -iluc_drop [0.05] | Drop criteria |
| | | -iluc_rate [5.0] | Ratio of Maximum fill-in |
| ILUT | -p {ilut 9} | -ilut_drop [0.05] | Drop criteria |
| | | -ilut_rate [5.0] | Ratio of Maximum fill-in |
| additive Schwarz | -adds true | -adds_iter [1] | Number of iterations |

Other Options

| Option | |
|----------------------|--|
| -maxiter [1000] | Maximum number of iterations |
| -tol [1.0e-12] | Convergence criteria |
| -print [0] | Display of the residual |
| | -print {none 0} None |
| | -print {mem 1} Saves the residual history in memory |
| | -print {out 2} Displays the residual history |
| | -print {all 3} Saves the residual history and displays it on the screen |
| -scale [0] | Selection of scaling. The result will overwrite the original matrix and vectors |
| | -scale {none 0} No scaling |
| | -scale {jacobi 1} Jacobi scaling $D^{-1}Ax = D^{-1}b$ D represents the diagonal of $A = (a_{ij})$ |
| | -scale {symm_diag 2} Diagonal scaling $D^{-1/2}AD^{-1/2}x = D^{-1/2}b$ $D^{-1/2}$ represents an diagonal matrix that has $1/\sqrt{a_{ii}}$ as an diagonal element |
| -initx_zeros [true] | Behavior of initial vector x_0 |
| | -initx_zeros {false 0} Given values |
| | -initx_zeros {true 1} All elements are set to 0. |
| -omp_num_threads [t] | Number of threads t represents the maximum number of threads |

Precision Default: -precision double

| Precision | Option | Auxiliary Option |
|-----------|-----------------------|------------------|
| DOUBLE | -precision {double 0} | |
| QUAD | -precision {quad 1} | |

Solving linear equation

To solve the linear equation $Ax = b$, the following functions are used:

- C `int lis_solve(LIS_MATRIX A, LIS_VECTOR b, LIS_VECTOR x, LIS_SOLVER solver)`
- Fortran subroutine `lis_solve(LIS_MATRIX A, LIS_VECTOR b, LIS_VECTOR x, LIS_SOLVER solver, integer ierr)`

3.5 Solving Eigenvalue Problem

The program to solve the eigenvalue problem $Ax = \lambda x$ with a specified solver is as follows:

C(Sequential, OpenMP, MPI)

```
1: LIS_MATRIX A;
2: LIS_VECTOR x;
3: LIS_REAL eval;
4: LIS_ESOLVER esolver;
5:
6: /* Create matrix and vector */
7:
8: lis_esolver_create(&esolver);
9: lis_esolver_set_option("-e ii -i bicg -p none",esolver);
10: lis_esolver_set_option("-etol 1.0e-12 -tol 1.0e-12",esolver);
11: lis_solve(A,x,eval,esolver);
```

Fortran(Sequential, OpenMP, MPI)

```
1: LIS_MATRIX A
2: LIS_VECTOR x
3: LIS_REAL eval
4: LIS_ESOLVER esolver
5:
6: /* Create matrix and vector */
7:
8: call lis_esolver_create(esolver,ierr)
9: call lis_esolver_set_option('-e ii -i bicg -p none',esolver,ierr)
10: call lis_esolver_set_option('-etol 1.0e-12 -tol 1.0e-12',esolver,ierr)
11: call lis_solve(A,x,eval,esolver,ierr)
```

Creating an ESOLVER

To create an ESOLVER, the following functions are used:

- C `int lis_esolver_create(LIS_ESOLVER *esolver)`
- Fortran subroutine `lis_esolver_create(LIS_ESOLVER esolver, integer ierr)`

Specifying options

To specify options such as a solver, the following functions are used:

- C `int lis_esolver_set_option(char *text, LIS_ESOLVER esolver)`
- Fortran subroutine `lis_esolver_set_option(character text, LIS_ESOLVER esolver, integer ierr)`

or,

- C `int lis_esolver_set_optionC(LIS_ESOLVER esolver)`
- Fortran subroutine `lis_esolver_set_optionC(LIS_ESOLVER esolver, integer ierr)`

ine opt `lis_esolver_set_optionC` is a function that sets the option specified in the command line to **ESOLVER**, when the user's program is run. When text is replaced with a desired command line option, the information will be stored in options and parameters.

The table below shows the allowable command line options, where `-e {pi|1}` means `-e pi` or `-e 1` and `-emaxiter [1000]` indicates that `-emaxiter` defaults to 1,000.

Specifying an Eigensolver Default: `-i bicg`

| Method | Option | Auxiliary Option |
|-------------------------------|-------------------------|---|
| Power Iteration | <code>-e {pi 1}</code> | |
| Inverse Iteration | <code>-e {ii 2}</code> | <code>-i [bicg]</code> Linear equation solver |
| Approximate Inverse Iteration | <code>-e {aii 3}</code> | |
| Conjugate Gradient | <code>-e {cg 4}</code> | |
| Lanczos Iteration | <code>-e {li 5}</code> | <code>-ss [10]</code> Size of subspace |
| Subspace Iteration | <code>-e {si 6}</code> | <code>-ss [10]</code> Size of subspace |
| Conjugate Residual | <code>-e {cr 7}</code> | |

Specifying a Preconditioner Default: `-p ilu`

| Preconditioner | Option | Auxiliary Option |
|------------------|----------------------------|--|
| None | <code>-p {none 0}</code> | |
| Jacobi | <code>-p {jacobi 1}</code> | |
| ILU(k) | <code>-p {ilu 2}</code> | <code>-ilu_fill [0]</code> Fill level k |
| SSOR | <code>-p {ssor 3}</code> | <code>-ssor_w [1.0]</code> Relaxation Coefficient ω ($0 < \omega < 2$) |
| hybrid | <code>-p {hybrid 4}</code> | <code>-hybrid_i [sor]</code> Linear Equation Solver |
| | | <code>-hybrid_maxiter [25]</code> Maximum number of iterations |
| | | <code>-hybrid_tol [1.0e-3]</code> Convergence criteria |
| | | <code>-hybrid_w [1.5]</code> Relaxation Coefficient ω for the SOR method ($0 < \omega < 2$) |
| | | <code>-hybrid_ell [2]</code> Value for l of the BiCGSTAB(l) method |
| | | <code>-hybrid_restart [40]</code> Restart values for GMRES and Orthomin |
| I+S | <code>-p {is 5}</code> | <code>-is_alpha [1.0]</code> Parameter α for preconditioner of a $I + \alpha S^{(m)}$ type |
| | | <code>-is_m [3]</code> Parameter m for preconditioner of a $I + \alpha S^{(m)}$ type |
| SAINV | <code>-p {sainv 6}</code> | <code>-sainv_drop [0.05]</code> Drop criteria |
| SA-AMG | <code>-p {saamg 7}</code> | <code>-saamg_unsym [false]</code> Selection of asymmetric version (Matrix structure must be symmetric) |
| Crout ILU | <code>-p {iluc 8}</code> | <code>-iluc_drop [0.05]</code> Drop criteria |
| | | <code>-iluc_rate [5.0]</code> Ratio of Maximum fill-in |
| ILUT | <code>-p {ilut 9}</code> | <code>-ilut_drop [0.05]</code> Drop criteria |
| | | <code>-ilut_rate [5.0]</code> Ratio of Maximum fill-in |
| additive Schwarz | <code>-adds true</code> | <code>-adds_iter [1]</code> Number of iterations |

Other Options

| Option | |
|-----------------------------------|---|
| <code>-emaxiter [1000]</code> | Maximum number of iterations |
| <code>-etol [1.0e-5]</code> | Convergence criteria |
| <code>-eprint [0]</code> | Display of the residual |
| | <code>-eprint {none 0}</code> None |
| | <code>-eprint {mem 1}</code> Saves the residual history in memory |
| | <code>-eprint {out 2}</code> Displays the residual history |
| | <code>-eprint {all 3}</code> Saves the residual history and displays it on the screen |
| <code>-ie [ii]</code> | Inner eigensolver used in Lanczos Iteration or Subspace Iteration |
| | <code>-ie {pi 1}</code> Power Iteration (Subspace Iteration only) |
| | <code>-ie {ii 2}</code> Inverse Iteration |
| | <code>-ie {aii 3}</code> Approximate Inverse Iteration |
| <code>-shift [0.0]</code> | Amount of shift |
| <code>-initx_ones [true]</code> | Behavior of initial vector x_0 |
| | <code>-initx_ones {false 0}</code> Given values |
| | <code>-initx_ones {true 1}</code> All elements are set to 1. |
| <code>-omp_num_threads [t]</code> | Number of threads |
| | <code>t</code> represents the maximum number of threads |

Solving eigenvalue problem

To solve the eigenvalue problem $Ax = \lambda x$, the following functions are used:

- C `int lis_esolve(LIS_MATRIX A, LIS_VECTOR x,
 LIS_REAL eval, LIS_ESOLVER esolver)`
- Fortran subroutine `lis_esolve(LIS_MATRIX A, LIS_VECTOR x,
 LIS_REAL eval, LIS_ESOLVER esolver, integer ierr)`

3.6 Sample Programs

This is a program for solving the linear equation $Ax = b$ with a specified solver to provide an approximate solution for the equation, where matrix A is a tridiagonal matrix of 12×12 .

$$A = \begin{pmatrix} 2 & 1 & & & \\ 1 & 2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & 2 & 1 \\ & & & 1 & 2 \end{pmatrix}$$

Vector b on the right-hand side of the equation is solved such that approximate solution x will be always 1.

This sample program is stored in the `lis-($VERSION)/test` directory.

Test program: test3.c

```
1: #include <stdio.h>
2: #include "lis.h"
3: main(int argc, char *argv[])
4: {
5:     int i,n,gn,is,ie,iter;
6:     LIS_MATRIX A;
7:     LIS_VECTOR b,x,u;
8:     LIS_SOLVER solver;
9:     n = 12;
10:    lis_initialize(&argc,&argv);
11:    lis_matrix_create(MPI_COMM_WORLD,&A);
12:    lis_matrix_set_size(A,0,n);
13:    lis_matrix_get_size(A,&n,&gn)
14:    lis_matrix_get_range(A,&is,&ie)
15:    for(i=is;i<ie;i++)
16:    {
17:        if( i>0 ) lis_matrix_set_value(LIS_INS_VALUE,i,i-1,1.0,A);
18:        if( i<gn-1 ) lis_matrix_set_value(LIS_INS_VALUE,i,i+1,1.0,A);
19:        lis_matrix_set_value(LIS_INS_VALUE,i,i,2.0,A);
20:    }
21:    lis_matrix_set_type(A,LIS_MATRIX_CRS);
22:    lis_matrix_assemble(A);
23:
24:    lis_vector_duplicate(A,u);
25:    lis_vector_duplicate(A,b);
26:    lis_vector_duplicate(A,x);
27:    lis_vector_set_all(1.0,u);
28:    lis_matvec(A,u,b);
29:
30:    lis_solver_create(&solver);
31:    lis_solver_set_optionC(solver);
32:    lis_solve(A,b,x,solver);
33:    lis_solver_get_iters(solver,&iter);
34:    printf("iter = %d\n",iter);
35:    lis_vector_print(x);
36:    lis_matrix_destroy(A);
37:    lis_vector_destroy(u);
38:    lis_vector_destroy(b);
39:    lis_vector_destroy(x);
40:    lis_solver_destroy(solver);
41:    lis_finalize();
42:    return 0;
43: }
```


Test program: test3f.f

```

1:      implicit none
2:
3: #include "lisf.h"
4:
5:      integer          i,n,gn,is,ie,iter,ierr
6:      LIS_MATRIX       A
7:      LIS_VECTOR       b,x,u
8:      LIS_SOLVER       solver
9:      n = 12
10:     call lis_initialize(ierr)
11:     call lis_matrix_create(LIS_COMM_WORLD,A,ierr)
12:     call lis_matrix_set_size(A,0,n,ierr)
13:     call lis_matrix_get_size(A,n,gn,ierr)
14:     call lis_matrix_get_range(A,is,ie,ierr)
15:     do i=is,ie-1
16:         if( i>1 ) call lis_matrix_set_value(LIS_INS_VALUE,i,i-1,1.0d0,
17:                                             A,ierr)
18:         if( i<gn ) call lis_matrix_set_value(LIS_INS_VALUE,i,i+1,1.0d0,
19:                                             A,ierr)
20:         call lis_matrix_set_value(LIS_INS_VALUE,i,i,2.0d0,A,ierr)
21:     enddo
22:     call lis_matrix_set_type(A,LIS_MATRIX_CRS,ierr)
23:     call lis_matrix_assemble(A,ierr)
24:
25:     call lis_vector_duplicate(A,u,ierr)
26:     call lis_vector_duplicate(A,b,ierr)
27:     call lis_vector_duplicate(A,x,ierr)
28:     call lis_vector_set_all(1.0d0,u,ierr)
29:     call lis_matvec(A,u,b,ierr)
30:
31:     call lis_solver_create(solver,ierr)
32:     call lis_solver_set_optionC(solver,ierr)
33:     call lis_solve(A,b,x,solver,ierr)
34:     call lis_solver_get_iters(solver,iter,ierr)
35:     write(*,*) 'iter = ',iter
36:     call lis_vector_print(x,ierr)
37:     call lis_matrix_destroy(A,ierr)
38:     call lis_vector_destroy(b,ierr)
39:     call lis_vector_destroy(x,ierr)
40:     call lis_vector_destroy(u,ierr)
41:     call lis_solver_destroy(solver,ierr)
42:     call lis_finalize(ierr)
43:
44:     stop
45:     end

```

3.7 Compiling and Linking

Provided below are examples for cases in which the test programs `test3.c` located in the `lis-($VERSION)/test` directory are compiled on SGI Altix 3700 using Intel C/C++ Compiler 8.1 (icc) and Intel Fortran Compiler 8.1 (ifort). Since the library includes the Fortran 90 code if the SA-AMG preconditioner is used, the link must be processed with the Fortran 90 compiler.

Sequential

Compile

```
>icc -c -I$(INSTALLDIR)/include test3.c
```

Link

```
>icc -o test3 test3.o -llis
```

Link(Use SA-AMG)

```
>ifort -nofor_main -o test3 test3.o -llis
```

OpenMP

Compile

```
>icc -c -openmp -I$(INSTALLDIR)/include test3.c
```

Link

```
>icc -openmp -o test3 test3.o -llis
```

Link(Use SA-AMG)

```
>ifort -nofor_main -openmp -o test3 test3.o -llis
```

MPI

Compile

```
>icc -c -DUSE_MPI -I$(INSTALLDIR)/include test3.c
```

Link

```
>icc -o test3 test3.o -llis -lmpi
```

Link(Use SA-AMG)

```
>ifort -nofor_main -o test3 test3.o -llis -lmpi
```

OpenMP + MPI

Compile

```
>icc -c -openmp -DUSE_MPI -I$(INSTALLDIR)/include test3.c
```

Link

```
>icc -openmp -o test3 test3.o -llis -lmpi
```

Link(Use SA-AMG)

```
>ifort -nofor_main -openmp -o test3 test3.o -llis -lmpi
```

Provided below are examples for cases in which the test programs `test3f.f` located in the `lis-($VERSION)/test` directory are compiled on SGI Altix 3700 using Intel Fortran Compiler 8.1 (ifort). Since the `#include` statement is used for the user's Fortran program, the compiler option must be specified to use the pre-processor. The option for ifort is `-fpp`.

Sequential

Compile

```
>ifort -c -fpp -I$(INSTALLDIR)/include test3f.f
```

Link

```
>ifort -o test3 test3.o -llis
```

OpenMP

Compile

```
>ifort -c -fpp -openmp -I$(INSTALLDIR)/include test3f.f
```

Link

```
>ifort -openmp -o test3 test3.o -llis
```

MPI

Compile

```
>ifort -c -fpp -DUSE_MPI -I$(INSTALLDIR)/include test3f.f
```

Link

```
>ifort -o test3 test3.o -llis -lmpi
```

OpenMP + MPI

Compile

```
>ifort -c -fpp -openmp -DUSE_MPI -I$(INSTALLDIR)/include test3f.f
```

Link

```
>ifort -openmp -o test3 test3.o -llis -lmpi
```

3.8 Running

Run the test programs `test3.c` and `test3f.f` in the `lis-($VERSION)/test` directory by entering the following:

sequential

```
>./test3 -i bicgstab
```

OpenMP

```
>env OMP_NUM_THREADS=2 ./test3 -i bicgstab
```

MPI

```
>mpirun -np 2 ./test3 -i bicgstab
```

OpenMP + MPI

```
>mpirun -np 2 env OMP_NUM_THREADS=2 ./test3 -i bicgstab
```

Then, the following results will be returned:

```
SOLVER : BiCGSTAB
```

```
PRECON : None
```

```
lis_solve is normal end
```

```
iter = 6
```

```
0 1.000000e+000
1 1.000000e+000
2 1.000000e+000
3 1.000000e+000
4 1.000000e+000
5 1.000000e+000
6 1.000000e+000
7 1.000000e+000
8 1.000000e+000
9 1.000000e+000
10 1.000000e+000
11 1.000000e+000
```

4 Quadruple Precision Operations

The double precision operation sometimes requires a large number of iterations for convergence because of the rounding error. The high-precision operation is effective for the improvement of convergence[15]. In this library, we implement the quadruple precision operations, which have "double-double" precision[16, 17] by combining two double precision floating point numbers. To use quadruple precision by the same interface as double precision, coefficient matrix A , solution x , and b of the right-hand side are assumed to be double precision. Acceleration was achieved by using the SSE2 SIMD instruction[25].

4.1 Quadruple Precision Operations

Run the test programs `test4.c` on an environment which supports SSE2 in the `lis-($VERSION)/test` directory by entering the following:

Double precision

```
>./test4 200 2.0 -precision double
```

Then, the following results will be returned:

```
n=200 gamma=2.000000
Initial vector x = 0
PRECISION : DOUBLE
SOLVER     : BiCG 2
PRECON     : None
STORAGE    : CRS
lis_solve is LIS_MAXITER(code=4)
BiCG: iter      = 1001 iter_double = 1001 iter_quad = 0
BiCG: times     = 2.044368e-02
BiCG: p_times   = 4.768372e-06 (p_c = 4.768372e-06 p_i = 0.000000e+00 )
BiCG: i_times   = 2.043891e-02
BiCG: Residual  = 8.917591e+01
```

Quadruple precision

```
>./test4 200 2.0 -precision quad
```

Then, the following results will be returned:

```
n=200 gamma=2.000000
Initial vector x = 0
PRECISION : QUAD
SOLVER     : BiCG 2
PRECON     : None
STORAGE    : CRS
lis_solve is normal end
BiCG: iter      = 230 iter_double = 0 iter_quad = 230
BiCG: times     = 2.267408e-02
BiCG: p_times   = 4.549026e-04 (p_c = 5.006790e-06 p_i = 4.498959e-04 )
BiCG: i_times   = 2.221918e-02
BiCG: Residual  = 6.499145e-11
```

5 Matrix Storage Format

This section describes the matrix storage types that can be used for the library. Assume that the matrix row (column) number begins with 0 and that the number of non-zero elements of matrix A of $n \times n = (a_{ij})$ is nnz .

5.1 Compressed Row Storage (CRS)

The CRS format uses three arrays (`ptr`, `index`, `value`) to store data.

- The `value` array, a double-precision array with a length of nnz , stores non-zero elements of matrix A along the row.
- The `index` array, an integer array with a length of nnz , stores the column numbers of the non-zero elements stored in the `value` array.
- The `ptr` array, an integer array with a length of $n + 1$, stores the starting points of the rows of the `value` and `index` arrays.

5.1.1 Creating a Matrix (Sequential and OpenMP)

The right-hand diagram in Figure 2 shows how matrix A in Figure 2 is stored in the CRS format. The program to create this matrix in the CRS format is as follows:

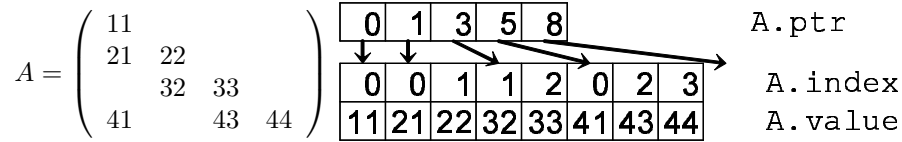


Figure 2: Data structures of CRS.

Sequential and OpenMP

```

1: int      n, nnz;
2: int      *ptr, *index;
3: LIS_SCALAR *value;
4: LIS_MATRIX A;
5: n = 4; nnz = 8;
6: ptr = (int *)malloc( (n+1)*sizeof(int) );
7: index = (int *)malloc( nnz*sizeof(int) );
8: value = (LIS_SCALAR *)malloc( nnz*sizeof(LIS_SCALAR) );
9: lis_matrix_create(0, &A);
10: lis_matrix_set_size(A, 0, n);
11:
12: ptr[0] = 0; ptr[1] = 1; ptr[2] = 3; ptr[3] = 5; ptr[4] = 8;
13: index[0] = 0; index[1] = 0; index[2] = 1; index[3] = 1;
14: index[4] = 2; index[5] = 0; index[6] = 2; index[7] = 3;
15: value[0] = 11; value[1] = 21; value[2] = 22; value[3] = 32;
16: value[4] = 33; value[5] = 41; value[6] = 43; value[7] = 44;
17:
18: lis_matrix_set_crs(nnz, ptr, index, value, A);
19: lis_matrix_assemble(A);

```

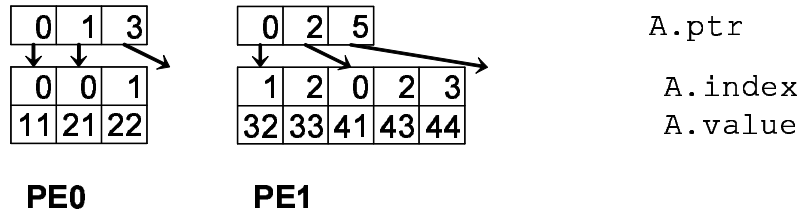


Figure 3: Data structures of CRS.

5.1.2 Creating a Matrix (MPI)

Figure 3 shows how matrix *A* in Figure 2 is stored in the CRS format with two processors. The program to create this matrix in the CRS format with two processors is as follows:

```

MPI
1: int      i,k,n,nnz,my_rank;
2: int      *ptr,*index;
3: LIS_SCALAR *value;
4: LIS_MATRIX A;
5: MPI_Comm_rank(MPI_COMM_WORLD,&my_rank);
6: if( my_rank==0 ) {n = 2; nnz = 3;}
7: else {n = 2; nnz = 5;}
8: ptr = (int *)malloc( (n+1)*sizeof(int) );
9: index = (int *)malloc( nnz*sizeof(int) );
10: value = (LIS_SCALAR *)malloc( nnz*sizeof(LIS_SCALAR) );
11: lis_matrix_create(MPI_COMM_WORLD,&A);
12: lis_matrix_set_size(A,n,0);
13: if( my_rank==0 ) {
14:     ptr[0] = 0; ptr[1] = 1; ptr[2] = 3;
15:     index[0] = 0; index[1] = 0; index[2] = 1;
16:     value[0] = 11; value[1] = 21; value[2] = 22;}
17: else {
18:     ptr[0] = 0; ptr[1] = 2; ptr[2] = 5;
19:     index[0] = 1; index[1] = 2; index[2] = 0; index[3] = 2; index[4] = 3;
20:     value[0] = 32; value[1] = 33; value[2] = 41; value[3] = 43; value[4] = 44;}
21: lis_matrix_set_crs(nnz,ptr,index,value,A);
22: lis_matrix_assemble(A);

```

5.1.3 Associating Arrays

To associate the arrays required by the CRS format with matrix *A*, the following functions are used:

- C `int lis_matrix_set_crs(int nnz, int row[], int index[], LIS_SCALAR value[], LIS_MATRIX A)`
- Fortran subroutine `lis_matrix_set_crs(integer nnz, integer row(), integer index(), LIS_SCALAR value(), LIS_MATRIX A, integer ierr)`

5.2 Compressed Column Storage (CCS)

The CSS format uses three arrays (`ptr`, `index`, `value`) to store data.

- The `value` array, a double-precision array with a length of nnz , stores the values for the non-zero elements of matrix A along the column.
- The `index` array, an integer array with a length of nnz , stores the row numbers of the non-zero elements stored in the `value` array.
- The `ptr` array, an integer array with a length of $n + 1$, stores the starting points of the rows of the `value` and `index` arrays.

5.2.1 Creating a Matrix (Sequential and OpenMP)

The right-hand diagram in Figure 4 shows how matrix A in Figure 4 is stored in the CCS format. The program to create this matrix in the CCS format is as follows:

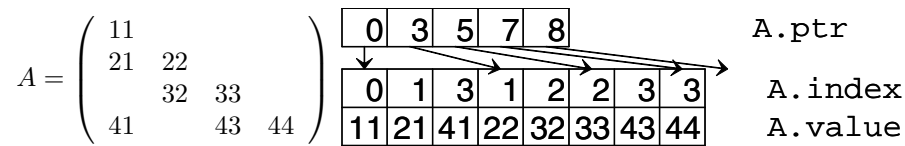


Figure 4: Data structures of CCS.

Sequential and OpenMP

```

1: int      n,nnz;
2: int      *ptr,*index;
3: LIS_SCALAR *value;
4: LIS_MATRIX A;
5: n = 4; nnz = 8;
6: ptr = (int *)malloc( (n+1)*sizeof(int) );
7: index = (int *)malloc( nnz*sizeof(int) );
8: value = (LIS_SCALAR *)malloc( nnz*sizeof(LIS_SCALAR) );
9: lis_matrix_create(0,&A);
10: lis_matrix_set_size(A,0,n);
11:
12: ptr[0] = 0; ptr[1] = 3; ptr[2] = 5; ptr[3] = 7; ptr[4] = 8;
13: index[0] = 0; index[1] = 1; index[2] = 3; index[3] = 1;
14: index[4] = 2; index[5] = 2; index[6] = 3; index[7] = 3;
15: value[0] = 11; value[1] = 21; value[2] = 41; value[3] = 22;
16: value[4] = 32; value[5] = 33; value[6] = 43; value[7] = 44;
17:
18: lis_matrix_set_ccs(nnz,ptr,index,value,A);
19: lis_matrix_assemble(A);

```

5.2.2 Creating a Matrix (MPI)

Figure 5 shows how matrix A in Figure 4 is stored with two processors. The program to create this matrix in the CCS format with two processors is as follows:

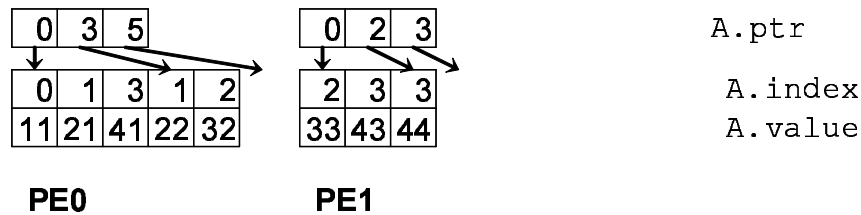


Figure 5: Data structures of CCS.

MPI

```

1: int      i,k,n,nnz,my_rank;
2: int      *ptr,*index;
3: LIS_SCALAR *value;
4: LIS_MATRIX A;
5: MPI_Comm_rank(MPI_COMM_WORLD,&my_rank);
6: if( my_rank==0 ) {n = 2; nnz = 3;}
7: else {n = 2; nnz = 5;}
8: ptr = (int *)malloc( (n+1)*sizeof(int) );
9: index = (int *)malloc( nnz*sizeof(int) );
10: value = (LIS_SCALAR *)malloc( nnz*sizeof(LIS_SCALAR) );
11: lis_matrix_create(MPI_COMM_WORLD,&A);
12: lis_matrix_set_size(A,n,0);
13: if( my_rank==0 ) {
14:     ptr[0] = 0; ptr[1] = 3; ptr[2] = 5;
15:     index[0] = 0; index[1] = 1; index[2] = 3; index[3] = 1; index[4] = 2;
16:     value[0] = 11; value[1] = 21; value[2] = 41; value[3] = 22; value[4] = 32;
17: } else {
18:     ptr[0] = 0; ptr[1] = 2; ptr[2] = 3;
19:     index[0] = 2; index[1] = 3; index[2] = 3;
20:     value[0] = 33; value[1] = 43; value[2] = 44;
21: lis_matrix_set_ccs(nnz,ptr,index,value,A);
22: lis_matrix_assemble(A);

```

5.2.3 Associating Arrays

To associate the arrays required by the CCS format with matrix A , the following functions are used:

- C `int lis_matrix_set_ccs(int nnz, int row[], int index[], LIS_SCALAR value[],`
- Fortran subroutine `lis_matrix_set_ccs(integer nnz, integer row(), integer index(),`
`LIS_SCALAR value(), LIS_MATRIX A, integer ierr)`

5.3 Modified Compressed Sparse Row (MSR)

The MSR format is a modified version of the CRS format. The MSR format is different in that it divides the diagonal before storing it. The MSR format uses two arrays (**index,value**) to store data. Assume that ndz represents the number of zero elements of the diagonal.

- The **value** array, a double-precision array with a length of $nnz + ndz + 1$, stores the diagonal of matrix A down to the n -th element. The $n + 1$ -th element is not used. For the $n + 2$ -th and later elements, the values of non-zero elements except the diagonal of matrix A are stored along the row.
- The **index** array, an integer array with a length of $nnz + ndz + 1$, stores the starting points of the rows of the non-diagonals of matrix A down to the $n + 1$ -th element. For the $n + 2$ -th and later elements, it stores the row numbers of the non-diagonals of matrix A stored in the **value** array.

5.3.1 Creating a Matrix (Sequential and OpenMP)

The right-hand diagram in Figure 6 shows how matrix A is stored in the MSR format. The program to create this matrix in the MSR format is as follows:

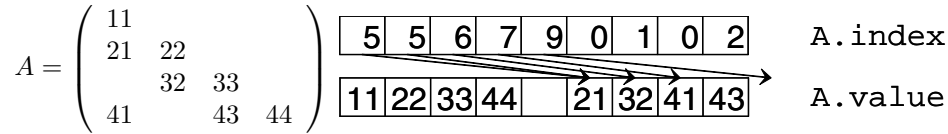


Figure 6: Data structures of MSR.

Sequential and OpenMP

```

1: int      n,nnz,ndz;
2: int      *index;
3: LIS_SCALAR *value;
4: LIS_MATRIX A;
5: n = 4; nnz = 8; ndz = 0;
6: index = (int *)malloc( (nnz+ndz+1)*sizeof(int) );
7: value = (LIS_SCALAR *)malloc( (nnz+ndz+1)*sizeof(LIS_SCALAR) );
8: lis_matrix_create(0,&A);
9: lis_matrix_set_size(A,0,n);
10:
11: index[0] = 5; index[1] = 5; index[2] = 6; index[3] = 7;
12: index[4] = 9; index[5] = 0; index[6] = 1; index[7] = 0; index[8] = 2;
13: value[0] = 11; value[1] = 22; value[2] = 33; value[3] = 44;
14: value[4] = 0; value[5] = 21; value[6] = 32; value[7] = 41; value[8] = 43;
15:
16: lis_matrix_set_msr(nnz,ndz,index,value,A);
17: lis_matrix_assemble(A);

```

5.3.2 Creating a Matrix (MPI)

Figure 7 shows how matrix A in Figure 6 is stored in the MSR format with two processors. The program to create this matrix in the MSR format with two processors is as follows:

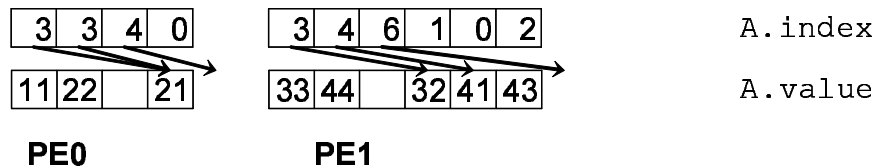


Figure 7: Data structures of MSR.

MPI

```

1: int      i,k,n,nnz,ndz,my_rank;
2: int      *index;
3: LIS_SCALAR *value;
4: LIS_MATRIX A;
5: MPI_Comm_rank(MPI_COMM_WORLD,&my_rank);
6: if( my_rank==0 ) {n = 2; nnz = 3; ndz = 0;}
7: else          {n = 2; nnz = 5; ndz = 0;}
8: index = (int *)malloc( (nnz+ndz+1)*sizeof(int) );
9: value = (LIS_SCALAR *)malloc( (nnz+ndz+1)*sizeof(LIS_SCALAR) );
10: lis_matrix_create(MPI_COMM_WORLD,&A);
11: lis_matrix_set_size(A,n,0);
12: if( my_rank==0 ) {
13:     index[0] = 3; index[1] = 3; index[2] = 4; index[3] = 0;
14:     value[0] = 11; value[1] = 22; value[2] = 0; value[3] = 21;}
15: else {
16:     index[0] = 3; index[1] = 4; index[2] = 6; index[3] = 1;
17:     index[4] = 0; index[5] = 2;
18:     value[0] = 33; value[1] = 44; value[2] = 0; value[3] = 32;
19:     value[4] = 41; value[5] = 43;}
20: lis_matrix_set_msr(nnz,ndz,index,value,A);
21: lis_matrix_assemble(A);

```

5.3.3 Associating Arrays

To associate the arrays required by the MSR format with matrix A , the following functions are used:

- C `int lis_matrix_set_msr(int nnz, int ndz, int index[], LIS_SCALAR value[], LIS_MATRIX A)`
- Fortran subroutine `lis_matrix_set_msr(integer nnz, integer ndz, integer index(), LIS_SCALAR value(), LIS_MATRIX A, integer ierr)`

5.4 Diagonal (DIA)

DIA uses two arrays (**index**, **value**) to store data. Assume that nnd represents the number of non-zero diagonals of matrix A .

- The **value** array, a double-precision array with a length of $nnd \times n$, stores non-zero diagonals of matrix A .
- The **index** array, an integer array with a length of nnd , stores the offsets from the main diagonal to the other diagonals.

For OpenMP, the following modifications have been made: DIA uses two arrays (**index**, **value**) to store data. Assume that $nprocs$ represents the number of threads. nnd_p is the number of non-zero diagonals of the partial matrix into which the row block of matrix A has been divided. $maxnnd$ is the maximum value nnd_p .

- The **value** array, a double-precision array with a length of $maxnnd \times n$, stores non-zero diagonals of matrix A .
- The **index** array, an integer array with a length of $nprocs \times maxnnd$, stores the offsets from the main diagonal to the other diagonals.

5.4.1 Creating a Matrix (Sequential)

The right-hand diagram in Figure 8 shows how matrix A in Figure 8 is stored in DIA format. The program to create this matrix in the DIA format is as follows:

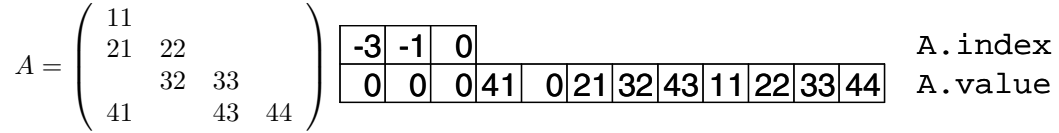


Figure 8: Data structures of DIA.

Sequential

```

1: int      n,nnd;
2: int      *index;
3: LIS_SCALAR *value;
4: LIS_MATRIX A;
5: n = 4; nnd = 3;
6: index = (int *)malloc( nnd*sizeof(int) );
7: value = (LIS_SCALAR *)malloc( n*nnd*sizeof(LIS_SCALAR) );
8: lis_matrix_create(0,&A);
9: lis_matrix_set_size(A,0,n);
10:
11: index[0] = -3; index[1] = -1; index[2] = 0;
12: value[0] = 0; value[1] = 0; value[2] = 0; value[3] = 41;
13: value[4] = 0; value[5] = 21; value[6] = 32; value[7] = 43;
14: value[8] = 11; value[9] = 22; value[10] = 33; value[11] = 44;
15:
16: lis_matrix_set_dia(nnd,index,value,A);
17: lis_matrix_assemble(A);

```


5.4.3 Creating a Matrix (MPI)

Figure 10 shows how matrix A in Figure 8 is stored in the DIA format with two processors. The program to create this matrix in the DIA format with two processors is as follows:

| | | | | | | | | | | | | |
|---|-----|----|---|----|---|----|---------|---|---|----|----|---------|
| <table><tr><td>-1</td><td>0</td></tr><tr><td>0</td><td>21</td></tr></table> | -1 | 0 | 0 | 21 | <table><tr><td>-3</td><td>-1</td><td>0</td></tr><tr><td>0</td><td>41</td><td>32</td></tr></table> | -3 | -1 | 0 | 0 | 41 | 32 | A.index |
| -1 | 0 | | | | | | | | | | | |
| 0 | 21 | | | | | | | | | | | |
| -3 | -1 | 0 | | | | | | | | | | |
| 0 | 41 | 32 | | | | | | | | | | |
| <table><tr><td>11</td><td>22</td></tr></table> | 11 | 22 | <table><tr><td>43</td><td>33</td><td>44</td></tr></table> | 43 | 33 | 44 | A.value | | | | | |
| 11 | 22 | | | | | | | | | | | |
| 43 | 33 | 44 | | | | | | | | | | |
| PE0 | PE1 | | | | | | | | | | | |

Figure 10: Data structures of DIA.

MPI

```

1: int          i,n,nnd,my_rank;
2: int          *index;
3: LIS_SCALAR   *value;
4: LIS_MATRIX   A;
5: MPI_Comm_rank(MPI_COMM_WORLD,&my_rank);
6: if( my_rank==0 ) {n = 2; nnd = 2;}
7: else          {n = 2; nnd = 3;}
8: index = (int *)malloc( nnd*sizeof(int) );
9: value = (LIS_SCALAR *)malloc( n*nnd*sizeof(LIS_SCALAR) );
10: lis_matrix_create(MPI_COMM_WORLD,&A);
11: lis_matrix_set_size(A,n,0);
12: if( my_rank==0 ) {
13:     index[0] = -1; index[1] = 0;
14:     value[0] = 0; value[1] = 21; value[2] = 11; value[3] = 22;}
15: else {
16:     index[0] = -3; index[1] = -1; index[2] = 0;
17:     value[0] = 0; value[1] = 41; value[2] = 32; value[3] = 43; value[4] = 33;
18:     value[5] = 44;}
19: lis_matrix_set_dia(nnd,index,value,A);
20: lis_matrix_assemble(A);

```

5.4.4 Associating Arrays

To associate the arrays required by the DIA format with matrix A , the following functions are used:

- C `int lis_matrix_set_dia(int nnd, int index[], LIS_SCALAR value[], LIS_MATRIX A)`
- Fortran subroutine `lis_matrix_set_dia(integer nnd, integer index(), LIS_SCALAR value(), LIS_MATRIX A, integer ierr)`

5.5 Ellpack-Itpack generalized diagonal (ELL)

ELL uses two arrays (`index`, `value`) to store data. Assume that *maxnzc* is the maximum value for the number of non-zero elements in the rows of matrix *A*.

- The `value` array, a double-precision array with a length of $\text{maxnzc} \times n$, stores non-zero elements of the rows of matrix *A* along the column. The first column consists of the number of first non-zero elements of the rows. If there is no number of non-zero elements to be stored, then 0 is stored.
- The `index` array, an integer array with a length of $\text{maxnzc} \times n$, stores the column numbers of the non-zero elements stored in the `value` array. If the number of non-zero elements in the *i*-th row is *nnz*, then `index[nnzi*n + i]` stores row number *i*.

5.5.1 Creating a Matrix (Sequential and OpenMP)

The right-hand diagram in Figure 11 shows how matrix *A* in Figure 11 is stored in the ELL format. The program to create this matrix in the ELL format is as follows:

$$A = \begin{pmatrix} 11 & & & & \\ 21 & 22 & & & \\ & 32 & 33 & & \\ 41 & & 43 & 44 & \end{pmatrix} \quad \begin{array}{|c|c|c|c|c|c|c|c|c|c|c|c|} \hline 0 & 0 & 1 & 0 & 0 & 1 & 2 & 2 & 0 & 1 & 2 & 3 \\ \hline 11 & 21 & 32 & 41 & 0 & 22 & 33 & 43 & 0 & 0 & 0 & 44 \\ \hline \end{array} \quad \begin{array}{l} \text{A.index} \\ \text{A.value} \end{array}$$

Figure 11: Data structures of ELL.

Sequential and OpenMP

```

1: int          n,maxnzc;
2: int          *index;
3: LIS_SCALAR   *value;
4: LIS_MATRIX   A;
5: n = 4; maxnzc = 3;
6: index = (int *)malloc( n*maxnzc*sizeof(int) );
7: value = (LIS_SCALAR *)malloc( n*maxnzc*sizeof(LIS_SCALAR) );
8: lis_matrix_create(0,&A);
9: lis_matrix_set_size(A,0,n);
10:
11: index[0] = 0; index[1] = 0; index[2] = 1; index[3] = 0; index[4] = 0; index[5] = 1;
12: index[6] = 2; index[7] = 2; index[8] = 0; index[9] = 1; index[10] = 2; index[11] = 3;
13: value[0] = 11; value[1] = 21; value[2] = 32; value[3] = 41; value[4] = 0; value[5] = 22;
14: value[6] = 33; value[7] = 43; value[8] = 0; value[9] = 0; value[10] = 0; value[11] = 44;
15:
16: lis_matrix_set_ell(maxnzc,index,value,A);
17: lis_matrix_assemble(A);

```

5.5.2 Creating a Matrix (MPI)

Figure 12 shows how matrix A in Figure 11 is stored in the ELL format. The program to create this matrix in the ELL format with two processors is as follows:

| | | | | | | | | | | | | | | | | | | | | | | |
|--|-----|----|----|---|----|----|---|----|--|---|---|---|---|---|---|----|----|----|----|---|----|--------------------|
| <table><tr><td>0</td><td>0</td><td>0</td><td>1</td></tr><tr><td>11</td><td>21</td><td>0</td><td>22</td></tr></table> | 0 | 0 | 0 | 1 | 11 | 21 | 0 | 22 | <table><tr><td>1</td><td>0</td><td>2</td><td>2</td><td>2</td><td>3</td></tr><tr><td>32</td><td>41</td><td>33</td><td>43</td><td>0</td><td>44</td></tr></table> | 1 | 0 | 2 | 2 | 2 | 3 | 32 | 41 | 33 | 43 | 0 | 44 | A.index A.value |
| 0 | 0 | 0 | 1 | | | | | | | | | | | | | | | | | | | |
| 11 | 21 | 0 | 22 | | | | | | | | | | | | | | | | | | | |
| 1 | 0 | 2 | 2 | 2 | 3 | | | | | | | | | | | | | | | | | |
| 32 | 41 | 33 | 43 | 0 | 44 | | | | | | | | | | | | | | | | | |
| PE0 | PE1 | | | | | | | | | | | | | | | | | | | | | |

Figure 12: Data structures of ELL.

MPI

```

1: int      i,n,maxnzs,my_rank;
2: int      *index;
3: LIS_SCALAR *value;
4: LIS_MATRIX A;
5: MPI_Comm_rank(MPI_COMM_WORLD,&my_rank);
6: if( my_rank==0 ) {n = 2; maxnzs = 2;}
7: else           {n = 2; maxnzs = 3;}
8: index = (int *)malloc( n*maxnzs*sizeof(int) );
9: value = (LIS_SCALAR *)malloc( n*maxnzs*sizeof(LIS_SCALAR) );
10: lis_matrix_create(MPI_COMM_WORLD,&A);
11: lis_matrix_set_size(A,n,0);
12: if( my_rank==0 ) {
13:     index[0] = 0; index[1] = 0; index[2] = 0; index[3] = 1;
14:     value[0] = 11; value[1] = 21; value[2] = 0; value[3] = 22;}
15: else {
16:     index[0] = 1; index[1] = 0; index[2] = 2; index[3] = 2; index[4] = 2;
17:     index[5] = 3;
18:     value[0] = 32; value[1] = 41; value[2] = 33; value[3] = 43; value[4] = 0;
19:     value[5] = 44;}
20: lis_matrix_set_ell(maxnzs,index,value,A);
21: lis_matrix_assemble(A);

```

5.5.3 Associating Arrays

To associate an array required for the ELL format with matrix A , the following functions are used:

- C `int lis_matrix_set_ell(int maxnzs, int index[], LIS_SCALAR value[], LIS_MATRIX A)`
- Fortran subroutine `lis_matrix_set_ell(integer maxnzs, integer index(), LIS_SCALAR value(), LIS_MATRIX A, integer ierr)`

5.6 Jagged Diagonal (JDS)

JDS first sorts the non-zero elements of the rows in decreasing order of size, and then stores them along the column. JDS uses four arrays (**perm**, **ptr**, **index**, **value**) to store the elements. Assume that $maxn_zr$ represents the maximum value for the number of non-zero elements of matrix A .

- The **perm** array, an integer array with a length of n , stores the sorted row numbers.
- The **value** array, a double-precision array with a length of nnz , stores jagged diagonals of sorted matrix A . The first jagged diagonals consist of the first non-zero elements of the rows. The next jagged diagonals, as well as later jagged diagonals, consist of the second non-zero elements.
- The **index** array, an integer array with a length of nnz , stores the row numbers of the non-zero elements stored in the **value** array.
- The **ptr** array, an integer array with a length of $maxn_zr + 1$, stores the starting points of the jagged diagonals.

For OpenMP, the following modifications have been made: JDS uses four arrays (**perm**, **ptr**, **index**, **value**) to store data. Assume that $nprocs$ is the number of threads. $maxn_zr_p$ is the number of non-zero diagonals of the partial matrix into which the row block of matrix A has been divided. $maxmaxn_zr$ is the maximum value of $maxn_zr_p$.

- The **perm** array, an integer array with a length of n , stores the sorted row numbers.
- The **value** array, a double-precision array with a length of nnz , stores jagged diagonals of sorted matrix A . The first jagged diagonals consist of the first non-zero elements of the rows. The next jagged diagonals, as well as the later diagonals, consist of the second non-zero elements.
- The **index** array, an integer array with a length of nnz , stores the row numbers of the non-zero elements stored in the **value** array.
- The **ptr** array, an integer array with a length of $nprocs \times (maxmaxn_zr + 1)$, stores the starting points of the jagged diagonals.

5.6.1 Creating a Matrix (Sequential)

The right-hand diagram in Figure 13 shows how matrix A in Figure 13 is stored in the JDS format. The program to create this matrix in the JDS format is as follows:

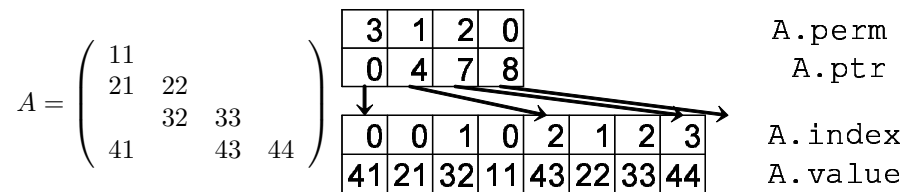


Figure 13: Data structures of JDS.

Sequential

```

1: int      n, nnz, maxnzs;
2: int      *perm, *ptr, *index;
3: LIS_SCALAR *value;
4: LIS_MATRIX A;
5: n = 4; nnz = 8; maxnzs = 3;
6: perm = (int *)malloc( n*sizeof(int) );
7: ptr = (int *)malloc( (maxnzs+1)*sizeof(int) );
8: index = (int *)malloc( nnz*sizeof(int) );
9: value = (LIS_SCALAR *)malloc( nnz*sizeof(LIS_SCALAR) );
10: lis_matrix_create(0, &A);
11: lis_matrix_set_size(A, 0, n);
12:
13: perm[0] = 3; perm[1] = 1; perm[2] = 2; perm[3] = 0;
14: ptr[0] = 0; ptr[1] = 4; ptr[2] = 7; ptr[3] = 8;
15: index[0] = 0; index[1] = 0; index[2] = 1; index[3] = 0;
16: index[4] = 2; index[5] = 1; index[6] = 2; index[7] = 3;
17: value[0] = 41; value[1] = 21; value[2] = 32; value[3] = 11;
18: value[4] = 43; value[5] = 22; value[6] = 33; value[7] = 44;
19:
20: lis_matrix_set_jds(nnz, maxnzs, perm, ptr, index, value, A);
21: lis_matrix_assemble(A);

```

5.6.2 Creating a Matrix (OpenMP)

Figure 14 shows how matrix A in Figure 13 is stored in the JDS format with two threads. The program to create this matrix in the JDS format with two threads is as follows:

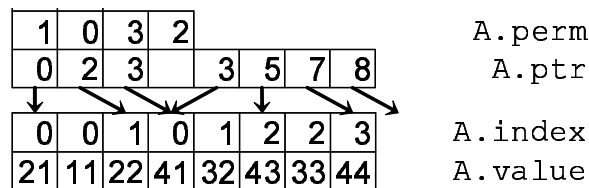


Figure 14: Data structures of JDS.

OpenMP

```

1: int      n,nnz,maxmaxnzs,nprocs;
2: int      *perm,*ptr,*index;
3: LIS_SCALAR *value;
4: LIS_MATRIX A;
5: n = 4; nnz = 8; maxmaxnzs = 3; nprocs = 2;
6: perm = (int *)malloc( n*sizeof(int) );
7: ptr = (int *)malloc( nprocs*(maxmaxnzs+1)*sizeof(int) );
8: index = (int *)malloc( nnz*sizeof(int) );
9: value = (LIS_SCALAR *)malloc( nnz*sizeof(LIS_SCALAR) );
10: lis_matrix_create(0,&A);
11: lis_matrix_set_size(A,0,n);
12:
13: perm[0] = 1; perm[1] = 0; perm[2] = 3; perm[3] = 2;
14: ptr[0] = 0; ptr[1] = 2; ptr[2] = 3; ptr[3] = 0;
15: ptr[4] = 3; ptr[5] = 5; ptr[6] = 7; ptr[7] = 8;
16: index[0] = 0; index[1] = 0; index[2] = 1; index[3] = 0;
17: index[4] = 1; index[5] = 2; index[6] = 2; index[7] = 3;
18: value[0] = 21; value[1] = 11; value[2] = 22; value[3] = 41;
19: value[4] = 32; value[5] = 43; value[6] = 33; value[7] = 44;
20:
21: lis_matrix_set_jds(nnz,maxmaxnzs,perm,ptr,index,value,A);
22: lis_matrix_assemble(A);

```

5.6.3 Creating a Matrix (MPI)

Figure 15 shows how matrix A in Figure 13 is stored in the JDS format with two processors. The program to create this matrix in the JDS format with two processors is as follows:

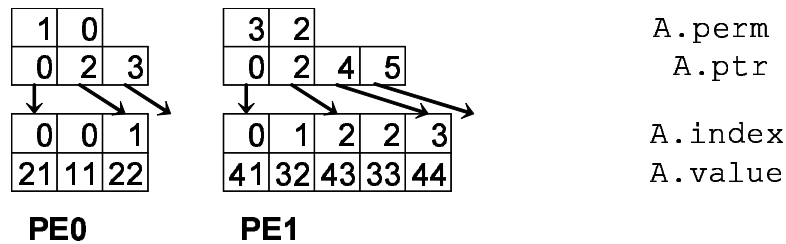


Figure 15: Data structures of JDS.

MPI

```

1: int          i,n,nnz,maxnzs,my_rank;
2: int          *perm,*ptr,*index;
3: LIS_SCALAR   *value;
4: LIS_MATRIX   A;
5: MPI_Comm_rank(MPI_COMM_WORLD,&my_rank);
6: if( my_rank==0 ) {n = 2; nnz = 3; maxnzs = 2;}
7: else         {n = 2; nnz = 5; maxnzs = 3;}
8: perm = (int *)malloc( n*sizeof(int) );
9: ptr = (int *)malloc( (maxnzs+1)*sizeof(int) );
10: index = (int *)malloc( nnz*sizeof(int) );
11: value = (LIS_SCALAR *)malloc( nnz*sizeof(LIS_SCALAR) );
12: lis_matrix_create(MPI_COMM_WORLD,&A);
13: lis_matrix_set_size(A,n,0);
14: if( my_rank==0 ) {
15:     perm[0] = 1; perm[1] = 0;
16:     ptr[0] = 0; ptr[1] = 2; ptr[2] = 3;
17:     index[0] = 0; index[1] = 0; index[2] = 1;
18:     value[0] = 21; value[1] = 11; value[2] = 22;}
19: else {
20:     perm[0] = 3; perm[1] = 2;
21:     ptr[0] = 0; ptr[1] = 2; ptr[2] = 4; ptr[3] = 5;
22:     index[0] = 0; index[1] = 1; index[2] = 2; index[3] = 2; index[4] = 3;
23:     value[0] = 41; value[1] = 32; value[2] = 43; value[3] = 33; value[4] = 44;}
24: lis_matrix_set_jds(nnz,maxnzs,perm,ptr,index,value,A);
25: lis_matrix_assemble(A);

```

5.6.4 Associating Arrays

To associate an array required for the JDS format with matrix A , the following functions are used:

- C `int lis_matrix_set_jds(int nnz, int maxnzs, int perm[], int ptr[], int index[], LIS_SCALAR value[], LIS_MATRIX A)`
- Fortran subroutine `lis_matrix_set_jds(integer nnz, integer maxnzs, integer ptr(), integer index(), LIS_SCALAR value(), LIS_MATRIX A, integer ierr)`

5.7 Block Sparse Row (BSR)

BSR breaks down each matrix into partial matrixes (called blocks) with a size of $r \times c$. BSR stores non-zero blocks (blocks in which at least one non-zero element exists) with the same step as that for the CRS format. Assume that $nr = n/r$ and $nnzb$ are the numbers of non-zero blocks of A . BSR uses three arrays (`bp`, `bind`, `value`) to store matrices.

- The `value` array, a double-precision array with a length of $nnzb \times r \times c$, stores all elements of the non-zero blocks.
- The `bind` array, an integer array with a length of $nnzb$, stores block column numbers of the non-zero blocks.
- The `bp` array, an integer array with a length of $nr + 1$, stores the starting points of the block rows in the `bind` array.

5.7.1 Creating a Matrix (Sequential and OpenMP)

The right-hand diagram in Figure 16 shows how matrix A in Figure 16 is stored in the BSR format. The program to create this matrix in the BSR format is as follows:

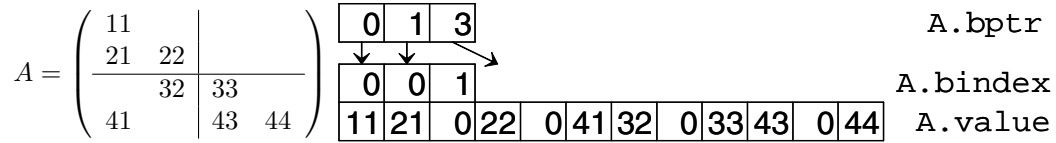


Figure 16: Data structures of BSR.

Sequential and OpenMP

```

1: int          n, bnr, bnc, nr, nc, bnnz;
2: int          *bp, *bind;
3: LIS_SCALAR   *value;
4: LIS_MATRIX   A;
5: n = 4; bnr = 2; bnc = 2; bnnz = 3; nr = (n-1)/bnr+1; nc = (n-1)/bnc+1;
6: bp = (int *)malloc( (nr+1)*sizeof(int) );
7: bind = (int *)malloc( bnnz*sizeof(int) );
8: value = (LIS_SCALAR *)malloc( bnr*bnc*bnnz*sizeof(LIS_SCALAR) );
9: lis_matrix_create(0, &A);
10: lis_matrix_set_size(A, 0, n);
11:
12: bp[0] = 0; bp[1] = 1; bp[2] = 3;
13: bind[0] = 0; bind[1] = 0; bind[2] = 1;
14: value[0] = 11; value[1] = 21; value[2] = 0; value[3] = 22;
15: value[4] = 0; value[5] = 41; value[6] = 32; value[7] = 0;
16: value[8] = 33; value[9] = 43; value[10] = 0; value[11] = 44;
17:
18: lis_matrix_set_bsr(bnr, bnc, bnnz, bp, bind, value, A);
19: lis_matrix_assemble(A);

```

5.7.2 Creating a Matrix (MPI)

Figure 17 shows how matrix A in Figure 16 is stored in the BSR format with two processors. The program to create this matrix in the BSR format with two processors is as follows:

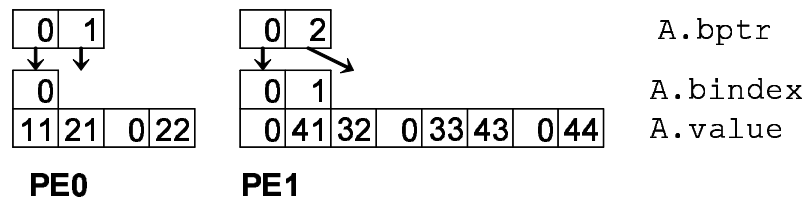


Figure 17: Data structures of BSR.

MPI

```

1: int      n, bnr, bnc, nr, nc, bnnz, my_rank;
2: int      *bptr, *bindex;
3: LIS_SCALAR *value;
4: LIS_MATRIX A;
5: MPI_Comm_rank(MPI_COMM_WORLD, &my_rank);
6: if( my_rank==0 ) {n = 2; bnr = 2; bnc = 2; bnnz = 1; nr = (n-1)/bnr+1; nc = (n-1)/bnc+1;}
7: else      {n = 2; bnr = 2; bnc = 2; bnnz = 2; nr = (n-1)/bnr+1; nc = (n-1)/bnc+1;}
8: bptr = (int *)malloc( (nr+1)*sizeof(int) );
9: bindex = (int *)malloc( bnnz*sizeof(int) );
10: value = (LIS_SCALAR *)malloc( bnr*bnc*bnnz*sizeof(LIS_SCALAR) );
11: lis_matrix_create(MPI_COMM_WORLD, &A);
12: lis_matrix_set_size(A, n, 0);
13: if( my_rank==0 ) {
14:     bptr[0] = 0; bptr[1] = 1;
15:     bindex[0] = 0;
16:     value[0] = 11; value[1] = 21; value[2] = 0; value[3] = 22;}
17: else {
18:     bptr[0] = 0; bptr[1] = 2;
19:     bindex[0] = 0; bindex[1] = 1;
20:     value[0] = 0; value[1] = 41; value[2] = 32; value[3] = 0;
21:     value[4] = 33; value[5] = 43; value[6] = 0; value[7] = 44;}
22: lis_matrix_set_bsr(bnr, bnc, bnnz, bptr, bindex, value, A);
23: lis_matrix_assemble(A);

```

5.7.3 Associating Arrays

To associate the arrays required by the BSR format with matrix A , the following functions are used:

- C `int lis_matrix_set_bsr(int bnr, int bnc, int bnnz, int bptr[], int bindex[], LIS_SCALAR value[], LIS_MATRIX A)`
- Fortran subroutine `lis_matrix_set_bsr(integer bnr, integer bnc, integer bnnz, integer bptr(), integer bindex(), LIS_SCALAR value(), LIS_MATRIX A, integer ierr)`

5.8 Block Sparse Column (BSC)

BSC breaks down each matrix into partial matrixes (called blocks) with a size of $r \times c$. BSC stores non-zero blocks (blocks in which at least one non-zero block exists) in the same step as that for the CCS format. Assume that $nc = n/c$ and $nnzb$ are the numbers of non-zero blocks of A. BSC uses three arrays (**bp**tr, **bin**dex, **val**ue) to store matrices.

- The **value** array, a double-precision array with a length of $nnzb \times r \times c$, stores all elements of the non-zero blocks.
- The **bin**dex array, an integer array with a length of $nnzb$, stores block row numbers of the non-zero blocks.
- The **bp**tr array, an integer array with a length of $nc + 1$, stores the starting points of the block columns in the **bin**dex array.

5.8.1 Creating a Matrix (Sequential and OpenMP)

The right-hand diagram in Figure 18 shows how matrix A in Figure 18 is stored in the BSC format. The program to create this matrix in the BSC format is as follows:

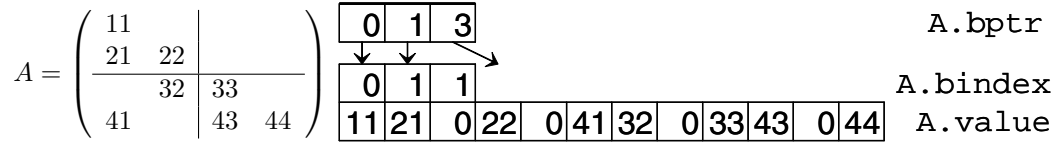


Figure 18: Data structures of BSC.

Sequential and OpenMP

```

1: int          n, bnr, bnc, nr, nc, bnnz;
2: int          *bpctr, *bindex;
3: LIS_SCALAR   *value;
4: LIS_MATRIX   A;
5: n = 4; bnr = 2; bnc = 2; bnnz = 3; nr = (n-1)/bnr+1; nc = (n-1)/bnc+1;
6: bpctr = (int *)malloc( (nc+1)*sizeof(int) );
7: bindex = (int *)malloc( bnnz*sizeof(int) );
8: value = (LIS_SCALAR *)malloc( bnr*bnc*bnnz*sizeof(LIS_SCALAR) );
9: lis_matrix_create(0, &A);
10: lis_matrix_set_size(A, 0, n);
11:
12: bpctr[0] = 0; bpctr[1] = 1; bpctr[2] = 3;
13: bindex[0] = 0; bindex[1] = 1; bindex[2] = 1;
14: value[0] = 11; value[1] = 21; value[2] = 0; value[3] = 22;
15: value[4] = 0; value[5] = 41; value[6] = 32; value[7] = 0;
16: value[8] = 33; value[9] = 43; value[10] = 0; value[11] = 44;
17:
18: lis_matrix_set_bsc(bnr, bnc, bnnz, bpctr, bindex, value, A);
19: lis_matrix_assemble(A);

```

5.8.2 Creating a Matrix (MPI)

Figure 19 shows how matrix A in Figure 18 is stored in the BSC format with two processors. The program to create this matrix in the BSC format with two processors is as follows:

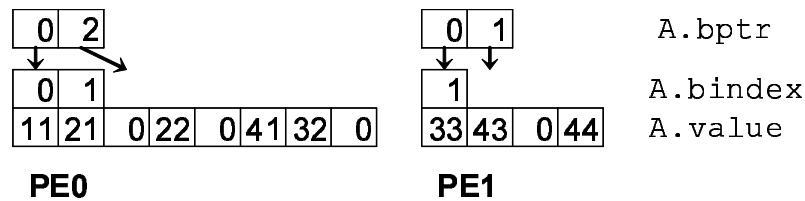


Figure 19: Data structures of BSC.

MPI

```

1: int      n, bnr, bnc, nr, nc, bnnz, my_rank;
2: int      *bptr, *bindex;
3: LIS_SCALAR *value;
4: LIS_MATRIX A;
5: MPI_Comm_rank(MPI_COMM_WORLD, &my_rank);
6: if( my_rank==0 ) {n = 2; bnr = 2; bnc = 2; bnnz = 2; nr = (n-1)/bnr+1; nc = (n-1)/bnc+1;}
7: else      {n = 2; bnr = 2; bnc = 2; bnnz = 1; nr = (n-1)/bnr+1; nc = (n-1)/bnc+1;}
8: bptr = (int *)malloc( (nr+1)*sizeof(int) );
9: bindex = (int *)malloc( bnnz*sizeof(int) );
10: value = (LIS_SCALAR *)malloc( bnr*bnc*bnnz*sizeof(LIS_SCALAR) );
11: lis_matrix_create(MPI_COMM_WORLD, &A);
12: lis_matrix_set_size(A, n, 0);
13: if( my_rank==0 ) {
14:     bptr[0] = 0; bptr[1] = 2;
15:     bindex[0] = 0; bindex[1] = 1;
16:     value[0] = 11; value[1] = 21; value[2] = 0; value[3] = 22;
17:     value[4] = 0; value[5] = 41; value[6] = 32; value[7] = 0;}
18: else {
19:     bptr[0] = 0; bptr[1] = 1;
20:     bindex[0] = 1;
21:     value[0] = 33; value[1] = 43; value[2] = 0; value[3] = 44;}
22: lis_matrix_set_bsc(bnr, bnc, bnnz, bptr, bindex, value, A);
23: lis_matrix_assemble(A);

```

5.8.3 Associating Arrays

To associate the arrays required by the BSC format with matrix A , the following functions are used:

- C `int lis_matrix_set_bsc(int bnr, int bnc, int bnnz, int bptr[], int bindex[], LIS_SCALAR value[], LIS_MATRIX A)`
- Fortran subroutine `lis_matrix_set_bsc(integer bnr, integer bnc, integer bnnz, integer bptr(), integer bindex(), LIS_SCALAR value(), LIS_MATRIX A, integer ierr)`

5.9 Variable Block Row (VBR)

VBR is a generalized version of BSR. The division points of the rows and columns are given by the arrays (`row` and `col`). VBR stores non-zero blocks (blocks in which at least one non-zero block exists) in the same step as that for the CRS format. Assume that nr and nc are the numbers of row and column divisions, respectively, and that $nnzb$ denotes the number of non-zero blocks of A , and nnz denotes the total number of elements of the non-zero blocks. VBR uses six arrays (`bptr`, `bindex`, `row`, `col`, `ptr` and `value`) to store matrices.

- The `row` array, an integer array with a length of $nr + 1$, stores the starting row number of the block rows.
- The `col` array, an integer array with a length of $nc + 1$, stores the starting column number of the block columns.
- The `bindex` array, an integer array with a length of $nnzb$, stores the block column numbers of the non-zero blocks.
- The `bptr` array, an integer array with a length of $nr + 1$, stores the starting point of the block rows in the `bindex` array.
- The `value` array, a double-precision array with a length of nnz , stores all elements of the non-zero blocks.
- The `ptr` array, an integer array with a length of $nnzb + 1$, stores the starting points of the non-zero blocks in the `value` array.

5.9.1 Creating a Matrix (Sequential and OpenMP)

The right-hand diagram in Figure 20 shows how matrix A in Figure 20 is stored in the VBR format. The program to create this matrix in the VBR format is as follows:

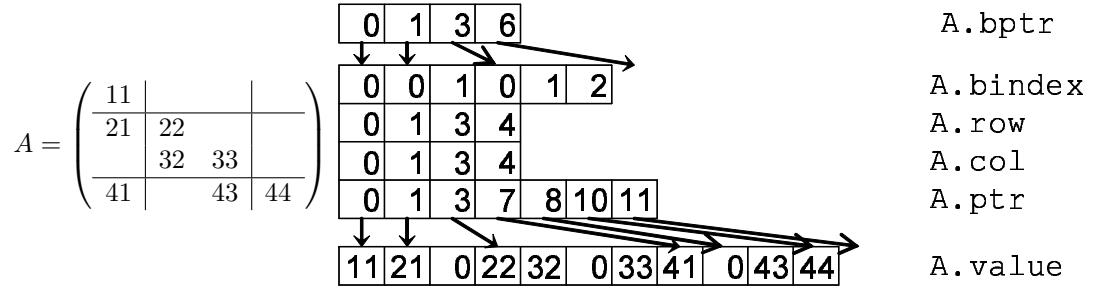


Figure 20: Data structures of VBR.


```

1: int          n,nnz,nr,nc,bnnz;
2: int          *row,*col,*ptr,*bptr,*bindex;
3: LIS_SCALAR   *value;
4: LIS_MATRIX   A;
5: n = 4; nnz = 11; bnnz = 6; nr = 3; nc = 3;
6: bptr  = (int *)malloc( (nr+1)*sizeof(int) );
7: row   = (int *)malloc( (nr+1)*sizeof(int) );
8: col   = (int *)malloc( (nc+1)*sizeof(int) );
9: ptr   = (int *)malloc( (bnnz+1)*sizeof(int) );
10: bindex = (int *)malloc( bnnz*sizeof(int) );
11: value = (LIS_SCALAR *)malloc( nnz*sizeof(LIS_SCALAR) );
12: lis_matrix_create(0,&A);
13: lis_matrix_set_size(A,0,n);
14:
15: bptr[0] = 0; bptr[1] = 1; bptr[2] = 3; bptr[3] = 6;
16: row[0]  = 0; row[1]  = 1; row[2]  = 3; row[3]  = 4;
17: col[0]  = 0; col[1]  = 1; col[2]  = 3; col[3]  = 4;
18: bindex[0] = 0; bindex[1] = 0; bindex[2] = 1; bindex[3] = 0;
19: bindex[4] = 1; bindex[5] = 2;
20: ptr[0]   = 0; ptr[1]   = 1; ptr[2]   = 3; ptr[3]   = 7;
21: ptr[4]   = 8; ptr[5]   = 10; ptr[6]   = 11;
22: value[0] = 11; value[1] = 21; value[2] = 0; value[3] = 22;
23: value[4] = 32; value[5] = 0; value[6] = 33; value[7] = 41;
24: value[8] = 0; value[9] = 43; value[10] = 44;
25:
26: lis_matrix_set_vbr(nnz,nr,nc,bnnz,row,col,ptr,bptr,bindex,value,A);
27: lis_matrix_assemble(A);

```

5.9.2 Creating a Matrix (MPI)

Figure 21 shows how matrix A in Figure 20 is stored in the VBR format with two processors. The program to create this matrix in the VBR format with two processors is as follows:

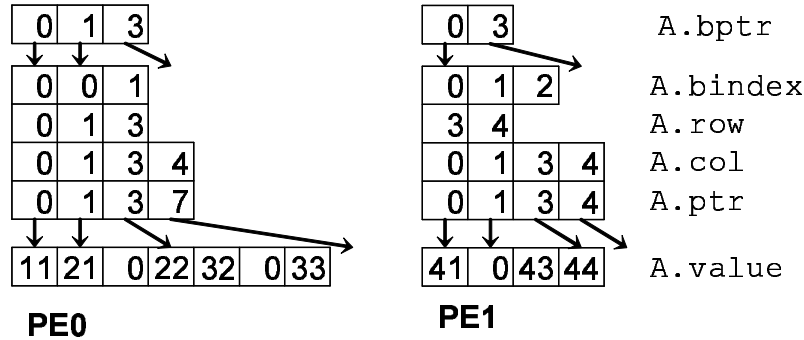


Figure 21: Data structures of VBR.

MPI

```

1: int          n,nnz,nr,nc,bnnz,my_rank;
2: int          *row,*col,*ptr,*bptr,*bindex;
3: LIS_SCALAR   *value;
4: LIS_MATRIX   A;
5: MPI_Comm_rank(MPI_COMM_WORLD,&my_rank);
6: if( my_rank==0 ) {n = 2; nnz = 7; bnnz = 3; nr = 2; nc = 3;}
7: else          {n = 2; nnz = 4; bnnz = 3; nr = 1; nc = 3;}
8: bptr  = (int *)malloc( (nr+1)*sizeof(int) );
9: row   = (int *)malloc( (nr+1)*sizeof(int) );
10: col   = (int *)malloc( (nc+1)*sizeof(int) );
11: ptr   = (int *)malloc( (bnnz+1)*sizeof(int) );
12: bindex = (int *)malloc( bnnz*sizeof(int) );
13: value = (LIS_SCALAR *)malloc( nnz*sizeof(LIS_SCALAR) );
14: lis_matrix_create(MPI_COMM_WORLD,&A);
15: lis_matrix_set_size(A,n,0);
16: if( my_rank==0 ) {
17:     bptr[0] = 0; bptr[1] = 1; bptr[2] = 3;
18:     row[0]  = 0; row[1]  = 1; row[2]  = 3;
19:     col[0]  = 0; col[1]  = 1; col[2]  = 3; col[3] = 4;
20:     bindex[0] = 0; bindex[1] = 0; bindex[2] = 1;
21:     ptr[0]   = 0; ptr[1]   = 1; ptr[2]   = 3; ptr[3]   = 7;
22:     value[0] = 11; value[1] = 21; value[2] = 0; value[3] = 22;
23:     value[4] = 32; value[5] = 0; value[6] = 33;}
24: else {
25:     bptr[0] = 0; bptr[1] = 3;
26:     row[0]  = 3; row[1]  = 4;
27:     col[0]  = 0; col[1]  = 1; col[2]  = 3; col[3] = 4;
28:     bindex[0] = 0; bindex[1] = 1; bindex[2] = 2;
29:     ptr[0]   = 0; ptr[1]   = 1; ptr[2]   = 3; ptr[3]   = 4;
30:     value[0] = 41; value[1] = 0; value[2] = 43; value[3] = 44;}
31: lis_matrix_set_vbr(nnz,nr,nc,bnnz,row,col,ptr,bptr,bindex,value,A);
32: lis_matrix_assemble(A);

```

5.9.3 Associating Arrays

To associate the arrays required by the VBR format with matrix A, the following functions are used:

- C `int lis_matrix_set_vbr(int nnz, int nr, int nc, int bnnz, int row[], int col[], int ptr[], int bptr[], int bindex[], LIS_SCALAR value[], LIS_MATRIX A)`
- Fortran subroutine `lis_matrix_set_vbr(integer nnz, integer nr, integer nc, integer bnnz, integer row(), integer col(), integer ptr(), integer bptr(), integer bindex(), LIS_SCALAR value(), LIS_MATRIX A, integer ierr)`

5.10 Coordinate (COO)

COO uses three arrays (`row`, `col` and `value`) to store data.

- The `value` array, a double-precision array with a length of nnz , stores non-zero elements.
- The `row` array, an integer array with a length of nnz , stores the row numbers of the non-zero elements.
- The `col` array, an integer array with a length of nnz , stores the column numbers of the non-zero elements.

5.10.1 Creating a Matrix (Sequential and OpenMP)

The right-hand diagram in Figure 22 shows how matrix A in Figure 22 is stored in the COO format. The program to create this matrix in the COO format is as follows:

$$A = \begin{pmatrix} 11 & & & & \\ 21 & 22 & & & \\ & 32 & 33 & & \\ 41 & & 43 & 44 & \end{pmatrix} \quad \begin{array}{|c|c|c|c|c|c|c|c|} \hline 0 & 1 & 3 & 1 & 2 & 2 & 3 & 3 \\ \hline 0 & 0 & 0 & 1 & 1 & 2 & 2 & 3 \\ \hline 11 & 21 & 41 & 22 & 32 & 33 & 43 & 44 \\ \hline \end{array} \quad \begin{array}{l} A.\text{row} \\ A.\text{col} \\ A.\text{value} \end{array}$$

Figure 22: Data structures of COO.

Sequential and OpenMP

```

1: int          n,nnz;
2: int          *row,*col;
3: LIS_SCALAR   *value;
4: LIS_MATRIX   A;
5: n = 4; nnz = 8;
6: row = (int *)malloc( nnz*sizeof(int) );
7: col = (int *)malloc( nnz*sizeof(int) );
8: value = (LIS_SCALAR *)malloc( nnz*sizeof(LIS_SCALAR) );
9: lis_matrix_create(0,&A);
10: lis_matrix_set_size(A,0,n);
11:
12: row[0] = 0; row[1] = 1; row[2] = 3; row[3] = 1;
13: row[4] = 2; row[5] = 2; row[6] = 3; row[7] = 3;
14: col[0] = 0; col[1] = 0; col[2] = 0; col[3] = 1;
15: col[4] = 1; col[5] = 2; col[6] = 2; col[7] = 3;
16: value[0] = 11; value[1] = 21; value[2] = 41; value[3] = 22;
17: value[4] = 32; value[5] = 33; value[6] = 43; value[7] = 44;
18:
19: lis_matrix_set_coo(nnz,row,col,value,A);
20: lis_matrix_assemble(A);

```

5.10.2 Creating a Matrix (MPI)

Figure 23 shows how matrix A in Figure 22 is stored in the COO format with two processors. The program to create this matrix in the COO format with two processors is as follows:

| | | | | | | | | | | | | | | | | | | | | | | | | | | |
|---|-----|----|----|----|---|---|----|----|----|---|---|---|---|---|---|---|---|---|---|---|----|----|----|----|----|---------------------------|
| <table><tr><td>0</td><td>1</td><td>1</td></tr><tr><td>0</td><td>0</td><td>1</td></tr><tr><td>11</td><td>21</td><td>22</td></tr></table> | 0 | 1 | 1 | 0 | 0 | 1 | 11 | 21 | 22 | <table><tr><td>3</td><td>2</td><td>2</td><td>3</td><td>3</td></tr><tr><td>0</td><td>1</td><td>2</td><td>2</td><td>3</td></tr><tr><td>41</td><td>32</td><td>33</td><td>43</td><td>44</td></tr></table> | 3 | 2 | 2 | 3 | 3 | 0 | 1 | 2 | 2 | 3 | 41 | 32 | 33 | 43 | 44 | A.row A.col A.value |
| 0 | 1 | 1 | | | | | | | | | | | | | | | | | | | | | | | | |
| 0 | 0 | 1 | | | | | | | | | | | | | | | | | | | | | | | | |
| 11 | 21 | 22 | | | | | | | | | | | | | | | | | | | | | | | | |
| 3 | 2 | 2 | 3 | 3 | | | | | | | | | | | | | | | | | | | | | | |
| 0 | 1 | 2 | 2 | 3 | | | | | | | | | | | | | | | | | | | | | | |
| 41 | 32 | 33 | 43 | 44 | | | | | | | | | | | | | | | | | | | | | | |
| PE0 | PE1 | | | | | | | | | | | | | | | | | | | | | | | | | |

Figure 23: Data structures of COO.

MPI

```

1: int      n,nnz,my_rank;
2: int      *row,*col;
3: LIS_SCALAR *value;
4: LIS_MATRIX A;
5: MPI_Comm_rank(MPI_COMM_WORLD,&my_rank);
6: if( my_rank==0 ) {n = 2; nnz = 3;}
7: else {n = 2; nnz = 5;}
8: row = (int *)malloc( nnz*sizeof(int) );
9: col = (int *)malloc( nnz*sizeof(int) );
10: value = (LIS_SCALAR *)malloc( nnz*sizeof(LIS_SCALAR) );
11: lis_matrix_create(MPI_COMM_WORLD,&A);
12: lis_matrix_set_size(A,n,0);
13: if( my_rank==0 ) {
14:     row[0] = 0; row[1] = 1; row[2] = 1;
15:     col[0] = 0; col[1] = 0; col[2] = 1;
16:     value[0] = 11; value[1] = 21; value[2] = 22;}
17: else {
18:     row[0] = 3; row[1] = 2; row[2] = 2; row[3] = 3; row[4] = 3;
19:     col[0] = 0; col[1] = 1; col[2] = 2; col[3] = 2; col[4] = 3;
20:     value[0] = 41; value[1] = 32; value[2] = 33; value[3] = 43; value[4] = 44;}
21: lis_matrix_set_coo(nnz,row,col,value,A);
22: lis_matrix_assemble(A);

```

5.10.3 Associating Arrays

To associate the arrays required by the COO format with matrix A , the following functions are used:

- C `int lis_matrix_set_coo(int nnz, int row[], int col[], LIS_SCALAR value[], LIS_MATRIX A)`
- Fortran subroutine `lis_matrix_set_coo(integer nnz, integer row(), integer col(), LIS_SCALAR value(), LIS_MATRIX A, integer ierr)`

5.11 Dense (DNS)

DNS uses one array (**value**) to store data.

- The **value** array, a double-precision array with a length of $n \times n$, stores elements with priority given to columns.

5.11.1 Creating a Matrix (Sequential and OpenMP)

The right-hand diagram in Figure 24 shows how matrix A in Figure 24 is stored in the DNS format. The program to create this matrix in the DNS format is as follows:

$$A = \begin{pmatrix} 11 & & & & \\ 21 & 22 & & & \\ & 32 & 33 & & \\ 41 & & 43 & 44 & \end{pmatrix} \quad \begin{array}{|c|c|c|c|c|c|c|c|} \hline 11 & 21 & 0 & 41 & 0 & 22 & 32 & 0 \\ \hline 0 & 0 & 33 & 43 & 0 & 0 & 0 & 44 \\ \hline \end{array} \quad \text{A.Value}$$

Figure 24: Data structures of DNS.

Sequential and OpenMP

```

1: int          n;
2: LIS_SCALAR   *value;
3: LIS_MATRIX   A;
4: n = 4;
5: value = (LIS_SCALAR *)malloc( n*n*sizeof(LIS_SCALAR) );
6: lis_matrix_create(0,&A);
7: lis_matrix_set_size(A,0,n);
8:
9: value[0] = 11; value[1] = 21; value[2] = 0; value[3] = 41;
10: value[4] = 0; value[5] = 22; value[6] = 32; value[7] = 0;
11: value[8] = 0; value[9] = 0; value[10] = 33; value[11] = 43;
12: value[12] = 0; value[13] = 0; value[14] = 0; value[15] = 44;
13:
14: lis_matrix_set_dns(value,A);
15: lis_matrix_assemble(A);

```

5.11.2 Creating a Matrix (MPI)

Figure 25 shows how matrix A in Figure 24 is stored in the DNS format with two processors. The program to create this matrix in the DNS format with two processors is as follows:

| | | | | | | | | |
|------------|-----------|----------|-----------|------------|-----------|-----------|-----------|---------|
| 11 | 21 | 0 | 22 | 0 | 41 | 32 | 0 | A.Value |
| 0 | 0 | 0 | 0 | 33 | 43 | 0 | 44 | |
| PE0 | | | | PE1 | | | | |

Figure 25: Data structures of DNS.

```

MPI
1: int          n,my_rank;
2: LIS_SCALAR   *value;
3: LIS_MATRIX   A;
4: MPI_Comm_rank(MPI_COMM_WORLD,&my_rank);
5: if( my_rank==0 ) {n = 2;}
6: else          {n = 2;}
7: value = (LIS_SCALAR *)malloc( n*n*sizeof(LIS_SCALAR) );
8: lis_matrix_create(MPI_COMM_WORLD,&A);
9: lis_matrix_set_size(A,n,0);
10: if( my_rank==0 ) {
11:     value[0] = 11; value[1] = 21; value[2] = 0; value[3] = 22;
12:     value[4] = 0; value[5] = 0; value[6] = 0; value[7] = 0;}
13: else {
14:     value[0] = 0; value[1] = 41; value[2] = 32; value[3] = 0;
15:     value[4] = 33; value[5] = 43; value[6] = 0; value[7] = 44;}
16: lis_matrix_set_dns(value,A);
17: lis_matrix_assemble(A);

```

5.11.3 Associating Arrays

To associate the arrays required by the DNS format with matrix A , the following functions are used:

- C `int lis_matrix_set_dns(LIS_SCALAR value[], LIS_MATRIX A)`
- Fortran subroutine `lis_matrix_set_dns(LIS_SCALAR value(), LIS_MATRIX A, integer ierr)`

6 Functions

This section describes the functions that can be employed by users. The return value of the function in C and the value of `ierr` in Fortran are as follows:

Return value

| | |
|-------------------------------------|--|
| <code>LIS_SUCCESS(0)</code> | Normal termination |
| <code>LIS_ILL_OPTION(1)</code> | Illegal option |
| <code>LIS_BREAKDOWN(2)</code> | Breakdown |
| <code>LIS_OUT_OF_MEMORY(3)</code> | Insufficient working memory |
| <code>LIS_MAXITER(4)</code> | Did not converge within the maximum number of iterations |
| <code>LIS_NOT_IMPLEMENTED(5)</code> | Not implemented |
| <code>LIS_ERR_FILE_IO(6)</code> | File I/O error |

6.1 Vector Operations

Assume that the order of vector v is `global_n` and that the row number of each block into which the row block of vector v has been divided with `nprocs` units of processors is `local_n`. `global_n` and `local_n` are called the global order and the local order, respectively.

6.1.1 `lis_vector_create`

```
C      int lis_vector_create(LIS_Comm comm, LIS_VECTOR *vec)
Fortran subroutine lis_vector_create(LIS_Comm comm, LIS_VECTOR vec, integer ierr)
```

Capability

Creating vector v

Input

| | |
|-----------------------|------------------|
| <code>LIS_Comm</code> | MPI communicator |
|-----------------------|------------------|

Output

| | |
|-------------------|-------------|
| <code>vec</code> | Vector |
| <code>ierr</code> | Return code |

Note

For sequential and OpenMP versions, the value for `comm` is ignored.

6.1.2 lis_vector_destroy

```
C      int lis_vector_destroy(LIS_VECTOR vec)
Fortran subroutine lis_vector_destroy(LIS_VECTOR vec, integer ierr)
```

Capability

Removing unwanted vectors from memory

Input

| | |
|-----|----------------------------------|
| vec | Vector to be removed from memory |
|-----|----------------------------------|

Output

| | |
|------|-------------|
| ierr | Return code |
|------|-------------|

6.1.3 lis_vector_duplicate

```
C      int lis_vector_duplicate(void *vin, LIS_VECTOR *vout)
Fortran subroutine lis_vector_duplicate(LIS_VECTOR vin, LIS_VECTOR vout,
      integer ierr)
```

Capability

Creating a vector that has the same information as an existing vector.

Input

| | |
|-----|---------------|
| vin | Source vector |
|-----|---------------|

Output

| | |
|------|--------------------|
| vout | Destination vector |
| ierr | Return code |

Note

The `lis_vector_duplicate` function does not copy the values, but only reserves an area. To copy the values as well, the function `lis_vector_copy` must be used after this function.

6.1.4 lis_vector_set_size

```
C      int lis_vector_set_size(LIS_VECTOR vec, int local_n, int global_n)
Fortran subroutine lis_vector_set_size(LIS_VECTOR vec, integer local_n,
                                     integer global_n, integer ierr)
```

Capability

Assigning vector size

Input

| | |
|----------|----------------------------|
| vec | Vector |
| local_n | Local order of the vector |
| global_n | Global order of the vector |

Output

| | |
|------|-------------|
| ierr | Return code |
|------|-------------|

Note

Either `local_n` or `global_n` must be provided. This function can create a vector in one of the following ways: Creating partial vectors of order `local_n` from `local_n`, or creating from `global_n` partial vectors into which the row block of the vector of order `global_n` has been divided from a given number of processors.

In the case of Sequential and OpenMP versions, `local_n = global_n`. This means that both `lis_vector_set_size(v,n,0)` and `lis_vector_set_size(v,0,n)` create a vector of order n .

6.1.5 lis_vector_get_size

```
C      int lis_vector_get_size(LIS_VECTOR v, int *local_n, int *global_n)
Fortran subroutine lis_vector_get_size(LIS_VECTOR v, integer local_n,
                                     integer global_n, integer ierr)
```

Capability

Ascertaining the size of vector v

Input

| | |
|---|--------|
| v | Vector |
|---|--------|

Output

| | |
|----------|----------------------------|
| local_n | Local order of the vector |
| global_n | Global order of the vector |
| ierr | Return code |

Note

In the case of Sequential and OpenMP versions, `local_n = global_n`.

6.1.6 lis_vector_get_range

```
C      int lis_vector_get_range(LIS_VECTOR v, int *is, int *ie)
Fortran subroutine lis_vector_get_range(LIS_VECTOR v, integer is, integer ie,
      integer ierr)
```

Capability

Ascertaining where in the whole vector the partial vector v is located

Input

| | |
|---|----------------|
| v | Partial vector |
|---|----------------|

Output

| | |
|------|--|
| is | Number of the row at which partial vector v starts in the whole vector. |
| ie | 1+ number of the row at which partial vector v ends in the whole vector. |
| ierr | Return code |

Note

For Sequential and OpenMP versions, an n -th order vector results in `is = 0` and `ie = n`.

6.1.7 lis_vector_set_value

```
C      int lis_vector_set_value(int flag, int i, LIS_SCALAR value, LIS_VECTOR v)
Fortran subroutine lis_vector_set_value(integer flag, integer i, LIS_SCALAR value,
      LIS_VECTOR v, integer ierr)
```

Capability

Assigning a scalar `value` to the i -th row of vector v

Input

| | |
|-------|--|
| flag | LIS_INS.VALUE Assignment : $v[i] = \text{value}$ LIS_ADD.VALUE Assignment add: $v[i] = v[i] + \text{value}$ |
| i | Place at which the value should be assigned |
| value | Scalar value to assign |
| v | Destination Vector |

Output

| | |
|------|--|
| v | Vector with the scalar <code>value</code> assigned to its i -th row. |
| ierr | Return code |

Note

For MPI, the i -th row of the whole vector must be specified instead of the i -th row of the partial vector.

6.1.8 lis_vector_get_value

```
C      int lis_vector_get_value(LIS_VECTOR v, int i, LIS_SCALAR *value)
Fortran subroutine lis_vector_get_value(LIS_VECTOR v, integer i, LIS_SCALAR value,
      integer ierr)
```

Capability

Ascertaining a scalar of the i -th row of vector v .

Input

| | |
|-----|---|
| i | Place to which the value should be assigned |
| v | Destination Vector |

Output

| | |
|-------|----------------------------|
| value | Scalar of its i -th row. |
| ierr | Return code |

Note

For MPI, the i -th row of the whole vector must be specified rather than the i -th row of the partial vector.

6.1.9 lis_vector_set_values

```
C      int lis_vector_set_values(int flag, int count, int index[],
                                LIS_SCALAR value[], LIS_VECTOR v)
Fortran subroutine lis_vector_set_values(integer flag, integer count,
                                         integer index(), LIS_SCALAR value(), LIS_VECTOR v, integer ierr)
```

Capability

Assigning a scalar `value[i]` to the `index[i]`-th row of vector `v`

Input

| | |
|-------|---|
| flag | <code>LIS_INS_VALUE</code> Assignment : <code>v[index[i]] = value[i]</code> <code>LIS_ADD_VALUE</code> Assignment add: <code>v[index[i]] = v[index[i]] + value[i]</code> |
| index | Number of elements of array which stores the scalar values to be assigned |
| index | Array which stores the places at which the value should be assigned |
| value | Array which stores scalar values to be assigned |
| v | Destination Vector |

Output

| | |
|------|---|
| v | Vector with the scalar <code>value[i]</code> assigned to its <code>index[i]</code> -th row. |
| ierr | Return code |

Note

For MPI, the `index[i]`-th row of the whole vector must be specified instead of the `index[i]`-th row of the partial vector.

6.1.10 lis_vector_get_values

```
C      int lis_vector_get_values(LIS_VECTOR v, int start, int count,
                                LIS_SCALAR value[])
Fortran subroutine lis_vector_get_values(LIS_VECTOR v, integer start,
                                         integer count, LIS_SCALAR value(), integer ierr)
```

Capability

Ascertaining scalar values of the `start + i`-th row of vector `v`, where $i = 0, 1, \dots, \text{start} - 1$.

Input

| | |
|-------|--|
| start | Start place to which the values should be assigned |
| count | Number of the values to be ascertained |
| v | Destination Vector |

Output

| | |
|-------|------------------------------------|
| value | Vector which stores scalar values. |
| ierr | Return code |

Note

For MPI, the `start + i`-th row of the whole vector must be specified rather than the `start + i`-th row of the partial vector.

6.1.11 lis_vector_copy

```
C      int lis_vector_copy(LIS_VECTOR x, LIS_VECTOR y)
Fortran subroutine lis_vector_copy(LIS_VECTOR x, LIS_VECTOR y, integer ierr)
```

Capability

Copying the value of a vector: $y \leftarrow x$

Input

| | |
|---|---------------|
| x | Source vector |
|---|---------------|

Output

| | |
|------|--------------------|
| y | Destination vector |
| ierr | Return code |

6.1.12 lis_vector_set_all

```
C      int lis_vector_set_all(LIS_SCALAR value, LIS_VECTOR x)
Fortran subroutine lis_vector_set_all(LIS_SCALAR value, LIS_VECTOR x, integer ierr)
```

Capability

Assigning a Scalar Value **value** to all elements of a vector

Input

| | |
|-------|------------------------|
| value | Scalar value to assign |
| v | Target vector |

Output

| | |
|------|---|
| v | Vector with the value assigned to all its elements |
| ierr | Return code |

6.2 Matrix Operations

Assume that the order of matrix A is `global_n` \times `global_n` and that the number of rows of each partial matrix into which the row block of matrix A has been divided with `nprocs` units of processors is `local_n`. Here, `global_n` and `local_n` are called the global number of rows and the local number of rows, respectively.

6.2.1 `lis_matrix_create`

```
C      int lis_matrix_create(LIS_Comm comm, LIS_MATRIX *A)
Fortran subroutine lis_matrix_create(LIS_Comm comm, LIS_MATRIX A, integer ierr)
```

Capability

Creating matrix A

Input

| | |
|-----------------------|------------------|
| <code>LIS_Comm</code> | MPI communicator |
|-----------------------|------------------|

Output

| | |
|-------------------|-------------|
| <code>A</code> | Matrix |
| <code>ierr</code> | Return code |

Note

For Sequential and OpenMP versions, the value for `comm` is ignored.

6.2.2 `lis_matrix_destroy`

```
C      int lis_matrix_destroy(LIS_MATRIX A)
Fortran subroutine lis_matrix_destroy(LIS_MATRIX A, integer ierr)
```

Capability

Removing unwanted matrixes from memory

Input

| | |
|----------------|------------------------------|
| <code>A</code> | Matrix to remove from memory |
|----------------|------------------------------|

Output

| | |
|-------------------|-------------|
| <code>ierr</code> | Return code |
|-------------------|-------------|

6.2.3 lis_matrix_duplicate

```
C      int lis_matrix_duplicate(LIS_MATRIX Ain, LIS_MATRIX *Aout)
Fortran subroutine lis_matrix_duplicate(LIS_MATRIX Ain, LIS_MATRIX Aout,
      integer ierr)
```

Capability

Creating a matrix that has the same information as an existing matrix.

Input

| | |
|-----|---------------|
| Ain | Source matrix |
|-----|---------------|

Output

| | |
|------|--------------------|
| Aout | Destination matrix |
| ierr | Return code |

Note

The `lis_matrix_duplicate` function does not copy the values of the elements of the matrix, but only reserves an area. To copy the values of the elements as well, the `lis_matrix_copy` function must be used.

6.2.4 lis_matrix_malloc

```
C      int lis_matrix_malloc(LIS_MATRIX A, int nnz_row, int nnz[])
Fortran subroutine lis_matrix_malloc(LIS_MATRIX A, integer nnz_row, integer nnz[],
      integer ierr)
```

Capability

The area where the matrix elements are stored is allocated.

Input

| | |
|---------|---|
| A | Matrix |
| nnz_row | Average of non-zero element numbers |
| nnz | Array of non-zero element numbers of each row |

Output

| | |
|------|-------------|
| ierr | Return code |
|------|-------------|

Note

Either `nnz_row` or `nnz` must be provided.

6.2.5 lis_matrix_set_value

```
C      int lis_matrix_set_value(int flag, int i, int j, LIS_SCALAR value,  
                             LIS_MATRIX A)  
Fortran subroutine lis_matrix_set_value(integer flag, integer i, integer j,  
                                       LIS_SCALAR value, LIS_MATRIX A, integer ierr)
```

Capability

Assigning an element to the cell of i -th row and j -th column of matrix **A**

Input

| | |
|-------|--|
| flag | LIS_INS.VALUE Assignment : $A(i,j) = \text{value}$ LIS_ADD.VALUE Assignment add: $A(i,j) = A(i,j) + \text{value}$ |
| i | Row number of the matrix |
| j | Column number of the matrix |
| value | Value to assign |
| A | Matrix |

Output

| | |
|------|--|
| A | Matrix with the element assigned to the cell of the i -th row and j -th column |
| ierr | Return code |

Note

For MPI, the i -th row and j -th column of the whole matrix must be specified, rather than the i -th row and j -th column of the partial matrix.

The `lis_matrix_set_value` function stores the assigned value in a temporary internal format. For this reason, when `lis_matrix_set_value` has been used, the `lis_matrix_assemble` function must be called.

6.2.6 lis_matrix_assemble

```
C      int lis_matrix_assemble(LIS_MATRIX A)  
Fortran subroutine lis_matrix_assemble(LIS_MATRIX A, integer ierr)
```

Capability

Building a matrix

Input

| | |
|---|--------|
| A | Matrix |
|---|--------|

Output

| | |
|------|--|
| A | Matrix built in the specified storage format |
| ierr | Return code |

6.2.7 lis_matrix_set_size

```
int lis_matrix_set_size(LIS_MATRIX A, int local_n, int global_n)
Fortran subroutine lis_matrix_set_size(LIS_MATRIX A, integer local_n,
integer global_n, integer ierr)
```

Capability

Assigning matrix size

Input

| | |
|----------|--|
| A | Matrix |
| local_n | Local number of rows of matrix <i>A</i> |
| global_n | Global number of rows of matrix <i>A</i> |

Output

| | |
|------|-------------|
| ierr | Return code |
|------|-------------|

Note

Either `local_n` or `global_n` must be provided. This function can create matrices in one of the following two ways: Creating partial matrices of order `local_n` x *N* from `local_n`, or creating partial matrices into which the row block of the vector of order `global_n` x `global_n` from `global_n` has been divided with a given number of processors. *N* represents the total sum of `local_n` of each processor.

In case of Sequential and OpenMP versions, `local_n = global_n`. This means that both `lis_matrix_set_size(A,n,0)` and `lis_matrix_set_size(A,0,n)` create a matrix of *n* x *n*.

For MPI version, `lis_matrix_set_size(A,n,0)` creates at each processor *p* a partial matrix of $n_p \times N$, where *N* is the total sum of n_p of each processor. On the other hand, `lis_matrix_set_size(A,0,n)` creates at each processor *p* a partial matrix of $m_p \times n$, where m_p is the number of the partial matrix, which is determined by the library.

6.2.8 lis_matrix_get_size

```
C      int lis_matrix_get_size(LIS_MATRIX A, int *local_n, int *global_n)
Fortran subroutine lis_matrix_get_size(LIS_MATRIX A, integer local_n,
integer global_n, integer ierr)
```

Capability

Ascertaining matrix size

Input

| | |
|---|--------|
| A | Matrix |
|---|--------|

Output

| | |
|----------|--|
| local_n | Local number of rows of matrix <i>A</i> |
| global_n | Global number of rows of matrix <i>A</i> |
| ierr | Return code |

Note

In case of Sequential and OpenMP versions, `local_n = global_n`.

6.2.9 lis_matrix_get_range

```
C      int lis_matrix_get_range(LIS_MATRIX A, int *is, int *ie)
Fortran subroutine lis_matrix_get_range(LIS_MATRIX A, integer is, integer ie,
      integer ierr)
```

Capability

Ascertaining where in the whole matrix partial matrix A is located.

Input

| | |
|---|----------------|
| A | Partial matrix |
|---|----------------|

Output

| | |
|------|---|
| is | Number of the row at which partial matrix A starts in the whole matrix. |
| ie | 1+ the number of the row at which partial matrix A ends in the whole matrix |
| ierr | Return code |

Note

For Sequential and OpenMP versions, a matrix of $n \times n$ results in **is** = 0 and **ie** = **n**.

6.2.10 lis_matrix_set_type

```
C      int lis_matrix_set_type(LIS_MATRIX A, int matrix_type)
Fortran subroutine lis_matrix_set_type(LIS_MATRIX A, int matrix_type, integer ierr)
```

Capability

Assigning storage format

Input

| | |
|-------------|----------------|
| A | Matirx |
| matrix_type | Storage format |

Output

| | |
|------|-------------|
| ierr | Return code |
|------|-------------|

Note

`matrix_type` of A is `LIS_MATRIX_CRS` when the matrix is created. The table below shows the allowable storage formats for `matrix_type`.

| storage format | | matrix_type |
|-------------------------------------|-------|----------------|
| Compressed Row Storage | (CRS) | LIS_MATRIX_CRS |
| Compressed Column Storage | (CCS) | LIS_MATRIX_CCS |
| Modified Compressed Sparse Row | (MSR) | LIS_MATRIX_MSR |
| Diagonal | (DIA) | LIS_MATRIX_DIA |
| Ellpack-Itpack generalized diagonal | (ELL) | LIS_MATRIX_ELL |
| Jagged Diagonal | (JDS) | LIS_MATRIX_JDS |
| Block Sparse Row | (BSR) | LIS_MATRIX_BSR |
| Block Sparse Column | (BSC) | LIS_MATRIX_BSC |
| Variable Block Row | (VBR) | LIS_MATRIX_VBR |
| Dense | (DNS) | LIS_MATRIX_DNS |
| Coordinate | (COO) | LIS_MATRIX_COO |

6.2.11 lis_matrix_get_type

```
C      int lis_matrix_get_type(LIS_MATRIX A, int *matrix_type)
Fortran subroutine lis_matrix_get_type(LIS_MATRIX A, integer matrix_type,
      integer ierr)
```

Capability

Ascertaining storage format

Input

| | |
|---|--------|
| A | Matrix |
|---|--------|

Output

| | |
|-------------|----------------|
| matrix_type | Storage format |
| ierr | Return code |

6.2.12 lis_matrix_set_blocksize

```
C      int lis_matrix_set_blocksize(LIS_MATRIX A, int bnr, int bnc, int row[],
                                   int col[])
Fortran subroutine lis_matrix_set_blocksize(LIS_MATRIX A, integer bnr, integer bnc,
                                           integer row[], integer col[], integer ierr)
```

Capability

Assigning block size for BSR, BSC, and VBR

Input

| | |
|-----|--|
| A | Matrix |
| bnr | Row block size for BSR (BSC) or the number of row blocks for VBR |
| bnc | Column block size for BSR (BSC) or the number of column blocks for VBR |
| row | Array of the row division information about VBR |
| col | Array of the column division information about VBR |

Output

| | |
|------|-------------|
| ierr | Return code |
|------|-------------|

6.2.13 lis_matrix_convert

```
C      int lis_matrix_convert(LIS_MATRIX Ain, LIS_MATRIX Aout)
Fortran subroutine lis_matrix_convert(LIS_MATRIX Ain, LIS_MATRIX Aout, integer ierr)
```

Capability

Converting the storage type of matrix *Ain* into a desired type to create matrix *Aout*.

Input

| | |
|-----|---------------|
| Ain | Source matrix |
|-----|---------------|

Output

| | |
|------|--|
| Aout | Matrix with the storage type converted into the specified type |
| ierr | Return code |

Note

The specification of the converted storage format is set to *Aout* by using `lis_matrix_set_type`. The specification of the block size of BSR, BSC, and VBR is set to *Aout* by using `lis_matrix_set_blocksize`.

In converting the storage type of the source matrix into a specified type, the conversions indicated by 1 in the table below are performed directly, and the other conversions are made via the indicated types. The conversions with no indication are made via the CRS type.

| Src \ Dst | CRS | CCS | MSR | DIA | ELL | JDS | BSR | BSC | VBR | DNS | COO |
|-----------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| CRS | 1 | 1 | 1 | 1 | 1 | 1 | 1 | CCS | 1 | 1 | 1 |
| COO | 1 | 1 | 1 | CRS | CRS | CRS | CRS | CCS | CRS | CRS | 1 |

6.2.14 lis_matrix_copy

```
C      int lis_matrix_copy(LIS_MATRIX Ain, LIS_MATRIX Aout)
Fortran subroutine lis_matrix_copy(LIS_MATRIX Ain, LIS_MATRIX Aout, integer ierr)
```

Capability

Copies the values of the elements

Input

| | |
|-----|---------------|
| Ain | Source matrix |
|-----|---------------|

Output

| | |
|------|--------------------|
| Aout | Destination matrix |
| ierr | Return code |

6.2.15 lis_matrix_get_diagonal

```
C      int lis_matrix_get_diagonal(LIS_MATRIX A, LIS_VECTOR d)
Fortran subroutine lis_matrix_get_diagonal(LIS_MATRIX A, LIS_VECTOR d, integer ierr)
```

Capability

Storing the diagonals of matrix A in vector d

Input

| | |
|---|--------|
| A | Matrix |
|---|--------|

Output

| | |
|------|--|
| d | Vector that contains the diagonals of the matrix |
| ierr | Return code |

6.2.16 lis_matrix_set_crs

```
C      int lis_matrix_set_crs(int nnz, int ptr[], int index[], LIS_SCALAR value[],
                             LIS_MATRIX A)
Fortran subroutine lis_matrix_set_crs(integer nnz, integer row(), integer index(),
                                     LIS_SCALAR value(), LIS_MATRIX A, integer ierr)
```

Capability

Associating the arrays required by the CRS format created by the user with matrix A

Input

| | |
|-------------------|-----------------------------|
| nnz | Number of non-zero elements |
| ptr, index, value | Arrays for the CRS format |
| A | Matrix |

Output

| | |
|---|------------------------------|
| A | Matrix and associated arrays |
|---|------------------------------|

Note

When the `lis_matrix_set_crs` function has been used, the `lis_matrix_assemble` function must be called.

6.2.17 lis_matrix_set_ccs

```
C      int lis_matrix_set_ccs(int nnz, int ptr[], int index[], LIS_SCALAR value[],
                             LIS_MATRIX A)
Fortran subroutine lis_matrix_set_ccs(integer nnz, integer row(), integer index(),
                                     LIS_SCALAR value(), LIS_MATRIX A, integer ierr)
```

Capability

Associating the arrays required by the CCS format created by the user with matrix A

Input

| | |
|-------------------|-----------------------------|
| nnz | Number of non-zero elements |
| ptr, index, value | Arrays for the CCS format |
| A | Matrix |

Output

| | |
|---|------------------------------|
| A | Matrix and associated arrays |
|---|------------------------------|

Note

When the `lis_matrix_set_ccs` function has been used, the `lis_matrix_assemble` function must be called.

6.2.18 lis_matrix_set_msr

```
C      int lis_matrix_set_msr(int nnz, int ndz, int index[], LIS_SCALAR value[],
                             LIS_MATRIX A)
Fortran subroutine lis_matrix_set_msr(integer nnz, integer ndz, integer index(),
                                     LIS_SCALAR value(), LIS_MATRIX A, integer ierr)
```

Capability

Associating the arrays required by the MSR format created by the user with matrix A

Input

| | |
|--------------|---|
| nnz | Number of non-zero elements |
| ndz | Number of non-zero elements at the diagonal |
| index, value | Arrays for the MSR format |
| A | Matrix |

Output

| | |
|---|------------------------------|
| A | Matrix and associated arrays |
|---|------------------------------|

Note

When the `lis_matrix_set_msr` function has been used, the `lis_matrix_assemble` function must be called.

6.2.19 lis_matrix_set_dia

```
C      int lis_matrix_set_dia(int nnd, int index[], LIS_SCALAR value[],
                             LIS_MATRIX A)
Fortran subroutine lis_matrix_set_dia(integer nnd, integer index(),
                                     LIS_SCALAR value(), LIS_MATRIX A, integer ierr)
```

Capability

Associating the arrays required by the DIA format created by the user with matrix A

Input

| | |
|--------------|------------------------------|
| nnd | Number of non-zero diagonals |
| index, value | Arrays for the DIA format |
| A | Matrix |

Output

| | |
|---|------------------------------|
| A | Matrix and associated arrays |
|---|------------------------------|

Note

When the `lis_matrix_set_dia` function has been used, the `lis_matrix_assemble` function must be called.

6.2.20 lis_matrix_set_ell

```
C      int lis_matrix_set_ell(int maxnzs, int index[], LIS_SCALAR value[],
                             LIS_MATRIX A)
Fortran subroutine lis_matrix_set_ell(integer maxnzs, integer index(),
                                     LIS_SCALAR value(), LIS_MATRIX A, integer ierr)
```

Capability

Associating the arrays required by the ELL format created by the user with matrix A

Input

| | |
|--------------|---|
| maxnzs | Maximum number of non-zero elements at each row |
| index, value | Arrays for the ELL format |
| A | Matrix |

Output

| | |
|---|------------------------------|
| A | Matrix and associated arrays |
|---|------------------------------|

Note

When the `lis_matrix_set_ell` function has been used, the `lis_matrix_assemble` function must be called.

6.2.21 lis_matrix_set_jds

```
C      int lis_matrix_set_jds(int nnz, int maxnzs, int perm[], int ptr[],
                             int index[], LIS_SCALAR value[], LIS_MATRIX A)
Fortran subroutine lis_matrix_set_jds(integer nnz, integer maxnzs, integer ptr(),
                                     integer index(), LIS_SCALAR value(), LIS_MATRIX A, integer ierr)
```

Capability

Associating the arrays required by the JDS format created by the user with matrix A

Input

| | |
|-------------------------|---|
| nnz | Number of non-zero elements |
| maxnzs | Maximum number of non-zero elements in each row |
| perm, ptr, index, value | Arrays for the JDS format |
| A | Matrix |

Output

| | |
|---|------------------------------|
| A | Matrix and associated arrays |
|---|------------------------------|

Note

When the `lis_matrix_set_jds` function has been used, the `lis_matrix_assemble` function must be called.

6.2.22 lis_matrix_set_bsr

```
C      int lis_matrix_set_bsr(int bnr, int bnc, int bnnz, int bptr[], int bindx[],
                             LIS_SCALAR value[], LIS_MATRIX A)
Fortran subroutine lis_matrix_set_bsr(integer bnr, integer bnc, integer bnnz,
                                     integer bptr(), integer bindx(), LIS_SCALAR value(), LIS_MATRIX A,
                                     integer ierr)
```

Capability

Associating the arrays required by the BSR format created by the user with matrix A

Input

| | |
|--------------------|---------------------------|
| bnr | Row block size |
| bnc | Column block size |
| bnnz | Number of non-zero blocks |
| bptr, bindx, value | Arrays for the BSR format |
| A | Matrix |

Output

| | |
|---|------------------------------|
| A | Matrix and associated arrays |
|---|------------------------------|

Note

When the `lis_matrix_set_bsr` function has been used, the `lis_matrix_assemble` function must be called.

6.2.23 lis_matrix_set_bsc

```
C      int lis_matrix_set_bsc(int bnr, int bnc, int bnnz, int bptr[], int bindex[],
        LIS_SCALAR value[], LIS_MATRIX A)
Fortran subroutine lis_matrix_set_bsc(integer bnr, integer bnc, integer bnnz,
        integer bptr(), integer bindex(), LIS_SCALAR value(), LIS_MATRIX A,
        integer ierr)
```

Capability

Associating the arrays required by the BSC format created by the user with matrix A

Input

| | |
|---------------------|---------------------------|
| bnr | Row block size |
| bnc | Column block size |
| bnnz | Number of non-zero blocks |
| bptr, bindex, value | Arrays for the BSC format |
| A | Matrix |

Output

| | |
|---|------------------------------|
| A | Matrix and associated arrays |
|---|------------------------------|

Note

When the `lis_matrix_set_bsc` function has been used, the `lis_matrix_assemble` function must be called.

6.2.24 lis_matrix_set_vbr

```
C      int lis_matrix_set_vbr(int nnz, int nr, int nc, int bnnz, int row[],
                             int col[], int ptr[], int bptr[], int bindex[], LIS_SCALAR value[],
                             LIS_MATRIX A)
Fortran subroutine lis_matrix_set_vbr(integer nnz, integer nr, integer nc,
                                     integer bnnz, integer row(), integer col(), integer ptr(), integer bptr(),
                                     integer bindex(), LIS_SCALAR value(), LIS_MATRIX A, integer ierr)
```

Capability

Associating the arrays required by the VBR format created by the user with matrix A

Input

| | |
|------------------------------------|---------------------------------|
| nnz | Number of all non-zero elements |
| nr | Number of row blocks |
| nc | Number of column blocks |
| bnnz | Number of non-zero blocks |
| row, col, ptr, bptr, bindex, value | Arrays for the VBR format |
| A | Matrix |

Output

| | |
|---|------------------------------|
| A | Matrix and associated arrays |
|---|------------------------------|

Note

When the `lis_matrix_set_vbr` function has been used, the `lis_matrix_assemble` function must be called.

6.2.25 lis_matrix_set_coo

```
C      int lis_matrix_set_coo(int nnz, int row[], int col[], LIS_SCALAR value[],
                             LIS_MATRIX A)
Fortran subroutine lis_matrix_set_coo(integer nnz, integer row(), integer col(),
                                     LIS_SCALAR value(), LIS_MATRIX A, integer ierr)
```

Capability

Associating the arrays required by the COO format created by the user with matrix A

Input

| | |
|-----------------|-----------------------------|
| nnz | Number of non-zero elements |
| row, col, value | Arrays for the COO format |
| A | Matrix |

Output

| | |
|---|------------------------------|
| A | Matrix and associated arrays |
|---|------------------------------|

Note

When the `lis_matrix_set_coo` function has been used, the `lis_matrix_assemble` function must be called.

6.2.26 lis_matrix_set_dns

```
C      int lis_matrix_set_dns(LIS_SCALAR value[], LIS_MATRIX A)
Fortran subroutine lis_matrix_set_dns(LIS_SCALAR value(), LIS_MATRIX A, integer ierr)
```

Capability

Associating the arrays required by the DNS format created by the user with matrix A

Input

| | |
|-------|---------------------------|
| value | Arrays for the DNS format |
| A | Matrix |

Output

| | |
|---|------------------------------|
| A | Matrix and associated arrays |
|---|------------------------------|

Note

When the `lis_matrix_set_dns` function has been used, the `lis_matrix_assemble` function must be called.

6.3 Vector and Matrix Operations

6.3.1 lis_vector_scale

```
C      int lis_vector_scale(LIS_SCALAR alpha, LIS_VECTOR x)
Fortran subroutine lis_vector_scale(LIS_SCALAR alpha, LIS_VECTOR x, integer ierr)
```

Capability

Multiplying all values of a vector by **alpha**: $x \leftarrow \alpha x$

Input

| | |
|-------|------------------------------------|
| alpha | Scalar value |
| x | Vector to multiply by alpha |

Output

| | |
|------|---|
| x | Vector with all its elements multiplied by alpha |
| ierr | Return code |

6.3.2 lis_vector_dot

```
C      int lis_vector_dot(LIS_VECTOR x, LIS_VECTOR y, LIS_SCALAR *val)
Fortran subroutine lis_vector_dot(LIS_VECTOR x, LIS_VECTOR y, LIS_SCALAR val,
                                integer ierr)
```

Capability

Calculating the inner product: $val \leftarrow x^T y$

Input

| | |
|---|--------|
| x | Vector |
| y | Vector |

Output

| | |
|------|---------------------|
| val | Inner product value |
| ierr | Return code |

6.3.3 lis_vector_nrm2

```
C      int lis_vector_nrm2(LIS_VECTOR x, LIS_SCALAR *val)
Fortran subroutine lis_vector_nrm2(LIS_VECTOR x, LIS_SCALAR val, integer ierr)
```

Capability

Calculating 2-norms of a vector: $val \leftarrow \|x\|_2$

Input

| | |
|---|--------|
| x | Vector |
|---|--------|

Output

| | |
|------|-----------------------|
| val | 2-norms of the vector |
| ierr | Return code |

6.3.4 lis_vector_nrm1

```
C      int lis_vector_nrm1(LIS_VECTOR x, LIS_SCALAR *val)
Fortran subroutine lis_vector_nrm1(LIS_VECTOR x, LIS_SCALAR val, integer ierr)
```

Capability

Calculating 1-norms of a vector: $val \leftarrow ||x||_2$

Input

| | |
|---|--------|
| x | Vector |
|---|--------|

Output

| | |
|------|-----------------------|
| val | 1-norms of the vector |
| ierr | Return code |

6.3.5 lis_vector_axpy

```
C      int lis_vector_axpy(LIS_SCALAR alpha, LIS_VECTOR x, LIS_VECTOR y)
Fortran subroutine lis_vector_axpy(LIS_SCALAR alpha, LIS_VECTOR x, LIS_VECTOR y,
                                   integer ierr)
```

Capability

Calculating $y \leftarrow \alpha x + y$

Input

| | |
|-------|--------------|
| alpha | Scalar value |
| x, y | Vector |

Output

| | |
|------|---|
| y | Calculation result of $\alpha x + y$ (the value of vector y is overwritten) |
| ierr | Return code |

6.3.6 lis_vector_xpay

```
C      int lis_vector_xpay(LIS_VECTOR x, LIS_SCALAR alpha, LIS_VECTOR y)
Fortran subroutine lis_vector_xpay(LIS_VECTOR x, LIS_SCALAR alpha, LIS_VECTOR y,
                                   integer ierr)
```

Capability

Calculating $y \leftarrow x + \alpha y$

Input

| | |
|-------|--------------|
| alpha | Scalar value |
| x, y | Vector |

Output

| | |
|------|---|
| y | Calculation result of $x + \alpha y$ (the value of vector y is overwritten) |
| ierr | Return code |

6.3.7 lis_vector_axpyz

```
C      int lis_vector_axpyz(LIS_SCALAR alpha, LIS_VECTOR x, LIS_VECTOR y,  
                           LIS_VECTOR z)  
Fortran subroutine lis_vector_axpyz(LIS_SCALAR alpha, LIS_VECTOR x, LIS_VECTOR y,  
                                   LIS_VECTOR z, integer ierr)
```

Capability

Calculating $z \leftarrow \alpha x + y$

Input

| | |
|-------|--------------|
| alpha | Scalar value |
| x, y | Vector |

Output

| | |
|------|--------------------------------------|
| z | Calculation result of $x + \alpha y$ |
| ierr | Return code |

6.3.8 lis_matrix_scaling

```
C      int lis_matrix_scaling(LIS_MATRIX A, LIS_VECTOR b, LIS_VECTOR d, int action)  
Fortran subroutine lis_matrix_scaling(LIS_MATRIX A, LIS_VECTOR b,  
                                   LIS_VECTOR d, integer action, integer ierr)
```

Capability

Performing matrix scaling

Input

| | |
|--------|--|
| A | Matrix |
| b | Vector |
| action | LIS_SCALE_JACOBI Jacobi scaling $D^{-1}Ax = D^{-1}b$, D represents the diagonal of $A = (a_{ij})$ LIS_SCALE_SYMM_DIAG Diagonal scaling $D^{-1/2}AD^{-1/2}x = D^{-1/2}b$, $D^{-1/2}$ represents an diagonal matrix that has $1/\sqrt{a_{ii}}$ as an diagonal element |

Output

| | |
|------|--|
| d | Vector that contains the diagonals of D^{-1} or $D^{-1/2}$ |
| ierr | Return code |

6.3.9 lis_matvec

```
C      void lis_matvec(LIS_MATRIX A, LIS_VECTOR x, LIS_VECTOR y)
Fortran subroutine lis_matvec(LIS_MATRIX A, LIS_VECTOR x, LIS_VECTOR y)
```

Capability

Performing the matrix vector product $y \leftarrow Ax$

Input

| | |
|---|--------|
| A | Matrix |
| x | Vector |

Output

| | |
|---|--------|
| y | Vector |
|---|--------|

6.3.10 lis_matvect

```
C      void lis_matvect(LIS_MATRIX A, LIS_VECTOR x, LIS_VECTOR y)
Fortran subroutine lis_matvect(LIS_MATRIX A, LIS_VECTOR x, LIS_VECTOR y)
```

Capability

Performing the transpose matrix vector product $y \leftarrow A^T x$

Input

| | |
|---|--------|
| A | Matrix |
| x | Vector |

Output

| | |
|---|--------|
| y | Vector |
|---|--------|

6.4 Solving Linear Equation

6.4.1 lis_solver_create

```
C      int lis_solver_create(LIS_SOLVER *solver)
Fortran subroutine lis_solver_create(LIS_SOLVER solver, integer ierr)
```

Capability

Creating SOLVER

Input

None

Output

| | |
|--------|-------------|
| solver | SOLVER |
| ierr | Return code |

Note

SOLVER has information on the solver, the preconditioner, etc.

6.4.2 lis_solver_destroy

```
C      int lis_solver_destroy(LIS_SOLVER solver)
Fortran subroutine lis_solver_destroy(LIS_SOLVER solver, integer ierr)
```

Capability

Removing unwanted SOLVER from memory

Input

| | |
|--------|------------------------------|
| solver | SOLVER to remove from memory |
|--------|------------------------------|

Output

| | |
|------|-------------|
| ierr | Return code |
|------|-------------|

```
C      int lis_solver_set_option(char *text, LIS_SOLVER solver)
Fortran subroutine lis_solver_set_option(character text, LIS_SOLVER solver,
      integer ierr)
```

Setting options for solvers, preconditioners, and others

| text | Command line option |
|------|---------------------|
| ... | ... |

| | |
|--------|-------------|
| solver | SOLVER |
| ierr | Return code |

The table below shows the allowable command line options, where `-i {cg|1}` means `-i cg` or `-i 1` and `-maxiter [1000]` indicates that `-maxiter` defaults to 1,000.

| Method | Option | Auxiliary Option | |
|--------------|------------------|------------------|--|
| CG | -i {cg 1} | | |
| BiCG | -i {bicg 2} | | |
| CGS | -i {cgs 3} | | |
| BiCGSTAB | -i {bicgstab 4} | | |
| BiCGSTAB(l) | -i {bicgstabl 5} | -ell [2] | Value for l |
| GPBiCG | -i {gpbicg 6} | | |
| TFQMR | -i {tfqmr 7} | | |
| Orthomin(m) | -i {orthomin 8} | -restart [40] | Value for Restart m |
| GMRES(m) | -i {gmres 9} | -restart [40] | Value for Restart m |
| Jacobi | -i {jacobi 10} | | |
| Gauss-Seidel | -i {gs 11} | | |
| SOR | -i {sor 12} | -omega [1.9] | Value for Relaxation Coefficient ω ($0 < \omega < 2$) |
| BiCGSafe | -i {bicgsafe 13} | | |
| CR | -i {cr 14} | | |
| BiCR | -i {bicr 15} | | |
| CRS | -i {crs 16} | | |
| BiCRSTAB | -i {bicrstab 17} | | |
| GPBiCR | -i {gpbicr 18} | | |
| BiCRSafe | -i {bicrsafe 19} | | |
| FGMRES(m) | -i {fgmres 20} | -restart [40] | Value for Restart m |
| IDR(s) | -i {idrs 21} | -restart [40] | Value for Restart s |
| MINRES | -i {minres 22} | | |

Specifying a Preconditioner Default: -p none

| Preconditioner | Option | Auxiliary Option | |
|------------------|---------------|----------------------|---|
| None | -p {none 0} | | |
| Jacobi | -p {jacobi 1} | | |
| ILU(k) | -p {ilu 2} | -ilu_fill [0] | Fill level k |
| SSOR | -p {ssor 3} | -ssor_w [1.0] | Relaxation Coefficient ω ($0 < \omega < 2$) |
| hybrid | -p {hybrid 4} | -hybrid_i [sor] | Linear Equation Solver |
| | | -hybrid_maxiter [25] | Maximum number of iterations |
| | | -hybrid_tol [1.0e-3] | Convergence criteria |
| | | -hybrid_w [1.5] | Relaxation Coefficient ω for the SOR method ($0 < \omega < 2$) |
| | | -hybrid_ell [2] | Value for l of the BiCGSTAB(l) method |
| | | -hybrid_restart [40] | Restart values for GMRES and Orthomin |
| I+S | -p {is 5} | -is_alpha [1.0] | Parameter α for preconditioner of a $I + \alpha S^{(m)}$ type |
| | | -is_m [3] | Parameter m for preconditioner of a $I + \alpha S^{(m)}$ type |
| SAINV | -p {sainv 6} | -sainv_drop [0.05] | Drop criteria |
| SA-AMG | -p {saamg 7} | -saamg_unsym [false] | Selection of asymmetric version (Matrix structure must be symmetric) |
| Crout ILU | -p {iluc 8} | -iluc_drop [0.05] | Drop criteria |
| | | -iluc_rate [5.0] | Ratio of Maximum fill-in |
| ILUT | -p {ilut 9} | -ilut_drop [0.05] | Drop criteria |
| | | -ilut_rate [5.0] | Ratio of Maximum fill-in |
| additive Schwarz | -adds true | -adds_iter [1] | Number of iterations |

Other Options

| Option | |
|----------------------|--|
| -maxiter [1000] | Maximum number of iterations |
| -tol [1.0e-12] | Convergence criteria |
| -print [0] | Display of the residual |
| | -print {none 0} None |
| | -print {mem 1} Saves the residual history in memory |
| | -print {out 2} Displays the residual history |
| | -print {all 3} Saves the residual history and displays it on the screen |
| -scale [0] | Selection of scaling. The result will overwrite the original matrix and vectors |
| | -scale {none 0} No scaling |
| | -scale {jacobi 1} Jacobi scaling $D^{-1}Ax = D^{-1}b$ D represents the diagonal of $A = (a_{ij})$ |
| | -scale {symm_diag 2} Diagonal scaling $D^{-1/2}AD^{-1/2}x = D^{-1/2}b$ $D^{-1/2}$ represents an diagonal matrix that has $1/\sqrt{a_{ii}}$ as an diagonal element |
| -initx_zeros [true] | Behavior of initial vector x_0 |
| | -initx_zeros {false 0} Given values |
| | -initx_zeros {true 1} All elements are set to 0. |
| -omp_num_threads [t] | Number of threads t represents the maximum number of threads |

Precision Default: -precision double

| Precision | Option | Auxiliary Option |
|-----------|-----------------------|------------------|
| DOUBLE | -precision {double 0} | |
| QUAD | -precision {quad 1} | |

6.4.4 lis_solver_set_optionC

```
C      int lis_solver_set_optionC(LIS_SOLVER solver)
Fortran subroutine lis_solver_set_optionC(LIS_SOLVER solver, integer ierr)
```

Capability

Setting options for solvers, preconditioners, and other options on the command line

Input

None

Output

| | |
|--------|-------------|
| solver | SOLVER |
| ierr | Return code |

6.4.5 lis_solve

```
C      int lis_solve(LIS_MATRIX A, LIS_VECTOR b, LIS_VECTOR x, LIS_SOLVER solver)
Fortran subroutine lis_solve(LIS_MATRIX A, LIS_VECTOR b, LIS_VECTOR x,
                             LIS_SOLVER solver, integer ierr)
```

Capability

Solving the linear equation $Ax = b$ with a desired solver

Input

| | |
|--------|--------------------|
| A | Coefficient matrix |
| b | Right-side vector |
| x | Initial vector |
| solver | SOLVER |

Output

| | |
|--------|--|
| x | Approximate solution |
| solver | Number of iterations, Execution time, etc. |
| ierr | Return code |

6.4.6 lis_solver_get_iters

```
C      int lis_solver_get_iters(LIS_SOLVER solver, int *iters)
Fortran subroutine lis_solver_get_iters(LIS_SOLVER solver, integer iters,
                                     integer ierr)
```

Capability

Ascertaining number of iterations from SOLVER

Input

| | |
|--------|--------|
| solver | SOLVER |
|--------|--------|

Output

| | |
|-------|----------------------|
| iters | Number of iterations |
| ierr | Return code |

6.4.7 lis_solver_get_itersex

```
C      int lis_solver_get_itersex(LIS_SOLVER solver, int *iters, int *iters_double,
                                int *iters_quad)
Fortran subroutine lis_solver_get_itersex(LIS_SOLVER solver, integer iters,
                                     integer iters_double, integer iters_quad, integer ierr)
```

Capability

Ascertaining number of iterations from SOLVER

Input

| | |
|--------|--------|
| solver | SOLVER |
|--------|--------|

Output

| | |
|--------------|--|
| iters | Number of iterations |
| iters_double | Number of double precision iterations |
| iters_quad | Number of quadruple precision iterations |
| ierr | Return code |

6.4.8 lis_solver_get_time

```
C      int lis_solver_get_time(LIS_SOLVER solver, double *times, double *itimes,  
                             double *ptimes)  
Fortran subroutine lis_solver_get_time(LIS_SOLVER solver, real*8 times,  
                                     real*8 itimes, real*8 ptimes, integer ierr)
```

Capability

Ascertaining execution time from SOLVER

Input

| | |
|--------|--------|
| solver | SOLVER |
|--------|--------|

Output

| | |
|-------|-------------------------------|
| times | Execution time (seconds) |
| times | Iteration time (seconds) |
| times | Preconditioner time (seconds) |
| ierr | Return code |

6.4.9 lis_solver_get_timeex

```
C      int lis_solver_get_timeex(LIS_SOLVER solver, double *times, double *itimes,  
                                double *ptimes, double *p_c_times, double *p_i_times)  
Fortran subroutine lis_solver_get_timeex(LIS_SOLVER solver, real*8 times,  
                                         real*8 itimes, real*8 ptimes, real*8 p_c_times, real*8 p_i_times,  
                                         integer ierr)
```

Capability

Ascertaining execution time from SOLVER

Input

| | |
|--------|--------|
| solver | SOLVER |
|--------|--------|

Output

| | |
|-----------|--|
| times | Total time (seconds) |
| itimes | Iteration time (seconds) |
| ptimes | Preconditioner time (seconds) |
| p_c.times | Preconditioner in creation time (seconds) |
| p_i.times | Preconditioner in iteration time (seconds) |
| ierr | Return code |

6.4.10 lis_solver_get_residualnorm

```
C      int lis_solver_get_residualnorm(LIS_SOLVER solver, LIS_REAL *residual)
Fortran subroutine lis_solver_get_residualnorm(LIS_SOLVER solver, LIS_REAL residual,
      integer ierr)
```

Capability

Ascertaining 2-norms of $b - Ax$ from SOLVER

Input

| | |
|--------|--------|
| solver | SOLVER |
|--------|--------|

Output

| | |
|----------|---------------------|
| residual | 2-norms of $b - Ax$ |
| ierr | Return code |

6.4.11 lis_solver_get_rhistory

```
C      int lis_solver_get_rhistory(VECTOR v)
Fortran subroutine lis_solver_get_rhistory(LIS_VECTOR v, integer ierr)
```

Capability

Storing the residual norm history in a vector

Input

| |
|------|
| None |
|------|

Output

| | |
|------|-------------|
| v | Vector |
| ierr | Return code |

Note

Vector **v** must be created in advance with the `lis_vector_create` function. When vector **v** is shorter than the residual history, it stores the residual history from the beginning for the length of vector **v**.

6.4.12 lis_solver_get_solver

```
C      int lis_solver_get_solver(LIS_SOLVER solver, int *nsol)
Fortran subroutine lis_solver_get_solver(LIS_SOLVER solver, integer nsol,
      integer ierr)
```

Capability

Ascertaining solver number from SOLVER

Input

solver SOLVER

Output

nsol Solver number

ierr Return code

Note

The number of the solver is as follows:

| Solver | Number | Solver | Number |
|-------------|--------|--------------|--------|
| CG | 1 | Gauss-Seidel | 11 |
| BiCG | 2 | SOR | 12 |
| CGS | 3 | BiCGSafe | 13 |
| BiCGSTAB | 4 | CR | 14 |
| BiCGSTAB(l) | 5 | BiCR | 15 |
| GPBiCG | 6 | CRS | 16 |
| TFQMR | 7 | BiCRSTAB | 17 |
| Orthomin(m) | 8 | GPBiCR | 18 |
| GMRES(m) | 9 | BiCRSafe | 19 |
| Jacobi | 10 | FGMRES(m) | 20 |
| IDR(s) | 21 | MINRES | 22 |

6.4.13 lis_solver_get_solvername

```
C      int lis_get_solvername(int nsol, char *name)
Fortran subroutine lis_get_solvername(integer nsol, character name, integer ierr)
```

Capability

Ascertaining solver name from solver number

Input

nsol Solver number

Output

name Solver name

ierr Return code

6.5 Solving Eigenvalue Problem

6.5.1 lis_esolver_create

```
C      int lis_esolver_create(LIS_ESOLVER *esolver)
Fortran subroutine lis_esolver_create(LIS_ESOLVER esolver, integer ierr)
```

Capability

Creating ESOLVER

Input

None

Output

| | |
|---------|-------------|
| esolver | ESOLVER |
| ierr | Return code |

Note

ESOLVER has information on the eigensolver, the preconditioner, etc.

6.5.2 lis_esolver_destroy

```
C      int lis_esolver_destroy(LIS_ESOLVER esolver)
Fortran subroutine lis_esolver_destroy(LIS_ESOLVER esolver, integer ierr)
```

Capability

Removing unwanted ESOLVER from memory

Input

| | |
|---------|-------------------------------|
| esolver | ESOLVER to remove from memory |
|---------|-------------------------------|

Output

| | |
|------|-------------|
| ierr | Return code |
|------|-------------|

6.5.3 lis_esolver_set_option

```
C      int lis_esolver_set_option(char *text, LIS_ESOLVER esolver)
Fortran subroutine lis_esolver_set_option(character text, LIS_ESOLVER esolver,
      integer ierr)
```

Capability

Setting options for solvers, preconditioners, and others

Input

text Command line option

Output

esolver ESOLVER

ierr Return code

Note

The table below shows the allowable command line options, where `-e {pi|1}` means `-e pi` or `-e 1` and `-emaxiter [1000]` indicates that `-emaxiter` defaults to 1,000.

Specifying an Eigensolver Default: `-e pi`

| Method | Option | Auxiliary Option | |
|--------------------------------|-------------------------|------------------------|------------------------|
| Power Iteration | <code>-e {pi 1}</code> | | |
| Inverse Iteration | <code>-e {ii 2}</code> | <code>-i [bicg]</code> | Linear equation solver |
| Preconditioned Power Iteration | <code>-e {aii 3}</code> | | |
| Conjugate Gradient | <code>-e {cg 4}</code> | | |
| Lanczos Iteration | <code>-e {li 5}</code> | <code>-ss [10]</code> | Size of subspace |
| Subspace Iteration | <code>-e {si 6}</code> | <code>-ss [10]</code> | Size of subspace |
| Conjugate Residual | <code>-e {cr 7}</code> | | |

Specifying a Preconditioner Default: -p ilu

| Preconditioner | Option | Auxiliary Option | |
|------------------|---------------|----------------------|---|
| None | -p {none 0} | | |
| Jacobi | -p {jacobi 1} | | |
| ILU(k) | -p {ilu 2} | -ilu_fill [0] | Fill level k |
| SSOR | -p {ssor 3} | -ssor_w [1.0] | Relaxation Coefficient ω ($0 < \omega < 2$) |
| hybrid | -p {hybrid 4} | -hybrid_i [sor] | Linear Equation Solver |
| | | -hybrid_maxiter [25] | Maximum number of iterations |
| | | -hybrid_tol [1.0e-3] | Convergence criteria |
| | | -hybrid_w [1.5] | Relaxation Coefficient ω for the SOR method ($0 < \omega < 2$) |
| | | -hybrid_ell [2] | Value for l of the BiCGSTAB(l) method |
| | | -hybrid_restart [40] | Restart values for GMRES and Orthomin |
| I+S | -p {is 5} | -is_alpha [1.0] | Parameter α for preconditioner of a $I + \alpha S^{(m)}$ type |
| | | -is_m [3] | Parameter m for preconditioner of a $I + \alpha S^{(m)}$ type |
| SAINV | -p {sainv 6} | -sainv_drop [0.05] | Drop criteria |
| SA-AMG | -p {saamg 7} | -saamg_unsym [false] | Selection of asymmetric version (Matrix structure must be symmetric) |
| Crout ILU | -p {iluc 8} | -iluc_drop [0.05] | Drop criteria |
| | | -iluc_rate [5.0] | Ratio of Maximum fill-in |
| ILUT | -p {ilut 9} | -ilut_drop [0.05] | Drop criteria |
| | | -ilut_rate [5.0] | Ratio of Maximum fill-in |
| additive Schwarz | -adds true | -adds_iter [1] | Number of iterations |

Other Options

| Option | |
|----------------------|--|
| -emaxiter [1000] | Maximum number of iterations |
| -etol [1.0e-5] | Convergence criteria |
| -eprint [0] | Display of the residual |
| | -eprint {none 0} None |
| | -eprint {mem 1} Saves the residual history in memory |
| | -eprint {out 2} Displays the residual history |
| | -eprint {all 3} Saves the residual history and displays it on the screen |
| -ie [ii] | Inner eigensolver used in Lanczos Iteration or Subspace Iteration |
| | -ie {pi 1} Power Iteration (Subspace Iteration only) |
| | -ie {ii 2} Inverse Iteration |
| -shift [0.0] | Amount of shift |
| | -ie {aii 3} Preconditioned Power Iteration |
| -initx_ones [true] | Behavior of initial vector x_0 |
| | -initx_ones {false 0} Given values |
| | -initx_ones {true 1} All elements are set to 1. |
| -omp_num_threads [t] | Number of threads |
| | t represents the maximum number of threads |

6.5.4 lis_esolver_set_optionC

```
C      int lis_esolver_set_optionC(LIS_ESOLVER esolver)
Fortran subroutine lis_esolver_set_optionC(LIS_ESOLVER esolver, integer ierr)
```

Capability

Setting options for eigensolvers and other options on the command line

Input

None

Output

| | |
|---------|-------------|
| esolver | ESOLVER |
| ierr | Return code |

6.5.5 lis_solve

```
C      int lis_solve(LIS_MATRIX A, LIS_VECTOR x,
                   LIS_REAL evalue, LIS_ESOLVER esolver)
Fortran subroutine lis_solve(LIS_MATRIX A, LIS_VECTOR x,
                           LIS_REAL evalue, LIS_ESOLVER esolver, integer ierr)
```

Capability

Solving the eigenvalue problem $Ax = \lambda x$ with a desired eigensolver

Input

| | |
|---------|----------------|
| A | Matrix |
| x | Initial vector |
| esolver | ESOLVER |

Output

| | |
|---------|--|
| evalue | Approximate extreme eigenvalue |
| x | Approximate extreme eigenvector |
| esolver | Number of iterations, Execution time, etc. |
| ierr | Return code |

6.5.6 lis_esolver_get_iters

```
C      int lis_esolver_get_iters(LIS_ESOLVER esolver, int *iters)
Fortran subroutine lis_esolver_get_iters(LIS_ESOLVER esolver, integer iters,
                                         integer ierr)
```

Capability

Ascertaining number of iterations from ESOLVER

Input

| | |
|---------|---------|
| esolver | ESOLVER |
|---------|---------|

Output

| | |
|-------|----------------------|
| iters | Number of iterations |
| ierr | Return code |

6.5.7 lis_esolver_get_itersex

```
C      int lis_esolver_get_itersex(LIS_ESOLVER esolver, int *iters,
                                   int *iters_double, int *iters_quad)
Fortran subroutine lis_esolver_get_itersex(LIS_ESOLVER esolver, integer iters,
                                           integer iters_double, integer iters_quad, integer ierr)
```

Capability

Ascertaining number of iterations from ESOLVER

Input

| | |
|---------|---------|
| esolver | ESOLVER |
|---------|---------|

Output

| | |
|--------------|--|
| iters | Number of iterations |
| iters_double | Number of double precision iterations |
| iters_quad | Number of quadruple precision iterations |
| ierr | Return code |

6.5.8 lis_esolver_get_time

```
C      int lis_esolver_get_time(LIS_ESOLVER esolver, double *times, double *itimes,  
                             double *ptimes)  
Fortran subroutine lis_esolver_get_time(LIS_ESOLVER esolver, real*8 times,  
                                       real*8 itimes, real*8 ptimes, integer ierr)
```

Capability

Ascertaining execution time from ESOLVER

Input

| | |
|---------|---------|
| esolver | ESOLVER |
|---------|---------|

Output

| | |
|-------|-------------------------------|
| times | Execution time (seconds) |
| times | Iteration time (seconds) |
| times | Preconditioner time (seconds) |
| ierr | Return code |

6.5.9 lis_esolver_get_timeex

```
C      int lis_esolver_get_timeex(LIS_ESOLVER esolver, double *times,  
                                double *itimes, double *ptimes, double *p_c_times, double *p_i_times)  
Fortran subroutine lis_esolver_get_timeex(LIS_ESOLVER esolver, real*8 times,  
                                       real*8 itimes, real*8 ptimes, real*8 p_c_times, real*8 p_i_times,  
                                       integer ierr)
```

Capability

Ascertaining execution time from ESOLVER

Input

| | |
|---------|---------|
| esolver | ESOLVER |
|---------|---------|

Output

| | |
|-----------|--|
| times | Total time (seconds) |
| itimes | Iteration time (seconds) |
| ptimes | Preconditioner time (seconds) |
| p_c.times | Preconditioner in creation time (seconds) |
| p_i.times | Preconditioner in iteration time (seconds) |
| ierr | Return code |

6.5.10 lis_esolver_get_residualnorm

```
C      int lis_esolver_get_residualnorm(LIS_ESOLVER esolver, LIS_REAL *residual)
Fortran subroutine lis_esolver_get_residualnorm(LIS_ESOLVER esolver,
        LIS_REAL residual, integer ierr)
```

Capability

Ascertaining 2-norms of $(\lambda x - Ax)/\lambda$ from ESOLVER

Input

| | |
|---------|---------|
| esolver | ESOLVER |
|---------|---------|

Output

| | |
|----------|---------------------------------------|
| residual | 2-norms of $(\lambda x - Ax)/\lambda$ |
| ierr | Return code |

6.5.11 lis_esolver_get_rhistory

```
C      int lis_esolver_get_rhistory(VECTOR v)
Fortran subroutine lis_esolver_get_rhistory(LIS_VECTOR v, integer ierr)
```

Capability

Storing the residual norm history in a vector

Input

None

Output

| | |
|------|-------------|
| v | Vector |
| ierr | Return code |

Note

Vector **v** must be created in advance with the `lis_vector_create` function. When vector **v** is shorter than the residual history, it stores the residual history from the beginning for the length of vector **v**.

6.5.12 lis_esolver_get_evalues

```
C      int lis_esolver_get_evalues(LIS_ESOLVER esolver, LIS_VECTOR v)
Fortran subroutine lis_esolver_get_evalues(LIS_ESOLVER esolver,
      LIS_VECTOR v, integer ierr)
```

Capability

Storing all the eigenvalues in a vector

Input

| | |
|---------|---------|
| esolver | ESOLVER |
|---------|---------|

Output

| | |
|------|--|
| v | Vector that contains all the eigenvalues |
| ierr | Return code |

Note

Vector **v** must be created in advance with the **lis_vector_create** function. When the length of the vector **v** is shorter than the number of eigenvalues, it stores the eigenvalues from the beginning for the length of vector **v**.

6.5.13 lis_esolver_get_evectors

```
C      int lis_esolver_get_evectors(LIS_ESOLVER esolver, LIS_VECTOR *v)
Fortran subroutine lis_esolver_get_evectors(LIS_ESOLVER esolver,
      LIS_VECTOR v, integer ierr)
```

Capability

Storing all the eigenvectors in an array

Input

| | |
|---------|---------|
| esolver | ESOLVER |
|---------|---------|

Output

| | |
|------|--|
| v | Array that contains all the eigenvectors |
| ierr | Return code |

Note

Array ***v** must be created in advance.

6.5.14 lis_esolver_get_esolver

```
C      int lis_esolver_get_esolver(LIS_ESOLVER esolver, int *nesol)
Fortran subroutine lis_esolver_get_esolver(LIS_ESOLVER esolver, integer nesol,
      integer ierr)
```

Capability

Ascertaining eigensolver number from ESOLVER

Input

esolver ESOLVER

Output

nesol Eigensolver number

ierr Return code

Note

The number of the eigensolver is as follows:

| Method | Number |
|-------------------------------|--------|
| Power Iteration | 1 |
| Inverse Iteration | 2 |
| Approximate Inverse Iteration | 3 |
| Conjugate Gradient | 4 |
| Lanczos Iteration | 5 |
| Subspace Iteration | 6 |
| Conjugate Residual | 7 |

6.5.15 lis_esolver_get_esolvername

```
C      int lis_get_esolvername(int nesol, char *ename)
Fortran subroutine lis_get_esolvername(integer nesol, character ename, integer ierr)
```

Capability

Ascertaining eigensolver name from eigensolver number

Input

nesol Eigensolver number

Output

name Eigensolver name

ierr Return code

6.6 File Input and Output

6.6.1 lis_input_matrix

```
C      int lis_input_matrix(LIS_MATRIX A, char *filename)
Fortran subroutine lis_input_matrix(LIS_MATRIX A, LIS_VECTOR x,
      character filename, integer ierr)
```

Capability

Reading matrix data from a file

Input

| | |
|----------|-------------------------|
| filename | Name of the source file |
|----------|-------------------------|

Output

| | |
|------|--|
| A | Matrix in the storage format specified |
| x | Solution vector |
| ierr | Return code |

Note

The supported file formats are shown below:

- MatrixMarket format (extended to allow vector data to be read)
- Harwell-Boeing format

6.6.2 lis_input

```
C      int lis_input(LIS_MATRIX A, LIS_VECTOR b, LIS_VECTOR x, char *filename)
Fortran subroutine lis_input(LIS_MATRIX A, LIS_VECTOR b, LIS_VECTOR x,
      character filename, integer ierr)
```

Capability

Reading matrix and vector data from a file

Input

| | |
|----------|-------------------------|
| filename | Name of the source file |
|----------|-------------------------|

Output

| | |
|------|--|
| A | Matrix in the storage format specified |
| b | Right-side vector |
| x | Solution vector |
| ierr | Return code |

Note

The supported file formats are shown below:

- MatrixMarket format (extended to allow vector data to be read)
- Harwell-Boeing format

6.6.3 lis_input_vector

```
C      int lis_input_vector(LIS_VECTOR v, char *filename)
Fortran subroutine lis_input_vector(LIS_VECTOR v, character filename, integer ierr)
```

Capability

Reading vector data from a file

Input

| | |
|----------|-------------------------|
| filename | Name of the source file |
|----------|-------------------------|

Output

| | |
|------|-------------|
| v | Vector |
| ierr | Return code |

Note

The supported file formats are shown below:

- PLAIN format
- MM format

6.6.4 lis_output

```
C      int lis_output(LIS_MATRIX A, LIS_VECTOR b, LIS_VECTOR x, int format,
                    char *filename)
Fortran subroutine lis_output(LIS_MATRIX A, LIS_VECTOR b, LIS_VECTOR x,
                             integer format, character path, integer ierr)
```

Capability

Writing matrix and vector data into a file

Input

| | |
|----------|--|
| A | Matrix |
| b | Right-side vector. If no vector will be written into a file, then NULL must be input |
| x | Solution vector. If no vector will be written into a file, then NULL must be input |
| format | File format |
| | LIS_FMT_MM MatrixMarket format |
| filename | Name of the target file |

Output

| | |
|------|-------------|
| ierr | Return code |
|------|-------------|

6.6.5 lis_output_vector

```
C      int lis_output_vector(LIS_VECTOR v, int format, char *filename)
Fortran subroutine lis_output_vector(LIS_VECTOR v, integer format,
      character filename, integer ierr)
```

Capability

Writing vector data into a file

Input

| | | |
|----------|-------------------------|-------------------|
| v | Vector | |
| format | File format | |
| | LIS_FMT_PLAIN | PLAIN format |
| | LIS_FMT_MM | MM format |
| | LIS_FMT_LIS | LIS format(ASCII) |
| filename | Name of the target file | |

Output

| | |
|------|-------------|
| ierr | Return code |
|------|-------------|

6.6.6 lis_esolver_output_rhistory

```
C      int lis_esolver_output_rhistory(LIS_ESOLVER esolver, char *filename)
Fortran subroutine lis_esolver_output_rhistory(LIS_ESOLVER esolver,
      character filename)
```

Capability

Writing residual history into a file

Input

| | |
|----------|-------------------------|
| esolver | ESOLVER |
| filename | Name of the target file |

Output

| | |
|------|-------------|
| ierr | Return code |
|------|-------------|

6.7 Other Functions

6.7.1 lis_initialize

```
C      int lis_initialize(int* argc, char** argv[])
Fortran subroutine lis_initialize(integer ierr)
```

Capability

Initialization

Input

| | |
|------|----------------------------------|
| argc | Number of command line arguments |
| argv | Command line argument |

Output

| | |
|------|-------------|
| ierr | Return code |
|------|-------------|

6.7.2 lis_finalize

```
C      void lis_finalize()
Fortran subroutine lis_finalize(integer ierr)
```

Capability

finalization

Input

None

Output

| | |
|------|-------------|
| ierr | Return code |
|------|-------------|

6.7.3 lis_wtime

```
C      double lis_wtime()
Fortran function lis_wtime()
```

Capability

Measuring elapsed time

Input

None

Output

Time (in seconds) elapsed from a given point is returned as double data type

Note

To measure the processing time, use `lis_wtime` to measure the time immediately before starting time measurement and immediately after ending time measurement, and then determine the difference.

References

- [1] S. Fujino, M. Fujiwara and M. Yoshida. BiCGSafe method based on minimization of associate residual (in Japanese). Transactions of JSCES, Paper No.20050028, 2005. <http://save.k.u-tokyo.ac.jp/jscs/trans/trans2005/No20050028.pdf>.
- [2] T. Sogabe, M. Sugihara and S. Zhang. An Extension of the Conjugate Residual Method for Solving Nonsymmetric Linear Systems(in Japanese). Transactions of the Japan Society for Industrial and Applied Mathematics, Vol. 15, No. 3, pp. 445–460, 2005.
- [3] K. Abe, T. Sogabe, S. Fujino and S. Zhang. A Product-type Krylov Subspace Method Based on Conjugate Residual Method for Nonsymmetric Coefficient Matrices (in Japanese). IPSJ Transactions on Advanced Computing Systems, Vol. 48, No. SIG8(ACS18), pp. 11–21, 2007.
- [4] S. Fujino and Y. Onoue. Estimation of BiCRSafe method based on residual of BiCR method (in Japanese). IPSJ SIG Technical Report, 2007-HPC-111, pp. 25–30, 2007.
- [5] Y. Saad. A Flexible Inner-outer Preconditioned GMRES Algorithm. SIAM J. Sci. Stat. Comput., Vol. 14, pp. 461–469, 1993.
- [6] Y. Saad. ILUT: a dual threshold incomplete LU factorization. Numerical linear algebra with applications, Vol. 1, No. 4, pp. 387–402, 1994.
- [7] ITSOL: ITERATIVE SOLVERS package
<http://www-users.cs.umn.edu/~saad/software/ITSOL/index.html>.
- [8] N. Li, Y. Saad and E. Chow. Crout version of ILU for general sparse matrices. SIAM J. Sci. Comput., Vol. 25, pp. 716–728, 2003.
- [9] Toshiyuki Kohno, Hisashi Kotakemori and Hiroshi Niki. Improving the Modified Gauss-Seidel Method for Z-matrices. Linear Algebra and its Applications, Vol. 267, pp. 113–123, 1997.
- [10] A. Fujii, A. Nishida, and Y. Oyanagi. Evaluation of Parallel Aggregate Creation Orders : Smoothed Aggregation Algebraic Multigrid Method. High Performance Computational Science And Engineering, pp. 99–122, Springer, 2005.
- [11] K. Abe, S. Zhang, H. Hasegawa and R. Himeno. A SOR-base Variable Preconditioned CGR Method (in Japanese). Trans. JSIAM, Vol. 11, No. 4, pp. 157–170, 2001.
- [12] R. Bridson and W.-P. Tang. Refining an approximate inverse. J. Comput. Appl. Math., Vol. 123, pp. 293–306, 2000.
- [13] P. Soonerveld and M. B. van Gijzen. IDR(s): a family of simple and fast algorithms for solving large nonsymmetric systems of linear equations. TR 07-07, Math. Anal., Delft Univ. of Tech., 2007. http://ta.twi.tudelft.nl/TWA_Reports/07-07.pdf.
- [14] A. Greenbaum. Iterative Methods for Solving Linear Systems. SIAM, 1997.
- [15] H. Hasegawa. Utilizing the Quadruple-Precision Floating-Point Arithmetic Operation for the Krylov Subspace Methods. the 8th SIAM Conference on Applied Linear Algebra, 2003.
- [16] D. H. Bailey. A fortran-90 double-double library. <http://www.nersc.gov/~dhbailey/mpdist/mpdist.html>.
- [17] Y. Hida, X. S. Li and D. H. Bailey. Algorithms for quad-double precision floating point arithmetic. Proceedings of the 15th Symposium on Computer Arithmetic, pp.155–162, 2001.
- [18] T. Dekker. A floating-point technique for extending the available precision. Numerische Mathematik, vol.18 pp.224–242, 1971.

- [19] A. V. Knyazev. Toward the Optimal Preconditioned Eigensolver: Locally Optimal Block Preconditioned Conjugate Gradient Method. *SIAM J. Sci. Comput.*, Vol. 23, No. 2, pp. 517-541, 2001.
- [20] A. Nishida. Performance Evaluation of Intel Processor based cc-NUMA Systems for Scalable Iterative Solvers. *Proceedings of 8th Copper Mountain Conference on Iterative Methods*, Copper Mountain, Mar. 2004.
- [21] E. Suetomi and H. Sekimoto. Application of ORTHOMIN(1) Method to Nonsymmetric Generalized Eigenvalue Problems Appearing in the Multi-Group Neutron Diffusion Equations (in Japanese). *IPSJ Transactions of Information Processing Society of Japan*, Vol. 30, No. 5, pp. 661-667, 1989.
- [22] D. E. Knuth. *The Art of Computer Programming: Seminumerical Algorithms*, vol.2. Addison-Wesley, 1969.
- [23] D. H. Bailey. High-Precision Floating-Point Arithmetic in Scientific Computation. *Computing in Science and Engineering*, Volume 7, Issue 3, pp. 54-61, IEEE, 2005.
- [24] Intel Fortran Compiler User's Guide Vol I.
- [25] H. Kotakemori, A. Fujii, H. Hasegawa and A. Nishida. Implementation of Fast Quad Precision Operation and Acceleration with SSE2 for Iterative Solver Library (in Japanese). *IPSJ Transactions on Advanced Computing Systems*, Vol. 1, No. 1, pp. 73-84, 2008.
- [26] R. Barrett, et al. *Templates for the Solution of Linear Systems: Building Blocks for Iterative Methods*. SIAM, 1994.
- [27] Z. Bai, et al. *Templates for the Solution of Algebraic Eigenvalue Problems*. SIAM, 2000.
- [28] Y. Saad. SPARSKIT: a basic tool kit for sparse matrix computations, version 2, June 1994. <http://www.cs.umn.edu/~saad/software/SPARSKIT/sparskit.html>.
- [29] S. Balay, et al. PETSc users manual. Technical Report ANL-95/11, Argonne National Laboratory, August 2004.
- [30] R. S. Tuminaro, et al. Official Aztec user's guide, version 2.1. Technical Report SAND99-8801J, Sandia National Laboratories, November 1999.
- [31] R. B. Lehoucq, D. C. Sorensen, and C. Yang. *ARPACK Users' Guide: Solution of Large-scale Eigenvalue Problems with implicitly-restarted Arnoldi Methods*. SIAM, 1998.
- [32] R. Bramley and X. Wang. SPLIB: A library of iterative methods for sparse linear system. Technical report, Indiana University-Bloomington, 1995.
- [33] Matrix Market. <http://math.nist.gov/MatrixMarket>.

A Appendix A: File Formats

This section describes the file formats available for the library.

A.1 MatrixMarket Format

The MatrixMarket format[33] is not designed to store vector data. For this library, it has been extended so that it can handle vector data. Assume that the number of non-zero elements for matrix $A = (a_{ij})$ of $M \times N$ is L and that $a_{ij} = A(I, J)$. The file is structured as follows:

```
%%MatrixMarket matrix coordinate real general <-- Header
%
% | Comment lines with 0 or more lines
%
% <--
M N L B X <-- Numbers of rows, columns, and
I1 J1 A(I1,J1) <-- non-zero elements (0 or 1) (0 or 1)
I2 J2 A(I2,J2) | Row and column number values
. . . | The index is 1-base
IL JL A(IL,JL) <--
I1 B(I1) <--
I2 B(I2) | Exists only when B=1
. . . | Row number value
IM B(IM) <--
I1 X(I1) <--
I2 X(I2) | Exists only when X=1
. . . | Row number value
IM X(IM) <--
```

The MatrixMarket file for matrix A and vector b in Equation (A.1) is structured as follows:

$$A = \begin{pmatrix} 2 & 1 & & \\ 1 & 2 & 1 & \\ & 1 & 2 & 1 \\ & & 1 & 2 \end{pmatrix} \quad b = \begin{pmatrix} 0 \\ 1 \\ 2 \\ 3 \end{pmatrix} \quad (\text{A.1})$$

```
%%MatrixMarket matrix coordinate real general
4 4 10 1 0
1 2 1.00e+00
1 1 2.00e+00
2 3 1.00e+00
2 1 1.00e+00
2 2 2.00e+00
3 4 1.00e+00
3 2 1.00e+00
3 3 2.00e+00
4 4 2.00e+00
4 3 1.00e+00
1 0.00e+00
2 1.00e+00
3 2.00e+00
4 3.00e+00
```

A.2 Harwell-Boeing Format

The Harwell-Boeing format inputs and outputs the matrix in the CCS storage format. Assume that the array `value` stores the value of non-zero elements of matrix A , the array `index` stores the row indices of the non-zero elements and the array `ptr` stores pointers to the beginning of each column in the arrays `value` and `index`. The file is structured as follows:

```

Line 1 (A72,A8)
  1 - 72 Title
  73 - 80 Key
Line 2 (5I14)
  1 - 14 Total number of lines excluding header
  15 - 28 Number of lines for ptr
  29 - 42 Number of lines for index
  43 - 56 Number of lines for value
  57 - 70 Number of lines for right-hand sides
Line 3 (A3,11X,4I14)
  1 - 3 Matrix type
      Col.1: R Real matrix
            C Complex matrix (Non-support)
            P Pattern only (Non-support)
      Col.2: S Symmetric
            U Unsymmetric
            H Hermitian (Non-support)
            Z Skew symmetric (Non-support)
            R Rectangular (Non-support)
      Col.3: A Assembled
            E Elemental matrices (Non-support)
  4 - 14 Blank space
  15 - 28 Number of rows
  29 - 42 Number of columns
  43 - 56 Number of non-zero elements
  57 - 70 0
Line 4 (2A16,2A20)
  1 - 16 Format for ptr
  17 - 32 Format for index
  33 - 52 Format for value
  53 - 72 Format for right-hand sides
Line 5 (A3,11X,2I14) Only present if there are right-hand sides present
  1   Right-hand side type
      F for full storage
      M for same format as matrix (Non-support)
  2   G if a starting vector is supplied
  3   X if an exact solution vector is supplied
  4 - 14 Blank space
  15 - 28 Number of right-hand sides
  29 - 42 Number of non-zero elements

```

The Harwell-Boeing file for matrix A and vector b in Equation (A.1) is structured as follows:

```

1-----10-----20-----30-----40-----50-----60-----70-----80
Harwell-Boeing format sample                                     Lis
      8              1              1              4              2
RUA              4              4              10             4
(11i7)          (13i6)          (3e26.18)          (3e26.18)
F              1              0
      1      3      6      9
      1      2      1      2      3      2      3      4      3      4
2.0000000000000000E+00  1.0000000000000000E+00  1.0000000000000000E+00
2.0000000000000000E+00  1.0000000000000000E+00  1.0000000000000000E+00
2.0000000000000000E+00  1.0000000000000000E+00  1.0000000000000000E+00
2.0000000000000000E+00
0.0000000000000000E+00  1.0000000000000000E+00  2.0000000000000000E+00
3.0000000000000000E+00

```

A.3 xMatrixMarket Format (for Vectors)

The MatrixMarket format[33] has been extended so that it can store vector data. Assume that vector $b = (b_i)$ is a vector of order N and that $b_i = B(I)$. The file is structured as follows:

```
%%MatrixMarket vector coordinate real general <-- Header
% <--+
% | Comment lines with 0 or more lines
% <--+
N <-- Number of rows
I1 B(I1) <--+
I2 B(I2) | Row number value
. . . | The index is 1-base
IN B(IN) <--+
```

The MatrixMarket file for vector b in Equation (A.1) is structured as follows:

```
%%MatrixMarket vector coordinate real general
4
1 0.00e+00
2 1.00e+00
3 2.00e+00
4 3.00e+00
```

A.4 PLAIN Format (for Vectors)

The PLAIN format is designed to write vector values from the beginning in order. Assume that vector $b = (b_i)$ is a vector of order N and that $b_i = B(I)$. The file is structured as follows:

```
B(1) <--+
B(2) | Vector value
. . . |
B(N) <--+
```

For vector b in Equation (A.1), the file is structured as follows:

```
0.00e+00
1.00e+00
2.00e+00
3.00e+00
```