

---

# PRIMME

large-scale eigenvalue and  
singular value solver

**Documentation**

*Release 3.2*

Andreas Stathopoulos  
Eloy Romero Alcalde  
Lingfei Wu  
James R. McCombs

Jan 30, 2021



# CONTENTS

<b>1</b>	<b>PRIMME: PReconditioned Iterative MultiMethod Eigensolver</b>	<b>1</b>
1.1	Incompatibilities . . . . .	2
1.2	Changelog . . . . .	3
1.3	License Information . . . . .	6
1.4	Citing the code . . . . .	7
1.5	Contact Information . . . . .	8
<b>2</b>	<b>Support</b>	<b>9</b>
2.1	Directory Structure . . . . .	10
2.2	Making and Linking . . . . .	11
2.3	Tested Systems . . . . .	13
2.4	Main Contributors . . . . .	14
<b>3</b>	<b>Eigenvalue Problems</b>	<b>15</b>
3.1	C Library Interface . . . . .	15
3.2	FORTRAN 77 Library Interface . . . . .	25
3.3	FORTRAN 90 Library Interface . . . . .	37
3.4	Python Interface . . . . .	44
3.5	MATLAB Interface . . . . .	48
3.6	Parameters Description . . . . .	52
3.7	Preset Methods . . . . .	74
3.8	Error Codes . . . . .	77
<b>4</b>	<b>Singular Value Problems</b>	<b>79</b>
4.1	C Library Interface . . . . .	79
4.2	FORTRAN Library Interface . . . . .	87
4.3	FORTRAN 90 Library Interface . . . . .	97
4.4	Python Interface . . . . .	103
4.5	MATLAB Interface . . . . .	106
4.6	Parameter Description . . . . .	109
4.7	Preset Methods . . . . .	125
4.8	Error Codes . . . . .	126
<b>5</b>	<b>Indices</b>	<b>127</b>
	<b>Bibliography</b>	<b>129</b>
	<b>Index</b>	<b>131</b>



## **PRIMME: PRECONDITIONED ITERATIVE MULTIMETHOD EIGENSOLVER**

PRIMME, pronounced as *prime*, is a high-performance library for computing a few eigenvalues/eigenvectors, and singular values/vectors. PRIMME is especially optimized for large, difficult problems. Real symmetric and complex Hermitian problems, standard  $Ax = \lambda x$  and generalized  $Ax = \lambda Bx$ , are supported. Besides standard eigenvalue problems with a normal matrix are supported. It can find largest, smallest, or interior singular/eigenvalues, and can use preconditioning to accelerate convergence. PRIMME is written in C99, but complete interfaces are provided for Fortran, MATLAB, Python, and R.

## 1.1 Incompatibilities

From PRIMME 2.2 to 3.0:

- Removed constants `primme_thick` and `primme_dtr`, and the member `scheme` from `restarting_params`.
- Added members `numBroadcast`, `volumeBroadcast`, `flopsDense`, `timeBroadcast`, `timeDense`, `estimateBNorm`, `estimateInvBNorm`, and `lockingIssue` to `primme_stats`.
- Added members `matrixMatvec_type`, `applyPreconditioner_type`, `massMatrixMatvec_type`, `globalSumReal_type`, `broadcastReal`, `broadcastReal_type`, `BNorm`, `invBNorm`, `orth`, `internalPrecision`, `massMatrix`, `convTestFun_type`, `monitorFun_type`, `queue`, and `profile` to `primme_params`.
- Added members `matrixMatvec_type`, `applyPreconditioner_type`, `globalSumReal_type`, `broadcastReal`, `broadcastReal_type`, `internalPrecision`, `convTestFun_type`, `monitorFun_type`, `queue`, and `profile` to `primme_svds_params`.
- Changed callbacks `monitorFun` and `monitorFun`.
- Changed the value of all constants; see `primme_get_member_f77()`, `primme_set_member_f77()`, `primme_svds_get_member_f77()`, and `primme_svds_set_member_f77()`.
- Removed `intWorkSize`, `realWorkSize`, `intWork`, `realWork` from `primme_params` and `primme_svds_params`.

From PRIMME 2.0 to 2.1:

- Added members `monitorFun` and `monitor` to `primme_params`.
- Added members `monitorFun` and `monitor` to `primme_svds_params`.
- Renamed `PRIMME_SUBSPACE_ITERATION` as `PRIMME_STEEPEST_DESCENT`.

From PRIMME 1.x to 2.0:

- Prototype of callbacks has changed: `matrixMatvec`, `applyPreconditioner`, `massMatrixMatvec` and `globalSumReal`.
- The next parameters are `PRIMME_INT`: `n`, `nLocal`, `maxMatvecs`, `iseed`, `numOuterIterations`, `numRestarts`, `numMatvecs` and `numMatvecs`; use the macro `PRIMME_INT_P` to print the values.
- Rename the values of the enum `primme_preset_method`.
- Rename `primme_Free` to `primme_free()`.
- Integer parameters in Fortran functions are of the same size as `PRIMME_INT`, which is `integer*8` by default.
- Extra parameter in many Fortran functions to return the error code.
- Removed `primme_display_stats_f77`.

## 1.2 Changelog

Changes in PRIMME 3.2 (released on Jan 29, 2021):

- Fixed Intel 2021 compiler error "Unsupported combination of types for <tgmath.h>."
- Fixed compiling issues with PGI compiler also about `tgmath.h`.
- Fixed `dprimme()` and other variants not returning error code `PRIMME_MAIN_ITER_FAILURE` when it should do in some corner cases.
- Fixed warnings from gcc/clang undefined behavior sanitizers.
- Matlab: renamed `disp` to `reportLevel`.
- Matlab: add flag `returnUnconverged` to return unconverged pairs optionally.
- Matlab: return `primme_params/primme_svds_params`.

Changes in PRIMME 3.1 (released on May 2, 2020):

- Fixed compilation issues in F90 interface and examples.
- Fixed bug in block orthogonalization.
- Updated Python interface to Python version 3.8.

Changes in PRIMME 3.0 (released on December 14, 2019):

- Added support for the generalized Hermitian eigenvalue problem (see `massMatrixMatvec`) and the standard normal eigenvalue problem (see `zprimme_normal()`).
- Added support for GPU (see `magma_dprimme()`, `magma_zprimme_normal()`, and `magma_dprimme_svds()`).
- Added support for half precision (see `hprimme()` and `kprimme()`, and other variants for normal eigenproblems and singular value problems).
- Added block orthogonalization (see `orth`).
- Resolution of all linear system of equations simultaneously in Jacobi-Davidson.
- Added interface for Fortran 90.
- Added an optional callback for broadcasting (see `broadcastReal` and `broadcastReal`).
- The callbacks can work with different precision than the main call (see for instance `matrixMatvec_type` and `globalSumReal_type`).
- Added new counters: `numGlobalSum`, `volumeGlobalSum`, `numBroadcast`, `volumeGlobalSum`, `timeOrtho`, `timeGlobalSum`, `timeBroadcast`.
- Added `primme_params_create()`, `primme_params_destroy()`, `primme_svds_params_create()`, and `primme_svds_params_destroy()`.

Changes in PRIMME 2.2 (released on October 26, 2018):

- Improved stability for single precision.
- Improved support for the shared library.
- Updated PETSc examples in Fortran; added new examples in single precision.
- Improved support for FreeBSD and MacOS.
- New install and uninstall actions.

- MATLAB interface support for user-defined stopping criterion (see `convTestFun` and `convTestFun`) and stopping with `ctr+c`.
- Optional suffix on **BLAS/LAPACK** function names (for OpenBLAS, see `PRIMME_BLAS_SUFFIX`).
- Replaced XHEGV by XHEGVX (to support ESSL).
- Fixed bugs in the library and in the Matlab interface.

Changes in PRIMME 2.1 (released on April 4, 2017):

- Improved robustness by broadcasting the result of critical **LAPACK** operations instead of replicating them on every process; this is useful when using a threaded **BLAS/LAPACK** or when some parallel processes may run on different architectures or libraries.
- New stopping criteria in QMR that improve performance for interior problems.
- MATLAB interface reimplementations with support for singular value problems, `primme_svds()`, with double and single precision, and compatible with Octave.
- R interface
- Proper reporting of convergence history for singular value solvers.

Changes in PRIMME 2.0 (released on September 19, 2016):

- Changed license to BSD 3-clause.
- New support for singular value problems; see `dprimme_svds()`.
- New support for `float` and `complex float` arithmetic.
- Support for problem dimensions larger than  $2^{31}$ , without requiring **BLAS** and **LAPACK** compiled with 64-bits integers.
- Improve robustness and performance for interior problems; implemented advanced refined and harmonic-Ritz extractions.
- Python interface compatible with **NumPy** and **SciPy Library**.
- Added parameter to indicate the leading dimension of the input/output matrices and to return an error code in callbacks `matrixMatvec`, `applyPreconditioner`, `massMatrixMatvec` and `globalSumReal`.
- Changed to type `PRIMME_INT` the options `n`, `nLocal`, `maxMatvecs` and `iseed`, and the stats counters `numOuterIterations`, `numRestarts`, `numMatvecs`, `numPreconds`. Also changed `realWorkSize` to `size_t`. Fortran interface functions will expect an integer of size compatible with `PRIMME_INT` for all parameters with integer type: `int`, `PRIMME_INT` and `size_t`; see also parameter value in functions `primmetop_set_member_f77()`, `primmetop_get_member_f77()`, `primme_set_member_f77()` and `primme_get_member_f77()`.
- Added parameter to return an error code in Fortran interface functions: `primmetop_set_member_f77()`, `primmetop_get_member_f77()`, `primme_set_member_f77()` and `primme_get_member_f77()`.
- Added leading dimension for `evecs` `ldevecs` and preferred leading dimension for the operators `ldOps`, such as `matrixMatvec`.
- Optional user-defined convergence function, `convTestFun`.
- Prefixed methods with `PRIMME_`. Rename Fortran constants from `PRIMMEF77_` to `PRIMME_`.
- Removed `primme_display_stats_f77`.

Changes in PRIMME 1.2.2 (released on October 13, 2015):

- Fixed wrong symbols in `libdprimme.a` and `libzprimme.a`.



- `primme_set_method()` sets `PRIMME_JDQMR` instead of `PRIMME_JDQMR_ETol` for preset methods `PRIMME_DEFAULT_MIN_TIME` and `PRIMME_DYNAMIC` when seeking interior values.
- Fixed compilation of driver with a `PETSc` installation without `HYPRE`.
- Included the content of the environment variable `INCLUDE` for compiling the driver.

Changes in PRIMME 1.2.1 (released on September 7, 2015):

- Added MATLAB interface to full PRIMME functionality.
- Support for `BLAS/LAPACK` with 64bits integers (`-DPRIMME_BLASINT_SIZE=64`).
- Simplified configuration of `Make_flags` and `Make_links` (removed `TOP` variable and replaced defines `NUM_SUM` and `NUM_IBM` by `F77UNDERSCORE`).
- Replaced directories `DTEST` and `ZTEST` by `TEST`, that has:
  - `driver.c`: read matrices in MatrixMarket format and `PETSc` binary and call PRIMME with the parameters specified in a file; support complex arithmetic and MPI and can use `PETSc` preconditioners.
  - `ex*.c` and `ex*.f`: small, didactic examples of usage in C and Fortran and in parallel (with `PETSc`).
- Fixed a few minor bugs and improved documentation (especially the F77 interface).
- Using `Sphinx` to manage documentation.

Changes in PRIMME 1.2 (released on December 21, 2014):

- A Fortran compiler is no longer required for building the PRIMME library. Fortran programs can still be linked to PRIMME's F77 interface.
- Fixed some uncommon issues with the F77 interface.
- PRIMME can be called now multiple times from the same program.
- Performance improvements in the QMR inner solver, especially for complex arithmetic.
- Fixed a couple of bugs with the locking functionality.
  - In certain extreme cases where all eigenvalues of a matrix were needed.
  - The order of selecting interior eigenvalues.

The above fixes have improved robustness and performance.

- PRIMME now assigns unique random seeds per parallel process for up to  $4096^3$  (140 trillion) processes.
- For the `PRIMME_DYNAMIC` method, fixed issues with initialization and synchronization decisions across multiple processes.
- Fixed uncommon library interface bugs, coordinated better setting the method and the user setting of parameters, and improved the interface in the sample programs and makefiles.
- Other performance and documentation improvements.

## 1.3 License Information

PRIMME is licensed under the 3-clause license BSD. Python and MATLAB interfaces have BSD-compatible licenses. Source code under `tests` is compatible with LGPLv3. Details can be taken from `COPYING.txt`:

```
Copyright (c) 2018, College of William & Mary  
All rights reserved.
```

## 1.4 Citing the code

Please cite [r1] and [r6]. Find the BibTeX in the following and also in `doc/primme.bib`:

```
@Article{PRIMME,
  author = {Andreas Stathopoulos and James R. McCombs},
  title = {{PRIMME}: {PR}econditioned {I}terative {M}ulti{M}ethod
           {E}igensolver: Methods and software description},
  journal = {ACM Transactions on Mathematical Software},
  volume = {37},
  number = {2},
  year = {2010},
  pages = {21:1--21:30},
}

@Article{svds_software,
  author = {Lingfei Wu and Eloy Romero and Andreas Stathopoulos},
  title = {PRIMME{\_}SVDS: {A} High-Performance Preconditioned {SVD} Solver for
           Accurate Large-Scale Computations},
  journal = {SIAM Journal on Scientific Computing},
  volume = {39},
  number = {5},
  pages = {S248--S271},
  year = {2017},
  doi = {10.1137/16M1082214},
  url = { https://doi.org/10.1137/16M1082214 },
}
```

More information on the algorithms and research that led to this software can be found in the rest of the papers [r2], [r3], [r4], [r5], [r7]. The work has been supported by a number of grants from the National Science Foundation.

## 1.5 Contact Information

For reporting bugs or questions about functionality contact [Andreas Stathopoulos](#) by email, *andreas* at *cs.wm.edu*. See further information in the webpage <http://www.cs.wm.edu/~andreas/software> and on [github](#).

**SUPPORT**

- National Science Foundation through grants CCF 1218349, ACI SI2-SSE 1440700, and NSCI 1835821
- Department of Energy through grant Exascale Computing Project 17-SC-20-SC

## 2.1 Directory Structure

The next directories and files should be available:

- `COPYING.txt`, license;
- `Make_flags`, flags to be used by makefiles to compile library and tests;
- `Link_flags`, flags needed in making and linking the test programs;
- `include/`, directory with headers files;
- `src/`, directory with the source code for `libprimme`:
  - `include/`, common headers;
  - `eigs/`, eigenvalue interface and implementation;
  - `svds/`, singular value interface and implementation;
  - `tools/`, tools used to generated some headers;
- `Matlab/`, MATLAB interface;
- `Python/`, Python interface;
- `examples/`, sample programs in C, C++ and F77, both sequential and parallel;
- `tests/`, drivers for testing purpose and test cases;
- `lib/libprimme.a`, the PRIMME library (to be made);
- `makefile` main make file;
- `readme.txt` text version of the documentation;
- `doc/` directory with the HTML and PDF versions of the documentation.

## 2.2 Making and Linking

`Make_flags` has the flags and compilers used to make `libprimme.a`:

- *CC*, compiler program such as `gcc`, `clang` or `icc`.
- *CFLAGS*, compiler options such as `-g` or `-O3` and macro definitions like the ones described next.

Compiler flags for the *BLAS* and *LAPACK* libraries:

- `-DF77UNDERSCORE`, if Fortran appends an underscore to function names (usually it does).
- `-DPRIMME_BLASINT_SIZE=64`, if the library integers are 64-bit integer (`kind=8`) type, aka ILP64 interface; usually integers are 32-bits even in 64-bit architectures (aka LP64 interface).
- `-DPRIMME_BLAS_SUFFIX=<suffix>`, set a suffix to BLAS/LAPACK function names; for instance, OpenBlas compiled with ILP64 may append `_64` to the function names.

By default PRIMME sets the integer type for matrix dimensions and counters (*PRIMME\_INT*) to 64 bits integer `int64_t`. This can be changed by setting the macro `PRIMME_INT_SIZE` to one of the following values:

- 0: use the regular `int` of your compiler.
- 32: use C99 `int32_t`.
- 64: use C99 `int64_t`.

---

**Note:** When `-DPRIMME_BLASINT_SIZE=64` is set the code uses the type `int64_t` supported by the C99 standard. In case the compiler doesn't honor the standard, you can set the corresponding type name supported, for instance `-DPRIMME_BLASINT_SIZE=__int64`.

---

After customizing `Make_flags`, type this to generate `libprimme.a`:

```
make lib
```

Making can be also done at the command line:

```
make lib CC=clang CFLAGS='-O3'
```

`Link_flags` has the flags for linking with external libraries and making the executables located in `examples` and `tests`:

- *LDFLAGS*, linker flags such as `-framework Accelerate`.
- *LIBS*, flags to link with libraries (*BLAS* and *LAPACK* are required), such as `-lprimme -llapack -lblas -lgfortran -lm`.

After that, type this to compile and execute a simple test:

```
$ make test
...
Test passed!
...
Test passed!
```

In case of linking problems check flags in *LDFLAGS* and *LIBS* and consider to add/remove `-DF77UNDERSCORE` from *CFLAGS*. If the execution fails consider to add/remove `-DPRIMME_BLASINT_SIZE=64` from *CFLAGS*.

Full description of actions that *make* can take:

- *make lib*, builds the static library `libprimme.a`.

- *make solib*, builds the shared library `libprimme.so`.
- *make install*, installs header files and the static and dynamic libraries.
- *make uninstall*, uninstalls header files and the static and dynamic libraries.
- *make matlab*, builds `libprimme.a` compatible with MATLAB and the MATLAB module.
- *make octave*, builds `libprimme.a` and the Octave module.
- *make python*, builds `libprimme.a` and the Python module.
- *make python\_install*, install the Python module.
- *make R\_install*, builds and installs the R package.
- *make test*, build and execute simple examples.
- *make clean*, removes all `*.o`, `a.out`, and core files from `src`.

### 2.2.1 Considerations using an IDE

PRIMME can be built in other environments such as Anjuta, Eclipse, KDevelop, Qt Creator, Visual Studio and XCode. To build the PRIMME library do the following:

1. Create a new project and include the source files under the directory `src`.
2. Add the directories `include` and `src/include` as include directories.

To build an example code using PRIMME make sure:

- to add a reference for PRIMME, [BLAS](#) and [LAPACK](#) libraries;
- to add the directory `include` as an include directory.



## 2.3 Tested Systems

PRIMME is primary developed with GNU gcc, g++ and gfortran (versions 4.8 and later). Many users have reported builds on several other platforms/compilers:

- SUSE 13.1 & 13.2
- CentOS 6.6
- Ubuntu 18.04
- MacOS X 10.9 & 10.10
- Cygwin & MinGW
- Cray XC30
- FreeBSD 11.2

## 2.4 Main Contributors

- James R. McCombs
- Eloy Romero Alcalde
- Andreas Stathopoulos
- Lingfei Wu

## EIGENVALUE PROBLEMS

### 3.1 C Library Interface

The PRIMME interface is composed of the following functions. To solve real symmetric and complex Hermitian problems, standard  $Ax = \lambda x$  and generalized  $Ax = \lambda Bx$ , call:

```
int dprimme (double *evals, double *evecs, double *resNorms,  
             primme_params *primme)  
int zprimme (double *evals, PRIMME_COMPLEX_DOUBLE *evecs,  
             double *resNorms, primme_params *primme)
```

There are more versions for matrix problems working in other precisions:

Precision	Real	Complex
half	<i>hprimme()</i> <i>hsprimme()</i>	<i>kprimme()</i> <i>ksprimme()</i>
single	<i>sprimme()</i>	<i>cprimme()</i>
double	<i>dprimme()</i>	<i>zprimme()</i>

To solve standard eigenproblems with normal but not necessarily Hermitian matrices call:

```
int zprimme_normal (PRIMME_COMPLEX_DOUBLE *evals,  
                   PRIMME_COMPLEX_DOUBLE *evecs,  
                   double *resNorms, primme_params *primme)
```

There are more versions for matrix problems working in other precisions:

Precision	Complex
half	<i>kprimme_normal()</i> <i>kcprimme_normal()</i>
single	<i>cprimme_normal()</i>
double	<i>zprimme_normal()</i>

Other useful functions:

```
void primme_initialize (primme_params *primme)  
int primme_set_method (primme_preset_method method,  
                      primme_params *params)  
void primme_display_params (primme_params primme)  
void primme_free (primme_params *primme)
```

PRIMME stores its data on the structure *primme\_params*. See *Parameters Guide* for an introduction about its fields.

### 3.1.1 Running

To use PRIMME, follow these basic steps.

1. Include:

```
#include "primme.h" /* header file is required to run primme */
```

2. Initialize a PRIMME parameters structure for default settings:

```
primme_params primme;  
primme_initialize (&primme);
```

3. Set problem parameters (see also *Parameters Guide*), and, optionally, set one of the *preset methods*:

```
primme.matrixMatvec = LaplacianMatrixMatvec; /* MV product */  
primme.n = 100; /* set problem dimension */  
primme.numEvals = 10; /* Number of wanted eigenpairs */  
ret = primme_set_method (method, &primme);  
...
```

4. Then call the solver:

```
ret = dprimme (evals, vecs, resNorms, &primme);
```

The call arguments are:

- *evals*, array to return the found eigenvalues;
- *vecs*, array to return the found eigenvectors;
- *resNorms*, array to return the residual norms of the found eigenpairs; and
- *ret*, returned error code.

5. To free the work arrays in PRIMME:

```
primme_free (&primme);
```

See usage examples at the directory *examples*.

### 3.1.2 Parameters Guide

PRIMME stores the data on the structure *primme\_params*, which has the next fields:

#### *Basic*

PRIMME\_INT *n*, matrix dimension.

void (\**matrixMatvec*) (...), matrix-vector product.

void (\**massMatrixMatvec*) (...), mass matrix-vector product (null for standard problems).

int *numEvals*, how many eigenpairs to find.

primme\_target *target*, which eigenvalues to find.

int *numTargetShifts*, for targeting interior eigenpairs.

double \**targetShifts*

double *eps*, tolerance of the residual norm of converged eigenpairs.

#### *For parallel programs*

int *numProcs*, number of processes

int *procID*, rank of this process

PRIMME\_INT *nLocal*, number of rows stored in this process  
 void (\* *globalSumReal*) (...), sum reduction among processes  
 void (\* *broadcastReal*) (...), broadcast array among processes

#### *Accelerate the convergence*

void (\* *applyPreconditioner*) (...), preconditioner-vector product.  
 int *initSize*, initial vectors as approximate solutions.  
 int *maxBasisSize*  
 int *minRestartSize*  
 int *maxBlockSize*

#### *User data*

void \* *commInfo*  
 void \* *matrix*  
 void \* *massMatrix*  
 void \* *preconditioner*  
 void \* *convtest*  
 void \* *monitor*

#### *Advanced options*

PRIMME\_INT *ldevecs*, leading dimension of the evecs.  
 int *numOrthoConst*, orthogonal constrains to the eigenvectors.  
 int *dynamicMethodSwitch*  
 int *locking*  
 PRIMME\_INT *maxMatvecs*  
 PRIMME\_INT *maxOuterIterations*  
 PRIMME\_INT *iseed* [4]  
 double *aNorm*  
 double *BNorm*  
 double *invBNorm*  
 int *printLevel*  
 FILE \* *outputFile*  
 double \* *ShiftsForPreconditioner*  
 primme\_init *initBasisMode*  
 struct projection\_params *projectionParams*  
 struct restarting\_params *restartingParams*  
 struct correction\_params *correctionParams*  
 struct primme\_stats *stats*  
 void (\* *convTestFun*) (...), custom convergence criterion.  
 PRIMME\_INT *ldOPs*, leading dimension to use in *matrixMatvec*.  
 void (\* *monitorFun*) (...), custom convergence history.  
 primme\_op\_datatype *matrixMatvec\_type*  
 primme\_op\_datatype *massMatrixMatvec\_type*  
 primme\_op\_datatype *applyPreconditioner\_type*  
 primme\_op\_datatype *globalSumReal\_type*  
 primme\_op\_datatype *broadcastReal\_type*  
 primme\_op\_datatype *internalPrecision*

```
primme_orth orth
```

PRIMME requires the user to set at least the dimension of the matrix (*n*) and the matrix-vector product (*matrixMatvec*), as they define the problem to be solved. For parallel programs, *nLocal*, *procID* and *globalSumReal* are also required.

In addition, most users would want to specify how many eigenpairs to find, *numEvals*, and provide a preconditioner *applyPreconditioner* (if available).

It is useful to have set all these before calling *primme\_set\_method()*. Also, if users have a preference on *maxBasisSize*, *maxBlockSize*, etc, they should also provide them into *primme\_params* prior to the *primme\_set\_method()* call. This helps *primme\_set\_method()* make the right choice on other parameters. It is sometimes useful to check the actual parameters that PRIMME is going to use (before calling it) or used (on return) by printing them with *primme\_display\_params()*.

### 3.1.3 Interface Description

The next enumerations and functions are declared in *primme.h*.

#### ?primme

```
int hprimme (PRIMME_HALF *evals, PRIMME_HALF *evecs, PRIMME_HALF *resNorms,
             primme_params *primme)
```

```
int hsprimme (float *evals, PRIMME_HALF *evecs, float *resNorms, primme_params *primme)
```

```
int kprimme (PRIMME_HALF *evals, PRIMME_COMPLEX_HALF *evecs, PRIMME_HALF *resNorms,
             primme_params *primme)
```

```
int ksprimme (float *evals, PRIMME_COMPLEX_HALF *evecs, float *resNorms, primme_params
              *primme)
    New in version 3.0.
```

```
int sprimme (float *evals, float *evecs, float *resNorms, primme_params *primme)
```

```
int cprimme (float *evals, PRIMME_COMPLEX_FLOAT *evecs, float *resNorms, primme_params
            *primme)
    New in version 2.0.
```

```
int dprimme (double *evals, double *evecs, double *resNorms, primme_params *primme)
```

```
int zprimme (double *evals, PRIMME_COMPLEX_DOUBLE *evecs, double *resNorms, primme_params
            *primme)
    Solve a real symmetric/Hermitian standard or generalized eigenproblem.
```

All arrays should be hosted on CPU. The computations are performed on CPU (see *magma\_dprimme()* for using GPUs).

#### Parameters

- **evals** – array at least of size *numEvals* to store the computed eigenvalues; all processes in a parallel run return this local array with the same values.
- **evecs** – array at least of size *nLocal* times (*numOrthoConst* + *numEvals*) with leading dimension *ldevecs* to store column-wise the (local part for this process of the) computed eigenvectors.
- **resNorms** – array at least of size *numEvals* to store the residual norms of the computed eigenpairs; all processes in parallel run return this local array with the same values.

- **primme** – parameters structure.

**Returns** error indicator; see *Error Codes*.

On input, `evecs` should start with the content of the `numOrthoConst` vectors, followed by the `initSize` vectors.

On return, the  $i$ -th eigenvector starts at `evecs[( numOrthoConst + i)* ldevecs ]`, with value `evals[i]` and associated residual 2-norm `resNorms[i]`. The first vector has index  $i=0$ . The number of eigenpairs marked as converged (see *eps*) is returned on `initSize`. Since version 4.0, if the returned error code is `PRIMME_MAIN_ITER_FAILURE`, PRIMME may return also unconverged eigenpairs and its residual norms in `evecs`, `evals`, and `resNorms` starting at  $i=\text{initSize}$  and going up to either `numEvals-1` or the last `resNorms[i]` with non-negative value.

All internal operations are performed at the same precision than `evecs` unless the user sets `internalPrecision` otherwise. The functions `hsprimme()` and `ksprimme()` perform all computations in half precision by default and report the eigenvalues and the residual norms in single precision. These functions may help in applications that may be not built with a compiler supporting half precision.

The type and precision of the callbacks is also the same as `evecs`. Although this can be changed. See details for `matrixMatvec`, `massMatrixMatvec`, `applyPreconditioner`, `globalSumReal`, `broadcastReal`, and `convTestFun`.

### *magma\_?primme*

```
int magma_hprimme (PRIMME_HALF *evals, PRIMME_HALF *evecs, PRIMME_HALF *resNorms,
                  primme_params *primme)
int magma_hsprimme (float *evals, PRIMME_HALF *evecs, float *resNorms, primme_params *primme)
int magma_kprimme (PRIMME_HALF *evals, PRIMME_COMPLEX_HALF *evecs, PRIMME_HALF
                  *resNorms, primme_params *primme)
int magma_sprimme (float *evals, float *evecs, float *resNorms, primme_params *primme)
int magma_ksprimme (float *evals, PRIMME_COMPLEX_HALF *evecs, float *resNorms, primme_params
                  *primme)
int magma_cprimme (float *evals, PRIMME_COMPLEX_FLOAT *evecs, float *resNorms, primme_params
                  *primme)
int magma_dprimme (double *evals, double *evecs, double *resNorms, primme_params *primme)
int magma_zprimme (double *evals, PRIMME_COMPLEX_DOUBLE *evecs, double *resNorms,
                  primme_params *primme)
```

Solve a real symmetric/Hermitian standard or generalized eigenproblem.

Most of the computations are performed on GPU (see `dprimme()` for using only the CPU).

#### Parameters

- **evals** – CPU array at least of size `numEvals` to store the computed eigenvalues; all processes in a parallel run return this local array with the same values.
- **evecs** – GPU array at least of size `nLocal` times  $(\text{numOrthoConst} + \text{numEvals})$  with leading dimension `ldevecs` to store column-wise the (local part for this process of the) computed eigenvectors.
- **resNorms** – CPU array at least of size `numEvals` to store the residual norms of the computed eigenpairs; all processes in parallel run return this local array with the same values.
- **primme** – parameters structure.

**Returns** error indicator; see *Error Codes*.

On input, `evects` should start with the content of the `numOrthoConst` vectors, followed by the `initSize` vectors.

On return, the  $i$ -th eigenvector starts at `evects[( numOrthoConst + i)* ldevecs ]`, with value `evals[i]` and associated residual 2-norm `resNorms[i]`. The first vector has index  $i=0$ . The number of eigenpairs marked as converged (see `eps`) is returned on `initSize`. Since version 4.0, if the returned error code is `PRIMME_MAIN_ITER_FAILURE`, PRIMME may return also unconverged eigenpairs and its residual norms in `evects`, `evals`, and `resNorms` starting at  $i=\text{initSize}$  and going up to either `numEvals-1` or the last `resNorms[i]` with non-negative value.

All internal operations are performed at the same precision than `evects` unless the user sets `internalPrecision` otherwise. The functions `hsprimme()` and `ksprimme()` perform all computations in half precision by default and report the eigenvalues and the residual norms in single precision. These functions may help in applications that may be not built with a compiler supporting half precision.

The type and precision of the callbacks is also the same as `evects`. Although this can be changed. See details for `matrixMatvec`, `massMatrixMatvec`, `applyPreconditioner`, `globalSumReal`, `broadcastReal`, and `convTestFun`.

New in version 3.0.

### ?primme\_normal

```
int kprimme_normal (PRIMME_COMPLEX_HALF *evals, PRIMME_COMPLEX_HALF *evects,
                   PRIMME_HALF *resNorms, primme_params *primme)
int kcprimme_normal (PRIMME_COMPLEX_FLOAT *evals, PRIMME_COMPLEX_HALF *evects, float
                    *resNorms, primme_params *primme)
int cprimme_normal (PRIMME_COMPLEX_FLOAT *evals, PRIMME_COMPLEX_FLOAT *evects, float
                  *resNorms, primme_params *primme)
int zprimme_normal (PRIMME_COMPLEX_DOUBLE *evals, PRIMME_COMPLEX_DOUBLE *evects,
                  double *resNorms, primme_params *primme)
```

Solve a normal standard eigenproblem, which may not be Hermitian.

All arrays should be hosted on CPU. The computations are performed on CPU (see `magma_zprimme_normal()` for using GPUs).

#### Parameters

- **evals** – array at least of size `numEvals` to store the computed eigenvalues; all processes in a parallel run return this local array with the same values.
- **evects** – array at least of size `nLocal` times  $(\text{numOrthoConst} + \text{numEvals})$  with leading dimension `ldevecs` to store column-wise the (local part for this process of the) computed eigenvectors.
- **resNorms** – array at least of size `numEvals` to store the residual norms of the computed eigenpairs; all processes in parallel run return this local array with the same values.
- **primme** – parameters structure.

**Returns** error indicator; see [Error Codes](#).

On input, `evects` should start with the content of the `numOrthoConst` vectors, followed by the `initSize` vectors.

On return, the  $i$ -th eigenvector starts at `evects[( numOrthoConst + i)* ldevecs ]`, with value `evals[i]` and associated residual 2-norm `resNorms[i]`. The first vector has index  $i=0$ . The number of eigenpairs marked as converged (see `eps`) is returned on `initSize`. Since version 4.0, if the returned error code is `PRIMME_MAIN_ITER_FAILURE`, PRIMME may return also unconverged eigenpairs and its residual norms in



*evects*, *evals*, and *resNorms* starting at *i=initSize* and going up to either *numEvals*-1 or the last *resNorms[i]* with non-negative value.

All internal operations are performed at the same precision than *evects* unless the user sets *internalPrecision* otherwise. The functions *hsprimme()* and *ksprimme()* perform all computations in half precision by default and report the eigenvalues and the residual norms in single precision. These functions may help in applications that may be not built with a compiler supporting half precision.

The type and precision of the callbacks is also the same as *evects*. Although this can be changed. See details for *matrixMatvec*, *applyPreconditioner*, *globalSumReal*, *broadcastReal*, and *convTestFun*.

New in version 3.0.

### *magma\_?primme\_normal*

```
int magma_kprimme_normal (PRIMME_COMPLEX_HALF *evals, PRIMME_COMPLEX_HALF *evects,
                          PRIMME_HALF *resNorms, primme_params *primme)
int magma_kcprimme_normal (PRIMME_COMPLEX_FLOAT *evals, PRIMME_COMPLEX_HALF
                           *evects, float *resNorms, primme_params *primme)
int magma_cpprimme_normal (PRIMME_COMPLEX_FLOAT *evals, PRIMME_COMPLEX_FLOAT
                           *evects, float *resNorms, primme_params *primme)
int magma_zprimme_normal (PRIMME_COMPLEX_DOUBLE *evals, PRIMME_COMPLEX_DOUBLE
                           *evects, double *resNorms, primme_params *primme)
```

Solve a normal standard eigenproblem, which may not be Hermitian.

Most of the computations are performed on GPU (see *zprimme\_normal()* for using only the CPU).

#### Parameters

- **evals** – CPU array at least of size *numEvals* to store the computed eigenvalues; all processes in a parallel run return this local array with the same values.
- **evects** – GPU array at least of size *nLocal* times (*numOrthoConst* + *numEvals*) with leading dimension *ldevects* to store column-wise the (local part for this process of the) computed eigenvectors.
- **resNorms** – CPU array at least of size *numEvals* to store the residual norms of the computed eigenpairs; all processes in parallel run return this local array with the same values.
- **primme** – parameters structure.

**Returns** error indicator; see *Error Codes*.

On input, *evects* should start with the content of the *numOrthoConst* vectors, followed by the *initSize* vectors.

On return, the *i*-th eigenvector starts at *evects[( numOrthoConst + i)\* ldevects ]*, with value *evals[i]* and associated residual 2-norm *resNorms[i]*. The first vector has index *i=0*. The number of eigenpairs marked as converged (see *eps*) is returned on *initSize*. Since version 4.0, if the returned error code is *PRIMME\_MAIN\_ITER\_FAILURE*, PRIMME may return also unconverged eigenpairs and its residual norms in *evects*, *evals*, and *resNorms* starting at *i=initSize* and going up to either *numEvals*-1 or the last *resNorms[i]* with non-negative value.

All internal operations are performed at the same precision than *evects* unless the user sets *internalPrecision* otherwise. The functions *hsprimme()* and *ksprimme()* perform all computations in half precision by default and report the eigenvalues and the residual norms in single precision. These functions may help in applications that may be not built with a compiler supporting half precision.

The type and precision of the callbacks is also the same as *evcs*. Although this can be changed. See details for *matrixMatvec*, *applyPreconditioner*, *globalSumReal*, *broadcastReal*, and *convTestFun*.

New in version 3.0.

### **primme\_initialize**

void **primme\_initialize** (*primme\_params* \**primme*)

Initialize a PRIMME parameters structure to the default values.

After calling *dprimme()* (or a variant), call *primme\_free()* to release allocated resources by PRIMME.

#### **Parameters**

- **primme** – parameters structure.

Example:

```
primme_params primme;
primme_initialize(&primme);

primme.n = 100;
...
dprimme(evals, evcs, rnorms, &primme);
...

primme_free(&primme);
```

See the alternative function *primme\_params\_create()* that also allocates the *primme\_params* structure.

### **primme\_params\_create**

*primme\_params* \***primme\_params\_create** (void)

Allocate and initialize a parameters structure to the default values.

After calling *dprimme()* (or a variant), call *primme\_params\_destroy()* to release allocated resources by PRIMME.

**Returns** pointer to a parameters structure.

Example:

```
primme_params *primme = primme_params_create();

primme->n = 100;
...
dprimme(evals, evcs, rnorms, primme);
...

primme_params_destroy(primme);
```

See the alternative function *primme\_initialize()* that only initializes the structure.

New in version 3.0.

## primme\_set\_method

int **primme\_set\_method** (*primme\_preset\_method method, primme\_params \*primme*)  
 Set PRIMME parameters to one of the preset configurations.

### Parameters

- **method** – preset configuration; one of

*PRIMME\_DYNAMIC*  
*PRIMME\_DEFAULT\_MIN\_TIME*  
*PRIMME\_DEFAULT\_MIN\_MATVECS*  
*PRIMME\_Arnoldi*  
*PRIMME\_GD*  
*PRIMME\_GD\_plusK*  
*PRIMME\_GD\_Olsen\_plusK*  
*PRIMME\_JD\_Olsen\_plusK*  
*PRIMME\_RQI*  
*PRIMME\_JDQR*  
*PRIMME\_JDQMR*  
*PRIMME\_JDQMR\_ETol*  
*PRIMME\_STEEPEST\_DESCENT*  
*PRIMME\_LOBPCG\_OrthoBasis*  
*PRIMME\_LOBPCG\_OrthoBasis\_Window*

- **primme** – parameters structure.

See also *Preset Methods*.

## primme\_display\_params

void **primme\_display\_params** (*primme\_params primme*)  
 Display all printable settings of `primme` into the file descriptor *outputFile*.

### Parameters

- **primme** – parameters structure.

## primme\_free

void **primme\_free** (*primme\_params \*primme*)  
 Free memory allocated by PRIMME.

### Parameters

- **primme** – parameters structure.

### **primme\_params\_destroy**

int **primme\_params\_destroy** (*primme\_params* \**primme*)

Free memory allocated by PRIMME associated to a parameters structure created with *primme\_params\_create()*.

#### **Parameters**

- **primme** – parameters structure.

**Returns** nonzero value if the call is not successful.

New in version 3.0.

## 3.2 FORTRAN 77 Library Interface

The next enumerations and functions are declared in `primme_f77.h`.

### **type ptr**

Fortran datatype with the same size as a pointer. Use `integer*4` when compiling in 32 bits and `integer*8` in 64 bits.

### 3.2.1 `primme_initialize_f77`

#### **subroutine primme\_initialize\_f77 (primme)**

Allocate and initialize a PRIMME parameters structure to the default values.

After calling `dprimme_f77()` (or a variant), call `primme_free_f77()` to release allocated resources by PRIMME.

**Parameters** `primme [ptr]` :: (output) parameters structure.

### 3.2.2 `primme_set_method_f77`

#### **subroutine primme\_set\_method\_f77 (method, primme, ierr)**

Set PRIMME parameters to one of the preset configurations.

##### **Parameters**

- **method** [*integer*] :: (input) preset configuration. One of:

```
PRIMME_DYNAMIC
PRIMME_DEFAULT_MIN_TIME
PRIMME_DEFAULT_MIN_MATVECS
PRIMME_Arnoldi
PRIMME_GD
PRIMME_GD_plusK
PRIMME_GD_Olsen_plusK
PRIMME_JD_Olsen_plusK
PRIMME_RQI
PRIMME_JDQR
PRIMME_JDQMR
PRIMME_JDQMR_ETol
PRIMME_STEEPEST_DESCENT
PRIMME_LOBPCG_OrthoBasis
PRIMME_LOBPCG_OrthoBasis_Window
```

See `primme_preset_method`.

- **primme** [*ptr*] :: (input) parameters structure.
- **ierr** [*integer*] :: (output) if 0, successful; if negative, something went wrong.

### 3.2.3 primme\_free\_f77

**subroutine primme\_free\_f77** (*primme*)

Free memory allocated by PRIMME and delete all values set.

**Parameters** *primme* [*ptr*] :: (input/output) parameters structure.

### 3.2.4 sprimme\_f77

**subroutine sprimme\_f77** (*evals*, *evects*, *resNorms*, *primme*, *ierr*)

Solve a real symmetric standard or generalized eigenproblem.

All arrays should be hosted on CPU. The computations are performed on CPU (see *magma\_sprimme\_f77()* for using GPUs).

**Parameters**

- **evals** (\*) [*real*] :: (output) array at least of size *numEvals* to store the computed eigenvalues; all parallel calls return the same value in this array.
- **evects** (\*) [*real*] :: (input/output) array at least of size *nLocal* times (*numOrthoConst* + *numEvals*) with leading dimension *ldevects* to store column-wise the (local part for this process of the) computed eigenvectors.
- **resNorms** (\*) [*real*] :: (output) array at least of size *numEvals* to store the residual norms of the computed eigenpairs; all parallel calls return the same value in this array.
- **primme** [*ptr*] :: parameters structure.
- **ierr** [*integer*] :: (output) error indicator; see *Error Codes*.

Further descriptions of *evals*, *evects*, and *resNorms* on notes in subroutine *dprimme\_f77()*.

New in version 2.0.

### 3.2.5 cprimme\_f77

**subroutine cprimme\_f77** (*evals*, *evects*, *resNorms*, *primme*, *ierr*)

Solve a Hermitian standard or generalized eigenproblem.

All arrays should be hosted on CPU. The computations are performed on CPU (see *magma\_cprimme\_f77()* for using GPUs).

**Parameters**

- **evals** (\*) [*real*] :: (output) array at least of size *numEvals* to store the computed eigenvalues; all parallel calls return the same value in this array.
- **evects** (\*) [*complex real*] :: (input/output) array at least of size *nLocal* times (*numOrthoConst* + *numEvals*) with leading dimension *ldevects* to store column-wise the (local part for this process of the) computed eigenvectors.
- **resNorms** (\*) [*real*] :: (output) array at least of size *numEvals* to store the residual norms of the computed eigenpairs; all parallel calls return the same value in this array.
- **primme** [*ptr*] :: (input) parameters structure.
- **ierr** [*integer*] :: (output) error indicator; see *Error Codes*.

Further descriptions of *evals*, *evects*, and *resNorms* on notes in subroutine *dprimme\_f77()*.

New in version 2.0.

### 3.2.6 dprimme\_f77

**subroutine dprimme\_f77** (*evals*, *evects*, *resNorms*, *primme*, *ierr*)

Solve a real symmetric standard or generalized eigenproblem.

All arrays should be hosted on CPU. The computations are performed on CPU (see `magma_dprimme_f77()` for using GPUs).

#### Parameters

- **evals** (\*) [*double precision*] :: (output) array at least of size `numEvals` to store the computed eigenvalues; all parallel calls return the same value in this array.
- **evects** (\*) [*double precision*] :: (input/output) array at least of size `nLocal` times (`numOrthoConst` + `numEvals`) with leading dimension `ldevects` to store column-wise the (local part for this process of the) computed eigenvectors.
- **resNorms** (\*) [*double precision*] :: (output) array at least of size `numEvals` to store the residual norms of the computed eigenpairs; all parallel calls return the same value in this array.
- **primme** [*ptr*] :: parameters structure.
- **ierr** [*integer*] :: (output) error indicator; see *Error Codes*.

On input, *evects* should start with the content of the `numOrthoConst` vectors, followed by the `initSize` vectors.

On return, the *i*-th eigenvector starts at `evects(( numOrthoConst + i - 1)* ldevects + 1)`, with value `evals(i)` and associated residual 2-norm `resNorms(i)`. The first vector has index *i*=1. The number of eigenpairs marked as converged (see *eps*) is returned on `initSize`. Since version 4.0, if the returned error code is `PRIMME_MAIN_ITER_FAILURE`, PRIMME may return also unconverged eigenpairs and its residual norms in *evects*, *evals*, and *resNorms* starting at *i* = `initSize` + 1 and going up to either `numEvals` or the last `resNorms(i)` with non-negative value.

All internal operations are performed at the same precision than *evects* unless the user sets `internalPrecision` otherwise.

The type and precision of the callbacks is also the same as *evects*. Although this can be changed. See details for `matrixMatvec`, `massMatrixMatvec`, `applyPreconditioner`, `globalSumReal`, `broadcastReal`, and `convTestFun`.

### 3.2.7 zprimme\_f77

**subroutine zprimme\_f77** (*evals*, *evects*, *resNorms*, *primme*, *ierr*)

Solve a Hermitian standard or generalized eigenproblem.

All arrays should be hosted on CPU. The computations are performed on CPU (see `magma_zprimme_f77()` for using GPUs).

#### Parameters

- **evals** (\*) [*double precision*] :: (output) array at least of size `numEvals` to store the computed eigenvalues; all parallel calls return the same value in this array.
- **evects** (\*) [*complex double precision*] :: (input/output) array at least of size `nLocal` times (`numOrthoConst` + `numEvals`) with leading dimension `ldevects` to store column-wise the (local part for this process of the) computed eigenvectors.

- **resNorms** (\*) [*double precision*] :: (output) array at least of size *numEvals* to store the residual norms of the computed eigenpairs; all parallel calls return the same value in this array.
- **primme** [*ptr*] :: parameters structure.
- **ierr** [*integer*] :: (output) error indicator; see *Error Codes*.

Further descriptions of *evals*, *evects*, and *resNorms* on notes in subroutine *dprimme\_f77()*.

### 3.2.8 magma\_sprimme\_f77

**subroutine magma\_sprimme\_f77** (*evals*, *evects*, *resNorms*, *primme*, *ierr*)

Solve a real symmetric standard or generalized eigenproblem.

Most of the computations are performed on GPU (see *sprimme\_f77()* for using only the CPU).

#### Parameters

- **evals** (\*) [*real*] :: (output) CPU array at least of size *numEvals* to store the computed eigenvalues; all parallel calls return the same value in this array.
- **evects** (\*) [*real*] :: (input/output) GPU array at least of size *nLocal* times (*numOrthoConst* + *numEvals*) with leading dimension *ldevects* to store column-wise the (local part for this process of the) computed eigenvectors.
- **resNorms** (\*) [*real*] :: (output) CPU array at least of size *numEvals* to store the residual norms of the computed eigenpairs; all parallel calls return the same value in this array.
- **primme** [*ptr*] :: parameters structure.
- **ierr** [*integer*] :: (output) error indicator; see *Error Codes*.

Further descriptions of *evals*, *evects*, and *resNorms* on notes in subroutine *dprimme\_f77()*.

New in version 3.0.

### 3.2.9 magma\_cprimme\_f77

**subroutine magma\_cprimme\_f77** (*evals*, *evects*, *resNorms*, *primme*, *ierr*)

Solve a Hermitian standard or generalized eigenproblem.

Most of the computations are performed on GPU (see *cprimme\_f77()* for using only the CPU).

#### Parameters

- **evals** (\*) [*real*] :: (output) CPU array at least of size *numEvals* to store the computed eigenvalues; all parallel calls return the same value in this array.
- **evects** (\*) [*complex real*] :: (input/output) GPU array at least of size *nLocal* times (*numOrthoConst* + *numEvals*) with leading dimension *ldevects* to store column-wise the (local part for this process of the) computed eigenvectors.
- **resNorms** (\*) [*real*] :: (output) CPU array at least of size *numEvals* to store the residual norms of the computed eigenpairs; all parallel calls return the same value in this array.
- **primme** [*ptr*] :: (input) parameters structure.
- **ierr** [*integer*] :: (output) error indicator; see *Error Codes*.

Further descriptions of *evals*, *evects*, and *resNorms* on notes in subroutine *dprimme\_f77()*.

New in version 3.0.



### 3.2.10 magma\_dprimme\_f77

**subroutine magma\_dprimme\_f77** (*evals*, *evects*, *resNorms*, *primme*, *ierr*)

Solve a real symmetric standard or generalized eigenproblem.

Most of the computations are performed on GPU (see [dprimme\\_f77\(\)](#) for using only the CPU).

#### Parameters

- **evals** (\*) [*double precision*] :: (output) CPU array at least of size *numEvals* to store the computed eigenvalues; all parallel calls return the same value in this array.
- **evects** (\*) [*double precision*] :: (input/output) GPU array at least of size *nLocal* times (*numOrthoConst* + *numEvals*) with leading dimension *ldevects* to store column-wise the (local part for this process of the) computed eigenvectors.
- **resNorms** (\*) [*double precision*] :: (output) CPU array at least of size *numEvals* to store the residual norms of the computed eigenpairs; all parallel calls return the same value in this array.
- **primme** [*ptr*] :: parameters structure.
- **ierr** [*integer*] :: (output) error indicator; see [Error Codes](#).

Further descriptions of *evals*, *evects*, and *resNorms* on notes in subroutine [dprimme\\_f77\(\)](#).

New in version 3.0.

### 3.2.11 magma\_zprimme\_f77

**subroutine magma\_zprimme\_f77** (*evals*, *evects*, *resNorms*, *primme*, *ierr*)

Solve a Hermitian standard or generalized eigenproblem.

Most of the computations are performed on GPU (see [zprimme\\_f77\(\)](#) for using only the CPU).

#### Parameters

- **evals** (\*) [*double precision*] :: (output) CPU array at least of size *numEvals* to store the computed eigenvalues; all parallel calls return the same value in this array.
- **evects** (\*) [*complex double precision*] :: (input/output) GPU array at least of size *nLocal* times (*numOrthoConst* + *numEvals*) with leading dimension *ldevects* to store column-wise the (local part for this process of the) computed eigenvectors.
- **resNorms** (\*) [*double precision*] :: (output) CPU array at least of size *numEvals* to store the residual norms of the computed eigenpairs; all parallel calls return the same value in this array.
- **primme** [*ptr*] :: (input) parameters structure.
- **ierr** [*integer*] :: (output) error indicator; see [Error Codes](#).

Further descriptions of *evals*, *evects*, and *resNorms* on notes in subroutine [dprimme\\_f77\(\)](#).

New in version 3.0.

### 3.2.12 cprimme\_normal\_f77

**subroutine cprimme\_normal\_f77** (*evals*, *evects*, *resNorms*, *primme*, *ierr*)

Solve a normal standard eigenproblem, which may not be Hermitian.

All arrays should be hosted on CPU. The computations are performed on CPU (see `magma_cprimme_normal_f77()` for using GPUs).

#### Parameters

- **evals** (\*) [*real*] :: (output) array at least of size `numEvals` to store the computed eigenvalues; all parallel calls return the same value in this array.
- **evects** (\*) [*complex real*] :: (input/output) array at least of size `nLocal` times (`numOrthoConst` + `numEvals`) with leading dimension `ldevects` to store column-wise the (local part for this process of the) computed eigenvectors.
- **resNorms** (\*) [*real*] :: (output) array at least of size `numEvals` to store the residual norms of the computed eigenpairs; all parallel calls return the same value in this array.
- **primme** [*ptr*] :: (input) parameters structure.
- **ierr** [*integer*] :: (output) error indicator; see *Error Codes*.

Further descriptions of *evals*, *evects*, and *resNorms* on notes in subroutine `dprimme_f77()`.

New in version 3.0.

### 3.2.13 zprimme\_normal\_f77

**subroutine zprimme\_normal\_f77** (*evals*, *evects*, *resNorms*, *primme*, *ierr*)

Solve a normal standard eigenproblem, which may not be Hermitian.

All arrays should be hosted on CPU. The computations are performed on CPU (see `magma_zprimme_normal_f77()` for using GPUs).

#### Parameters

- **evals** (\*) [*double precision*] :: (output) array at least of size `numEvals` to store the computed eigenvalues; all parallel calls return the same value in this array.
- **evects** (\*) [*complex double precision*] :: (input/output) array at least of size `nLocal` times (`numOrthoConst` + `numEvals`) with leading dimension `ldevects` to store column-wise the (local part for this process of the) computed eigenvectors.
- **resNorms** (\*) [*double precision*] :: (output) array at least of size `numEvals` to store the residual norms of the computed eigenpairs; all parallel calls return the same value in this array.
- **primme** [*ptr*] :: parameters structure.
- **ierr** [*integer*] :: (output) error indicator; see *Error Codes*.

Further descriptions of *evals*, *evects*, and *resNorms* on notes in subroutine `dprimme_f77()`.

New in version 3.0.

### 3.2.14 magma\_cprimme\_normal\_f77

**subroutine magma\_cprimme\_normal\_f77** (*evals*, *evects*, *resNorms*, *primme*, *ierr*)

Solve a normal standard eigenproblem, which may not be Hermitian.

Most of the arrays are stored on GPU, and also most of the computations are done on GPU (see [cprimme\\_normal\\_f77\(\)](#) for using only the CPU).

#### Parameters

- **evals** (\*) [*real*] :: (output) CPU array at least of size *numEvals* to store the computed eigenvalues; all parallel calls return the same value in this array.
- **evects** (\*) [*complex real*] :: (input/output) GPU array at least of size *nLocal* times (*numOrthoConst* + *numEvals*) with leading dimension *ldevects* to store column-wise the (local part for this process of the) computed eigenvectors.
- **resNorms** (\*) [*real*] :: (output) CPU array at least of size *numEvals* to store the residual norms of the computed eigenpairs; all parallel calls return the same value in this array.
- **primme** [*ptr*] :: (input) parameters structure.
- **ierr** [*integer*] :: (output) error indicator; see [Error Codes](#).

Further descriptions of *evals*, *evects*, and *resNorms* on notes in subroutine [dprimme\\_f77\(\)](#).

New in version 3.0.

### 3.2.15 magma\_zprimme\_normal\_f77

**subroutine magma\_zprimme\_normal\_f77** (*evals*, *evects*, *resNorms*, *primme*, *ierr*)

Solve a normal standard eigenproblem, which may not be Hermitian.

Most of the arrays are stored on GPU, and also most of the computations are done on GPU (see [zprimme\\_normal\\_f77\(\)](#) for using only the CPU).

#### Parameters

- **evals** (\*) [*double precision*] :: (output) CPU array at least of size *numEvals* to store the computed eigenvalues; all parallel calls return the same value in this array.
- **evects** (\*) [*complex double precision*] :: (input/output) GPU array at least of size *nLocal* times (*numOrthoConst* + *numEvals*) with leading dimension *ldevects* to store column-wise the (local part for this process of the) computed eigenvectors.
- **resNorms** (\*) [*double precision*] :: (output) CPU array at least of size *numEvals* to store the residual norms of the computed eigenpairs; all parallel calls return the same value in this array.
- **primme** [*ptr*] :: (input) parameters structure.
- **ierr** [*integer*] :: (output) error indicator; see [Error Codes](#).

Further descriptions of *evals*, *evects*, and *resNorms* on notes in subroutine [dprimme\\_f77\(\)](#).

New in version 3.0.

### 3.2.16 primme\_set\_member\_f77

**subroutine primme\_set\_member\_f77** (*primme*, *label*, *value*)

Set a value in some field of the parameter structure.

#### Parameters

- **primme** [*ptr*] :: (input) parameters structure.
- **label** [*integer*] :: field where to set value. One of:

*PRIMME\_n*  
*PRIMME\_matrixMatvec*  
*PRIMME\_matrixMatvec\_type*  
*PRIMME\_applyPreconditioner*  
*PRIMME\_applyPreconditioner\_type*  
*PRIMME\_massMatrixMatvec*  
*PRIMME\_massMatrixMatvec\_type*  
*PRIMME\_numProcs*  
*PRIMME\_procID*  
*PRIMME\_commInfo*  
*PRIMME\_nLocal*  
*PRIMME\_globalSumReal*  
*PRIMME\_globalSumReal\_type*  
*PRIMME\_broadcastReal*  
*PRIMME\_broadcastReal\_type*  
*PRIMME\_numEvals*  
*PRIMME\_target*  
*PRIMME\_numTargetShifts*  
*PRIMME\_targetShifts*  
*PRIMME\_locking*  
*PRIMME\_initSize*  
*PRIMME\_numOrthoConst*  
*PRIMME\_maxBasisSize*  
*PRIMME\_minRestartSize*  
*PRIMME\_maxBlockSize*  
*PRIMME\_maxMatvecs*  
*PRIMME\_maxOuterIterations*  
*PRIMME\_iseed*  
*PRIMME\_aNorm*  
*PRIMME\_BNorm*  
*PRIMME\_invBNorm*  
*PRIMME\_eps*  
*PRIMME\_orth*  
*PRIMME\_internalPrecision*  
*PRIMME\_printLevel*  
*PRIMME\_outputFile*  
*PRIMME\_matrix*  
*PRIMME\_massMatrix*

```

PRIMME_preconditioner
PRIMME_initBasisMode
PRIMME_projectionParams_projection
PRIMME_restartingParams_maxPrevRetain
PRIMME_correctionParams_precondition
PRIMME_correctionParams_robustShifts
PRIMME_correctionParams_maxInnerIterations
PRIMME_correctionParams_projectors_LeftQ
PRIMME_correctionParams_projectors_LeftX
PRIMME_correctionParams_projectors_RightQ
PRIMME_correctionParams_projectors_RightX
PRIMME_correctionParams_projectors_SkewQ
PRIMME_correctionParams_projectors_SkewX
PRIMME_correctionParams_convTest
PRIMME_correctionParams_relTolBase
PRIMME_stats_numOuterIterations
PRIMME_stats_numRestarts
PRIMME_stats_numMatvecs
PRIMME_stats_numPreconds
PRIMME_stats_numGlobalSum
PRIMME_stats_volumeGlobalSum
PRIMME_stats_numBroadcast
PRIMME_stats_volumeBroadcast
PRIMME_stats_flopsDense
PRIMME_stats_numOrthoInnerProds
PRIMME_stats_elapsedTime
PRIMME_stats_timeMatvec
PRIMME_stats_timePrecond
PRIMME_stats_timeOrtho
PRIMME_stats_timeGlobalSum
PRIMME_stats_timeBroadcast
PRIMME_stats_timeDense
PRIMME_stats_estimateMinEval
PRIMME_stats_estimateMaxEval
PRIMME_stats_estimateLargestSVal
PRIMME_stats_estimateBNorm
PRIMME_stats_estimateInvBNorm
PRIMME_stats_maxConvTol
PRIMME_stats_lockingIssue
PRIMME_dynamicMethodSwitch
PRIMME_convTestFun
PRIMME_convTestFun_type
PRIMME_convtest
PRIMME_ldevecs
PRIMME_ldOPs
PRIMME_monitorFun
PRIMME_monitorFun_type

```

*PRIMME\_monitor*  
*PRIMME\_queue*

- **value** :: (input) value to set.

If the type of the option is integer (int, *PRIMME\_INT*, size\_t), the type of value should be as long as *PRIMME\_INT*, which is integer\*8 by default.

---

**Note:**    **Don't use** this subroutine inside PRIMME's callback functions, e.g., *matrixMatvec* or *applyPreconditioner*, or in functions called by these functions.

---

### 3.2.17 primmetop\_get\_member\_f77

**subroutine primmetop\_get\_member\_f77** (*primme*, *label*, *value*)

Get the value in some field of the parameter structure.

#### Parameters

- **primme** [*ptr*] :: (input) parameters structure.
- **label** [*integer*] :: (input) field where to get value. One of the detailed in subroutine *primmetop\_set\_member\_f77* ().
- **value** :: (output) value of the field.

If the type of the option is integer (int, *PRIMME\_INT*, size\_t), the type of value should be as long as *PRIMME\_INT*, which is integer\*8 by default.

---

**Note:**    **Don't use** this subroutine inside PRIMME's callback functions, e.g., *matrixMatvec* or *applyPreconditioner*, or in functions called by these functions. In those cases use *primme\_get\_member\_f77* ().

---

---

**Note:**    When label is one of *PRIMME\_matrixMatvec*, *PRIMME\_applyPreconditioner*, *PRIMME\_commInfo*, *PRIMME\_matrix* and *PRIMME\_preconditioner*, the returned value is a C pointer (void\*). Use Fortran pointer or other extensions to deal with it. For instance:

```
use iso_c_binding
MPI_Comm comm

comm = MPI_COMM_WORLD
call primme_set_member_f77(primme, PRIMME_commInfo, comm)
...
subroutine par_GlobalSumDouble(x,y,k,primme)
use iso_c_binding
implicit none
...
MPI_Comm, pointer :: comm
type(c_ptr) :: pcomm

call primme_get_member_f77(primme, PRIMME_commInfo, pcomm)
call c_f_pointer(pcomm, comm)
call MPI_Allreduce(x,y,k,MPI_DOUBLE,MPI_SUM,comm,ierr)
```

---

Most users would not need to retrieve these pointers in their programs.

---

### 3.2.18 primmetop\_get\_prec\_shift\_f77

**subroutine primmetop\_get\_prec\_shift\_f77** (*primme*, *index*, *value*)

Get the value in some position of the array *ShiftsForPreconditioner*.

#### Parameters

- **primme** [*ptr*] :: (input) parameters structure.
- **index** [*integer*] :: (input) position of the array; the first position is 1.
- **value** :: (output) value of the array at that position.

### 3.2.19 primme\_get\_member\_f77

**subroutine primme\_get\_member\_f77** (*primme*, *label*, *value*)

Get the value in some field of the parameter structure.

#### Parameters

- **primme** [*ptr*] :: (input) parameters structure.
- **label** [*integer*] :: (input) field where to get value. One of the detailed in subroutine `primmetop_set_member_f77()`.
- **value** :: (output) value of the field.

If the type of the option is integer (int, `PRIMME_INT`, `size_t`), the type of value should be as long as `PRIMME_INT`, which is `integer*8` by default.

---

**Note:** Use this subroutine exclusively inside PRIMME's callback functions, e.g., `matrixMatvec` or `applyPreconditioner`, or in functions called by these functions. Otherwise, e.g., from the main program, use the subroutine `primmetop_get_member_f77()`.

---



---

**Note:** When label is one of `PRIMME_matrixMatvec`, `PRIMME_applyPreconditioner`, `PRIMME_commInfo`, `PRIMME_matrix` and `PRIMME_preconditioner`, the returned value is a C pointer (void\*). Use Fortran pointer or other extensions to deal with it. For instance:

```
use iso_c_binding
MPI_Comm comm

comm = MPI_COMM_WORLD
call primme_set_member_f77(primme, PRIMME_commInfo, comm)
...
subroutine par_GlobalSumDouble(x,y,k,primme)
use iso_c_binding
implicit none
...
MPI_Comm, pointer :: comm
type(c_ptr) :: pcomm

call primme_get_member_f77(primme, PRIMME_commInfo, pcomm)
```

(continues on next page)

(continued from previous page)

```
call c_f_pointer(pcomm, comm)
call MPI_Allreduce(x,y,k,MPI_DOUBLE,MPI_SUM,comm,ierr)
```

Most users would not need to retrieve these pointers in their programs.

---

### 3.2.20 primme\_get\_prec\_shift\_f77

**subroutine** `primme_get_prec_shift_f77` (*primme*, *index*, *value*)

Get the value in some position of the array *ShiftsForPreconditioner*.

**Parameters**

- **primme** [*ptr*] :: (input) parameters structure.
- **index** [*integer*] :: (input) position of the array; the first position is 1.
- **value** :: (output) value of the array at that position.

---

**Note:** Use this subroutine exclusively inside the subroutine *matrixMatvec*, *massMatrixMatvec*, or *applyPreconditioner*. Otherwise use the subroutine *primmetop\_get\_prec\_shift\_f77()*.

---



### 3.3 FORTRAN 90 Library Interface

New in version 3.0.

The next enumerations and functions are declared in `primme_f90.inc`.

**type c\_ptr**

Fortran datatype for C pointers in module `iso_c_binding`.

**subroutine primme\_eigs\_matvec** (*x*, *ldx*, *y*, *ldy*, *blockSize*, *primme*, *ierr*)

Abstract interface for the callbacks `matrixMatvec`, `massMatrixMatvec`, and `applyPreconditioner`.

#### Parameters

- **x** (*ldx*,\*) [*type*(\*),*in*] :: matrix of size `nLocal` x `blockSize` in column-major order with leading dimension `ldx`.
- **ldx** [*c\_int64\_t*] :: the leading dimension of the array `x`.
- **y** (*ldy*,\*) [*type*(\*),*out*] :: matrix of size `nLocal` x `blockSize` in column-major order with leading dimension `ldy`.
- **ldy** [*c\_int64\_t*] :: the leading dimension of the array `y`.
- **blockSize** [*c\_int*,*in*] :: number of columns in `x` and `y`.
- **primme** [*c\_ptr*,*in*] :: parameters structure created by `primme_params_create()`.
- **ierr** [*c\_int*,*out*] :: output error code; if it is set to non-zero, the current call to PRIMME will stop.

See more details about the precision and type for `x` and `y` in the documentation of the callbacks.

#### 3.3.1 primme\_params\_create

**function primme\_params\_create** ()

Allocate and initialize a parameters structure to the default values.

After calling `xprimme()` (or a variant), call `primme_params_destroy()` to release allocated resources by PRIMME.

**Return** `primme_params_create [c_ptr]` :: pointer to a parameters structure.

#### 3.3.2 primme\_set\_method

**function primme\_set\_method** (*method*, *primme*)

Set PRIMME parameters to one of the preset configurations.

#### Parameters

- **method** [*c\_int*,*in*] :: preset configuration. One of:

```
PRIMME_DYNAMIC
PRIMME_DEFAULT_MIN_TIME
PRIMME_DEFAULT_MIN_MATVECS
PRIMME_Arnoldi
PRIMME_GD
```

```
PRIMME_GD_plusK
PRIMME_GD_Olsen_plusK
PRIMME_JD_Olsen_plusK
PRIMME_RQI
PRIMME_JDQR
PRIMME_JDQMR
PRIMME_JDQMR_ETol
PRIMME_STEEPEST_DESCENT
PRIMME_LOBPCG_OrthoBasis
PRIMME_LOBPCG_OrthoBasis_Window
```

See [primme\\_preset\\_method](#).

- **primme** [*c\_ptr*,*in*] :: parameters structure created by [primme\\_params\\_create\(\)](#).

**Return** **primme\_set\_method** [*c\_int*] :: nonzero value if the call is not successful.

### 3.3.3 primme\_params\_destroy

**function** **primme\_params\_destroy** (*primme*)

Free memory allocated by PRIMME associated to a parameters structure created with [primme\\_params\\_create\(\)](#).

**Parameters** **primme** [*c\_ptr*] :: parameters structure.

**Return** **primme\_params\_destroy** :: nonzero value if the call is not successful.

### 3.3.4 xprimme

**function** **xprimme** (*evals*, *evecs*, *resNorms*, *primme*)

Solve a real symmetric/Hermitian standard or generalized eigenproblem.

All arrays should be hosted on CPU. The computations are performed on CPU (see [magma\\_xprimme\(\)](#) for using GPUs).

**Parameters**

- **evals** (\*) [*real(kind)*,*out*] :: array at least of size [numEvals](#) to store the computed eigenvalues; all processes in a parallel run return this local array with the same values.
- **evecs** (\*) [*real(kind)* or *complex(kind)*] :: array at least of size [nLocal](#) times ([numOrthoConst](#) + [numEvals](#)) with leading dimension [ldevecs](#) to store column-wise the (local part for this process of the) computed eigenvectors.
- **resNorms** (\*) [*real(kind)*,*out*] :: array at least of size [numEvals](#) to store the residual norms of the computed eigenpairs; all processes in parallel run return this local array with the same values.
- **primme** [*c\_ptr*,*in*] :: parameters structure created by [primme\\_params\\_create\(\)](#).

**Return** **xprimme** [*c\_int*] :: error indicator; see [Error Codes](#).

The arrays *evals*, *evecs*, and *resNorms* should have the same kind.

On input, *evecs* should start with the content of the [numOrthoConst](#) vectors, followed by the [initSize](#) vectors.

On return, the  $i$ -th eigenvector starts at `evects(( numOrthoConst + i - 1)* ldevecs + 1)`, with value `evals(i)` and associated residual 2-norm `resNorms(i)`. The first vector has index  $i=1$ . The number of eigenpairs marked as converged (see `eps`) is returned on `initSize`. Since version 4.0, if the returned error code is `PRIMME_MAIN_ITER_FAILURE`, PRIMME may return also unconverged eigenpairs and its residual norms in `evects`, `evals`, and `resNorms` starting at  $i = \text{initSize} + 1$  and going up to either `numEvals` or the last `resNorms(i)` with non-negative value.

All internal operations are performed at the same precision than `evects` unless the user sets `internalPrecision` otherwise.

The type and precision of the callbacks is also the same as `evects`. Although this can be changed. See details for `matrixMatvec`, `massMatrixMatvec`, `applyPreconditioner`, `globalSumReal`, `broadcastReal`, and `convTestFun`.

### 3.3.5 magma\_xprimme

**function magma\_xprimme** (*evals*, *evects*, *resNorms*, *primme*)

Solve a real symmetric/Hermitian standard or generalized eigenproblem.

Most of the computations are performed on GPU (see `xprimme()` for using only the CPU).

#### Parameters

- **evals** (\*) [*real(kind),out*] :: CPU array at least of size `numEvals` to store the computed eigenvalues; all processes in a parallel run return this local array with the same values.
- **evects** :: GPU array at least of size `nLocal` times (`numOrthoConst + numEvals`) with leading dimension `ldevecs` to store column-wise the (local part for this process of the) computed eigenvectors.
- **resNorms** (\*) [*real(kind),out*] :: CPU array at least of size `numEvals` to store the residual norms of the computed eigenpairs; all processes in parallel run return this local array with the same values.
- **primme** [*c\_ptr,in*] :: parameters structure created by `primme_params_create()`.

**Return** `magma_xprimme [c_int]` :: error indicator; see *Error Codes*.

The arrays `evals`, `evects`, and `resNorms` should have the same kind.

Further descriptions of `evals`, `evects`, and `resNorms` on notes in function `xprimme()`.

### 3.3.6 xprimme\_normal

**function xprimme\_normal** (*evals*, *evects*, *resNorms*, *primme*)

Solve a normal standard eigenproblem, which may not be Hermitian.

All arrays should be hosted on CPU. The computations are performed on CPU (see `magma_xprimme_normal()` for using GPUs).

#### Parameters

- **evals** (\*) [*complex(kind),out*] :: array at least of size `numEvals` to store the computed eigenvalues; all processes in a parallel run return this local array with the same values.
- **evects** :: array at least of size `nLocal` times (`numOrthoConst + numEvals`) with leading dimension `ldevecs` to store column-wise the (local part for this process of the) computed eigenvectors.

- **resNorms** (\*) [*real(kind),out*] :: array at least of size *numEvals* to store the residual norms of the computed eigenpairs; all processes in parallel run return this local array with the same values.
- **primme** [*c\_ptr,in*] :: parameters structure created by *primme\_params\_create()*.

**Return** *xprimme\_normal* [*c\_int*] :: error indicator; see *Error Codes*.

The arrays *evals*, *evects*, and *resNorms* should have the same kind.

Further descriptions of *evals*, *evects*, and *resNorms* on notes in function *xprimme()*.

### 3.3.7 magma\_xprimme\_normal

**function** *magma\_xprimme\_normal* (*evals*, *evects*, *resNorms*, *primme*)

Solve a normal standard eigenproblem, which may not be Hermitian.

Most of the arrays are stored on GPU, and also most of the computations are done on GPU (see *xprimme()* for using only the CPU).

#### Parameters

- **evals** (\*) [*complex(kind),out*] :: CPU array at least of size *numEvals* to store the computed eigenvalues; all processes in a parallel run return this local array with the same values.
- **evects** :: GPU array at least of size *nLocal* times (*numOrthoConst* + *numEvals*) with leading dimension *ldevects* to store column-wise the (local part for this process of the) computed eigenvectors.
- **resNorms** (\*) [*real(kind),out*] :: CPU array at least of size *numEvals* to store the residual norms of the computed eigenpairs; all processes in parallel run return this local array with the same values.
- **primme** [*c\_ptr,in*] :: parameters structure created by *primme\_params\_create()*.

**Return** *magma\_xprimme\_normal* [*c\_int*] :: error indicator; see *Error Codes*.

The arrays *evals*, *evects*, and *resNorms* should have the same kind.

Further descriptions of *evals*, *evects*, and *resNorms* on notes in function *xprimme()*.

### 3.3.8 primme\_set\_member

**function** *primme\_set\_member* (*primme*, *label*, *value*)

Set a value in some field of the parameter structure.

#### Parameters

- **primme** [*c\_ptr,in*] :: parameters structure created by *primme\_params\_create()*.
- **label** [*c\_int,in*] :: field where to set value. One of:

*PRIMME\_n*  
*PRIMME\_matrixMatvec*  
*PRIMME\_matrixMatvec\_type*  
*PRIMME\_applyPreconditioner*  
*PRIMME\_applyPreconditioner\_type*  
*PRIMME\_massMatrixMatvec*

*PRIMME\_massMatrixMatvec\_type*  
*PRIMME\_numProcs*  
*PRIMME\_procID*  
*PRIMME\_commInfo*  
*PRIMME\_nLocal*  
*PRIMME\_globalSumReal*  
*PRIMME\_globalSumReal\_type*  
*PRIMME\_broadcastReal*  
*PRIMME\_broadcastReal\_type*  
*PRIMME\_numEvals*  
*PRIMME\_target*  
*PRIMME\_numTargetShifts*  
*PRIMME\_targetShifts*  
*PRIMME\_locking*  
*PRIMME\_initSize*  
*PRIMME\_numOrthoConst*  
*PRIMME\_maxBasisSize*  
*PRIMME\_minRestartSize*  
*PRIMME\_maxBlockSize*  
*PRIMME\_maxMatvecs*  
*PRIMME\_maxOuterIterations*  
*PRIMME\_iseed*  
*PRIMME\_aNorm*  
*PRIMME\_BNorm*  
*PRIMME\_invBNorm*  
*PRIMME\_eps*  
*PRIMME\_orth*  
*PRIMME\_internalPrecision*  
*PRIMME\_printLevel*  
*PRIMME\_outputFile*  
*PRIMME\_matrix*  
*PRIMME\_massMatrix*  
*PRIMME\_preconditioner*  
*PRIMME\_initBasisMode*  
*PRIMME\_projectionParams\_projection*  
*PRIMME\_restartingParams\_maxPrevRetain*  
*PRIMME\_correctionParams\_precondition*  
*PRIMME\_correctionParams\_robustShifts*  
*PRIMME\_correctionParams\_maxInnerIterations*  
*PRIMME\_correctionParams\_projectors\_LeftQ*  
*PRIMME\_correctionParams\_projectors\_LeftX*  
*PRIMME\_correctionParams\_projectors\_RightQ*  
*PRIMME\_correctionParams\_projectors\_RightX*  
*PRIMME\_correctionParams\_projectors\_SkewQ*  
*PRIMME\_correctionParams\_projectors\_SkewX*  
*PRIMME\_correctionParams\_convTest*  
*PRIMME\_correctionParams\_relTolBase*

*PRIMME\_stats\_numOuterIterations*  
*PRIMME\_stats\_numRestarts*  
*PRIMME\_stats\_numMatvecs*  
*PRIMME\_stats\_numPreconds*  
*PRIMME\_stats\_numGlobalSum*  
*PRIMME\_stats\_volumeGlobalSum*  
*PRIMME\_stats\_numBroadcast*  
*PRIMME\_stats\_volumeBroadcast*  
*PRIMME\_stats\_flopsDense*  
*PRIMME\_stats\_numOrthoInnerProds*  
*PRIMME\_stats\_elapsedTime*  
*PRIMME\_stats\_timeMatvec*  
*PRIMME\_stats\_timePrecond*  
*PRIMME\_stats\_timeOrtho*  
*PRIMME\_stats\_timeGlobalSum*  
*PRIMME\_stats\_timeBroadcast*  
*PRIMME\_stats\_timeDense*  
*PRIMME\_stats\_estimateMinEval*  
*PRIMME\_stats\_estimateMaxEval*  
*PRIMME\_stats\_estimateLargestSVal*  
*PRIMME\_stats\_estimateBNorm*  
*PRIMME\_stats\_estimateInvBNorm*  
*PRIMME\_stats\_maxConvTol*  
*PRIMME\_stats\_lockingIssue*  
*PRIMME\_dynamicMethodSwitch*  
*PRIMME\_convTestFun*  
*PRIMME\_convTestFun\_type*  
*PRIMME\_convtest*  
*PRIMME\_ldevecs*  
*PRIMME\_ldOPs*  
*PRIMME\_monitorFun*  
*PRIMME\_monitorFun\_type*  
*PRIMME\_monitor*  
*PRIMME\_queue*

- **value [in]** :: value to set. The allowed types are *c\_int64*, *c\_double*, *c\_ptr*, *c\_funptr* and *procedure (primme\_eigs\_matvec)*

**Return** *primme\_set\_member [c\_int]* :: nonzero value if the call is not successful.

Examples:

```
type(c_ptr) :: primme
integer :: ierr
...

integer(c_int64_t) :: n = 100
ierr = primme_set_member(primme, PRIMME_n, n)
```

(continues on next page)

(continued from previous page)

```

ierr = primme_set_member(primme, PRIMME_correctionParams_precondition,
                        1_c_int64_t)

real(c_double) :: tol = 1.0D-12
ierr = primme_set_member(primme, PRIMME_eps, tol)

integer(c_int64_t), parameter :: numTargetShifts = 2
real(c_double) :: TargetShifts(numTargetShifts) = (/3.0D0, 5.1D0/)
ierr = primme_set_member(primme, PRIMME_numTargetShifts,
                        ↪numTargetShifts)
ierr = primme_set_member(primme, PRIMME_targetShifts, TargetShifts)

ierr = primme_set_member(primme, PRIMME_target, primme_closest_abs)

procedure(primme_eigs_matvec) :: MV, ApplyPrecon
ierr = primme_set_member(primme, PRIMME_matrixMatvec, MV)

ierr = primme_set_member(primme, PRIMME_applyPreconditioner,
                        c_funloc(ApplyPrecon))

```

### 3.3.9 primme\_get\_member

**function** `primme_get_member` (*primme, label, value*)

Get the value in some field of the parameter structure.

#### Parameters

- **primme** [*c\_ptr, in*] :: parameters structure created by `primme_params_create()`.
- **label** [*integer, in*] :: field where to get value. One of the detailed in function `primme_set_member()`.
- **value** [*out*] :: value of the field. The allowed types are `c_int64`, `c_double`, and `c_ptr`.

**Return** `primme_get_member` [*c\_int*] :: nonzero value if the call is not successful.

Examples:

```

type(c_ptr) :: primme
integer :: ierr
...

integer(c_int64_t) :: n
ierr = primme_get_member(primme, PRIMME_n, n)

real(c_double) :: aNorm
ierr = primme_get_member(primme, PRIMME_aNorm, aNorm)

real(c_double), pointer :: shifts(:)
type(c_ptr) :: pshifts
ierr = primme_get_member(primme, PRIMME_ShiftsForPreconditioner, pshifts)
call c_f_pointer(pshifts, shifts, shape=[k])

```

## 3.4 Python Interface

`primme.eigsh(A, k=6, M=None, sigma=None, which='LM', v0=None, ncv=None, maxiter=None, tol=0, return_eigenvectors=True, Minv=None, OPinv=None, mode='normal', lock=None, return_stats=False, maxBlockSize=0, minRestartSize=0, maxPrevRetain=0, method=None, return_history=False, convtest=None, **kargs)`

Find  $k$  eigenvalues and eigenvectors of the real symmetric square matrix or complex Hermitian matrix  $A$ .

Solves  $A * x[i] = w[i] * x[i]$ , the standard eigenvalue problem for  $w[i]$  eigenvalues with corresponding eigenvectors  $x[i]$ .

If  $M$  is specified, solves  $A * x[i] = w[i] * M * x[i]$ , the generalized eigenvalue problem for  $w[i]$  eigenvalues with corresponding eigenvectors  $x[i]$

### Parameters

- **A** (*An  $N \times N$  matrix, array, sparse matrix, or LinearOperator*) – the operation  $A * x$ , where  $A$  is a real symmetric matrix or complex Hermitian.
- **k** (*int, optional*) – The number of eigenvalues and eigenvectors to be computed. Must be  $1 \leq k < \min(A.shape)$ .
- **M** (*An  $N \times N$  matrix, array, sparse matrix, or LinearOperator*) – the operation  $M * x$  for the generalized eigenvalue problem

$$A * x = w * M * x.$$

$M$  must represent a real, symmetric matrix if  $A$  is real, and must represent a complex, Hermitian matrix if  $A$  is complex. For best results, the data type of  $M$  should be the same as that of  $A$ .

- **sigma** (*real, optional*) – Find eigenvalues near  $\sigma$ .
- **v0** ( *$N \times 1$ , ndarray, optional*) – Initial guesses to the eigenvectors.
- **ncv** (*int, optional*) – The maximum size of the basis
- **which** (*str ['LM' | 'SM' | 'LA' | 'SA' | number]*) – Which  $k$  eigenvectors and eigenvalues to find:

'LM' : Largest in magnitude eigenvalues; the farthest from  $\sigma$

'SM' : Smallest in magnitude eigenvalues; the closest to  $\sigma$

'LA' : Largest algebraic eigenvalues

'SA' : Smallest algebraic eigenvalues

'CLT' : closest but left to  $\sigma$

'CGT' : closest but greater than  $\sigma$

number : the closest to which

When  $\sigma == \text{None}$ , 'LM', 'SM', 'CLT', and 'CGT' treat  $\sigma$  as zero.

- **maxiter** (*int, optional*) – Maximum number of iterations.
- **tol** (*float*) – Tolerance for eigenpairs (stopping criterion). The default value is  $\sqrt{\text{machine precision}}$ .

An eigenpair  $(\lambda, v)$  is marked as converged when  $\|A*v - \lambda*B*v\| < \max(\text{leig}(A, B)) * \text{tol}$ .

The value is ignored if `convtest` is provided.



- **Minv** (*(not supported yet)*) – The inverse of  $M$  in the generalized eigenproblem.
- **OPinv** ( $N \times N$  matrix, array, sparse matrix, or *LinearOperator*, optional) – Preconditioner to accelerate the convergence. Usually it is an approximation of the inverse of  $(A - \sigma M)$ .
- **return\_eigenvectors** (*bool*, optional) – Return eigenvectors (True) in addition to eigenvalues
- **mode** (*string* ['normal' | 'buckling' | 'cayley']) – Only 'normal' mode is supported.
- **lock** ( $N \times i$ , ndarray, optional) – Seek the eigenvectors orthogonal to these ones. The provided vectors *should* be orthonormal. Useful to avoid converging to previously computed solutions.
- **maxBlockSize** (*int*, optional) – Maximum number of vectors added at every iteration.
- **minRestartSize** (*int*, optional) – Number of approximate eigenvectors kept during restart.
- **maxPrevRetain** (*int*, optional) – Number of approximate eigenvectors kept from previous iteration in restart. Also referred as +k vectors in GD+k.
- **method** (*int*, optional) – Preset method, one of:
  - **DEFAULT\_MIN\_TIME** : a variant of JDQMR,
  - **DEFAULT\_MIN\_MATVECS** : GD+k
  - **DYNAMIC** : choose dynamically between these previous methods.
 See a detailed description of the methods and other possible values in<sup>2</sup>.
- **convtest** (*callable*) – User-defined function to mark an approximate eigenpair as converged.  
 The function is called as `convtest(eval, evec, resNorm)` and returns True if the eigenpair with value *eval*, vector *evec* and residual norm *resNorm* is considered converged.
- **return\_stats** (*bool*, optional) – If True, the function returns extra information (see stats in Returns).
- **return\_history** (*bool*, optional) – If True, the function returns performance information at every iteration (see hist in Returns).

### Returns

- **w** (*array*) – Array of  $k$  eigenvalues ordered to best satisfy “which”.
- **v** (*array*) – An array representing the  $k$  eigenvectors. The column  $v[:, i]$  is the eigenvector corresponding to the eigenvalue  $w[i]$ .
- **stats** (*dict*, optional (if *return\_stats*)) – Extra information reported by PRIMME:
  - “numOuterIterations”: number of outer iterations
  - “numRestarts”: number of restarts
  - “numMatvecs”: number of  $A*v$
  - “numPreconds”: number of  $OPinv*v$
  - “elapsedTime”: time that took

<sup>2</sup> Preset Methods, <http://www.cs.wm.edu/~andreas/software/doc/readme.html#preset-methods>

- "estimateMinEval": the leftmost Ritz value seen
- "estimateMaxEval": the rightmost Ritz value seen
- "estimateLargestSVal": the largest singular value seen
- "rnorms":  $\|A*x[i] - x[i]*w[i]\|$
- "hist": (if return\_history) report at every outer iteration of:
  - \* "elapsedTime": time spent up to now
  - \* "numMatvecs": number of  $A*v$  spent up to now
  - \* "nconv": number of converged pair
  - \* "eval": eigenvalue of the first unconverged pair
  - \* "resNorm": residual norm of the first unconverged pair

**Raises `PrimmeError`** – When the requested convergence is not obtained.

The PRIMME error code can be found as `err` attribute of the exception object.

See also:

**`scipy.sparse.linalg.eigs()`** eigenvalues and eigenvectors for a general (nonsymmetric) matrix  $A$   
**`primme.svds()`** singular value decomposition for a matrix  $A$

## Notes

This function is a wrapper to PRIMME functions to find the eigenvalues and eigenvectors<sup>1</sup>.

## References

## Examples

```
>>> import primme, scipy.sparse
>>> A = scipy.sparse.spdiags(range(100), [0], 100, 100) # sparse diag. matrix
>>> evals, evecs = primme.eigsh(A, 3, tol=1e-6, which='LA')
>>> evals # the three largest eigenvalues of A
array([99., 98., 97.])
>>> new_evals, new_evecs = primme.eigsh(A, 3, tol=1e-6, which='LA', lock=evecs)
>>> new_evals # the next three largest eigenvalues
array([96., 95., 94.])
>>> evals, evecs = primme.eigsh(A, 3, tol=1e-6, which=50.1)
>>> evals # the three closest eigenvalues to 50.1
array([50., 51., 49.])
>>> M = scipy.sparse.spdiags(np.asarray(range(99,-1,-1)), [0], 100, 100)
>>> # the smallest eigenvalues of the eigenproblem (A,M)
>>> evals, evecs = primme.eigsh(A, 3, M=M, tol=1e-6, which='SA')
>>> evals
array([1.0035e-07, 1.0204e-02, 2.0618e-02])
```

---

<sup>1</sup> PRIMME Software, <https://github.com/primme/primme>

```
>>> # Giving the matvec as a function
>>> import primme, scipy.sparse, numpy as np
>>> Adiag = np.arange(0, 100).reshape((100,1))
>>> def Amatmat(x):
...     if len(x.shape) == 1: x = x.reshape((100,1))
...     return Adiag * x # equivalent to diag(Adiag).dot(x)
...
>>> A = scipy.sparse.linalg.LinearOperator((100,100), matvec=Amatmat,
↪matmat=Amatmat)
>>> evals, evecs = primme.eigsh(A, 3, tol=1e-6, which='LA')
>>> evals
array([99., 98., 97.] )
```

## 3.5 MATLAB Interface

**function [varargout] = primme\_eigs(varargin)**

`primme_eigs()` finds a few eigenvalues and their corresponding eigenvectors of a symmetric/Hermitian matrix,  $A$ , or of a generalized problem  $(A, B)$ , by calling `PRIMME`.

`D = primme_eigs(A)` returns a vector of  $A$ 's 6 largest magnitude eigenvalues.

`D = primme_eigs(A, B)` returns a vector of the 6 largest magnitude eigenvalues of  $(A, B)$

`D = primme_eigs(Afun, Bfun, dim)` `D = primme_eigs(Afun, dim)` accepts a functions `Afun` and `Bfun` instead of matrices. `Afun` and `Bfun` are function handles. `Afun(x)` and `Bfun(x)` return the matrix-vector product  $A*x$  and  $B*x$ .

`D = primme_eigs(..., k)` finds the  $k$  largest magnitude eigenvalues.  $k$  must be less than the dimension of the matrix  $A$ .

`D = primme_eigs(..., k, target)` returns  $k$  eigenvalues such that: If `target` is a real number, it finds the closest eigenvalues to `target`. If `target` is

- 'LA' or 'SA', eigenvalues with the largest or smallest algebraic value.
- 'LM' or 'SM', eigenvalues with the largest or smallest magnitude if `OPTS.targetShifts` is empty. If `target` is a real or complex scalar including 0, `primme_eigs()` finds the eigenvalues closest to `target`.

In addition, if some values are provided in `OPTS.targetShifts`, it finds eigenvalues that are farthest ('LM') or closest ('SM') in absolute value from the given values.

Examples:

`k=1, 'LM', OPTS.targetShifts=[]` returns the largest magnitude `eig(A)`. `k=1, 'SM', OPTS.targetShifts=[]` returns the smallest magnitude `eig(A)`. `k=3, 'SM', OPTS.targetShifts=[2, 5]` returns the closest eigenvalue in absolute sense to 2, and the two closest eigenvalues to 5.

- 'CLT' or 'CGT', find eigenvalues closest to but less or greater than the given values in `OPTS.targetShifts`.

`D = primme_eigs(..., k, target, OPTS)` specifies extra solver parameters. Some default values are indicated in brackets {}:

- `aNorm`: the estimated 2-norm of  $A$  {0.0 (estimate the norm internally)}
- `tol`: convergence tolerance:  $\text{NORM}(A*X(:,i) - X(:,i)*D(i,i)) < \text{tol} * \text{NORM}(A)$  (see `eps`)  $\{10^4 \text{ times the machine precision}\}$
- `maxBlockSize`: maximum block size (useful for high multiplicities) {1}
- `reportLevel`: reporting level (0-3) (see `HIST`) {no reporting 0}
- `display`: whether displaying reporting on screen (see `HIST`) {0 if `HIST` provided}
- `isreal`: whether  $A$  represented by `Afun` is real or complex {false}
- `isdouble`: whether the class of in/out vectors in `Afun` are double or single {false}
- `isgpu`: whether the class of in/out vectors in `Afun` are `gpuArray` {false}
- `ishermitian`: whether  $A$  is Hermitian; otherwise it is considered normal {true}
- `targetShifts`: shifts for interior eigenvalues (see `target`) {[]}
- `v0`: any number of initial guesses to the eigenvectors (see `initSize`) {[]}

- `orthoConst`: external orthogonalization constraints (see `numOrthoConst` {})
- `locking`: 1, hard locking; 0, soft locking
- `p`: maximum size of the search subspace (see `maxBasisSize`)
- `minRestartSize`: minimum Ritz vectors to keep in restarting
- `maxMatvecs`: maximum number of matrix vector multiplications {Inf}
- `maxit`: maximum number of outer iterations (see `maxOuterIterations`) {Inf}
- `maxPrevRetain`: number of Ritz vectors from previous iteration that are kept after restart {typically >0}
- `robustShifts`: setting to true may avoid stagnation or misconvergence
- `maxInnerIterations`: maximum number of inner solver iterations
- `LeftQ`: use the locked vectors in the left projector
- `LeftX`: use the approx. eigenvector in the left projector
- `RightQ`: use the locked vectors in the right projector
- `RightX`: use the approx. eigenvector in the right projector
- `SkewQ`: use the preconditioned locked vectors in the right projector
- `SkewX`: use the preconditioned approx. eigenvector in the right projector
- `relTolBase`: a legacy from classical JDQR (not recommended)
- `convTest`: how to stop the inner QMR Method
- `convTestFun`: function handler with an alternative convergence criterion. If `FUN(EVAL, EVEC, RNORM)` returns a nonzero value, the pair (EVAL, EVEC) with residual norm RNORM is considered converged
- `iseed`: random seed
- `returnUnconverged`: whether to return unconverged pairs if maximum iterations or matvecs is reached.

`D = primme_eigs(A, k, target, OPTS, METHOD)` specifies the eigensolver method. `METHOD` can be one of the next strings:

- `'PRIMME_DYNAMIC'`, (default) switches dynamically to the best method
- `'PRIMME_DEFAULT_MIN_TIME'`, best method for low-cost matrix-vector product
- `'PRIMME_DEFAULT_MIN_MATVECS'`, best method for heavy matvec/preconditioner
- `'PRIMME_Arnoldi'`, Arnoldi not implemented efficiently
- `'PRIMME_GD'`, classical block Generalized Davidson
- `'PRIMME_GD_plusK'`, GD+k block GD with recurrence restarting
- `'PRIMME_GD_Olsen_plusK'`, GD+k with approximate Olsen precondition.
- `'PRIMME_JD_Olsen_plusK'`, GD+k, exact Olsen (two precondition per step)
- `'PRIMME_RQI'`, Rayleigh Quotient Iteration. Also INVIT, but for INVIT provide `OPTS.targetShifts`
- `'PRIMME_JDQR'`, Original block, Jacobi Davidson
- `'PRIMME_JDQMR'`, Our block JDQMR method (similar to JDCG)
- `'PRIMME_JDQMR_ETol'`, Slight, but efficient JDQMR modification

- `'PRIMME_STEEPEST_DESCENT'`, equivalent to `GD(block,2*block)`
- `'PRIMME_LOBPCG_OrthoBasis'`, equivalent to `GD(nev,3*nev)+nev`
- `'PRIMME_LOBPCG_OrthoBasis_Window'` equivalent to `GD(block,3*block)+block nev>block`

`D = primme_eigs(A,k,target,OPTS,METHOD,P)`

`D = primme_eigs(A,k,target,OPTS,METHOD,P1,P2)` uses preconditioner `P` or `P = P1*P2` to accelerate convergence of the method. Applying `P\X` should approximate  $(A - \sigma \cdot \text{eye}(N)) \backslash X$ , for  $\sigma$  near the wanted eigenvalue(s). If `P` is `[]` then a preconditioner is not applied. `P` may be a function handle `PFUN` such that `PFUN(X)` returns `P\X`.

`[X,D] = primme_eigs(...)` returns a diagonal matrix `D` with the eigenvalues and a matrix `X` whose columns are the corresponding eigenvectors.

`[X,D,R] = primme_eigs(...)` also returns an array of the residual norms of the computed eigenpairs.

`[X,D,R,STATS] = primme_eigs(...)` returns a struct to report statistical information about number of matvecs, elapsed time, and estimates for the largest and smallest algebraic eigenvalues of `A`.

`[X,D,R,STATS,HIST] = primme_eigs(...)` it returns the convergence history, instead of printing it. Every row is a record, and the columns report:

- `HIST(:,1)`: number of matvecs
- `HIST(:,2)`: time
- `HIST(:,3)`: number of converged/locked pairs
- `HIST(:,4)`: block index
- `HIST(:,5)`: approximate eigenvalue
- `HIST(:,6)`: residual norm
- `HIST(:,7)`: QMR residual norm

`OPTS.reportLevel` controls the granularity of the record. If `OPTS.reportLevel == 1`, `HIST` has one row per converged eigenpair and only the first three columns together with the fifth and the sixth are reported. If `OPTS.reportLevel == 2`, `HIST` has one row per outer iteration and converged value, and only the first six columns are reported. Otherwise `HIST` has one row per QMR iteration, outer iteration and converged value, and all columns are reported.

The convergence history is displayed if `OPTS.reportLevel > 0` and either `HIST` is not returned or `OPTS.display == 1`.

Examples:

```
A = diag(1:100);

d = primme_eigs(A,10) % the 10 largest magnitude eigenvalues

d = primme_eigs(A,10,'SM') % the 10 smallest magnitude eigenvalues

d = primme_eigs(A,10,25.0) % the 10 closest eigenvalues to 25.0

opts.targetShifts = [2 20];
d = primme_eigs(A,10,'SM',opts) % 1 eigenvalue closest to 2 and
                                % 9 eigenvalues closest to 20

B = diag(100:-1:1);
d = primme_eigs(A,B,10,'SM') % the 10 smallest magnitude eigenvalues
```

(continues on next page)

(continued from previous page)

```

opts = struct();
opts.tol = 1e-4; % set tolerance
opts.maxBlockSize = 2; % set block size
[x,d] = primme_eigs(A,10,'SA',opts,'DEFAULT_MIN_TIME')

opts.orthoConst = x;
[d,rnorms] = primme_eigs(A,10,'SA',opts) % find another 10 with the default method

% Compute the 6 eigenvalues closest to 30.5 using ILU(0) as a preconditioner
% by passing the matrices L and U.
A = sparse(diag(1:50) + diag(ones(49,1), 1) + diag(ones(49,1), -1));
[L,U] = ilu(A, struct('type', 'nofill'));
d = primme_eigs(A, k, 30.5, [], [], L, U);

% Compute the 6 eigenvalues closest to 30.5 using Jacobi preconditioner
% by passing a function.
Pfun = @(x) (diag(A) - 30.5)\x;
d = primme_eigs(A,6,30.5,[],[],Pfun) % find the closest 5 to 30.5

```

See also: `MATLAB eigs`, `primme_svds()`

## 3.6 Parameters Description

### 3.6.1 Types

The following data types are macros used in PRIMME as followed.

**type PRIMME\_INT**

Integer type used in matrix dimensions (such as *n* and *nLocal*) and counters (such as *numMatvecs*).

The integer size is controlled by the compilation flag `PRIMME_INT_SIZE`, see [Making and Linking](#).

**type PRIMME\_HALF**

Macro that is `__fp16` if half precision is supported by the compiler. Otherwise it is a struct with the same size as `int short`.

New in version 3.0.

**type PRIMME\_COMPLEX\_HALF**

Macro that is a struct with fields `r` and `i` with type `PRIMME_HALF`.

New in version 3.0.

**type PRIMME\_COMPLEX\_FLOAT**

Macro that is `complex float` in C and `std::complex<float>` in C++.

New in version 2.0.

**type PRIMME\_COMPLEX\_DOUBLE**

Macro that is `complex double` in C and `std::complex<double>` in C++.

New in version 2.0.

### 3.6.2 Other macros

**PRIMME\_VERSION\_MAJOR**

Constant `int` with the major version number.

For instance, the value of the macro is 3 for version 3.0.

New in version 3.0.

**PRIMME\_VERSION\_MINOR**

Constant `int` with the minor version number.

For instance, the value of the macro is 0 for version 3.0.

New in version 3.0.

### 3.6.3 primme\_params

**type primme\_params**

Structure to set the problem matrices and eigensolver options.

**PRIMME\_INT n**

Dimension of the matrix.

Input/output:

`primme_initialize()` sets this field to 0;  
this field is read by `dprimme()`.



void (\***matrixMatvec**)(void \*x, *PRIMME\_INT* \*ldx, void \*y, *PRIMME\_INT* \*ldy, int \*blockSize, *primme\_params* \*primme, int \*ierr)  
 Block matrix-multivector multiplication,  $y = Ax$  in solving  $Ax = \lambda x$  or  $Ax = \lambda Bx$ .

#### Parameters

- **x** – matrix of size *nLocal* x blockSize in column-major order with leading dimension ldx.
- **ldx** – the leading dimension of the array x.
- **y** – matrix of size *nLocal* x blockSize in column-major order with leading dimension ldy.
- **ldy** – the leading dimension of the array y.
- **blockSize** – number of columns in x and y.
- **primme** – parameters structure.
- **ierr** – output error code; if it is set to non-zero, the current call to PRIMME will stop.

The actual type of x and y matches the type of *evecs* of the calling *dprimme()* (or a variant), unless the user sets *matrixMatvec\_type* to another precision.

Input/output:

*primme\_initialize()* sets this field to NULL;  
 this field is read by *dprimme()*.

---

**Note:** If you have performance issues with leading dimension different from *nLocal*, set *ldOps* to *nLocal*.

---

Changed in version 2.0.

primme\_op\_datatype **matrixMatvec\_type**

Precision of the vectors x and y passed to *matrixMatvec*.

If it is *primme\_op\_default*, the vectors' type matches the calling *dprimme()* (or a variant). Otherwise, the user can force the precision of the vectors x and y to be a particular precision regardless of the calling *dprimme()* (or a variant) function: half, single, or double, if *matrixMatvec\_type* is *primme\_half*, *primme\_float* or *primme\_double* respectively.

It is not recommended to set a lower precision than the one required to converge. An example of this is calling *dprimme()* setting *eps* to 1e-10 and *matrixMatvec\_type* to *primme\_op\_half*.

Input/output:

*primme\_initialize()* sets this field to *primme\_op\_default*;  
 this field is read by *dprimme()*, and if it is *primme\_op\_default* it is set to the value that matches the precision of calling function.

New in version 3.0.

void (\***applyPreconditioner**)(void \*x, *PRIMME\_INT* \*ldx, void \*y, *PRIMME\_INT* \*ldy, int \*blockSize, *primme\_params* \*primme, int \*ierr)

Block preconditioner-multivector application,  $y = M^{-1}x$  where  $M$  is usually an approximation of  $A - \sigma I$  or  $A - \sigma B$  for finding eigenvalues close to  $\sigma$ .

#### Parameters

- **x** – matrix of size *nLocal* x blockSize in column-major order with leading dimension ldx.

- **ldx** – the leading dimension of the array  $x$ .
- **y** – matrix of size  $nLocal \times blockSize$  in **column-major** order with leading dimension  $ldy$ .
- **ldy** – the leading dimension of the array  $y$ .
- **blockSize** – number of columns in  $x$  and  $y$ .
- **primme** – parameters structure.
- **ierr** – output error code; if it is set to non-zero, the current call to PRIMME will stop.

The actual type of  $x$  and  $y$  matches the type of `evects` of the calling `dprimme()` (or a variant), unless the user sets `applyPreconditioner_type` to another precision.

Input/output:

`primme_initialize()` sets this field to NULL;  
this field is read by `dprimme()`.

Changed in version 2.0.

#### `primme_op_datatype` **applyPreconditioner\_type**

Precision of the vectors  $x$  and  $y$  passed to `applyPreconditioner`.

If it is `primme_op_default`, the vectors' type matches the calling `dprimme()` (or a variant). Otherwise, the user can force the precision of the vectors  $x$  and  $y$  to be a particular precision regardless of the calling `dprimme()` (or a variant) function: half, single, or double, if `matrixMatvec_type` is `primme_half`, `primme_float` or `primme_double` respectively.

Input/output:

`primme_initialize()` sets this field to `primme_op_default`;  
this field is read by `dprimme()`, and if it is `primme_op_default` it is set to the value that matches the precision of calling function.

New in version 3.0.

`void (*massMatrixMatvec)` (`void *x`, `PRIMME_INT *ldx`, `void *y`, `PRIMME_INT *ldy`, `int *blockSize`, `primme_params *primme`, `int *ierr`)

Block matrix-multivector multiplication,  $y = Bx$  in solving  $Ax = \lambda Bx$ . If it is NULL, the standard eigenvalue problem  $Ax = \lambda x$  is solved.

#### Parameters

- **x** – matrix of size  $nLocal \times blockSize$  in **column-major** order with leading dimension  $ldx$ .
- **ldx** – the leading dimension of the array  $x$ .
- **y** – matrix of size  $nLocal \times blockSize$  in **column-major** order with leading dimension  $ldy$ .
- **ldy** – the leading dimension of the array  $y$ .
- **blockSize** – number of columns in  $x$  and  $y$ .
- **primme** – parameters structure.
- **ierr** – output error code; if it is set to non-zero, the current call to PRIMME will stop.

The actual type of  $x$  and  $y$  matches the type of `evects` of the calling `dprimme()` (or a variant), unless the user sets `matrixMatvec_type` to another precision.

Input/output:

`primme_initialize()` sets this field to NULL;  
this field is read by `dprimme()`.

Changed in version 2.0.

`primme_op_datatype` **massMatrixMatvec\_type**

Precision of the vectors  $x$  and  $y$  passed to `massMatrixMatvec`.

If it is `primme_op_default`, the vectors' type matches the calling `dprimme()` (or a variant). Otherwise, the user can force the precision of the vectors  $x$  and  $y$  to be a particular precision regardless of the calling `dprimme()` (or a variant) function: half, single, or double, if `massMatrixMatvec_type` is `primme_half`, `primme_float` or `primme_double` respectively.

It is not recommended to set a lower precision than the one required to converge. An example of this is calling `dprimme()` setting `eps` to 1e-10 and `massMatrixMatvec_type` to `primme_op_half`.

Input/output:

`primme_initialize()` sets this field to `primme_op_default`;  
this field is read by `dprimme()`, and if it is `primme_op_default` it is set to the value that matches the precision of calling function.

New in version 3.0.

`int` **numProcs**

Number of processes calling `dprimme()` or `zprimme()` in parallel.

Input/output:

`primme_initialize()` sets this field to 1;  
this field is read by `dprimme()`.

`int` **procID**

The identity of the local process within a parallel execution calling `dprimme()` or `zprimme()`. Only the process with id 0 prints information.

Input/output:

`primme_initialize()` sets this field to 0;  
`dprimme()` sets this field to 0 if `numProcs` is 1;  
this field is read by `dprimme()`.

`int` **nLocal**

Number of local rows on this process.

Input/output:

`primme_initialize()` sets this field to -1;  
`dprimme()` sets this field to  $n$  if `numProcs` is 1;  
this field is read by `dprimme()`.

`void *`**commInfo**

A pointer to whatever parallel environment structures needed. For example, with MPI, it could be a pointer to the MPI communicator. PRIMME does not use this. It is available for possible use in user functions defined in `matrixMatvec`, `applyPreconditioner`, `massMatrixMatvec`, `globalSumReal`, and `broadcastReal`.

Input/output:

`primme_initialize()` sets this field to NULL;

```
void (*globalSumReal)(void *sendBuf, void *recvBuf, int *count, primme_params *primme, int *ierr)
```

Global sum reduction function. No need to set for sequential programs.

#### Parameters

- **sendBuf** – array of size `count` with the local input values.
- **recvBuf** – array of size `count` with the global output values so that the *i*-th element of `recvBuf` is the sum over all processes of the *i*-th element of `sendBuf`.
- **count** – array size of `sendBuf` and `recvBuf`.
- **primme** – parameters structure.
- **ierr** – output error code; if it is set to non-zero, the current call to PRIMME will stop.

The actual type of `sendBuf` and `recvBuf` matches the type of `evects` of the calling `dprimme()` (or a variant), unless the user sets `globalSumReal_type` to another precision. See the recommendation about precision in `globalSumReal_type`.

Note that `count` is the number of values of the real type.

Input/output:

`primme_initialize()` sets this field to an internal function;  
`dprimme()` sets this field to an internal function if `numProcs` is 1 and `globalSumReal` is NULL;  
this field is read by `dprimme()`.

When MPI is used, this can be a simply wrapper to `MPI_Allreduce()` as shown below:

```
void par_GlobalSumForDouble(void *sendBuf, void *recvBuf, int *count,
                           primme_params *primme, int *ierr) {
    MPI_Comm communicator = *(MPI_Comm *) primme->commInfo;
    if (sendBuf == recvBuf) {
        *ierr = MPI_Allreduce(MPI_IN_PLACE, recvBuf, *count, MPIU_REAL, MPI_SUM,
        ↪communicator) != MPI_SUCCESS;
    } else {
        *ierr = MPI_Allreduce(sendBuf, recvBuf, *count, MPIU_REAL, MPI_SUM,
        ↪communicator) != MPI_SUCCESS;
    }
}
```

When calling `sprimme()` and `cprimme()` replace `MPI_DOUBLE` by ``MPI_FLOAT`.

Changed in version 2.0.

`primme_op_datatype` **globalSumReal\_type**

Precision of the vectors `sendBuf` and `recvBuf` passed to `globalSumReal`.

If it is `primme_op_default`, the vectors' type matches the calling `dprimme()` (or a variant). Otherwise, the user can force the precision of the vectors `sendBuf` and `recvBuf` to be a particular precision regardless of the calling `dprimme()` (or a variant) function: half, single, or double, if `globalSumReal_type` is `primme_half`, `primme_float` or `primme_double` respectively.

It is recommended to set a precision so that the machine precision times  $\log_2(\text{numProcs})$  is smaller than the precision required to converge. An example of this is calling `hprimme()` setting `eps` to 0.01 and `globalSumReal_type` to `primme_op_single` for 1000 processes.

Input/output:

`primme_initialize()` sets this field to `primme_op_default`;

this field is read by `dprimme()`, and if it is `primme_op_default` it is set to the value that matches the precision of calling function.

New in version 3.0.

void (**\*broadcastReal**) (void \*buffer, int \*count, *primme\_params* \*primme, int \*ierr)

Broadcast function from process with ID zero. It is optional in parallel executions, and not needed for sequential programs.

#### Parameters

- **buffer** – array of size `count` with the local input values.
- **count** – array size of `sendBuf` and `recvBuf`.
- **primme** – parameters structure.
- **ierr** – output error code; if it is set to non-zero, the current call to PRIMME will stop.

The actual type of `buffer` matches the type of `evects` of the calling `dprimme()` (or a variant), unless the user sets `broadcastReal_type` to another precision.

If `broadcastReal` is not provided, PRIMME uses `globalSumReal` for broadcasting, which is usually a bit more expensive.

Input/output:

`primme_initialize()` sets this field to NULL;  
this field is read by `dprimme()`.

When MPI is used, this can be a simply wrapper to `MPI_Bcast()` as shown below:

```
void broadcastForDouble(void *buffer, int *count,
                       primme_params *primme, int *ierr) {
    MPI_Comm communicator = *(MPI_Comm *) primme->commInfo;
    if (MPI_Bcast(buffer, *count, MPI_DOUBLE, 0 /* root */,
                  communicator) == MPI_SUCCESS) {
        *ierr = 0;
    } else {
        *ierr = 1;
    }
}
```

When calling `sprimme()` and `cprimme()` replace `MPI_DOUBLE` by `ˆMPI_FLOAT`.

New in version 3.0.

`primme_op_datatype` **broadcastReal\_type**

Precision of the vector `bufferˆ` passed to `broadcastReal`.

If it is `primme_op_default`, the vectors' type matches the calling `dprimme()` (or a variant). Otherwise, the user can force the precision of the vectors `x` and `y` to be a particular precision regardless of the calling `dprimme()` (or a variant) function: half, single, or double, if `matrixMatvec_type` is `primme_half`, `primme_float` or `primme_double` respectively.

It is not recommended to set a lower precision than the one required to converge. An example of this is calling `dprimme()` setting `eps` to 1e-10 and `broadcastReal_type` to `primme_op_half`.

Input/output:

`primme_initialize()` sets this field to `primme_op_default`;  
this field is read by `dprimme()`, and if it is `primme_op_default` it is set to the value that matches the precision of calling function.

New in version 3.0.

`primme_op_datatype` **internalPrecision**

Internal working precision.

If it is `primme_op_default`, most of the vectors are stored with the same precision as the calling `dprimme()` (or a variant), and most of the computations are done in that precision too. Otherwise, the working precision is changed to half, single, or double, if the user sets *internalPrecision* to `primme_half`, `primme_float` or `primme_double` respectively.

Input/output:

`primme_initialize()` sets this field to `primme_op_default`;  
this field is read by `dprimme()`.

New in version 3.0.

`int` **numEvals**

Number of eigenvalues wanted.

Input/output:

`primme_initialize()` sets this field to 1;  
this field is read by `primme_set_method()` (see *Preset Methods*) and `dprimme()`.

`primme_target` **target**

Which eigenpairs to find:

**primme\_smallest** Smallest algebraic eigenvalues; *targetShifts* is ignored.

**primme\_largest** Largest algebraic eigenvalues; *targetShifts* is ignored.

**primme\_closest\_geq** Closest to, but greater or equal than the shifts in *targetShifts*.

**primme\_closest\_leq** Closest to, but less or equal than the shifts in *targetShifts*.

**primme\_closest\_abs** Closest in absolute value to the shifts in *targetShifts*.

**primme\_largest\_abs** Furthest in absolute value to the shifts in *targetShifts*.

Input/output:

`primme_initialize()` sets this field to `primme_smallest`;  
this field is read by `dprimme()`.

`int` **numTargetShifts**

Size of the array *targetShifts*. Used only when *target* is `primme_closest_geq`, `primme_closest_leq`, `primme_closest_abs` or `primme_largest_abs`. The default values is 0.

Input/output:

`primme_initialize()` sets this field to 0;  
this field is read by `dprimme()`.

`double *`**targetShifts**

Array of shifts, at least of size *numTargetShifts*. Used only when *target* is `primme_closest_geq`, `primme_closest_leq`, `primme_closest_abs` or `primme_largest_abs`.

Eigenvalues are computed in order so that the *i*-th eigenvalue is the closest (or closest but left or closest but right, see *target*) to the *i*-th shift. If *numTargetShifts* < *numEvals*, the last shift given is used for all the remaining *i*'s.

Input/output:

`primme_initialize()` sets this field to NULL;  
this field is read by `dprimme()`.

---

**Note:** Considerations for interior problems:

- PRIMME will try to compute the eigenvalues in the order given in the `targetShifts`. However, for code efficiency and robustness, the shifts should be ordered. Order them in ascending (descending) order for shifts closer to the lower (higher) end of the spectrum.
  - If some shift is close to the lower (higher) end of the spectrum, use either `primme_closest_geq` (`primme_closest_leq`) or `primme_closest_abs`.
  - `primme_closest_leq` and `primme_closest_geq` are more efficient than `primme_closest_abs`.
  - For interior eigenvalues larger `maxBasisSize` is usually more robust.
  - To find the largest magnitude eigenvalues set `target` to `primme_largest_abs`, `numTargetShifts` to 1 and `targetShifts` to an array with a zero value.
- 

#### int `printLevel`

The level of message reporting from the code. All output is written in `outputFile`.

One of:

- 0: silent.
- 1: print some error messages when these occur.
- 2: as in 1, and info about targeted eigenpairs when they are marked as converged:

```
#Converged $1 eval[ $2 ]= $3 norm $4 Mvecs $5 Time $7
```

or locked:

```
#Lock epair[ $1 ]= $3 norm $4 Mvecs $5 Time $7
```

- 3: in as 2, and info about targeted eigenpairs every outer iteration:

```
OUT $6 conv $1 blk $8 MV $5 Sec $7 EV $3 |r| $4
```

Also, if it is used the dynamic method, show JDQMR/GDk performance ratio and the current method in use.

- 4: in as 3, and info about targeted eigenpairs every inner iteration:

```
INN MV $5 Sec $7 Eval $3 Lin|r| $9 EV|r| $4
```

- 5: in as 4, and verbose info about certain choices of the algorithm.

Output key:

\$1: Number of converged pairs up to now.  
\$2: The index of the pair currently converged.  
\$3: The eigenvalue.  
\$4: Its residual norm.  
\$5: The current number of matrix-vector products.  
\$6: The current number of outer iterations.

\$7: The current elapsed time.

\$8: Index within the block of the targeted pair .

\$9: QMR norm of the linear system residual.

In parallel programs, output is produced in call with *procID* 0 when *printLevel* is from 0 to 4. If *printLevel* is 5 output can be produced in any of the parallel calls.

Input/output:

*primme\_initialize()* sets this field to 1;  
this field is read by *dprimme()*.

---

**Note:** Convergence history for plotting may be produced simply by:

```
grep OUT outpufile | awk '{print $8" "$14}' > out
grep INN outpufile | awk '{print $3" "$11}' > inn
```

Then in gnuplot:

```
plot 'out' w lp, 'inn' w lp
```

---

double **aNorm**

An estimate of the norm of  $A$ , which is used in the default convergence criterion (see *eps*).

If *aNorm* is less than or equal to 0, the code uses the largest absolute Ritz value seen divided by *invBNorm*. On return, *aNorm* is then replaced with that value.

Input/output:

*primme\_initialize()* sets this field to 0.0;  
this field is read and written by *dprimme()*.

double **BNorm**

An estimate of the norm of  $B$ , which is used to estimate the conditioning number of the matrix  $B$ .

If *BNorm* is less than or equal to 0, the code uses the largest inner-product with  $B$  seen. On return, *BNorm* is then replaced with that value.

Input/output:

*primme\_initialize()* sets this field to 0.0;  
this field is read and written by *dprimme()*.

New in version 3.0.

double **invBNorm**

An estimate of the norm of the inverse of  $B$ , which is used in the default convergence criterion (see *eps*).

If *invBNorm* is less than or equal to 0, the code uses the inverse of the smallest inner-product with  $B$  seen. On return, *invBNorm* is then replaced with that value.

Input/output:

*primme\_initialize()* sets this field to 0.0;  
this field is read and written by *dprimme()*.

New in version 3.0.



**primme\_orth orth**

Selects the orthogonalization method used by PRIMME.

If the value is `primme_orth_implicit_I`, the bases are orthogonalized with classical Gram-Schmidt with reorthogonalization stopping when the new vector's norm is not reduced more than  $1/\sqrt{2}$  (Daniel's test) from the previous iteration. If several vectors are going to be orthogonalized, the algorithm is applied vector by vector.

If the value is `primme_orth_explicit_I`, the bases are orthogonalized with iterative Cholesky QR (or SVQB if Cholesky factorization fails), stopping when the conditioning of the basis is around  $\sqrt{3}$ . That deviation of the orthogonality level is taken into account in the Galerkin method.

The option `primme_orth_explicit_I` is usually more expensive in FLOPS, but it may be faster in time than `primme_orth_implicit_I` when `maxBlockSize` is large.

`primme_orth_implicit_I` is set by default if the precision is higher than single precision and `maxBlockSize` is 1. Otherwise, `primme_orth_explicit_I` is set by default.

Input/output:

`primme_initialize()` sets this field to `primme_orth_default`;  
this field is read and written by `dprimme()`.

New in version 3.0.

**double eps**

If `convTestFun` is NULL, an eigenpairs is marked as converged when the 2-norm of the residual vector is less than  $\text{eps} * a\text{Norm} * \text{invBNorm}$ . The residual vector is  $Ax - \lambda x$  or  $Ax - \lambda Bx$ .

The default value is machine precision times  $10^4$ .

Input/output:

`primme_initialize()` sets this field to 0.0;  
this field is read and written by `dprimme()`.

**FILE \*outputFile**

Opened file to write down the output.

Input/output:

`primme_initialize()` sets this field to the standard output;  
this field is read by `dprimme()` and `primme_display_params()`.

**int dynamicMethodSwitch**

If this value is 1, it alternates dynamically between `PRIMME_DEFAULT_MIN_TIME` and `PRIMME_DEFAULT_MIN_MATVECS`, trying to identify the fastest method.

On exit, it holds a recommended method for future runs on this problem:

- 1: use `PRIMME_DEFAULT_MIN_MATVECS` next time.
- 2: use `PRIMME_DEFAULT_MIN_TIME` next time.
- 3: close call, use `PRIMME_DYNAMIC` next time again.

Input/output:

`primme_initialize()` sets this field to 0;  
written by `primme_set_method()` (see *Preset Methods*);  
this field is read by `dprimme()`.

---

**Note:** Even for expert users we do not recommend setting `dynamicMethodSwitch` directly, but through `primme_set_method()`.

---

---

**Note:** The code obtains timings by the `gettimeofday` Unix utility. If a cheaper, more accurate timer is available, modify the `PRIMMESRC/COMMONSRC/wtime.c`

---

### int `locking`

If set to 1, hard locking will be used (locking converged eigenvectors out of the search basis). If set to 0, the code will try to use soft locking (à la ARPACK), when large enough `minRestartSize` is available.

Input/output:

`primme_initialize()` sets this field to -1;  
written by `primme_set_method()` (see *Preset Methods*);  
this field is read by `dprimme()`.

### int `initSize`

On input, the number of initial vector guesses provided in `evects` argument in `dprimme()` or `zprimme()`.

On output, `initSize` holds the number of converged eigenpairs. Without `locking` all `numEvals` approximations are in `evects` but only the `initSize` ones are converged.

During execution, it holds the current number of converged eigenpairs. In addition, if locking is used, these are accessible in `evals` and `evects`.

Input/output:

`primme_initialize()` sets this field to 0;  
this field is read and written by `dprimme()`.

### `PRIMME_INT` `ldevects`

The leading dimension of `evects`. The default is `nLocal`.

Input/output:

`primme_initialize()` sets this field to -1;  
this field is read by `dprimme()`.

New in version 2.0.

### int `numOrthoConst`

Number of vectors to be used as external orthogonalization constraints. These vectors are provided in the first `numOrthoConst` positions of the `evects` argument in `dprimme()` or `zprimme()` and must be orthonormal.

PRIMME finds new eigenvectors orthogonal to these constraints (equivalent to solving the problem with  $(I - YY^*)A(I - YY^*)$  and  $(I - YY^*)B(I - YY^*)$  matrices where  $Y$  are the given constraint vectors). This is a handy feature if some eigenvectors are already known, or for finding more eigenvalues after a call to `dprimme()` or `zprimme()`, possibly with different parameters (see an example in `TEST/ex_zseq.c`).

Input/output:

`primme_initialize()` sets this field to 0;  
this field is read by `dprimme()`.

**int `maxBasisSize`**

The maximum basis size allowed in the main iteration. This has memory implications.

Input/output:

`primme_initialize()` sets this field to 0;  
 this field is read and written by `primme_set_method()` (see *Preset Methods*);  
 this field is read by `dprimme()`.

**int `minRestartSize`**

Maximum Ritz vectors kept after restarting the basis.

Input/output:

`primme_initialize()` sets this field to 0;  
 this field is read and written by `primme_set_method()` (see *Preset Methods*);  
 this field is read by `dprimme()`.

**int `maxBlockSize`**

The maximum block size the code will try to use.

The user should set this based on the architecture specifics of the target computer, as well as any a priori knowledge of multiplicities. The code does *not* require that `maxBlockSize` > 1 to find multiple eigenvalues. For some methods, keeping to 1 yields the best overall performance.

Input/output:

`primme_initialize()` sets this field to 1;  
 this field is read and written by `primme_set_method()` (see *Preset Methods*);  
 this field is read by `dprimme()`.

---

**Note:** Inner iterations of QMR are not performed in a block fashion. Every correction equation from a block is solved independently.

---

***PRIMME\_INT* `maxMatvecs`**

Maximum number of matrix vector multiplications (approximately equal to the number of preconditioning operations) that the code is allowed to perform before it exits.

Input/output:

`primme_initialize()` sets this field to `INT_MAX`;  
 this field is read by `dprimme()`.

***PRIMME\_INT* `maxOuterIterations`**

Maximum number of outer iterations that the code is allowed to perform before it exits.

Input/output:

`primme_initialize()` sets this field to `INT_MAX`;  
 this field is read by `dprimme()`.

***PRIMME\_INT* `iseed`**

The `PRIMME_INT` `iseed[4]` is an array with the seeds needed by the `LAPACK` `dlarnv` and `zlarnv`.

The default value is an array with values -1, -1, -1 and -1. In that case, `iseed` is set based on the value of `procID` to avoid every parallel process generating the same sequence of pseudorandom numbers.

Input/output:

`primme_initialize()` sets this field to `[-1, -1, -1, -1]`;  
 this field is read and written by `dprimme()`.

void **\*matrix**

This field may be used to pass any required information in the matrix-vector product *matrixMatvec*.

Input/output:

*primme\_initialize()* sets this field to NULL;

void **\*massMatrix**

This field may be used to pass any required information in the matrix-vector product *massMatrixMatvec*.

Input/output:

*primme\_initialize()* sets this field to NULL;

New in version 3.0.

void **\*preconditioner**

This field may be used to pass any required information in the preconditioner function *applyPreconditioner*.

Input/output:

*primme\_initialize()* sets this field to NULL;

double **\*ShiftsForPreconditioner**

Array of size *blockSize* provided during execution of *dprimme()* and *zprimme()* holding the shifts to be used (if needed) in the preconditioning operation.

For example if the block size is 3, there will be an array of three shifts in *ShiftsForPreconditioner*. Then the user can invert a shifted preconditioner for each of the block vectors  $(M - \text{ShiftsForPreconditioner}_i)^{-1}x_i$ . Classical Davidson (diagonal) preconditioning is an example of this.

this field is read and written by *dprimme()*.

primme\_init **initBasisMode**

Select how the search subspace basis is initialized up to *minRestartSize* vectors if not enough initial vectors are provided (see *initSize*):

- *primme\_init\_krylov*, with a block Krylov subspace generated by the matrix problem and the last initial vectors if given or a random vector otherwise; the size of the block is *maxBlockSize*.
- *primme\_init\_random*, with random vectors.
- *primme\_init\_user*, the initial basis will have only initial vectors if given, or a single random vector.

Input/output:

*primme\_initialize()* sets this field to *primme\_init\_krylov*;

this field is read by *dprimme()*.

New in version 2.0.

primme\_projection **projectionParams.projection**

Select the extraction technique, i.e., how the approximate eigenvectors  $x_i$  and eigenvalues  $\lambda_i$  are computed from the search subspace  $\mathcal{V}$ :

- *primme\_proj\_RR*, Rayleigh-Ritz,  $Ax_i - Bx_i\lambda_i \perp \mathcal{V}$ .

- `primme_proj_harmonic`, Harmonic Rayleigh-Ritz,  $Ax_i - Bx_i\lambda_i \perp (A - \tau B)\mathcal{V}$ , where  $\tau$  is the current target shift (see *targetShifts*).
- `primme_proj_refined`, refined extraction, compute  $x_i$  with  $\|x_i\| = 1$  that minimizes  $\|(A - \tau B)x_i\|$ ; the eigenvalues are computed as the Rayleigh quotients,  $\lambda_i = \frac{x_i^* A x_i}{x_i^* B x_i}$ .

Input/output:

`primme_initialize()` sets this field to `primme_proj_default`;  
`primme_set_method()` and `dprimme()` sets it to `primme_proj_RR` if it is `primme_proj_default`.

`int restartingParams.maxPrevRetain`

Number of approximations from previous iteration to be retained after restart (this is the locally optimal restarting, see [r2]). The restart size is *minRestartSize* plus *maxPrevRetain*.

Input/output:

`primme_initialize()` sets this field to 0;  
 this field is read and written by `primme_set_method()` (see *Preset Methods*);  
 this field is read by `dprimme()`.

`int correctionParams.precondition`

Set to 1 to use preconditioning. Make sure *applyPreconditioner* is not NULL then!

Input/output:

`primme_initialize()` sets this field to 0;  
 this field is read and written by `primme_set_method()` (see *Preset Methods*);  
 this field is read by `dprimme()`.

`int correctionParams.robustShifts`

Set to 1 to use robust shifting. It tries to avoid stagnation and misconvergence by providing as shifts in *ShiftsForPreconditioner* the Ritz values displaced by an approximation of the eigenvalue error.

Input/output:

`primme_initialize()` sets this field to 0;  
 written by `primme_set_method()` (see *Preset Methods*);  
 this field is read by `dprimme()`.

`int correctionParams.maxInnerIterations`

Control the maximum number of inner QMR iterations:

- 0: no inner iterations;
- >0: perform at most that number of inner iterations per outer step;
- <0: perform at most the rest of the remaining matrix-vector products up to reach *maxMatvecs*.

Input/output:

`primme_initialize()` sets this field to 0;  
 this field is read and written by `primme_set_method()` (see *Preset Methods*);  
 this field is read by `dprimme()`.

See also *convTest*.

`double correctionParams.relTolBase`

Parameter used when *convTest* is *primme\_decreasing\_LTolerance*.

Input/output:

`primme_initialize()` sets this field to 0;  
 written by `primme_set_method()` (see *Preset Methods*);  
 this field is read by `dprimme()`.

`primme_convergentest` `correctionParams.convTest`

Set how to stop the inner QMR method:

- `primme_full_LTolerance`: stop by iterations only;
- `primme_decreasing_LTolerance`, stop when  $\text{relTolBase}^{-\text{outIts}}$  where `outIts` is the number of outer iterations and `relTolBase` is set in `relTolBase`; This is a legacy option from classical JDQR and we recommend **strongly** against its use.
- `primme_adaptive`, stop when the estimated eigenvalue residual has reached the required tolerance (based on Notay's JDCG).
- `primme_adaptive_ETolerance`, as `primme_adaptive` but also stopping when the estimated eigenvalue residual has reduced 10 times.

Input/output:

`primme_initialize()` sets this field to `primme_adaptive_ETolerance`;  
 written by `primme_set_method()` (see *Preset Methods*);  
 this field is read by `dprimme()`.

---

**Note:** Avoid to set `maxInnerIterations` to -1 and `convTest` to `primme_full_LTolerance`.

---

See also `maxInnerIterations`.

`int correctionParams.projectors.LeftQ`

`int correctionParams.projectors.LeftX`

`int correctionParams.projectors.RightQ`

`int correctionParams.projectors.RightX`

`int correctionParams.projectors.SkewQ`

`int correctionParams.projectors.SkewX`

Control the projectors involved in the computation of the correction appended to the basis every (outer) iteration.

Consider the current selected Ritz value  $\Lambda$  and vectors  $X$ , the residual associated vectors  $R = AX - X\Lambda$ , the previous locked vectors  $Q$ , and the preconditioner  $M^{-1}$ .

When `maxInnerIterations` is 0, the correction  $D$  appended to the basis in GD is:

RightX	SkewX	$D$
0	0	$M^{-1}R$ (Classic GD)
1	0	$M^{-1}(R - \Delta X)$ (cheap Olsen's Method)
1	1	$(I - M^{-1}X(X^*M^{-1}X)^{-1}X^*)M^{-1}R$ (Olsen's Method)
0	1	error

Where  $\Delta$  is a diagonal matrix that  $\Delta_{i,i}$  holds an estimation of the error of the approximate eigenvalue  $\Lambda_{i,i}$ .

The values of `RightQ`, `SkewQ`, `LeftX` and `LeftQ` are ignored.

When `maxInnerIterations` is not 0, the correction  $D$  in Jacobi-Davidson results from solving:

$$P_Q^l P_X^l (A - \sigma I) P_X^r P_Q^r M^{-1} D' = -R, \quad D = P_X^r P_Q^l M^{-1} D'.$$

For LeftQ:

- 0:  $P_Q^l = I$ ;
- 1:  $P_Q^l = I - QQ^*$ .

For LeftX:

- 0:  $P_X^l = I$ ;
- 1:  $P_X^l = I - XX^*$ .

For RightQ and SkewQ:

RightQ	SkewQ	$P_Q^r$
0	0	$I$
1	0	$I - QQ^*$
1	1	$I - KQ(Q^*KQ)^{-1}Q^*$
0	1	error

For RightX and SkewX:

RightX	SkewX	$P_X^r$
0	0	$I$
1	0	$I - XX^*$
1	1	$I - KX(X^*KX)^{-1}X^*$
0	1	error

Input/output:

`primme_initialize()` sets all of them to 0;  
 this field is written by `primme_set_method()` (see *Preset Methods*);  
 this field is read by `dprimme()`.

See [r3] for a study about different projector configurations in JD.

#### **PRIMME\_INT** **ldOPs**

Recommended leading dimension to be used in `matrixMatvec`, `applyPreconditioner` and `massMatrixMatvec`. The default value is zero, which means no user recommendation. In that case, PRIMME computes ldOPs internally to get better memory performance.

Input/output:

`primme_initialize()` sets this field to -1;  
 this field is read by `dprimme()`.

New in version 2.0.

`void (*monitorFun) (void *basisEvals, int *basisSize, int *basisFlags, int *iblock, int *blockSize, void *basisNorms, int *numConverged, void *lockedEvals, int *numLocked, int *lockedFlags, void *lockedNorms, int *inner_its, void *LSRes, const char *msg, double *time, primme_event *event, struct primme_params *primme, int *ierr)`

Convergence monitor. Used to customize how to report solver information during execution (iteration number, matvecs, time, unconverged and converged eigenvalues, residual norms, targets, etc).

#### **Parameters**

- **basisEvals** – array with approximate eigenvalues of the basis.
- **basisSize** – size of the arrays, `basisEvals`, `basisFlags` and `basisNorms`.

- **basisFlags** – state of every approximate pair in the basis.
- **iblock** – indices of the approximate pairs in the block targeted during current iteration.
- **blockSize** – size of array **iblock**.
- **basisNorms** – array with residual norms of the pairs in the basis.
- **numConverged** – number of pairs converged in the basis plus the number of the locked pairs (note that this value isn't monotonic).
- **lockedEvals** – array with the locked eigenvalues.
- **numLocked** – size of the arrays **lockedEvals**, **lockedFlags** and **lockedNorms**.
- **lockedFlags** – state of each locked eigenpair.
- **lockedNorms** – array with the residual norms of the locked pairs.
- **inner\_its** – number of performed QMR iterations in the current correction equation. It resets for each block vector.
- **LSRes** – residual norm of the linear system at the current QMR iteration.
- **msg** – output message or function name.
- **time** – time duration.
- **event** – event reported.
- **primme** – parameters structure; the counter in **stats** are updated with the current number of matrix-vector products, iterations, elapsed time, etc., since start.
- **ierr** – output error code; if it is set to non-zero, the current call to PRIMME will stop.

This function is called at the following events:

- `*event == primme_event_outer_iteration`: every outer iterations.

For this event the following inputs are provided: **basisEvals**, **basisNorms**, **basisSize**, **basisFlags**, **iblock** and **blockSize**.

**basisNorms[iblock[i]]** has the residual norm for the selected pair in the block. PRIMME avoids computing the residual of soft-locked pairs, **basisNorms[i]** for  $i < \text{iblock}[0]$ . So those values may correspond to previous iterations. The values **basisNorms[i]** for  $i > \text{iblock}[\text{blockSize}-1]$  are not valid.

If *locking* is enabled, **lockedEvals**, **numLocked**, **lockedFlags** and **lockedNorms** are also provided.

**inner\_its** and **LSRes** are not provided.

- `*event == primme_event_inner_iteration`: every QMR iteration.

**basisEvals[0]** and **basisNorms[0]** provides the approximate eigenvalue and the residual norm of the pair which is improved in the current correction equation. If *convTest* is *primme\_adaptive* or *primme\_adaptive\_ETolerance*, **basisEvals[0]** and **basisNorms[0]** are updated every QMR iteration.

**inner\_its** and **LSRes** are also provided.

**lockedEvals**, **numLocked**, **lockedFlags** and **lockedNorms** may not be provided.

- `*event == primme_event_converged`: a new eigenpair in the basis passed the convergence criterion.



`iblock[0]` is the index of the newly converged pair in the basis which will be locked or soft-locked. The following are provided: `basisEvals`, `basisNorms`, `basisSize`, `basisFlags` and `blockSize[0]==1`.

`lockedEvals`, `numLocked`, `lockedFlags` and `lockedNorms` may not be provided.

`inner_its` and `LSRes` are not provided.

- `*event == primme_event_locked`: new pair was added to the locked eigenvectors.

`lockedEvals`, `numLocked`, `lockedFlags` and `lockedNorms` are provided. The last element of `lockedEvals`, `lockedFlags` and `lockedNorms` corresponds to the recent locked pair.

`basisEvals`, `numConverged`, `basisFlags` and `basisNorms` may not be provided.

`inner_its` and `LSRes` are not provided.

- `*event == primme_event_message`: output message

`msg` is the message to print.

The rest of the arguments are not provided.

The values of `basisFlags` and `lockedFlags` are:

- 0: unconverged.
- 1: internal use; only in `basisFlags`.
- 2: passed convergence test `convTestFun`.
- 3: *practically converged* because the solver may not be able to reduce the residual norm further without recombining the locked eigenvectors.

The actual type of `basisEvals`, `basisNorms`, `lockedEvals`, `lockedNorms` and `LSRes` matches the type of `evects` of the calling `dprimme()` (or a variant), unless the user sets `monitorFun_type` to another precision.

Input/output:

`primme_initialize()` sets this field to NULL;  
`dprimme()` sets this field to an internal function if it is NULL;  
 this field is read by `dprimme()`.

Changed in version 3.0.

#### `primme_op_datatype` **`monitorFun_type`**

Precision of the vectors `basisEvals`, `basisNorms`, `lockedEvals`, `lockedNorms` and `LSRes` passed to `monitorFun`.

If it is `primme_op_default`, the vectors' type matches the calling `dprimme()` (or a variant). Otherwise, the precision is half, single, or double, if `monitorFun_type` is `primme_half`, `primme_float` or `primme_double` respectively.

Input/output:

`primme_initialize()` sets this field to `primme_op_default`;  
 this field is read by `dprimme()`, and if it is `primme_op_default` it is set to the value that matches the precision of calling function.

New in version 3.0.

#### `void *monitor`

This field may be used to pass any required information to the function `monitorFun`.

Input/output:

`primme_initialize()` sets this field to NULL;

New in version 2.0.

**PRIMME\_INT stats.numOuterIterations**

Hold the number of outer iterations. The value is available during execution and at the end.

Input/output:

`primme_initialize()` sets this field to 0;  
written by `dprimme()`.

**PRIMME\_INT stats.numRestarts**

Hold the number of restarts during execution and at the end.

Input/output:

`primme_initialize()` sets this field to 0;  
written by `dprimme()`.

**PRIMME\_INT stats.numMatvecs**

Hold how many vectors the operator in `matrixMatvec` has been applied on. The value is available during execution and at the end.

Input/output:

`primme_initialize()` sets this field to 0;  
written by `dprimme()`.

**PRIMME\_INT stats.numPreconds**

Hold how many vectors the operator in `applyPreconditioner` has been applied on. The value is available during execution and at the end.

Input/output:

`primme_initialize()` sets this field to 0;  
written by `dprimme()`.

**PRIMME\_INT stats.numGlobalSum**

Hold how many times `globalSumReal` has been called. The value is available during execution and at the end.

Input/output:

`primme_initialize()` sets this field to 0;  
written by `dprimme()`.

**double stats.volumeGlobalSum**

Hold how many REAL have been reduced by `globalSumReal`. The value is available during execution and at the end.

Input/output:

`primme_initialize()` sets this field to 0;  
written by `dprimme()`.

**PRIMME\_INT stats.numBroadcast**

Hold how many times `broadcastReal` has been called. The value is available during execution and at the end.

Input/output:

`primme_initialize()` sets this field to 0;  
written by `dprimme()`.

New in version 3.0.

`double stats.volumeBroadcast`

Hold how many REAL have been broadcast by *broadcastReal*. The value is available during execution and at the end.

Input/output:

*primme\_initialize()* sets this field to 0;  
written by *dprimme()*.

New in version 3.0.

*PRIMME\_INT* `stats.numOrthoInnerProds`

Hold how many inner products with vectors of length *nLocal* have been computed during orthogonalization. The value is available during execution and at the end.

Input/output:

*primme\_initialize()* sets this field to 0;  
written by *dprimme()*.

New in version 3.0.

`double stats.elapsedTime`

Hold the wall clock time spent by the call to *dprimme()* or *zprimme()*. The value is available at the end of the execution.

Input/output:

*primme\_initialize()* sets this field to 0;  
written by *dprimme()*.

`double stats.timeMatvec`

Hold the wall clock time spent by *matrixMatvec*. The value is available at the end of the execution.

Input/output:

*primme\_initialize()* sets this field to 0;  
written by *dprimme()*.

`double stats.timePrecond`

Hold the wall clock time spent by *applyPreconditioner*. The value is available at the end of the execution.

Input/output:

*primme\_initialize()* sets this field to 0;  
written by *dprimme()*.

`double stats.timeOrtho`

Hold the wall clock time spent by orthogonalization. The value is available at the end of the execution.

Input/output:

*primme\_initialize()* sets this field to 0;  
written by *dprimme()*.

`double stats.timeGlobalSum`

Hold the wall clock time spent by *globalSumReal*. The value is available at the end of the execution.

Input/output:

*primme\_initialize()* sets this field to 0;

written by `dprimme()`.

`double stats.timeBroadcast`

Hold the wall clock time spent by `broadcastReal`. The value is available at the end of the execution.

Input/output:

`primme_initialize()` sets this field to 0;  
written by `dprimme()`.

New in version 3.0.

`double stats.estimateMinEVal`

Hold the estimation of the smallest eigenvalue for the current eigenproblem. The value is available during execution and at the end.

Input/output:

`primme_initialize()` sets this field to 0;  
written by `dprimme()`.

`double stats.estimateMaxEVal`

Hold the estimation of the largest eigenvalue for the current eigenproblem. The value is available during execution and at the end.

Input/output:

`primme_initialize()` sets this field to 0;  
written by `dprimme()`.

`double stats.estimateLargestSVal`

Hold the estimation of the largest singular value (i.e., the absolute value of the eigenvalue with largest absolute value) for the current eigenproblem. The value is available during execution and at the end.

Input/output:

`primme_initialize()` sets this field to 0;  
written by `dprimme()`.

`double stats.maxConvTol`

Hold the maximum residual norm of the converged eigenvectors. The value is available during execution and at the end.

Input/output:

`primme_initialize()` sets this field to 0;  
written by `dprimme()`.

`PRIMME_INT stats.lockingIssue`

It is set to a nonzero value if some of the returned eigenpairs do not pass the convergence criterion. See `convTestFun` and `eps`.

Input/output:

`primme_initialize()` sets this field to 0;  
written by `dprimme()`.

New in version 3.0.

`void (*convTestFun)(double *eval, void *evec, double *resNorm, int *isconv, primme_params *primme, int *ierr)`

Function that evaluates if the approximate eigenpair has converged. If NULL, it is used the default convergence criteria (see `eps`).

### Parameters

- **eval** – the approximate value to evaluate.
- **vec** – one dimensional array of size `nLocal` containing the approximate vector; it can be NULL.
- **resNorm** – the norm of the residual vector.
- **isconv** – (output) the function sets zero if the pair is not converged and non zero otherwise.
- **primme** – parameters structure.
- **ierr** – output error code; if it is set to non-zero, the current call to PRIMME will stop.

The actual type of `vec` matches the type of `vecs` of the calling `dprimme()` (or a variant), unless the user sets `convTestFun_type` to another precision.

Input/output:

`primme_initialize()` sets this field to NULL;  
this field is read by `dprimme()`.

New in version 2.0.

`primme_op_datatype` **convTestFun\_type**

Precision of the vectors `vec` passed to `convTestFun`.

If it is `primme_op_default`, `vec`'s type matches the calling `dprimme()` (or a variant). Otherwise, the precision is half, single, or double, if `convTestFun_type` is `primme_half`, `primme_float` or `primme_double` respectively.

Input/output:

`primme_initialize()` sets this field to `primme_op_default`;  
this field is read by `dprimme()`, and if it is `primme_op_default` it is set to the value that matches the precision of calling function.

New in version 3.0.

`void` \***convtest**

This field may be used to pass any required information to the function `convTestFun`.

Input/output:

`primme_initialize()` sets this field to NULL;

New in version 2.0.

`void` \***queue**

Pointer to the accelerator's data structure.

If the main call is `dprimme_magma()` or a variant, this field should have the pointer to an initialized `magma_queue_t`.

See example `examples/ex_eigs_dmagma.c`.

Input/output:

`primme_initialize()` sets this field to NULL;  
this field is read by `dprimme_magma()`.

New in version 3.0.

## 3.7 Preset Methods

`enum primme_preset_method`

**enumerator PRIMME\_DEFAULT\_MIN\_TIME**

Set as `PRIMME_JDQMR_ETol` when *target* is either `primme_smallest` or `primme_largest`, and as `PRIMME_JDQMR` otherwise. This method is usually the fastest if the cost of the matrix vector product is inexpensive.

**enumerator PRIMME\_DEFAULT\_MIN\_MATVECS**

Currently set as `PRIMME_GD_Olsen_plusK`; this method usually performs fewer matrix vector products than other methods, so it's a good choice when this operation is expensive.

**enumerator PRIMME\_DYNAMIC**

Switches to the best method dynamically; currently, between methods `PRIMME_DEFAULT_MIN_TIME` and `PRIMME_DEFAULT_MIN_MATVECS`.

With `PRIMME_DYNAMIC primme_set_method()` sets `dynamicMethodSwitch = 1` and makes the same changes as for method `PRIMME_DEFAULT_MIN_TIME`.

**enumerator PRIMME\_Arnoldi**

Arnoldi implemented à la Generalized Davidson.

With `PRIMME_Arnoldi primme_set_method()` sets:

- `locking = 0;`
- `maxPrevRetain = 0;`
- `precondition = 0;`
- `maxInnerIterations = 0.`

**enumerator PRIMME\_GD**

Generalized Davidson.

With `PRIMME_GD primme_set_method()` sets:

- `locking = 0;`
- `maxPrevRetain = 0;`
- `robustShifts = 1;`
- `maxInnerIterations = 0;`
- `RightX = 0;`
- `SkewX = 0.`

**enumerator PRIMME\_GD\_plusK**

GD with locally optimal restarting.

With `PRIMME_GD_plusK primme_set_method()` sets `maxPrevRetain = 2` if `maxBlockSize` is 1 and `numEvals > 1`; otherwise it sets `maxPrevRetain` to `maxBlockSize`. Also:

- `locking = 0;`
- `maxInnerIterations = 0;`
- `RightX = 0;`
- `SkewX = 0.`

**enumerator PRIMME\_GD\_Olsen\_plusK**

GD+k and the cheap Olsen's Method.

With `PRIMME_GD_Olsen_plusK primme_set_method()` makes the same changes as for method `PRIMME_GD_plusK` and sets `RightX = 1`.

**enumerator PRIMME\_JD\_Olsen\_plusK**

GD+k and Olsen's Method.

With `PRIMME_JD_Olsen_plusK primme_set_method()` makes the same changes as for method `PRIMME_GD_plusK` and also sets `robustShifts = 1`, `RightX` to 1, and `SkewX` to 1.

**enumerator PRIMME\_RQI**

(Accelerated) Rayleigh Quotient Iteration.

With `PRIMME_RQI primme_set_method()` sets:

- `locking = 1;`
- `maxPrevRetain = 0;`
- `robustShifts = 1;`
- `maxInnerIterations = -1;`
- `LeftQ = 1;`
- `LeftX = 1;`
- `RightQ = 0;`
- `RightX = 1;`
- `SkewQ = 0;`
- `SkewX = 0;`
- `convTest = primme_full_LTolerance.`

---

**Note:** If `numTargetShifts > 0` and `targetShifts` are provided, the interior problem solved uses these shifts in the correction equation. Therefore RQI becomes INVIT (inverse iteration) in that case.

---

**enumerator PRIMME\_JDQR**

Jacobi-Davidson with fixed number of inner steps.

With `PRIMME_JDQR primme_set_method()` sets:

- `locking = 1;`
- `maxPrevRetain = 1;`
- `robustShifts = 0;`
- `maxInnerIterations = 10` if it is 0;
- `LeftQ = 0;`
- `LeftX = 1;`
- `RightQ = 1;`
- `RightX = 1;`
- `SkewQ = 1;`
- `SkewX = 1;`
- `relTolBase = 1.5;`
- `convTest = primme_full_LTolerance.`

**enumerator PRIMME\_JDQMR**

Jacobi-Davidson with adaptive stopping criterion for inner Quasi Minimum Residual (QMR).

With `PRIMME_JDQMR primme_set_method()` sets:

- `locking = 0;`
- `maxPrevRetain = 1` if it is 0
- `maxInnerIterations = -1;`
- `LeftQ = precondition;`
- `LeftX = 1;`
- `RightQ = 0;`
- `RightX = 0;`
- `SkewQ = 0;`

- *SkewX* = 1;
- *convTest* = *primme\_adaptive*.

**enumerator PRIMME\_JDQMR\_ETol**

JDQMR but QMR stops after residual norm reduces by a 0.1 factor.

With *PRIMME\_JDQMR\_ETol primme\_set\_method()* makes the same changes as for the method *PRIMME\_JDQMR* and sets *convTest* = *primme\_adaptive\_ETolerance*.

**enumerator PRIMME\_STEEPEST\_DESCENT**

Steepest descent.

With *PRIMME\_STEEPEST\_DESCENT primme\_set\_method()* sets:

- *locking* = 1;
- *maxBasisSize* = *numEvals* \* 2;
- *minRestartSize* = *numEvals*;
- *maxBlockSize* = *numEvals*;
- *maxPrevRetain* = 0;
- *robustShifts* = 0;
- *maxInnerIterations* = 0;
- *RightX* = 1;
- *SkewX* = 0.

**enumerator PRIMME\_LOBPCG\_OrthoBasis**

LOBPCG with orthogonal basis.

With *PRIMME\_LOBPCG\_OrthoBasis primme\_set\_method()* sets:

- *locking* = 0;
- *maxBasisSize* = *numEvals* \* 3;
- *minRestartSize* = *numEvals*;
- *maxBlockSize* = *numEvals*;
- *maxPrevRetain* = *numEvals*;
- *robustShifts* = 0;
- *maxInnerIterations* = 0;
- *RightX* = 1;
- *SkewX* = 0.

**enumerator PRIMME\_LOBPCG\_OrthoBasis\_Window**

LOBPCG with sliding window of *maxBlockSize* < 3 \* *numEvals*.

With *PRIMME\_LOBPCG\_OrthoBasis\_Window primme\_set\_method()* sets:

- *locking* = 0;
- *maxBasisSize* = *maxBlockSize* \* 3;
- *minRestartSize* = *maxBlockSize*;
- *maxPrevRetain* = *maxBlockSize*;
- *robustShifts* = 0;
- *maxInnerIterations* = 0;
- *RightX* = 1;
- *SkewX* = 0.



## 3.8 Error Codes

The functions `dprimme()` and `zprimme()` return one of the following error codes. Some of the error codes have a macro associated which is indicated in brackets.

- 0: success; usually all requested eigenpairs have converged.
- -1: (PRIMME\_UNEXPECTED\_FAILURE) unexpected internal error; please consider to set `printLevel` to a value larger than 0 to see the call stack and to report these errors because they may be bugs.
- -2: (PRIMME\_MALLOC\_FAILURE) failure in allocating memory; it can be either CPU or GPU.
- -3: (PRIMME\_MAIN\_ITER\_FAILURE) maximum number of outer iterations `maxOuterIterations` or matvecs `maxMatvecs` reached.
- -4: if argument `primme` is NULL.
- -5: if `n < 0` or `nLocal < 0` or `nLocal > n`.
- -6: if `numProcs < 1`.
- -7: if `matrixMatvec` is NULL.
- -8: if `applyPreconditioner` is NULL and `precondition > 0`.
- -10: if `numEvals > n`.
- -11: if `numEvals < 0`.
- -12: if `convTestFun` is not NULL and `eps > 0` and `eps < machine precision` given by `internalPrecision` and the precision of PRIMME call (`sprimme()`, `dprimme()`...).
- -13: if `target` is not properly defined.
- -14: if `target` is one of `primme_closest_geq`, `primme_closest_leq`, `primme_closest_abs` or `primme_largest_abs` but `numTargetShifts <= 0` (no shifts).
- -15: if `target` is one of `primme_closest_geq`, `primme_closest_leq`, `primme_closest_abs` or `primme_largest_abs` but `targetShifts` is NULL (no shifts array).
- -16: if `numOrthoConst < 0` or `numOrthoConst > n`. (no free dimensions left).
- -17: if `maxBasisSize < 2` and `n > 2`.
- -18: if `minRestartSize < 0`, or `minRestartSize` is zero but `n > 2` and `numEvals > 0`.
- -19: if `maxBlockSize < 0`, or `maxBlockSize` is zero but `numEvals > 0`.
- -20: if `maxPrevRetain < 0`.
- -22: if `initSize < 0`.
- -23: if `locking == 0` and `initSize > maxBasisSize`.
- -24: if `locking` and `initSize > numEvals`.
- -25: if `maxPrevRetain + minRestartSize >= maxBasisSize`, and `n > maxBasisSize`.
- -26: if `minRestartSize >= n`, and `n > 2`.
- -27: if `printLevel < 0` or `printLevel > 5`.
- -28: if `convTest` is not one of `primme_full_LTolerance`, `primme_decreasing_LTolerance`, `primme_adaptive_ETolerance` or `primme_adaptive`.
- -29: if `convTest == primme_decreasing_LTolerance` and `relTolBase <= 1`.
- -30: if `evals` is NULL.

- -31: if `evecs` is NULL, or is not a GPU pointer when calling a GPU variant (for instance `magma_dprimme`).
- -32: if `resNorms` is NULL.
- -33: if `locking == 0` and `minRestartSize < numEvals` and `n > 2`.
- -34: if `ldvecs < nLocal`.
- -35: if `ldOPs` is not zero and less than `nLocal`.
- -38: if `locking == 0` and `target` is `primme_closest_leq` or `primme_closest_geq`.
- -40: (PRIMME\_LAPACK\_FAILURE) some LAPACK function performing a factorization returned an error code; set `printLevel > 0` to see the error code and the call stack.
- -41: (PRIMME\_USER\_FAILURE) some of the user-defined functions (`matrixMatvec`, `applyPreconditioner`, ...) returned a non-zero error code; set `printLevel > 0` to see the call stack that produced the error.
- -42: (PRIMME\_ORTHO\_CONST\_FAILURE) the provided orthogonal constraints (see `numOrthoConst`) are not full rank.
- -43: (PRIMME\_PARALLEL\_FAILURE) some process has a different value in an input option than the process zero, or it is not acting coherently; set `printLevel > 0` to see the call stack that produced the error.
- -44: (PRIMME\_FUNCTION\_UNAVAILABLE) PRIMME was not compiled with support for the requesting precision or for GPUs.

## SINGULAR VALUE PROBLEMS

### 4.1 C Library Interface

New in version 2.0.

The PRIMME SVDS interface is composed of the following functions. To solve real and complex singular value problems call respectively:

```
int dprimme_svds (double *svals, double *svecs, double *resNorms,  
                 primme_svds_params *primme_svds)  
int zprimme_svds (double *svals, PRIMME_COMPLEX_DOUBLE *svecs,  
                 double *resNorms, primme_svds_params *primme_svds)
```

There are more versions for matrix problems working in other precisions:

Precision	Real	Complex
half	<i>hprimme_svds()</i> <i>hsprimme_svds()</i>	<i>kprimme_svds()</i> <i>ksprimme_svds()</i>
single	<i>sprimme_svds()</i>	<i>cprimme_svds()</i>
double	<i>dprimme_svds()</i>	<i>zprimme_svds()</i>

Other useful functions:

```
void primme_svds_initialize (primme_svds_params *primme_svds)  
int primme_svds_set_method (primme_svds_preset_method method,  
    primme_preset_method methodStage1,  
    primme_preset_method methodStage2, primme_svds_params *primme_svds)  
void primme_svds_display_params (primme_svds_params primme_svds)  
void primme_svds_free (primme_svds_params *primme_svds)
```

PRIMME SVDS stores its data on the structure *primme\_svds\_params*. See *Parameters Guide* for an introduction about its fields.

#### 4.1.1 Running

To use PRIMME SVDS, follow these basic steps.

1. Include:

```
#include "primme.h" /* header file is required to run primme */
```

2. Initialize a PRIMME SVDS parameters structure for default settings:

```
primme_svds_params primme_svds;  
primme_svds_initialize (&primme_svds);
```

3. Set problem parameters (see also *Parameters Guide*), and, optionally, set one of the *preset methods*:

```
primme_svds.matrixMatvec = matrixMatvec; /* MV product */
primme_svds.m = 1000; /* set the matrix dimensions */
primme_svds.n = 100;
primme_svds.numSvals = 10; /* Number of singular values */
primme_svds_set_method (primme_svds_hybrid, PRIMME_DEFAULT_METHOD,
                        PRIMME_DEFAULT_METHOD, &primme_svds);
...
```

4. Then to solve a real singular value problem call:

```
ret = dprimme_svds (svals, svecs, resNorms, &primme_svds);
```

The previous is the double precision call. There is available calls for complex double, single and complex single; check `zprimme_svds()`, `sprimme_svds()` and `cprimme_svds()`.

To solve complex singular value problems call:

```
ret = zprimme_svds (svals, svecs, resNorms, &primme_svds);
```

The call arguments are:

- *svals*, array to return the found singular values;
- *svecs*, array to return the found left and right singular vectors;
- *resNorms*, array to return the residual norms of the found triplets; and
- *ret*, returned error code.

5. To free the work arrays in PRIMME SVDS:

```
primme_svds_free (&primme_svds);
```

## 4.1.2 Parameters Guide

PRIMME SVDS stores the data on the structure `primme_svds_params`, which has the next fields:

### *Basic*

PRIMME\_INT *m*, number of rows of the matrix.  
PRIMME\_INT *n*, number of columns of the matrix.  
void (\**matrixMatvec*) (...), matrix-vector product.  
int *numSvals*, how many singular triplets to find.  
primme\_svds\_target *target*, which singular values to find.  
double *eps*, tolerance of the residual norm of converged triplets.

### *For parallel programs*

int *numProcs*, number of processes  
int *procID*, rank of this process  
PRIMME\_INT *mLocal*, number of rows stored in this process  
PRIMME\_INT *nLocal*, number of columns stored in this process  
void (\**globalSumReal*) (...), sum reduction among processes

### *Accelerate the convergence*

void (\**applyPreconditioner*) (...), preconditioner-vector product.

```

int initSize, initial vectors as approximate solutions.
int maxBasisSize
int minRestartSize
int maxBlockSize

```

#### *User data*

```

void * commInfo
void * matrix
void * preconditioner
void * convtest
void * monitor

```

#### *Advanced options*

```

int numTargetShifts, for targeting interior singular values.
double * targetShifts
int numOrthoConst, orthogonal constraints to the singular vectors.
int locking
PRIMME_INT maxMatvecs
PRIMME_INT iseed [4]
double aNorm
int printLevel
FILE * outputFile
primme_svds_operator method
primme_svds_operator methodStage2
primme_params primme
primme_params primmeStage2
void (* convTestFun) (...), custom convergence criterion.
void (* monitorFun) (...), custom convergence history.
primme_op_datatype matrixMatvec_type
primme_op_datatype applyPreconditioner_type
primme_op_datatype globalSumReal_type
primme_op_datatype broadcastReal_type
primme_op_datatype internalPrecision

```

PRIMME SVDS requires the user to set at least the matrix dimensions ( $m \times n$ ) and the matrix-vector product (*matrixMatvec*), as they define the problem to be solved. For parallel programs, *mLocal*, *nLocal*, *procID* and *globalSumReal* are also required.

In addition, most users would want to specify how many singular triplets to find, and provide a preconditioner (if available).

It is useful to have set all these before calling *primme\_svds\_set\_method()*. Also, if users have a preference on *maxBasisSize*, *maxBlockSize*, etc, they should also provide them into *primme\_svds\_params* prior to the *primme\_svds\_set\_method()* call. This helps *primme\_svds\_set\_method()* make the right choice on other parameters. It is sometimes useful to check the actual parameters that PRIMME SVDS is going to use (before calling it) or used (on return) by printing them with *primme\_svds\_display\_params()*.

### 4.1.3 Interface Description

The next enumerations and functions are declared in `primme.h`.

#### ?primme\_svds

```
int hprimme_svds (PRIMME_HALF *svals, PRIMME_HALF *svecs, PRIMME_HALF *resNorms,
                 primme_svds_params *primme_svds)
```

```
int hsprimme_svds (float *svals, PRIMME_HALF *svecs, float *resNorms, primme_svds_params
                  *primme_svds)
```

```
int kprimme_svds (PRIMME_HALF *svals, PRIMME_COMPLEX_HALF *svecs, PRIMME_HALF
                 *resNorms, primme_svds_params *primme_svds)
```

```
int ksprimme_svds (float *svals, PRIMME_COMPLEX_HALF *svecs, float *resNorms,
                  primme_svds_params *primme_svds)
```

New in version 3.0.

```
int sprimme_svds (float *svals, float *svecs, float *resNorms, primme_svds_params *primme_svds)
```

```
int cprimme_svds (float *svals, PRIMME_COMPLEX_FLOAT *svecs, float *resNorms,
                 primme_svds_params *primme_svds)
```

New in version 2.0.

```
int dprimme_svds (double *svals, double *svecs, double *resNorms, primme_svds_params *primme_svds)
```

```
int zprimme_svds (double *svals, PRIMME_COMPLEX_DOUBLE *svecs, double *resNorms,
                 primme_svds_params *primme_svds)
```

Solve a real singular value problem.

All arrays should be hosted on CPU. The computations are performed on CPU (see `magma_dprimme_svds()` for using GPUs).

#### Parameters

- **svals** – array at least of size `numSvals` to store the computed singular values; all processes in a parallel run return this local array with the same values.
- **svecs** – array at least of size  $(mLocal + nLocal)$  times  $(numOrthoConst + numSvals)$  to store column-wise the (local part for this process of the) computed left singular vectors and the right singular vectors.
- **resNorms** – array at least of size `numSvals` to store the residual norms of the computed triplets; all processes in parallel run return this local array with the same values.
- **primme\_svds** – parameters structure.

**Returns** error indicator; see *Error Codes*.

On input, `svecs` should start with the content of the `numOrthoConst` left vectors, followed by the `initSize` left vectors, followed by the `numOrthoConst` right vectors, and followed by the `initSize` right vectors.

On return, the *i*-th left singular vector starts at `svecs[(numOrthoConst + i)*mLocal]`. The *i*-th right singular vector starts at `svecs[(numOrthoConst + initSize)*mLocal + (numOrthoConst + i)*nLocal]`. The first vector has *i*=0.

All internal operations are performed at the same precision than `svecs` unless the user sets `internalPrecision` otherwise. The functions `hsprimme_svds()` and `ksprimme_svds()` perform all computations in half precision by default and report the eigenvalues and the residual norms in single precision. These functions may help in applications that may be not built with a compiler supporting half precision.

The type and precision of the callbacks depends on the type and precision of `svecs`. Although this can be changed. See details for `matrixMatvec`, `applyPreconditioner`, `globalSumReal`, `broadcastReal`, and `convTestFun`.

### **`magma_?primme_svds`**

```
int magma_hprimme_svds (PRIMME_HALF *svals, PRIMME_HALF *svecs, PRIMME_HALF
                        *resNorms, primme_svds_params *primme_svds)
int magma_hsprimme_svds (float *svals, PRIMME_HALF *svecs, float *resNorms, primme_svds_params
                        *primme_svds)
int magma_kprimme_svds (PRIMME_HALF *svals, PRIMME_COMPLEX_HALF *svecs,
                        PRIMME_HALF *resNorms, primme_svds_params *primme_svds)
int magma_ksprimme_svds (float *svals, PRIMME_COMPLEX_HALF *svecs, float *resNorms,
                        primme_svds_params *primme_svds)
int magma_sprimme_svds (float *svals, float *svecs, float *resNorms, primme_svds_params
                        *primme_svds)
int magma_cprimme_svds (float *svals, PRIMME_COMPLEX_FLOAT *svecs, float *resNorms,
                        primme_svds_params *primme_svds)
int magma_dprimme_svds (double *svals, double *svecs, double *resNorms, primme_svds_params
                        *primme_svds)
int magma_zprimme_svds (double *svals, PRIMME_COMPLEX_DOUBLE *svecs, double *resNorms,
                        primme_svds_params *primme_svds)
```

Solve a real singular value problem.

Most of the computations are performed on GPU (see `dprimme_svds()` for using only the CPU).

#### **Parameters**

- **`svals`** – CPU array at least of size `numSvals` to store the computed singular values; all processes in a parallel run return this local array with the same values.
- **`svecs`** – GPU array at least of size  $(mLocal + nLocal)$  times  $(numOrthoConst + numSvals)$  to store column-wise the (local part for this process of the) computed left singular vectors and the right singular vectors.
- **`resNorms`** – CPU array at least of size `numSvals` to store the residual norms of the computed triplets; all processes in parallel run return this local array with the same values.
- **`primme_svds`** – parameters structure.

**Returns** error indicator; see [Error Codes](#).

On input, `svecs` should start with the content of the `numOrthoConst` left vectors, followed by the `initSize` left vectors, followed by the `numOrthoConst` right vectors, and followed by the `initSize` right vectors.

On return, the *i*-th left singular vector starts at `svecs[( numOrthoConst +i)* mLocal ]`. The *i*-th right singular vector starts at `svecs[( numOrthoConst + initSize)* mLocal + ( numOrthoConst +i)* nLocal ]`. The first vector has *i*=0.

All internal operations are performed at the same precision than `svecs` unless the user sets `internalPrecision` otherwise. The functions `magma_hsprimme_svds()` and `magma_ksprimme_svds()` perform all computations in half precision by default and report the eigenvalues and the residual norms in single precision. These functions may help in applications that may be not built with a compiler supporting half precision.

The type and precision of the callbacks depends on the type and precision of `svecs`. Although this can be changed. See details for `matrixMatvec`, `applyPreconditioner`, `globalSumReal`, `broadcastReal`, and `convTestFun`.

New in version 3.0.

### **primme\_svds\_initialize**

void **primme\_svds\_initialize** (*primme\_svds\_params* \**primme\_svds*)

Initialize PRIMME SVDS parameters structure to the default values.

After calling `dprimme_svds()` (or a variant), call `primme_svds_free()` to release allocated resources by PRIMME.

#### **Parameters**

- **primme\_svds** – parameters structure.

Example:

```
primme_svds_params primme_svds;
primme_svds_initialize(&primme_svds);

primme_svds.n = 100;
...
dprimme_svds(svals, svecs, rnorms, &primme_svds);
...

primme_svds_free(&primme_svds);
```

See the alternative function `primme_svds_params_create()` that also allocates the structure.

### **primme\_svds\_create**

*primme\_svds\_params* \***primme\_svds\_params\_create** (void)

Allocate and initialize a parameters structure to the default values.

After calling `dprimme_svds()` (or a variant), call `primme_svds_params_destroy()` to release allocated resources by PRIMME.

#### **Parameters**

- **primme\_sv** – parameters structure.

Example:

```
primme_svds_params *primme_svds = primme_svds_params_create();

primme_svds->n = 100;
...
dprimme_svds(svals, svecs, rnorms, primme_svds);
...

primme_svds_params_destroy(primme_svds);
```

See the alternative function `primme_svds_initialize()` that only initializes the structure.

New in version 3.0.



## primme\_svds\_set\_method

int **primme\_svds\_set\_method** (*primme\_svds\_preset\_method method*, *primme\_preset\_method methodStage1*, *primme\_preset\_method methodStage2*, *primme\_svds\_params \*primme\_svds*)

Set PRIMME SVDS parameters to one of the preset configurations.

### Parameters

- **method** – preset method to compute the singular triplets; one of
  - *primme\_svds\_default*, currently set as *primme\_svds\_hybrid*.
  - *primme\_svds\_normalequations*, compute the eigenvectors of  $A^*A$  or  $AA^*$ .
  - *primme\_svds\_augmented*, compute the eigenvectors of the augmented matrix,  $\begin{pmatrix} 0 & A^* \\ A & 0 \end{pmatrix}$ .
  - *primme\_svds\_hybrid*, start with *primme\_svds\_normalequations*; use the resulting approximate singular vectors as initial vectors for *primme\_svds\_augmented* if the required accuracy was not achieved.
- **methodStage1** – preset method to compute the eigenpairs at the first stage; see available values at *primme\_set\_method()*.
- **methodStage2** – preset method to compute the eigenpairs with the second stage of *primme\_svds\_hybrid*; see available values at *primme\_set\_method()*.
- **primme\_svds** – parameters structure.

See also *Preset Methods*.

## primme\_svds\_display\_params

void **primme\_svds\_display\_params** (*primme\_svds\_params primme\_svds*)

Display all printable settings of *primme\_svds* into the file descriptor *outputFile*.

### Parameters

- **primme\_svds** – parameters structure.

## primme\_svds\_free

void **primme\_svds\_free** (*primme\_svds\_params \*primme\_svds*)

Free memory allocated by PRIMME SVDS.

### Parameters

- **primme\_svds** – parameters structure.

### **primme\_svds\_params\_destroy**

int **primme\_svds\_params\_destroy** (*primme\_svds\_params* \**primme*)

Free memory allocated by PRIMME associated to a parameters structure created with *primme\_svds\_params\_create()*.

#### **Parameters**

- **primme\_svds** – parameters structure.

**Returns** nonzero value if the call is not successful.

New in version 3.0.

## 4.2 FORTRAN Library Interface

New in version 2.0.

The next enumerations and functions are declared in `primme_svds_f77.h`.

### 4.2.1 sprimme\_svds\_f77

**subroutine sprimme\_svds\_f77** (*svals*, *svecs*, *resNorms*, *primme\_svds*, *ierr*)

Solve a real singular value problem using single precision.

All arrays should be hosted on CPU. The computations are performed on CPU (see `agma_sprimme_svds_f77()` for using GPUs).

#### Parameters

- **svals** (\*) [*real*] :: (output) array at least of size `numSvals` to store the computed singular values; all processes in a parallel run return this local array with the same values.
- **svecs** (\*) [*real*] :: array at least of size  $(mLocal + nLocal)$  times  $(numOrthoConst + numSvals)$  to store column-wise the (local part for this process of the) computed left singular vectors and the right singular vectors.
- **resNorms** (\*) [*real*] :: array at least of size `numSvals` to store the residual norms of the computed triplets; all processes in parallel run return this local array with the same values.
- **primme\_svds** [*ptr*] :: parameters structure.
- **ierr** [*integer*] :: (output) error indicator; see *Error Codes*.

On input, *svecs* should start with the content of the `numOrthoConst` left vectors, followed by the `initSize` left vectors, followed by the `numOrthoConst` right vectors and followed by the `initSize` right vectors.

On return, the *i*-th left singular vector starts at `svecs(( numOrthoConst + i - 1 ) * mLocal )`. The *i*-th right singular vector starts at `svecs(( numOrthoConst + initSize ) * mLocal + ( numOrthoConst + i - 1 ) * nLocal )`. The first vector has *i*=1.

All internal operations are performed at the same precision than *svecs* unless the user sets `internalPrecision` otherwise.

The type and precision of the callbacks depends on the type and precision of *svecs*. See details for `matrixMatvec`, `applyPreconditioner`, `globalSumReal`, `broadcastReal`, and `convTestFun`.

### 4.2.2 cprimme\_svds\_f77

**subroutine cprimme\_svds\_f77** (*svals*, *svecs*, *resNorms*, *primme\_svds*, *ierr*)

Solve a complex singular value problem using single precision.

All arrays should be hosted on CPU. The computations are performed on CPU (see `agma_cprimme_svds_f77()` for using GPUs).

#### Parameters

- **svals** (\*) [*real*] :: (output) array at least of size `numSvals` to store the computed singular values; all processes in a parallel run return this local array with the same values.

- **svecs** (\*) [*complex*] :: array at least of size  $(mLocal + nLocal)$  times  $(numOrthoConst + numSvals)$  to store column-wise the (local part for this process of the) computed left singular vectors and the right singular vectors.
- **resNorms** (\*) [*real*] :: array at least of size *numSvals* to store the residual norms of the computed triplets; all processes in parallel run return this local array with the same values.
- **primme\_svds** [*ptr*] :: parameters structure.
- **ierr** [*integer*] :: (output) error indicator; see *Error Codes*.

On input, *svecs* should start with the content of the *numOrthoConst* left vectors, followed by the *initSize* left vectors, followed by the *numOrthoConst* right vectors and followed by the *initSize* right vectors.

On return, the *i*-th left singular vector starts at *svecs*(( *numOrthoConst* + *i* - 1) \* *mLocal* ). The *i*-th right singular vector starts at *svecs*(( *numOrthoConst* + *initSize* ) \* *mLocal* + ( *numOrthoConst* + *i* - 1) \* *nLocal* ). The first vector has *i*=1.

All internal operations are performed at the same precision than *svecs* unless the user sets *internalPrecision* otherwise.

The type and precision of the callbacks depends on the type and precision of *svecs*. See details for *matrixMatvec*, *applyPreconditioner*, *globalSumReal*, *broadcastReal*, and *convTestFun*.

### 4.2.3 dprimme\_svds\_f77

**subroutine dprimme\_svds\_f77** (*svals*, *svecs*, *resNorms*, *primme\_svds*, *ierr*)

Solve a real singular value problem using double precision.

All arrays should be hosted on CPU. The computations are performed on CPU (see *gamma\_dprimme\_svds\_f77()* for using GPUs).

#### Parameters

- **svals** (\*) [*double precision*] :: (output) array at least of size *numSvals* to store the computed singular values; all processes in a parallel run return this local array with the same values.
- **svecs** (\*) [*double precision*] :: array at least of size  $(mLocal + nLocal)$  times  $(numOrthoConst + numSvals)$  to store column-wise the (local part for this process of the) computed left singular vectors and the right singular vectors.
- **resNorms** (\*) [*double precision*] :: array at least of size *numSvals* to store the residual norms of the computed triplets; all processes in parallel run return this local array with the same values.
- **primme\_svds** [*ptr*] :: parameters structure.
- **ierr** [*integer*] :: (output) error indicator; see *Error Codes*.

On input, *svecs* should start with the content of the *numOrthoConst* left vectors, followed by the *initSize* left vectors, followed by the *numOrthoConst* right vectors and followed by the *initSize* right vectors.

On return, the *i*-th left singular vector starts at *svecs*(( *numOrthoConst* + *i* - 1) \* *mLocal* ). The *i*-th right singular vector starts at *svecs*(( *numOrthoConst* + *initSize* ) \* *mLocal* + ( *numOrthoConst* + *i* - 1) \* *nLocal* ). The first vector has *i*=1.

All internal operations are performed at the same precision than *svecs* unless the user sets *internalPrecision* otherwise.

The type and precision of the callbacks depends on the type and precision of *svecs*. See details for *matrixMatvec*, *applyPreconditioner*, *globalSumReal*, *broadcastReal*, and *convTestFun*.

#### 4.2.4 zprimme\_svds\_f77

**subroutine zprimme\_svds\_f77** (*svals*, *svecs*, *resNorms*, *primme\_svds*, *ierr*)

Solve a complex singular value problem using double precision.

All arrays should be hosted on CPU. The computations are performed on CPU (see *magma\_zprimme\_svds\_f77()* for using GPUs).

##### Parameters

- **svals** (\*) [*double precision*] :: (output) array at least of size *numSvals* to store the computed singular values; all processes in a parallel run return this local array with the same values.
- **svecs** (\*) [*complex double precision*] :: array at least of size (*mLocal* + *nLocal*) times (*numOrthoConst* + *numSvals*) to store column-wise the (local part for this process of the) computed left singular vectors and the right singular vectors.
- **resNorms** (\*) [*double precision*] :: array at least of size *numSvals* to store the residual norms of the computed triplets; all processes in parallel run return this local array with the same values.
- **primme\_svds** [*ptr*] :: parameters structure.
- **ierr** [*integer*] :: (output) error indicator; see *Error Codes*.

On input, *svecs* should start with the content of the *numOrthoConst* left vectors, followed by the *initSize* left vectors, followed by the *numOrthoConst* right vectors and followed by the *initSize* right vectors.

On return, the *i*-th left singular vector starts at *svecs*((*numOrthoConst* + *i* - 1) \* *mLocal*). The *i*-th right singular vector starts at *svecs*((*numOrthoConst* + *initSize*) \* *mLocal* + (*numOrthoConst* + *i* - 1) \* *nLocal*). The first vector has *i*=1.

All internal operations are performed at the same precision than *svecs* unless the user sets *internalPrecision* otherwise.

The type and precision of the callbacks depends on the type and precision of *svecs*. See details for *matrixMatvec*, *applyPreconditioner*, *globalSumReal*, *broadcastReal*, and *convTestFun*.

#### 4.2.5 magma\_sprimme\_svds\_f77

**subroutine magma\_sprimme\_svds\_f77** (*svals*, *svecs*, *resNorms*, *primme\_svds*, *ierr*)

Solve a real singular value problem using single precision.

Most of the computations are performed on GPU (see *sprimme\_svds\_f77()* for using only the CPU).

##### Parameters

- **svals** (\*) [*real*] :: (output) CPU array at least of size *numSvals* to store the computed singular values; all processes in a parallel run return this local array with the same values.
- **svecs** (\*) [*real*] :: GPU array at least of size (*mLocal* + *nLocal*) times (*numOrthoConst* + *numSvals*) to store column-wise the (local part for this process of the) computed left singular vectors and the right singular vectors.

- **resNorms** (\*) [*real*] :: CPU array at least of size *numSvals* to store the residual norms of the computed triplets; all processes in parallel run return this local array with the same values.
- **primme\_svds** [*ptr*] :: parameters structure.
- **ierr** [*integer*] :: (output) error indicator; see *Error Codes*.

On input, *svecs* should start with the content of the *numOrthoConst* left vectors, followed by the *initSize* left vectors, followed by the *numOrthoConst* right vectors and followed by the *initSize* right vectors.

On return, the *i*-th left singular vector starts at *svecs*(( *numOrthoConst* + *i* - 1) \* *mLocal* ). The *i*-th right singular vector starts at *svecs*(( *numOrthoConst* + *initSize*)\* *mLocal* + ( *numOrthoConst* + *i* - 1)\* *nLocal* ). The first vector has *i*=1.

All internal operations are performed at the same precision than *svecs* unless the user sets *internalPrecision* otherwise.

The type and precision of the callbacks depends on the type and precision of *svecs*. See details for *matrixMatvec*, *applyPreconditioner*, *globalSumReal*, *broadcastReal*, and *convTestFun*.

New in version 3.0.

## 4.2.6 magma\_cprimme\_svds\_f77

**subroutine magma\_cprimme\_svds\_f77** (*svals*, *svecs*, *resNorms*, *primme\_svds*, *ierr*)

Solve a complex singular value problem using single precision.

Most of the computations are performed on GPU (see *cprimme\_svds\_f77()* for using only the CPU).

### Parameters

- **svals** (\*) [*real*] :: (output) CPU array at least of size *numSvals* to store the computed singular values; all processes in a parallel run return this local array with the same values.
- **svecs** (\*) [*complex*] :: GPU array at least of size (*mLocal* + *nLocal*) times (*numOrthoConst* + *numSvals*) to store column-wise the (local part for this process of the) computed left singular vectors and the right singular vectors.
- **resNorms** (\*) [*real*] :: CPU array at least of size *numSvals* to store the residual norms of the computed triplets; all processes in parallel run return this local array with the same values.
- **primme\_svds** [*ptr*] :: parameters structure.
- **ierr** [*integer*] :: (output) error indicator; see *Error Codes*.

On input, *svecs* should start with the content of the *numOrthoConst* left vectors, followed by the *initSize* left vectors, followed by the *numOrthoConst* right vectors and followed by the *initSize* right vectors.

On return, the *i*-th left singular vector starts at *svecs*(( *numOrthoConst* + *i* - 1) \* *mLocal* ). The *i*-th right singular vector starts at *svecs*(( *numOrthoConst* + *initSize*)\* *mLocal* + ( *numOrthoConst* + *i* - 1)\* *nLocal* ). The first vector has *i*=1.

All internal operations are performed at the same precision than *svecs* unless the user sets *internalPrecision* otherwise.

The type and precision of the callbacks depends on the type and precision of *svecs*. See details for *matrixMatvec*, *applyPreconditioner*, *globalSumReal*, *broadcastReal*, and *convTestFun*.

New in version 3.0.

## 4.2.7 magma\_dprimme\_svds\_f77

**subroutine magma\_dprimme\_svds\_f77** (*svals*, *svecs*, *resNorms*, *primme\_svds*, *ierr*)

Solve a real singular value problem using double precision.

Most of the computations are performed on GPU (see *dprimme\_svds\_f77()* for using only the CPU).

### Parameters

- **svals** (\*) [*double precision*] :: (output) CPU array at least of size *numSvals* to store the computed singular values; all processes in a parallel run return this local array with the same values.
- **svecs** (\*) [*double precision*] :: GPU array at least of size (*mLocal* + *nLocal*) times (*numOrthoConst* + *numSvals*) to store column-wise the (local part for this process of the) computed left singular vectors and the right singular vectors.
- **resNorms** (\*) [*double precision*] :: CPU array at least of size *numSvals* to store the residual norms of the computed triplets; all processes in parallel run return this local array with the same values.
- **primme\_svds** [*ptr*] :: parameters structure.
- **ierr** [*integer*] :: (output) error indicator; see *Error Codes*.

On input, *svecs* should start with the content of the *numOrthoConst* left vectors, followed by the *initSize* left vectors, followed by the *numOrthoConst* right vectors and followed by the *initSize* right vectors.

On return, the *i*-th left singular vector starts at *svecs*(( *numOrthoConst* + *i* - 1) \* *mLocal* ). The *i*-th right singular vector starts at *svecs*(( *numOrthoConst* + *initSize*)\* *mLocal* + ( *numOrthoConst* + *i* - 1)\* *nLocal* ). The first vector has *i*=1.

All internal operations are performed at the same precision than *svecs* unless the user sets *internalPrecision* otherwise.

The type and precision of the callbacks depends on the type and precision of *svecs*. See details for *matrixMatvec*, *applyPreconditioner*, *globalSumReal*, *broadcastReal*, and *convTestFun*.

New in version 3.0.

## 4.2.8 magma\_zprimme\_svds\_f77

**subroutine magma\_zprimme\_svds\_f77** (*svals*, *svecs*, *resNorms*, *primme\_svds*, *ierr*)

Solve a complex singular value problem using double precision.

Most of the computations are performed on GPU (see *zprimme\_svds\_f77()* for using only the CPU).

### Parameters

- **svals** (\*) [*double precision*] :: (output) CPU array at least of size *numSvals* to store the computed singular values; all processes in a parallel run return this local array with the same values.

- **svecs** (\*) [*complex double precision*] :: GPU array at least of size  $(mLocal + nLocal)$  times  $(numOrthoConst + numSvals)$  to store column-wise the (local part for this process of the) computed left singular vectors and the right singular vectors.
- **resNorms** (\*) [*double precision*] :: CPU array at least of size  $numSvals$  to store the residual norms of the computed triplets; all processes in parallel run return this local array with the same values.
- **primme\_svds** [ptr] :: parameters structure.
- **ierr** [integer] :: (output) error indicator; see *Error Codes*.

On input, **svecs** should start with the content of the  $numOrthoConst$  left vectors, followed by the *initSize* left vectors, followed by the  $numOrthoConst$  right vectors and followed by the *initSize* right vectors.

On return, the  $i$ -th left singular vector starts at **svecs**((  $numOrthoConst + i - 1$ ) \*  $mLocal$  ). The  $i$ -th right singular vector starts at **svecs**((  $numOrthoConst + initSize$ ) \*  $mLocal + (numOrthoConst + i - 1)$  \*  $nLocal$  ). The first vector has  $i=1$ .

All internal operations are performed at the same precision than **svecs** unless the user sets *internalPrecision* otherwise.

The type and precision of the callbacks depends on the type and precision of **svecs**. See details for *matrixMatvec*, *applyPreconditioner*, *globalSumReal*, *broadcastReal*, and *convTestFun*.

New in version 3.0.

## 4.2.9 primme\_svds\_initialize\_f77

**subroutine primme\_svds\_initialize\_f77** (*primme\_svds*, *ierr*)

Set PRIMME SVDS parameters structure to the default values.

After calling *dprimme\_svds\_f77*() (or a variant), call *primme\_svds\_free\_f77*() to release allocated resources by PRIMME.

**Parameters** **primme\_svds** [ptr] :: (output) parameters structure.

## 4.2.10 primme\_svds\_set\_method\_f77

**subroutine primme\_svds\_set\_method\_f77** (*method*, *methodStage1*, *methodStage2*, *primme\_svds*, *ierr*)

Set PRIMME SVDS parameters to one of the preset configurations.

**Parameters**

- **method** [integer] :: (input) preset configuration to compute the singular triplets; one of
  - *PRIMME\_SVDS\_default*, currently set as *PRIMME\_SVDS\_hybrid*.
  - *PRIMME\_SVDS\_normalequations*, compute the eigenvectors of  $A^*A$  or  $AA^*$ .
  - *PRIMME\_SVDS\_augmented*, compute the eigenvectors of the augmented matrix,  $\begin{pmatrix} 0 & A^* \\ A & 0 \end{pmatrix}$ .
  - *PRIMME\_SVDS\_hybrid*, start with *PRIMME\_SVDS\_normalequations*; use the resulting approximate singular vectors as initial vectors for *PRIMME\_SVDS\_augmented* if the required accuracy was not achieved.



- **methodStage1** [*primme\_preset\_method*] :: (input) preset method to compute the eigenpairs at the first stage; see available values at `primme_set_method_f77()`.
- **methodStage2** [*primme\_preset\_method*] :: (input) preset method to compute the eigenpairs with the second stage of *PRIMME\_SVDS\_hybrid*; see available values at `primme_set_method_f77()`.
- **primme\_svds** [*ptr*] :: (input/output) parameters structure.
- **ierr** [*integer*] :: (output) if 0, successful; if negative, something went wrong.

#### 4.2.11 primme\_svds\_display\_params\_f77

**subroutine primme\_svds\_display\_params\_f77** (*primme\_svds*)

Display all printable settings of *primme\_svds* into the file descriptor *outputFile*.

**Parameters** *primme\_svds* [*ptr*] :: (input) parameters structure.

#### 4.2.12 primme\_svds\_free\_f77

**subroutine primme\_svds\_free\_f77** (*primme\_svds*, *ierr*)

Free memory allocated by PRIMME SVDS and delete all values set.

**Parameters** *primme\_svds* [*ptr*] :: (input/output) parameters structure.

#### 4.2.13 primme\_svds\_set\_member\_f77

**subroutine primme\_svds\_set\_member\_f77** (*primme\_svds*, *label*, *value*, *ierr*)

Set a value in some field of the parameter structure.

**Parameters**

- **primme\_svds** [*ptr*] :: (input) parameters structure.
- **label** [*integer*] :: field where to set value. One of:

*PRIMME\_SVDS\_primme*  
*PRIMME\_SVDS\_primmeStage2*  
*PRIMME\_SVDS\_m*  
*PRIMME\_SVDS\_n*  
*PRIMME\_SVDS\_matrixMatvec*  
*PRIMME\_SVDS\_matrixMatvec\_type*  
*PRIMME\_SVDS\_applyPreconditioner*  
*PRIMME\_SVDS\_applyPreconditioner\_type*  
*PRIMME\_SVDS\_numProcs*  
*PRIMME\_SVDS\_procID*  
*PRIMME\_SVDS\_mLocal*  
*PRIMME\_SVDS\_nLocal*  
*PRIMME\_SVDS\_commInfo*  
*PRIMME\_SVDS\_globalSumReal*  
*PRIMME\_SVDS\_globalSumReal\_type*  
*PRIMME\_SVDS\_broadcastReal*

*PRIMME\_SVDS\_broadcastReal\_type*  
*PRIMME\_SVDS\_numSvals*  
*PRIMME\_SVDS\_target*  
*PRIMME\_SVDS\_numTargetShifts*  
*PRIMME\_SVDS\_targetShifts*  
*PRIMME\_SVDS\_method*  
*PRIMME\_SVDS\_methodStage2*  
*PRIMME\_SVDS\_matrix*  
*PRIMME\_SVDS\_preconditioner*  
*PRIMME\_SVDS\_locking*  
*PRIMME\_SVDS\_numOrthoConst*  
*PRIMME\_SVDS\_aNorm*  
*PRIMME\_SVDS\_eps*  
*PRIMME\_SVDS\_precondition*  
*PRIMME\_SVDS\_initSize*  
*PRIMME\_SVDS\_maxBasisSize*  
*PRIMME\_SVDS\_maxBlockSize*  
*PRIMME\_SVDS\_maxMatvecs*  
*PRIMME\_SVDS\_iseed*  
*PRIMME\_SVDS\_printLevel*  
*PRIMME\_SVDS\_outputFile*  
*PRIMME\_SVDS\_internalPrecision*  
*PRIMME\_SVDS\_convTestFun*  
*PRIMME\_SVDS\_convTestFun\_type*  
*PRIMME\_SVDS\_convtest*  
*PRIMME\_SVDS\_monitorFun*  
*PRIMME\_SVDS\_monitorFun\_type*  
*PRIMME\_SVDS\_monitor*  
*PRIMME\_SVDS\_queue*  
*PRIMME\_SVDS\_stats\_numOuterIterations*  
*PRIMME\_SVDS\_stats\_numRestarts*  
*PRIMME\_SVDS\_stats\_numMatvecs*  
*PRIMME\_SVDS\_stats\_numPreconds*  
*PRIMME\_SVDS\_stats\_numGlobalSum*  
*PRIMME\_SVDS\_stats\_numBroadcast*  
*PRIMME\_SVDS\_stats\_volumeGlobalSum*  
*PRIMME\_SVDS\_stats\_volumeBroadcast*  
*PRIMME\_SVDS\_stats\_elapsedTime*  
*PRIMME\_SVDS\_stats\_timeMatvec*  
*PRIMME\_SVDS\_stats\_timePrecond*  
*PRIMME\_SVDS\_stats\_timeOrtho*  
*PRIMME\_SVDS\_stats\_timeGlobalSum*  
*PRIMME\_SVDS\_stats\_timeBroadcast*  
*PRIMME\_SVDS\_stats\_lockingIssue*

- **value** :: (input) value to set.

---

**Note:** Don't use this subroutine inside PRIMME SVDS's callback functions, e.g., *matrixMatvec* or *applyPreconditioner*, or in functions called by these functions.

---

#### 4.2.14 primme\_svdstop\_get\_member\_f77

**subroutine** `primme_svdstop_get_member_f77` (*primme\_svds*, *label*, *value*, *ierr*)

Get the value in some field of the parameter structure.

##### Parameters

- **primme\_svds** [*ptr*] :: (input) parameters structure.
- **label** [*integer*] :: (input) field where to get value. One of the detailed in subroutine `primmesvds_top_set_member_f77()`.
- **value** :: (output) value of the field.

---

**Note:** Don't use this subroutine inside PRIMME SVDS's callback functions, e.g., *matrixMatvec* or *applyPreconditioner*, or in functions called by these functions. In those cases use *primme\_svds\_get\_member\_f77()*.

---



---

**Note:** When `label` is one of `PRIMME_SVDS_matrixMatvec`, `PRIMME_SVDS_applyPreconditioner`, `PRIMME_SVDS_commInfo`, `PRIMME_SVDS_intWork`, `PRIMME_SVDS_realWork`, `PRIMME_SVDS_matrix` and `PRIMME_SVDS_preconditioner`, the returned value is a C pointer (`void*`). Use Fortran pointer or other extensions to deal with it. For instance:

---

```

use iso_c_binding
MPI_Comm comm

comm = MPI_COMM_WORLD
call primme_svds_set_member_f77(primme_svds, PRIMME_SVDS_commInfo, comm)
...
subroutine par_GlobalSumDouble(x,y,k,primme_svds)
use iso_c_binding
implicit none
...
MPI_Comm, pointer :: comm
type(c_ptr) :: pcomm

call primme_svds_get_member_f77(primme_svds, PRIMME_SVDS_commInfo, pcomm)
call c_f_pointer(pcomm, comm)
call MPI_Allreduce(x,y,k,MPI_DOUBLE,MPI_SUM,comm,ierr)

```

Most users would not need to retrieve these pointers in their programs.

---

### 4.2.15 primme\_svds\_get\_member\_f77

**subroutine primme\_svds\_get\_member\_f77** (*primme\_svds*, *label*, *value*, *ierr*)

Get the value in some field of the parameter structure.

#### Parameters

- **primme\_svds** [*ptr*] :: (input) parameters structure.
- **label** [*integer*] :: (input) field where to get value. One of the detailed in subroutine `primme_svdstop_set_member_f77()`.
- **value** :: (output) value of the field.

---

**Note:** Use this subroutine exclusively inside PRIMME SVDS's callback functions, e.g., *matrixMatvec* or *applyPreconditioner*, or in functions called by these functions. Otherwise, e.g., from the main program, use the subroutine *primme\_svdstop\_get\_member\_f77()*.

---

---

**Note:** When `label` is one of `PRIMME_SVDS_matrixMatvec`, `PRIMME_SVDS_applyPreconditioner`, `PRIMME_SVDS_commInfo`, `PRIMME_SVDS_intWork`, `PRIMME_SVDS_realWork`, `PRIMME_SVDS_matrix` and `PRIMME_SVDS_preconditioner`, the returned value is a C pointer (`void*`). Use Fortran pointer or other extensions to deal with it. For instance:

---

```
use iso_c_binding
MPI_Comm comm

comm = MPI_COMM_WORLD
call primme_svds_set_member_f77(primme_svds, PRIMME_SVDS_commInfo, comm)
...
subroutine par_GlobalSumDouble(x,y,k,primme_svds)
use iso_c_binding
implicit none
...
MPI_Comm, pointer :: comm
type(c_ptr) :: pcomm

call primme_svds_get_member_f77(primme_svds, PRIMME_SVDS_commInfo, pcomm)
call c_f_pointer(pcomm, comm)
call MPI_Allreduce(x,y,k,MPI_DOUBLE,MPI_SUM,comm,ierr)
```

Most users would not need to retrieve these pointers in their programs.

---

## 4.3 FORTRAN 90 Library Interface

New in version 3.0.

The next enumerations and functions are declared in `primme_f90.inc`.

**subroutine primme\_svds\_matvec** (*x*, *ldx*, *y*, *ldy*, *blockSize*, *mode*, *primme\_svds*, *ierr*)

Abstract interface for the callbacks *matrixMatvec* and *applyPreconditioner*.

### Parameters

- **x** (*ldx*,\*) [*type*(\*),*in*] :: matrix with *blockSize* columns in *column-major* order with leading dimension *ldx*.
- **ldx** [*c\_int64\_t*] :: the leading dimension of the array *x*.
- **y** (*ldy*,\*) [*type*(\*),*out*] :: matrix with *blockSize* columns in *column-major* order with leading dimension *ldy*.
- **ldy** [*c\_int64\_t*] :: the leading dimension of the array *y*.
- **blockSize** [*c\_int*,*in*] :: number of columns in *x* and *y*.
- **mode** [*c\_int*,*in*] :: a flag.
- **primme\_svds** [*c\_ptr*,*in*] :: parameters structure created by *primme\_svds\_params\_create*() .
- **ierr** [*c\_int*,*out*] :: output error code; if it is set to non-zero, the current call to PRIMME will stop.

See more details about the precision and type and dimension for *x* and *y*, and the meaning of *mode* in the documentation of the callbacks.

### 4.3.1 primme\_svds\_params\_create

**function primme\_svds\_params\_create** ()

Allocate and initialize a parameters structure to the default values.

After calling *xprimme\_svds*() (or a variant), call *primme\_svds\_params\_destroy*() to release allocated resources by PRIMME.

**Return** *primme\_svds\_params\_create* [*c\_ptr*] :: pointer to a parameters structure.

### 4.3.2 primme\_svds\_set\_method

**function primme\_svds\_set\_method** (*method*, *methodStage1*, *methodStage2*, *primme\_svds*)

Set PRIMME SVDS parameters to one of the preset configurations.

### Parameters

- **method** [*integer*] :: (input) preset configuration to compute the singular triplets; one of
  - *PRIMME\_SVDS\_default*, currently set as *PRIMME\_SVDS\_hybrid*.
  - *PRIMME\_SVDS\_normalequations*, compute the eigenvectors of  $A^*A$  or  $AA^*$ .
  - *PRIMME\_SVDS\_augmented*, compute the eigenvectors of the augmented matrix,
 
$$\begin{pmatrix} 0 & A^* \\ A & 0 \end{pmatrix}.$$

- `PRIMME_SVDS_hybrid`, start with `PRIMME_SVDS_normalequations`; use the resulting approximate singular vectors as initial vectors for `PRIMME_SVDS_augmented` if the required accuracy was not achieved.
- **methodStage1** [*primme\_preset\_method*] :: (input) preset method to compute the eigenpairs at the first stage; see available values at `primme_set_method()`.
- **methodStage2** [*primme\_preset\_method*] :: (input) preset method to compute the eigenpairs with the second stage of `PRIMME_SVDS_hybrid`; see available values at `primme_set_method()`.
- **primme\_svds** [*ptr*] :: (input/output) parameters structure.
- **ierr** [*integer*] :: (output) if 0, successful; if negative, something went wrong.

### 4.3.3 xprimme\_svds

**function** `xprimme_svds` (*svals*, *svecs*, *resNorms*, *primme\_svds*)

Solve a real or complex singular value problem.

All arrays should be hosted on CPU. The computations are performed on CPU (see `magma_xprimme_svds()` for using GPUs).

#### Parameters

- **svals** (\*) [*out*] :: array at least of size `numSvals` to store the computed singular values; all processes in a parallel run return this local array with the same values.
- **svecs** (\*) :: array at least of size  $(mLocal + nLocal)$  times  $(numOrthoConst + numSvals)$  to store column-wise the (local part for this process of the) computed left singular vectors and the right singular vectors.
- **resNorms** (\*) [*out*] :: array at least of size `numSvals` to store the residual norms of the computed triplets; all processes in parallel run return this local array with the same values.
- **primme** [*c\_ptr,in*] :: parameters structure created by `primme_params_create_svds()`.

**Return** `xprimme_svds` [*c\_int*] :: error indicator; see *Error Codes*.

The arrays `svals`, `svecs`, and `resNorms` should have the same kind.

On input, `svecs` should start with the content of the `numOrthoConst` left vectors, followed by the `initSize` left vectors, followed by the `numOrthoConst` right vectors and followed by the `initSize` right vectors.

On return, the *i*-th left singular vector starts at `svecs(( numOrthoConst + i - 1 ) * mLocal )`. The *i*-th right singular vector starts at `svecs(( numOrthoConst + initSize ) * mLocal + ( numOrthoConst + i - 1 ) * nLocal )`. The first vector has *i*=1.

All internal operations are performed at the same precision than `svecs` unless the user sets `internalPrecision` otherwise.

The type and precision of the callbacks depends on the type and precision of `svecs`. See details for `matrixMatvec`, `applyPreconditioner`, `globalSumReal`, `broadcastReal`, and `convTestFun`.

### 4.3.4 magma\_xprimme\_svds

**function magma\_xprimme\_svds** (*svals*, *svecs*, *resNorms*, *primme\_svds*)

Solve a real or complex singular value problem.

Most of the computations are performed on GPU (see `xprimme_svds()` for using only the CPU).

#### Parameters

- **svals** (\*) [*out*] :: CPU array at least of size `numSvals` to store the computed singular values; all processes in a parallel run return this local array with the same values.
- **svecs** (\*) :: GPU array at least of size `(mLocal + nLocal)` times `(numOrthoConst + numSvals)` to store column-wise the (local part for this process of the) computed left singular vectors and the right singular vectors.
- **resNorms** (\*) [*out*] :: CPU array at least of size `numSvals` to store the residual norms of the computed triplets; all processes in parallel run return this local array with the same values.
- **primme** [*c\_ptr*,*in*] :: parameters structure created by `primme_params_create_svds()`.

**Return** `magma_xprimme_svds [c_int]` :: error indicator; see *Error Codes*.

The arrays `svals`, `svecs`, and `resNorms` should have the same kind.

On input, `svecs` should start with the content of the `numOrthoConst` left vectors, followed by the `initSize` left vectors, followed by the `numOrthoConst` right vectors and followed by the `initSize` right vectors.

On return, the *i*-th left singular vector starts at `svecs(( numOrthoConst + i - 1) * mLocal)`. The *i*-th right singular vector starts at `svecs(( numOrthoConst + initSize)* mLocal + ( numOrthoConst + i - 1)* nLocal)`. The first vector has *i*=1.

All internal operations are performed at the same precision than `svecs` unless the user sets `internalPrecision` otherwise.

The type and precision of the callbacks depends on the type and precision of `svecs`. See details for `matrixMatvec`, `applyPreconditioner`, `globalSumReal`, `broadcastReal`, and `convTestFun`.

### 4.3.5 primme\_svds\_params\_destroy

**function primme\_svds\_params\_destroy** (*primme\_svds*)

Free memory allocated by PRIMME associated to a parameters structure created with `primme_svds_params_create()`.

**Parameters** `primme_svds [c_ptr]` :: parameters structure.

**Return** `primme_svds_params_destroy` :: nonzero value if the call is not successful.

### 4.3.6 `primme_svds_set_member`

**function** `primme_svds_set_member` (*primme\_svds*, *label*, *value*)

Set a value in some field of the parameter structure.

#### Parameters

- **`primme_svds`** [*ptr*] :: (input) parameters structure.
- **`label`** [*integer*] :: field where to set value. One of:

`PRIMME_SVDS_primme`  
`PRIMME_SVDS_primmeStage2`  
`PRIMME_SVDS_m`  
`PRIMME_SVDS_n`  
`PRIMME_SVDS_matrixMatvec`  
`PRIMME_SVDS_matrixMatvec_type`  
`PRIMME_SVDS_applyPreconditioner`  
`PRIMME_SVDS_applyPreconditioner_type`  
`PRIMME_SVDS_numProcs`  
`PRIMME_SVDS_procID`  
`PRIMME_SVDS_mLocal`  
`PRIMME_SVDS_nLocal`  
`PRIMME_SVDS_commInfo`  
`PRIMME_SVDS_globalSumReal`  
`PRIMME_SVDS_globalSumReal_type`  
`PRIMME_SVDS_broadcastReal`  
`PRIMME_SVDS_broadcastReal_type`  
`PRIMME_SVDS_numSvals`  
`PRIMME_SVDS_target`  
`PRIMME_SVDS_numTargetShifts`  
`PRIMME_SVDS_targetShifts`  
`PRIMME_SVDS_method`  
`PRIMME_SVDS_methodStage2`  
`PRIMME_SVDS_matrix`  
`PRIMME_SVDS_preconditioner`  
`PRIMME_SVDS_locking`  
`PRIMME_SVDS_numOrthoConst`  
`PRIMME_SVDS_aNorm`  
`PRIMME_SVDS_eps`  
`PRIMME_SVDS_precondition`  
`PRIMME_SVDS_initSize`  
`PRIMME_SVDS_maxBasisSize`  
`PRIMME_SVDS_maxBlockSize`  
`PRIMME_SVDS_maxMatvecs`  
`PRIMME_SVDS_iseed`  
`PRIMME_SVDS_printLevel`  
`PRIMME_SVDS_outputFile`  
`PRIMME_SVDS_internalPrecision`



```

PRIMME_SVDS_convTestFun
PRIMME_SVDS_convTestFun_type
PRIMME_SVDS_convtest
PRIMME_SVDS_monitorFun
PRIMME_SVDS_monitorFun_type
PRIMME_SVDS_monitor
PRIMME_SVDS_queue
PRIMME_SVDS_stats_numOuterIterations
PRIMME_SVDS_stats_numRestarts
PRIMME_SVDS_stats_numMatvecs
PRIMME_SVDS_stats_numPreconds
PRIMME_SVDS_stats_numGlobalSum
PRIMME_SVDS_stats_numBroadcast
PRIMME_SVDS_stats_volumeGlobalSum
PRIMME_SVDS_stats_volumeBroadcast
PRIMME_SVDS_stats_elapsedTime
PRIMME_SVDS_stats_timeMatvec
PRIMME_SVDS_stats_timePrecond
PRIMME_SVDS_stats_timeOrtho
PRIMME_SVDS_stats_timeGlobalSum
PRIMME_SVDS_stats_timeBroadcast
PRIMME_SVDS_stats_lockingIssue

```

- **value** :: (input) value to set. The allowed types are *c\_int64*, *c\_double*, *c\_ptr*, *c\_funptr* and *procedure* (*primme\_svds\_matvec*)

**Return** *primme\_svds\_set\_member* [*c\_int*] :: nonzero value if the call is not successful.

Examples:

```

type(c_ptr) :: primme_svds
integer :: ierr
...

integer(c_int64_t) :: m = 100
ierr = primme_svds_set_member(primme_svds, PRIMME_SVDS_m, m)
ierr = primme_svds_set_member(primme_svds, PRIMME_SVDS_n, m)

real(c_double) :: tol = 1.0D-12
ierr = primme_svds_set_member(primme, PRIMME_SVDS_eps, tol)

integer(c_int64_t), parameter :: numTargetShifts = 2
real(c_double) :: TargetShifts(numTargetShifts) = (/3.0D0, 5.1D0/)
ierr = primme_svds_set_member(primme_svds, PRIMME_SVDS_
↳numTargetShifts, numTargetShifts)
ierr = primme_svds_set_member(primme_svds, PRIMME_SVDS_targetShifts,
↳TargetShifts)

ierr = primme_svds_set_member(primme_svds, PRIMME_SVDS_target, primme_
↳svds_closest_abs)

procedure(primme_svds_matvec) :: MV, ApplyPrecon

```

(continues on next page)

(continued from previous page)

```

ierr = primme_svds_set_member(primme_svds, PRIMME_SVDS_matrixMatvec, u
↪MV)

ierr = primme_svds_set_member(primme_svds, PRIMME_SVDS_
↪applyPreconditioner,
                                c_funloc(ApplyPrecon))

type(c_ptr) :: primme
ierr = primme_svds_get_member(primme_svds, PRIMME_SVDS_primme, primme)
ierr = primme_set_member(primme, PRIMME_correctionParams_precondition,
                        1_c_int64_t)

```

### 4.3.7 primme\_get\_member

**function** `primme_svds_get_member` (*primme*, *label*, *value*)

Get the value in some field of the parameter structure.

#### Parameters

- **primme** [*c\_ptr*,*in*] :: parameters structure created by `primme_svds_params_create()`.
- **label** [*integer*,*in*] :: field where to get value. One of the detailed in function `primme_svds_set_member()`.
- **value** [*out*] :: value of the field. The allowed types are `c_int64`, `c_double`, and `c_ptr`.

**Return** `primme_svds_get_member` [*c\_int*] :: nonzero value if the call is not successful.

Examples:

```

type(c_ptr) :: primme_svds
integer :: ierr
...

integer(c_int64_t) :: m
ierr = primme_svds_get_member(primme_svds, PRIMME_SVDS_m, m)

real(c_double) :: aNorm
ierr = primme_svds_get_member(primme_svds, PRIMME_SVDS_aNorm, aNorm)

type(c_ptr) :: primme
ierr = primme_svds_get_member(primme_svds, PRIMME_SVDS_primme, primme)
ierr = primme_set_member(primme, PRIMME_correctionParams_precondition,
                        1_c_int64_t)

```

## 4.4 Python Interface

`primme.svds(A, k=6, ncv=None, tol=0, which='LM', v0=None, maxiter=None, return_singular_vectors=True, precAHA=None, precAAH=None, precAug=None, u0=None, orthou0=None, orthov0=None, return_stats=False, maxBlockSize=0, method=None, methodStage1=None, methodStage2=None, return_history=False, convtest=None, **kargs)`  
 Compute  $k$  singular values and vectors of the matrix  $A$ .

### Parameters

- **A** (*{sparse matrix, LinearOperator}*) – Array to compute the SVD on, of shape  $(M, N)$
- **k** (*int, optional*) – Number of singular values and vectors to compute. Must be  $1 \leq k < \min(A.shape)$ .
- **ncv** (*int, optional*) – The maximum size of the basis
- **tol** (*float, optional*) – Tolerance for singular values. Zero (default) means  $10^{*4}$  times the machine precision.

A triplet  $(u, \sigma, v)$  is marked as converged when  $(\|A*v - \sigma*u\|^2 + \|A.H*u - \sigma*v\|^2)^{*.5}$  is less than “tol” \*  $\|A\|$ , or close to the minimum tolerance that the method can achieve. See the note.

The value is ignored if convtest is provided.

- **which** (*str ['LM' | 'SM'] or number, optional*) – Which  $k$  singular values to find:
  - ‘LM’ : largest singular values
  - ‘SM’ : smallest singular values
  - number : closest singular values to (referred as sigma later)
- **u0** (*ndarray, optional*) – Initial guesses for the left singular vectors.  
 If only u0 or v0 is provided, the other is computed. If both are provided, u0 and v0 should have the same number of columns.
- **v0** (*ndarray, optional*) – Initial guesses for the right singular vectors.
- **maxiter** (*int, optional*) – Maximum number of matvecs with  $A$  and  $A.H$ .
- **precAHA** (*{N x N matrix, array, sparse matrix, LinearOperator}, optional*) – Approximate inverse of  $(A.H*A - \sigma^{*2}*I)$ . If provided and  $M \geq N$ , it usually accelerates the convergence.
- **precAAH** (*{M x M matrix, array, sparse matrix, LinearOperator}, optional*) – Approximate inverse of  $(A*A.H - \sigma^{*2}*I)$ . If provided and  $M < N$ , it usually accelerates the convergence.
- **precAug** (*{(M+N) x (M+N) matrix, array, sparse matrix, LinearOperator}, optional*) – Approximate inverse of  $([zeros() A.H; zeros() A] - \sigma^{*2}*I)$ .

- **orthou0** (*ndarray, optional*) – Left orthogonal vector constrain.

Seek singular triplets orthogonal to orthou0 and orthov0. The provided vectors *should* be orthonormal. If only orthou0 or orthov0 is provided, the other is computed. Useful to avoid converging to previously computed solutions.

- **orthov0** (*ndarray, optional*) – Right orthogonal vector constrain. See orthou0.

- **maxBlockSize** (*int*, *optional*) – Maximum number of vectors added at every iteration.
- **convtest** (*callable*) – User-defined function to mark an approximate singular triplet as converged.  
The function is called as `convtest(sval, svecleft, svecright, resNorm)` and returns True if the triplet with value *sval*, left vector *svecleft*, right vector *svecright*, and residual norm *resNorm* is considered converged.
- **return\_stats** (*bool*, *optional*) – If True, the function returns extra information (see stats in Returns).
- **return\_history** (*bool*, *optional*) – If True, the function returns performance information at every iteration

### Returns

- **u** (*ndarray*, *shape*=(*M*, *k*), *optional*) – Unitary matrix having left singular vectors as columns. Returned if *return\_singular\_vectors* is True.
- **s** (*ndarray*, *shape*=(*k*,)) – The singular values.
- **vt** (*ndarray*, *shape*=(*k*, *N*), *optional*) – Unitary matrix having right singular vectors as rows. Returned if *return\_singular\_vectors* is True.
- **stats** (*dict*, *optional* (if *return\_stats*)) – Extra information reported by PRIMME:
  - “numOuterIterations”: number of outer iterations
  - “numRestarts”: number of restarts
  - “numMatvecs”: number of matvecs with A and A.H
  - “numPreconds”: cumulative number of applications of `precAHA`, `precAAH` and `precAug`
  - “elapsedTime”: time that took
  - “rnorms”:  $(\|A*v[:,i] - \sigma[i]*u[:,i]\|^2 + \|A.H*u[:,i] - \sigma[i]*v[:,i]\|^2)^{.5}$
  - “hist”: (if *return\_history*) report at every outer iteration of:
    - \* “elapsedTime”: time spent up to now
    - \* “numMatvecs”: number of  $A*v$  and  $A.H*v$  spent up to now
    - \* “nconv”: number of converged triplets
    - \* “sval”: singular value of the first unconverged triplet
    - \* “resNorm”: residual norm of the first unconverged triplet

### Notes

The default method used is the hybrid method, which first solves the equivalent eigenvalue problem  $A.H*A$  or  $A*A.H$  (normal equations) and then refines the solution solving the augmented problem. The minimum tolerance that this method can achieve is  $\|A\|*\epsilon$ , where  $\epsilon$  is the machine precision. However it may not return triplets with singular values smaller than  $\|A\|*\epsilon$  if “tol” is smaller than  $\|A\|*\epsilon/\sigma$ .

This function is a wrapper to PRIMME functions to find singular values and vectors<sup>1</sup>.

---

<sup>1</sup> PRIMME Software, <https://github.com/primme/primme>

## References

See also:

`primme.eigsh()` eigenvalue decomposition for a sparse symmetric/complex Hermitian matrix A

`scipy.sparse.linalg.eigs()` eigenvalues and eigenvectors for a general (nonsymmetric) matrix A

## Examples

```
>>> import primme, scipy.sparse
>>> A = scipy.sparse.spdiags(range(1, 11), [0], 100, 10) # sparse diag. rect.
↳matrix
>>> svecs_left, svals, svecs_right = primme.svds(A, 3, tol=1e-6, which='LM')
>>> svals # the three largest singular values of A
array([10., 9., 8.])

>>> import primme, scipy.sparse, numpy as np
>>> A = scipy.sparse.rand(10000, 100, random_state=10)
>>> prec = scipy.sparse.spdiags(np.reciprocal(A.multiply(A).sum(axis=0)),
...                             [0], 100, 100) # square diag. preconditioner
>>> # the three smallest singular values of A, using preconditioning
>>> svecs_left, svals, svecs_right = primme.svds(A, 3, which='SM', tol=1e-6,
↳precAHA=prec)
>>> ["%.5f" % x for x in svals.flat]
['4.57263', '4.78752', '4.82229']

>>> # Giving the matvecs as functions
>>> import primme, scipy.sparse, numpy as np
>>> Bdiag = np.arange(0, 100).reshape((100,1))
>>> Bdiagr = np.concatenate((np.arange(0, 100).reshape((100,1)).astype(np.
↳float32), np.zeros((100,1), dtype=np.float32)), axis=None).reshape((200,1))
>>> def Bmatmat(x):
...     if len(x.shape) == 1: x = x.reshape((100,1))
...     return np.vstack((Bdiag * x, np.zeros((100, x.shape[1]), dtype=np.
↳float32)))
...
>>> def Brmatmat(x):
...     if len(x.shape) == 1: x = x.reshape((200,1))
...     return (Bdiagr * x)[0:100,:]
...
>>> B = scipy.sparse.linalg.LinearOperator((200,100), matvec=Bmatmat,
↳matmat=Brmatmat, rmatvec=Brmatmat, dtype=np.float32)
>>> svecs_left, svals, svecs_right = primme.svds(B, 5, which='LM', tol=1e-6)
>>> svals
array([99., 98., 97., 96., 95.]
```

## 4.5 MATLAB Interface

**function [varargout] = primme\_svds(varargin)**

`primme_svds()` finds a few singular values and vectors of a matrix  $A$  by calling `PRIMME`.  $A$  is typically large and sparse.

`S = primme_svds(A)` returns a vector with the 6 largest singular values of  $A$ .

`S = primme_svds(AFUN, M, N)` accepts the function handle `AFUN` to perform the matrix vector products with an  $M$ -by- $N$  matrix  $A$ . `AFUN(X, 'notransp')` returns  $A*X$  while `AFUN(X, 'transp')` returns  $A' * X$ . In all the following,  $A$  can be replaced by `AFUN, M, N`.

`S = primme_svds(A, k)` computes the  $k$  largest singular values of  $A$ .

`S = primme_svds(A, k, sigma)` computes the  $k$  singular values closest to the scalar shift `sigma`.

- If `sigma` is a vector, find the singular value  $S(i)$  closest to each  $\text{sigma}(i)$ , for  $i \leq k$ .
- If `sigma` is 'L', it computes the largest singular values.
- if `sigma` is 'S', it computes the smallest singular values.

`S = primme_svds(A, k, sigma, OPTIONS)` specifies extra solver parameters. Some default values are indicated in brackets `{ }`:

- `aNorm`: estimation of the 2-norm of  $A$  {0.0 (estimate the norm internally)}
- `tol`: convergence tolerance  $\text{NORM}([A*V-U*S; A'*U-V*S]) \leq \text{tol} * \text{NORM}(A)$  (see `eps`) { $1e-10$  for double precision and  $1e-3$  for single precision}
- `maxit`: maximum number of matvecs with  $A$  and  $A'$  (see `maxMatVecs`) {inf}
- `p`: maximum basis size (see `maxBasisSize`)
- `reportLevel`: reporting level (0-3) (see `HIST`) {no reporting 0}
- `display`: whether displaying reporting on screen (see `HIST`) {0 if `HIST` provided}
- `isreal`: if 0, the matrix is complex; else it's real {0: complex}
- `isdouble`: if 0, the matrix is single; else it's double {1: double}
- `method`: which equivalent eigenproblem to solve
  - '`primme_svds_normalequations`':  $A' * A$  or  $A * A'$
  - '`primme_svds_augmented`':  $[0 \ A'; A \ 0]$
  - '`primme_svds_hybrid`': first normal equations and then augmented (default)
- `u0`: initial guesses to the left singular vectors (see `initSize`) `{[]}`
- `v0`: initial guesses to the right singular vectors `{[]}`
- `orthoConst`: external orthogonalization constraints (see `numOrthoConst`) `{[]}`
- `locking`: 1, hard locking; 0, soft locking
- `maxBlockSize`: maximum block size
- `iseed`: random seed
- `primme`: options for first stage solver
- `primmeStage2`: options for second stage solver

- `convTestFun`: function handler with an alternative convergence criterion. If `FUN(SVAL, LSVEC, RSVEC, RNORM)` returns a nonzero value, the triplet `(SVAL, LSVEC, RSVEC)` with residual norm `RNORM` is considered converged.

The available options for `OPTIONS.primme` and `primmeStage2` are the same as `primme_eigs()`, plus the option `'method'`.

`S = primme_svds(A, k, sigma, OPTIONS, P)` applies a preconditioner `P` as follows:

- If `P` is a matrix it applies  $P \backslash X$  and  $P' \backslash X$  to approximate  $A \backslash X$  and  $A' \backslash X$ .
- If `P` is a function handle, `PFUN, PFUN(X, 'notransp')` returns  $P \backslash X$  and `PFUN(X, 'transp')` returns  $P' \backslash X$ , approximating  $A \backslash X$  and  $A' \backslash X$  respectively.
- **If `P` is a struct, it can have one or more of the following fields:** `P.AHA \ X` or `P.AHA(X)` returns an approximation of  $(A' * A) \backslash X$ , `P.AAH \ X` or `P.AAH(X)` returns an approximation of  $(A * A') \backslash X$ , `P.aug \ X` or `P.aug(X)` returns an approximation of  $\begin{bmatrix} \text{zeros}(N, N) & A' \\ A & \text{zeros}(M, M) \end{bmatrix} \backslash X$ .
- If `P` is `[]` then no preconditioner is applied.

`S = primme_svds(A, k, sigma, OPTIONS, P1, P2)` applies a factorized preconditioner:

- If both `P1` and `P2` are nonempty, apply  $(P1 * P2) \backslash X$  to approximate  $A \backslash X$ .
- If `P1` is `[]` and `P2` is nonempty, then  $(P2' * P2) \backslash X$  approximates  $A' * A$ . `P2` can be the `R` factor of an (incomplete) QR factorization of `A` or the `L` factor of an (incomplete) `LL'` factorization of  $A' * A$  (RIF).
- If both `P1` and `P2` are `[]` then no preconditioner is applied.

`[U, S, V] = primme_svds(...)` returns also the corresponding singular vectors. If `A` is `M`-by-`N` and `k` singular triplets are computed, then `U` is `M`-by-`k` with orthonormal columns, `S` is `k`-by-`k` diagonal, and `V` is `N`-by-`k` with orthonormal columns.

`[S, R] = primme_svds(...)`

`[U, S, V, R] = primme_svds(...)` returns the residual norm of each `k` triplet, `NORM([A * V(:, i) - S(i, i) * U(:, i); A' * U(:, i) - S(i, i) * V(:, i)])`.

`[U, S, V, R, STATS] = primme_svds(...)` returns how many times `A` and `P` were used and elapsed time. The application of `A` is counted independently from the application of  $A'$ .

`[U, S, V, R, STATS, HIST] = primme_svds(...)` returns the convergence history, instead of printing it. Every row is a record, and the columns report:

- `HIST(:, 1)`: number of matvecs
- `HIST(:, 2)`: time
- `HIST(:, 3)`: number of converged/locked triplets
- `HIST(:, 4)`: stage
- `HIST(:, 5)`: block index
- `HIST(:, 6)`: approximate singular value
- `HIST(:, 7)`: residual norm
- `HIST(:, 8)`: QMR residual norm

`OPTS.reportLevel` controls the granularity of the record. If `OPTS.reportLevel == 1`, `HIST` has one row per converged eigenpair and only the first three columns together with the fifth and the sixth are reported. If `OPTS.reportLevel == 2`, `HIST` has one row per outer iteration and converged value, and only the first six columns are reported. Otherwise `HIST` has one row per QMR iteration, outer iteration and converged value, and all columns are reported.

The convergence history is displayed if `OPTS.reportLevel > 0` and either `HIST` is not returned or `OPTS.display == 1`.

Examples:

```
A = diag(1:50); A(200,1) = 0; % rectangular matrix of size 200x50

s = primme_svds(A,10) % the 10 largest singular values

s = primme_svds(A,10,'S') % the 10 smallest singular values

s = primme_svds(A,10,25) % the 10 closest singular values to 25

opts = struct();
opts.tol = 1e-4; % set tolerance
opts.method = 'primme_svds_normalequations' % set svd solver method
opts.primme.method = 'DEFAULT_MIN_TIME' % set first stage eigensolver method
opts.primme.maxBlockSize = 2; % set block size for first stage
[u,s,v] = primme_svds(A,10,'S',opts); % find 10 smallest svd triplets

opts.orthoConst = {u,v};
[s,rnorms] = primme_svds(A,10,'S',opts) % find another 10

% Compute the 5 smallest singular values of a rectangular matrix using
% Jacobi preconditioner on (A'*A)
A = sparse(diag(1:50) + diag(ones(49,1), 1));
A(200,50) = 1; % size(A)=[200 50]
P = diag(sum(abs(A).^2));
precond.AHA = @(x)P\x;
s = primme_svds(A,5,'S',[],precond) % find the 5 smallest values

% Estimation of the smallest singular value
A = diag([1 repmat(2,1,1000) 3:100]);
[~,sval,~,rnorm] = primme_svds(A,1,'S',struct('convTestFun',@(s,u,v,r)r<s*.1));
sval - rnorm % approximate smallest singular value
```

See also: [MATLAB svds](#), [primme\\_eigs\(\)](#)



## 4.6 Parameter Description

### 4.6.1 primme\_svds\_params

**type primme\_svds\_params**

Structure to set the problem matrix and the solver options.

*PRIMME\_INT* **m**

Number of rows of the matrix.

Input/output:

`primme_svds_initialize()` sets this field to 0;  
this field is read by `dprimme_svds()`.

*PRIMME\_INT* **n**

Number of columns of the matrix.

Input/output:

`primme_svds_initialize()` sets this field to 0;  
this field is read by `dprimme_svds()`.

**void (\*matrixMatvec)** (void \*x, *PRIMME\_INT* ldx, void \*y, *PRIMME\_INT* ldy, int \*blockSize, int \*transpose, *primme\_svds\_params* \*primme\_svds, int \*ierr)

Block matrix-multivector multiplication,  $y = Ax$  if `transpose` is zero, and  $y = A^*x$  otherwise.

#### Parameters

- **x** – input array.
- **ldx** – leading dimension of x.
- **y** – output array.
- **ldy** – leading dimension of y.
- **blockSize** – number of columns in x and y.
- **transpose** – if non-zero, the transpose A should be applied.
- **primme\_svds** – parameters structure.
- **ierr** – output error code; if it is set to non-zero, the current call to PRIMME will stop.

If `transpose` is zero, then x and y are arrays of dimensions *nLocal* x `blockSize` and *mLocal* x `blockSize` respectively. Elsewhere they have dimensions *mLocal* x `blockSize` and *nLocal* x `blockSize`. Both arrays are in **column-major** order (elements in the same column with consecutive row indices are consecutive in memory).

The actual type of x and y matches the type of `evects` of the calling `dprimme_svds()` (or a variant), unless `matrixMatvec_type` sets another precision.

Input/output:

`primme_svds_initialize()` sets this field to NULL;  
this field is read by `dprimme_svds()` and `zprimme_svds()`.

---

**Note:** Integer arguments are passed by reference to make easier the interface to other languages (like Fortran).

---

primme\_op\_datatype **matrixMatvec\_type**

Precision of the vectors  $x$  and  $y$  passed to *matrixMatvec\_type*.

If it is `primme_op_default`, the vectors' type matches the calling *dprimme\_svds()* (or a variant). Otherwise, the precision is half, single, or double, if *matrixMatvec\_type* is `primme_half`, `primme_float` or `primme_double` respectively.

Input/output:

*primme\_svds\_initialize()* sets this field to `primme_op_default`;  
this field is read by *dprimme\_svds()*, and if it is `primme_op_default` it is set to the value that matches the precision of calling function.

New in version 3.0.

void (\***applyPreconditioner**)(void \*x, *PRIMME\_INT* ldx, void \*y, *PRIMME\_INT* ldy, int \*blockSize, int \*mode, *primme\_svds\_params* \*primme\_svds, int \*ierr)

Block preconditioner-multivector application,  $y = M^{-1}x$  for finding singular values close to  $\sigma$ . Depending on mode,  $M$  is expected to be an approximation of the following operators:

- `primme_svds_op_AtA`:  $M \approx A^*Ax - \sigma^2I$ ,
- `primme_svds_op_AAt`:  $M \approx AA^*x - \sigma^2I$ ,
- `primme_svds_op_augmented`:  $M \approx \begin{pmatrix} 0 & A^* \\ A & 0 \end{pmatrix} - \sigma I$ .

#### Parameters

- **x** – input array.
- **ldx** – leading dimension of  $x$ .
- **y** – output array.
- **ldy** – leading dimension of  $y$ .
- **blockSize** – number of columns in  $x$  and  $y$ .
- **mode** – one of `primme_svds_op_AtA`, `primme_svds_op_AAt` or `primme_svds_op_augmented`.
- **primme\_svds** – parameters structure.
- **ierr** – output error code; if it is set to non-zero, the current call to PRIMME will stop.

If mode is `primme_svds_op_AtA`, then  $x$  and  $y$  are arrays of dimensions *nLocal* x `blockSize`; if mode is `primme_svds_op_AAt`, they are *mLocal* x `blockSize`; and otherwise they are (*mLocal* + *nLocal*) x `blockSize`. Both arrays are in *column-major* order (elements in the same column with consecutive row indices are consecutive in memory).

The actual type of  $x$  and  $y$  matches the type of *evecs* of the calling *dprimme\_svds()* (or a variant), unless *matrixMatvec\_type* sets another precision.

Input/output:

*primme\_svds\_initialize()* sets this field to NULL;  
this field is read by *dprimme\_svds()* and *zprimme\_svds()*.

primme\_op\_datatype **applyPreconditioner\_type**

Precision of the vectors  $x$  and  $y$  passed to *applyPreconditioner\_type*.

If it is `primme_op_default`, the vectors' type matches the calling `dprimme_svds()` (or a variant). Otherwise, the precision is half, single, or double, if `applyPreconditioner_type` is `primme_half`, `primme_float` or `primme_double` respectively.

Input/output:

`primme_svds_initialize()` sets this field to `primme_op_default`;  
this field is read by `dprimme_svds()`, and if it is `primme_op_default` it is set to the value that matches the precision of calling function.

New in version 3.0.

#### int numProcs

Number of processes calling `dprimme_svds()` or `zprimme_svds()` in parallel.

Input/output:

`primme_svds_initialize()` sets this field to 1;  
this field is read by `dprimme_svds()` and `zprimme_svds()`.

#### int procID

The identity of the local process within a parallel execution calling `dprimme_svds()` or `zprimme_svds()`. Only the process with id 0 prints information.

Input/output:

`primme_svds_initialize()` sets this field to 0;  
`dprimme_svds()` sets this field to 0 if `numProcs` is 1;  
this field is read by `dprimme_svds()` and `zprimme_svds()`.

#### PRIMME\_INT mLocal

Number of local rows on this process. The value depends on how the matrix and preconditioner is distributed along the processes.

Input/output:

`primme_svds_initialize()` sets this field to -1;  
`dprimme_svds()` sets this field to `m` if `numProcs` is 1;  
this field is read by `dprimme_svds()` and `zprimme_svds()`.

See also: `matrixMatvec` and `applyPreconditioner`.

#### PRIMME\_INT nLocal

Number of local columns on this process. The value depends on how the matrix and preconditioner is distributed along the processes.

Input/output:

`primme_svds_initialize()` sets this field to -1;  
`dprimme_svds()` sets this field to `n` if `numProcs` is 1;  
this field is read by `dprimme_svds()` and `zprimme_svds()`.

#### void \*commInfo

A pointer to whatever parallel environment structures needed. For example, with MPI, it could be a pointer to the MPI communicator. PRIMME does not use this. It is available for possible use in user functions defined in `matrixMatvec`, `applyPreconditioner`, `globalSumReal`, and `broadcastReal`.

Input/output:

`primme_svds_initialize()` sets this field to NULL;

```
void (*globalSumReal)(double *sendBuf, double *recvBuf, int *count, primme_svds_params
                    *primme_svds, int *ierr)
```

Global sum reduction function. No need to set for sequential programs.

#### Parameters

- **sendBuf** – array of size `count` with the local input values.
- **recvBuf** – array of size `count` with the global output values so that the *i*-th element of `recvBuf` is the sum over all processes of the *i*-th element of `sendBuf`.
- **count** – array size of `sendBuf` and `recvBuf`.
- **primme\_svds** – parameters structure.
- **ierr** – output error code; if it is set to non-zero, the current call to PRIMME will stop.

The actual type of `sendBuf` and `recvBuf` depends on which function is being calling. For `dprimme_svds()` and `zprimme_svds()` it is double, and for `sprimme_svds()` and `cprimme_svds()` it is float. Note that `count` is the number of values of the actual type.

Input/output:

`primme_svds_initialize()` sets this field to an internal function;  
`dprimme_svds()` sets this field to an internal function if `numProcs` is 1 and `globalSumReal` is NULL;  
this field is read by `dprimme_svds()` and `zprimme_svds()`.

When MPI is used, this can be a simply wrapper to `MPI_Allreduce()` as shown below:

```
void par_GlobalSumForDouble(void *sendBuf, void *recvBuf, int *count,
                           primme_svds_params *primme_svds, int *ierr) {
    MPI_Comm communicator = *(MPI_Comm *) primme_svds->commInfo;
    if (sendBuf == recvBuf) {
        *ierr = MPI_Allreduce(MPI_IN_PLACE, recvBuf, *count, MPIU_REAL, MPI_SUM,
        ↪communicator) != MPI_SUCCESS;
    } else {
        *ierr = MPI_Allreduce(sendBuf, recvBuf, *count, MPIU_REAL, MPI_SUM,
        ↪communicator) != MPI_SUCCESS;
    }
}
```

When calling `sprimme_svds()` and `cprimme_svds()` replace `MPI_DOUBLE` by `MPI_FLOAT`.

`primme_op_datatype` **globalSumReal\_type**

Precision of the vectors `sendBuf` and `recvBuf` passed to `globalSumReal`.

If it is `primme_op_default`, the vectors' type matches the calling `dprimme_svds()` (or a variant). Otherwise, the precision is half, single, or double, if `globalSumReal_type` is `primme_half`, `primme_float` or `primme_double` respectively.

Input/output:

`primme_svds_initialize()` sets this field to `primme_op_default`;  
this field is read by `dprimme_svds()`, and if it is `primme_op_default` it is set to the value that matches the precision of calling function.

New in version 3.0.

```
void (*broadcastReal)(void *buffer, int *count, primme_svds_params *primme_svds, int *ierr)
```

Broadcast function from process with ID zero. It is optional in parallel executions, and not needed for sequential programs.

**Parameters**

- **buffer** – array of size `count` with the local input values.
- **count** – array size of `sendBuf` and `recvBuf`.
- **primme\_svds** – parameters structure.
- **ierr** – output error code; if it is set to non-zero, the current call to PRIMME will stop.

The actual type of `buffer` matches the type of `svecs` of the calling `dprimme_svds()` (or a variant), unless `globalSumReal_type` sets another precision.

Input/output:

`primme_svds_initialize()` sets this field to NULL;  
this field is read by `dprimme_svds()`.

When MPI is used, this can be a simply wrapper to `MPI_Bcast()` as shown below:

```
void broadcastForDouble(void *buffer, int *count,
                       primme_svds_params *primme_svds, int *ierr) {
    MPI_Comm communicator = *(MPI_Comm *) primme_svds->commInfo;
    if (MPI_Bcast(buffer, *count, MPI_DOUBLE, 0 /* root */,
                  communicator) == MPI_SUCCESS) {
        *ierr = 0;
    } else {
        *ierr = 1;
    }
}
```

When calling `sprimme_svds()` and `cprimme_svds()` replace `MPI_DOUBLE` by `MPI_FLOAT`.

New in version 3.0.

**int numSvals**

Number of singular triplets wanted.

Input/output:

`primme_svds_initialize()` sets this field to 1;  
this field is read by `primme_svds_set_method()` (see *Preset Methods*) and  
`dprimme_svds()`.

**primme\_op\_datatype broadcastReal\_type**

Precision of the vector `buffer` passed to `broadcastReal`.

If it is `primme_op_default`, the vectors' type matches the calling `dprimme_svds()` (or a variant). Otherwise, the precision is half, single, or double, if `broadcastReal_type` is `primme_half`, `primme_float` or `primme_double` respectively.

Input/output:

`primme_svds_initialize()` sets this field to `primme_op_default`;  
this field is read by `dprimme_svds()`, and if it is `primme_op_default` it is set to the  
value that matches the precision of calling function.

New in version 3.0.

**primme\_op\_datatype internalPrecision**

Internal working precision.

If it is `primme_op_default`, most of the vectors are stored with the same precision as the calling `dprimme_svds()` (or a variant), and most of the computations are done in that precision too. Otherwise,

the working precision is changed to half, single, or double, if *internalPrecision* is *primme\_half*, *primme\_float* or *primme\_double* respectively.

Input/output:

*primme\_svds\_initialize()* sets this field to *primme\_op\_default*;  
this field is read by *dprimme\_svds()*.

New in version 3.0.

**primme\_svds\_target target**

Which singular values to find:

**primme\_svds\_smallest** Smallest singular values; *targetShifts* is ignored.

**primme\_svds\_largest** Largest singular values; *targetShifts* is ignored.

**primme\_svds\_closest\_abs** Closest in absolute value to the shifts in *targetShifts*.

Input/output:

*primme\_svds\_initialize()* sets this field to *primme\_svds\_smallest*;  
this field is read by *dprimme\_svds()* and *zprimme\_svds()*.

**int numTargetShifts**

Size of the array *targetShifts*. Used only when *target* is *primme\_svds\_closest\_abs*. The default values is 0.

Input/output:

*primme\_svds\_initialize()* sets this field to 0;  
this field is read by *dprimme\_svds()* and *zprimme\_svds()*.

**double \*targetShifts**

Array of shifts, at least of size *numTargetShifts*. Used only when *target* is *primme\_svds\_closest\_abs*.

Singular values are computed in order so that the *i*-th singular value is the closest to the *i*-th shift. If *numTargetShifts* < *numSvals*, the last shift given is used for all the remaining *i*'s.

Input/output:

*primme\_svds\_initialize()* sets this field to NULL;  
this field is read by *dprimme\_svds()* and *zprimme\_svds()*.

---

**Note:** Eventually this is used by *dprimme\_svds()* and *zprimme\_svds()*. Please see considerations of *targetShifts*.

---

**int printLevel**

The level of message reporting from the code. All output is written in *outputFile*.

One of:

- 0: silent.
- 1: print some error messages when these occur.
- 2: as in 1, and info about targeted singular triplets when they are marked as converged:

*#Converged \$1 sval[ \$2 ]= \$3 norm \$4 Mvecs \$5 Time \$7 stage \$10*

or locked:

```
#Lock triplet[ $1 ]= $3 norm $4 Mvecs $5 Time $7 stage $10
```

- 3: as in 2, and info about targeted singular triplets every outer iteration:

```
OUT $6 conv $1 blk $8 MV $5 Sec $7 SV $3 |r| $4 stage $10
```

Also, if using `PRIMME_DYNAMIC`, show JDQMR/GD+k performance ratio and the current method in use.

- 4: as in 3, and info about targeted singular triplets every inner iteration:

```
INN MV $5 Sec $7 Sval $3 Lin|r| $9 SV|r| $4 stage $10
```

- 5: as in 4, and verbose info about certain choices of the algorithm.

Output key:

\$1: Number of converged triplets up to now.  
 \$2: The index of the triplet currently converged.  
 \$3: The singular value.  
 \$4: Its residual norm.  
 \$5: The current number of matrix-vector products.  
 \$6: The current number of outer iterations.  
 \$7: The current elapsed time.  
 \$8: Index within the block of the targeted triplet.  
 \$9: QMR norm of the linear system residual.  
 \$10: stage (1 or 2)

In parallel programs, when `printLevel` is 0 to 4 only `procID` 0 produces output. For `printLevel` 5 output can be produced in any of the parallel calls.

Input/output:

`primme_svds_initialize()` sets this field to 1;  
 this field is read by `dprimme_svds()` and `zprimme_svds()`.

---

**Note:** Convergence history for plotting may be produced simply by:

```
grep OUT outpufile | awk '{print $8" "$14}' > out
grep INN outpufile | awk '{print $3" "$11}' > inn
```

Or in gnuplot:

```
plot 'out' w lp, 'inn' w lp
```

---

double **aNorm**

An estimate of the 2-norm of  $A$ , which is used in the default convergence criterion (see [eps](#)).

If `aNorm` is less than or equal to 0, the code uses the largest absolute Ritz value seen. On return, `aNorm` is then replaced with that value.

Input/output:

`primme_svds_initialize()` sets this field to 0.0;

this field is read and written by `dprimme_svds()` and `zprimme_svds()`.

**double eps**

If `convTestFun` is NULL, a triplet  $(u, \sigma, v)$  is marked as converged when  $\sqrt{\|Av - \sigma u\|^2 + \|A^*u - \sigma v\|^2}$  is less than `eps * aNorm`, or close to the minimum tolerance that the selected method can achieve in the given machine precision. See *Preset Methods*.

The default value is machine precision times  $10^4$ .

Input/output:

`primme_svds_initialize()` sets this field to 0.0;  
this field is read by `dprimme_svds()` and `zprimme_svds()`.

**FILE \*outputFile**

Opened file to write down the output.

Input/output:

`primme_svds_initialize()` sets this field to the standard output;  
this field is read by `dprimme_svds()`, `zprimme_svds()` and  
`primme_svds_display_params()`

**int locking**

If set to 1, the underneath eigensolvers will use hard locking. See *locking*.

Input/output:

`primme_svds_initialize()` sets this field to -1;  
written by `primme_svds_set_method()` (see *Preset Methods*);  
this field is read by `dprimme_svds()` and `zprimme_svds()`.

**int initSize**

On input, the number of initial vector guesses provided in `svecs` argument in `dprimme_svds()` and `zprimme_svds()`.

On output, `initSize` holds the number of converged triplets. Without *locking* all `numSvals` approximations are in `svecs` but only the first `initSize` are converged.

During execution, it holds the current number of converged triplets.

Input/output:

`primme_svds_initialize()` sets this field to 0;  
this field is read and written by `dprimme_svds()` and `zprimme_svds()`.

**int numOrthoConst**

Number of vectors to be used as external orthogonalization constraints. The left and the right vector constraints are provided as input of the `svecs` argument in `sprimme_svds()` or other variant, and must be orthonormal.

PRIMME SVDS finds new triplets orthogonal to these constraints (equivalent to solving the problem  $(I - UU^*)A(I - VV^*)$  where  $U$  and  $V$  are the given left and right constraint vectors). This is a handy feature if some singular triplets are already known, or for finding more triplets after a call to `dprimme_svds()` or `zprimme_svds()`, possibly with different parameters (see an example in `TEST/exsvd_zseq.c`).

Input/output:

`primme_svds_initialize()` sets this field to 0;  
this field is read by `dprimme_svds()` and `zprimme_svds()`.



**int `maxBasisSize`**

The maximum basis size allowed in the main iteration. This has memory implications.

Input/output:

`primme_svds_initialize()` sets this field to 0;  
 this field is read and written by `primme_svds_set_method()` (see *Preset Methods*);  
 this field is read by `dprimme_svds()` and `zprimme_svds()`.

**int `maxBlockSize`**

The maximum block size the code will try to use.

The user should set this based on the architecture specifics of the target computer, as well as any a priori knowledge of multiplicities. The code does *not* require that `maxBlockSize` > 1 to find multiple triplets. For some methods, keeping to 1 yields the best overall performance.

Input/output:

`primme_svds_initialize()` sets this field to 1;  
 this field is read and written by `primme_svds_set_method()` (see *Preset Methods*);  
 this field is read by `dprimme_svds()` and `zprimme_svds()`.

***PRIMME\_INT* `maxMatvecs`**

Maximum number of matrix vector multiplications (approximately half the number of preconditioning operations) that the code is allowed to perform before it exits.

Input/output:

`primme_svds_initialize()` sets this field to `INT_MAX`;  
 this field is read by `dprimme_svds()` and `zprimme_svds()`.

***PRIMME\_INT* `iseed`**

The `PRIMME_INT iseed[4]` is an array with the seeds needed by the **LAPACK** `dlarnv` and `zlarnv`.

The default value is an array with values -1, -1, -1 and -1. In that case, `iseed` is set based on the value of `procID` to avoid every parallel process generating the same sequence of pseudorandom numbers.

Input/output:

`primme_svds_initialize()` sets this field to [-1, -1, -1, -1];  
 this field is read and written by `dprimme_svds()` and `zprimme_svds()`.

**void `*matrix`**

This field may be used to pass any required information in the matrix-vector product `matrixMatvec`.

Input/output:

`primme_svds_initialize()` sets this field to `NULL`;

**void `*preconditioner`**

This field may be used to pass any required information in the preconditioner function `applyPreconditioner`.

Input/output:

`primme_svds_initialize()` sets this field to `NULL`;

**int `precondition`**

Set to 1 to use preconditioning. Make sure `applyPreconditioner` is not `NULL` then!

Input/output:

`primme_svds_initialize()` sets this field to 0;  
 this field is read and written by `primme_svds_set_method()` (see *Preset Methods*);

this field is read by `dprimme_svds()` and `zprimme_svds()`.

#### `primme_svds_op_operator` **method**

Select the equivalent eigenvalue problem that will be solved:

- `primme_svds_op_AtA`:  $A^*Ax = \sigma^2x$ ,
- `primme_svds_op_AAt`:  $AA^*x = \sigma^2x$ ,
- `primme_svds_op_augmented`:  $\begin{pmatrix} 0 & A^* \\ A & 0 \end{pmatrix}x = \sigma x$ .

The options for this solver are stored in `primme`.

Input/output:

`primme_svds_initialize()` sets this field to `primme_svds_op_none`;  
this field is read and written by `primme_svds_set_method()` (see *Preset Methods*);  
this field is read by `dprimme_svds()` and `zprimme_svds()`.

#### `primme_svds_op_operator` **methodStage2**

Select the equivalent eigenvalue problem that will be solved to refine the solution. The allowed options are `primme_svds_op_none` to not refine the solution and `primme_svds_op_augmented` to refine the solution by solving the augmented problem with the current solution as the initial vectors. See *method*.

The options for this solver are stored in `primmeStage2`.

Input/output:

`primme_svds_initialize()` sets this field to `primme_svds_op_none`;  
this field is read and written by `primme_svds_set_method()` (see *Preset Methods*);  
this field is read by `dprimme_svds()` and `zprimme_svds()`.

#### `primme_params` **primme**

Parameter structure storing the options for underneath eigensolver that will be called at the first stage. See *method*.

Input/output:

`primme_svds_initialize()` initialize this structure;  
this field is read and written by `primme_svds_set_method()` (see *Preset Methods*);  
this field is read and written by `dprimme_svds()` and `zprimme_svds()`.

#### `primme_params` **primmeStage2**

Parameter structure storing the options for underneath eigensolver that will be called at the second stage. See *methodStage2*.

Input/output:

`primme_svds_initialize()` initialize this structure;  
this field is read and written by `primme_svds_set_method()` (see *Preset Methods*);  
this field is read and written by `dprimme_svds()` and `zprimme_svds()`.

`void (*convTestFun)(double *sval, void *leftsvec, void *rightsvec, double *rNorm, int *isconv, primme_svds_params *primme_svds, int *ierr)`

Function that evaluates if the approximate triplet has converged. If NULL, it is used the default convergence criteria (see *eps*).

#### **Parameters**

- `sval` – the approximate singular value to evaluate.

- **leftsvec** – one dimensional array of size *mLocal* containing the approximate left singular vector; it can be NULL.
- **rightsvec** – one dimensional array of size *nLocal* containing the approximate right singular vector; it can be NULL.
- **resNorm** – the norm of the residual vector.
- **isconv** – (output) the function sets zero if the pair is not converged and non zero otherwise.
- **primme\_svds** – parameters structure.
- **ierr** – output error code; if it is set to non-zero, the current call to PRIMME will stop.

The actual type of **leftsvec** and **rightsvec** matches the type of **svecs** of the calling *dprimme\_svds()* (or a variant), unless *convTestFun\_type* sets another precision.

**Warning:** When solving the augmented problem (for the method *primme\_svds\_augmented* and at the second stage in the method *primme\_svds\_hybrid*), the given residual vector norm **resNorm** is an approximation of the actual residual. Also **leftsvec** and **rightsvec** may not have length 1.

Input/output:

*svds\_primme\_initialize()* sets this field to NULL;  
this field is read and written by *dprimme\_svds()*.

**primme\_op\_datatype convTestFun\_type**

Precision of the vectors **leftsvec** and **rightsvec** passed to *convTestFun*.

If it is *primme\_op\_default*, the type matches the calling *dprimme\_svds()* (or a variant). Otherwise, the precision is half, single, or double, if *convTestFun\_type* is *primme\_half*, *primme\_float* or *primme\_double* respectively.

Input/output:

*primme\_svds\_initialize()* sets this field to *primme\_op\_default*;  
this field is read by *dprimme\_svds()*, and if it is *primme\_op\_default* it is set to the value that matches the precision of calling function.

New in version 3.0.

**void \*convtest**

This field may be used to pass any required information to the function *convTestFun*.

Input/output:

*primme\_svds\_initialize()* sets this field to NULL;

**void (\*monitorFun)** (void \*basisSvals, int \*basisSize, int \*basisFlags, int \*iblock, int \*blockSize, void \*basisNorms, int \*numConverged, void \*lockedSvals, int \*numLocked, int \*lockedFlags, void \*lockedNorms, int \*inner\_its, void \*LSRes, **const** char \*msg, double \*time, *primme\_event* \*event, int \*stage, *primme\_svds\_params* \*primme\_svds, int \*ierr)

Convergence monitor. Used to customize how to report solver information during execution (stage, iteration number, matvecs, time, residual norms, targets, etc).

**Parameters**

- **basisSvals** – array with approximate singular values of the basis.

- **basisSize** – size of the arrays `basisSvals`, `basisFlags` and `basisNorms`.
- **basisFlags** – state of every approximate triplet in the basis.
- **iblock** – indices of the approximate triplet in the block.
- **blockSize** – size of array `iblock`.
- **basisNorms** – array with residual norms of the triplets in the basis.
- **numConverged** – number of triplets converged in the basis plus the number of the locked triplets (note that this value isn't monotonic).
- **lockedSvals** – array with the locked triplets.
- **numLocked** – size of the arrays `lockedSvals`, `lockedFlags` and `lockedNorms`.
- **lockedFlags** – state of each locked triplets.
- **lockedNorms** – array with residual norms of the locked triplets.
- **inner\_its** – number of performed QMR iterations in the current correction equation.
- **LSRes** – residual norm of the linear system at the current QMR iteration.
- **msg** – output message or function name.
- **time** – time duration.
- **event** – event reported.
- **stage** – 0 for first stage, 1 for second stage.
- **primme\_svds** – parameters structure; the counter in `stats` are updated with the current number of matrix-vector products, iterations, elapsed time, etc., since start.
- **ierr** – output error code; if it is set to non-zero, the current call to PRIMME will stop.

This function is called at the next events:

- `*event == primme_event_outer_iteration`: every outer iterations.

It is provided `basisSvals`, `basisSize`, `basisFlags`, `iblock` and `blockSize`.

`basisNorms[iblock[i]]` has the residual norms for the selected triplets in the block. PRIMME avoids computing the residual of soft-locked triplets, `basisNorms[i]` for `i < iblock[0]`. So those values may correspond to previous iterations. The values `basisNorms[i]` for `i > iblock[blockSize-1]` are not valid.

If *locking* is enabled, `lockedSvals`, `numLocked`, `lockedFlags` and `lockedNorms` are also provided.

`inner_its` and `LSRes` are not provided.

- `*event == primme_event_inner_iteration`: every QMR iteration.

`basisSvals[0]` and `basisNorms[0]` provides the approximate singular value and the residual norm of the triplet which is improved in the current correction equation. If *convTest* is *primme\_adaptive* or *primme\_adaptive\_ETolerance*, `basisSvals[0]`, and `basisNorms[0]` are updated every QMR iteration.

`inner_its` and `LSRes` are also provided.

`lockedSvals`, `numLocked`, `lockedFlags`, and `lockedNorms` may not be provided.

- `*event == primme_event_converged`: a new triplet in the basis passed the convergence criterion

`iblock[0]` is the index of the newly converged triplet in the basis which will be locked or soft locked. The following are provided: `basisSvals`, `basisSize`, `basisFlags` and `blockSize[0]==1`.

`lockedSvals`, `numLocked`, `lockedFlags` and `lockedNorms` may not be provided.

`inner_its` and `LSRes` are not provided.

- `*event == primme_event_locked`: a new triplet added to the locked singular vectors.

`lockedSvals`, `numLocked`, `lockedFlags` and `lockedNorms` are provided. The last element of `lockedSvals`, `lockedFlags` and `lockedNorms` corresponds to the recent locked triplet.

`basisSvals`, `numConverged`, `basisFlags` and `basisNorms` may not be provided.

`inner_its` and `LSRes` are not provided.

- `*event == primme_event_message`: output message

`msg` is the message to print.

The rest of the arguments are not provided.

The values of `basisFlags` and `lockedFlags` are:

- 0: unconverged.
- 1: internal use; only in `basisFlags`.
- 2: passed convergence test (see [eps](#)).
- 3: converged because the solver may not be able to reduce the residual norm further.

The actual type of `basisEvals`, `basisNorms`, `lockedEvals`, `lockedNorms` and `LSRes` matches the type of `evects` of the calling `dprimme_svds()` (or a variant), unless `monitorFun_type` sets another precision.

Input/output:

`primme_svds_initialize()` sets this field to NULL;  
`dprimme_svds()` sets this field to an internal function if it is NULL;  
 this field is read by `dprimme_svds()` and `zprimme_svds()`.

Changed in version 3.0.

#### `primme_op_datatype` **monitorFun\_type**

Precision of the vectors `basisEvals`, `basisNorms`, `lockedEvals`, `lockedNorms` and `LSRes` passed to `monitorFun`.

If it is `primme_op_default`, the vectors' type matches the calling `dprimme_svds()` (or a variant). Otherwise, the precision is half, single, or double, if `monitorFun_type` is `primme_half`, `primme_float` or `primme_double` respectively.

Input/output:

`primme_svds_initialize()` sets this field to `primme_op_default`;  
 this field is read by `dprimme_svds()`, and if it is `primme_op_default` it is set to the value that matches the precision of calling function.

New in version 3.0.

#### `void *monitor`

This field may be used to pass any required information to the function `monitorFun`.

Input/output:

*primme\_svds\_initialize()* sets this field to NULL;

**PRIMME\_INT stats.numOuterIterations**

Hold the number of outer iterations.

Input/output:

*primme\_svds\_initialize()* sets this field to 0;  
written by *dprimme\_svds()* and *zprimme\_svds()*.

**PRIMME\_INT stats.numRestarts**

Hold the number of restarts.

Input/output:

*primme\_svds\_initialize()* sets this field to 0;  
written by *dprimme\_svds()* and *zprimme\_svds()*.

**PRIMME\_INT stats.numMatvecs**

Hold how many vectors the operator in *matrixMatvec* has been applied on.

Input/output:

*primme\_svds\_initialize()* sets this field to 0;  
written by *dprimme\_svds()* and *zprimme\_svds()*.

**PRIMME\_INT stats.numPreconds**

Hold how many vectors the operator in *applyPreconditioner* has been applied on.

Input/output:

*primme\_svds\_initialize()* sets this field to 0;  
written by *dprimme\_svds()* and *zprimme\_svds()*.

**PRIMME\_INT stats.numGlobalSum**

Hold how many times *globalSumReal* has been called. The value is available during execution and at the end.

Input/output:

*primme\_svds\_initialize()* sets this field to 0;  
written by *dprimme\_svds()*.

New in version 3.0.

**double stats.volumeGlobalSum**

Hold how many REAL have been reduced by *globalSumReal*. The value is available during execution and at the end.

Input/output:

*primme\_svds\_initialize()* sets this field to 0;  
written by *dprimme\_svds()*.

New in version 3.0.

**PRIMME\_INT stats.numBroadcast**

Hold how many times *broadcastReal* has been called. The value is available during execution and at the end.

Input/output:

*primme\_svds\_initialize()* sets this field to 0;  
written by *dprimme\_svds()*.

New in version 3.0.

`double stats.volumeBroadcast`

Hold how many REAL have been broadcast by *broadcastReal*. The value is available during execution and at the end.

Input/output:

*primme\_svds\_initialize()* sets this field to 0;  
written by *dprimme\_svds()*.

New in version 3.0.

*PRIMME\_INT* `stats.numOrthoInnerProds`

Hold how many inner products with vectors of length *mLocal* and *nLocal* have been computed during orthogonalization. The value is available during execution and at the end.

Input/output:

*primme\_svds\_initialize()* sets this field to 0;  
written by *dprimme\_svds()*.

New in version 3.0.

`double stats.elapsedTime`

Hold the wall clock time spent by the call to *dprimme\_svds()* or *zprimme\_svds()*.

Input/output:

*primme\_svds\_initialize()* sets this field to 0;  
written by *dprimme\_svds()* and *zprimme\_svds()*.

`double stats.timeMatvec`

Hold the wall clock time spent by *matrixMatvec*. The value is available at the end of the execution.

Input/output:

*primme\_svds\_initialize()* sets this field to 0;  
written by *dprimme\_svds()*.

New in version 3.0.

`double stats.timePrecond`

Hold the wall clock time spent by *applyPreconditioner*. The value is available at the end of the execution.

Input/output:

*primme\_svds\_initialize()* sets this field to 0;  
written by *dprimme\_svds()*.

New in version 3.0.

`double stats.timeOrtho`

Hold the wall clock time spent by orthogonalization. The value is available at the end of the execution.

Input/output:

*primme\_svds\_initialize()* sets this field to 0;  
written by *dprimme\_svds()*.

New in version 3.0.

`double stats.timeGlobalSum`

Hold the wall clock time spent by *globalSumReal*. The value is available at the end of the execution.

Input/output:

*primme\_svds\_initialize()* sets this field to 0;  
written by *dprimme\_svds()*.

New in version 3.0.

`double stats.timeBroadcast`

Hold the wall clock time spent by *broadcastReal*. The value is available at the end of the execution.

Input/output:

*primme\_svds\_initialize()* sets this field to 0;  
written by *dprimme\_svds()*.

New in version 3.0.

*PRIMME\_INT* `stats.lockingIssue`

It is set to a nonzero value if some of the returned triplets do not pass the convergence criterion. See *convTestFun* and *eps*.

Input/output:

*primme\_svds\_initialize()* sets this field to 0;  
written by *dprimme\_svds()*.

New in version 3.0.

`void *queue`

Pointer to the accelerator's data structure.

If the main call is *dprimme\_svds\_magma()* or a variant, this field should have the pointer to an initialized *magma\_queue\_t*.

See example *examples/ex\_svds\_dmagma.c*.

Input/output:

*primme\_svds\_initialize()* sets this field to NULL;  
this field is read by *dprimme\_svds\_magma()*.

New in version 3.0.



## 4.7 Preset Methods

**enum primme\_svds\_preset\_method**

**enumerator primme\_svds\_default**

Set as `primme_svds_hybrid`.

**enumerator primme\_svds\_normalequations**

Solve the equivalent eigenvalue problem  $A^*AV = \Sigma^2V$  and computes  $U$  by normalizing the vectors  $AV$ . If  $m$  is smaller than  $n$ ,  $AA^*$  is solved instead.

With `primme_svds_normalequations` `primme_svds_set_method()` sets `method` to `primme_svds_op_AtA` if  $m$  is larger or equal than  $n$ , and to `primme_svds_op_AAAt` otherwise; and `methodStage2` is set to `primme_svds_op_none`.

The minimum residual norm that this method can achieve is  $\|A\|\epsilon\sigma^{-1}$ , where  $\epsilon$  is the machine precision and  $\sigma$  the required singular value.

**enumerator primme\_svds\_augmented**

Solve the equivalent eigenvalue problem  $\begin{pmatrix} 0 & A^* \\ A & 0 \end{pmatrix} X = \sigma X$  with  $X = \begin{pmatrix} V \\ U \end{pmatrix}$ .

With `primme_svds_augmented` `primme_svds_set_method()` sets `method` to `primme_svds_op_augmented` and `methodStage2` to `primme_svds_op_none`.

The minimum residual norm that this method can achieve is  $\|A\|\epsilon$ , where  $\epsilon$  is the machine precision. However it may not return triplets with singular values smaller than  $\|A\|\epsilon$ .

**enumerator primme\_svds\_hybrid**

First solve the equivalent normal equations (see `primme_svds_normalequations`) and then refine the solution solving the augmented problem (see `primme_svds_augmented`).

With `primme_svds_normalequations` `primme_svds_set_method()` sets `method` to `primme_svds_op_AtA` if  $m$  is larger or equal than  $n$ , and to `primme_svds_op_AAAt` otherwise; and `methodStage2` is set to `primme_svds_op_augmented`.

The minimum residual norm that this method can achieve is  $\|A\|\epsilon$ , where  $\epsilon$  is the machine precision. However it may not return triplets with singular values smaller than  $\|A\|\epsilon$  if `eps` is smaller than  $\|A\|\epsilon\sigma^{-1}$ .

## 4.8 Error Codes

The functions `dprimme_svds()` and `zprimme_svds()` return one of the following error codes. Some of the error codes have a macro associated which is indicated in brackets.

- 0: success; usually all requested singular triplets have converged.
- -1: (PRIMME\_UNEXPECTED\_FAILURE) unexpected internal error; please consider to set `printLevel` to a value larger than 0 to see the call stack and to report these errors because they may be bugs.
- -2: (PRIMME\_MALLOC\_FAILURE) failure in allocating memory; it can be either CPU or GPU.
- -3: (PRIMME\_MAIN\_ITER\_FAILURE) maximum number of matvecs `maxMatvecs` reached.
- -4: `primme_svds` is NULL.
- -5: Wrong value for `m` or `n` or `mLocal` or `nLocal`.
- -6: Wrong value for `numProcs`.
- -7: `matrixMatvec` is not set.
- -8: `applyPreconditioner` is not set but `precondition == 1`.
- -9: `numProcs > 1` but `globalSumReal` is not set.
- -10: Wrong value for `numSvals`, it's larger than  $\min(m, n)$ .
- -11: Wrong value for `numSvals`, it's smaller than 1.
- -13: Wrong value for `target`.
- -14: Wrong value for `method`.
- -15: Not supported combination of method and `methodStage2`.
- -16: Wrong value for `printLevel`.
- -17: `svals` is not set.
- -18: `svecs` is not set.
- -19: `resNorms` is not set.
- -40: (PRIMME\_LAPACK\_FAILURE) some LAPACK function performing a factorization returned an error code; set `printLevel > 0` to see the error code and the call stack.
- -41: (PRIMME\_USER\_FAILURE) some of the user-defined functions (`matrixMatvec`, `applyPreconditioner`, ...) returned a non-zero error code; set `printLevel > 0` to see the call stack that produced the error.
- -42: (PRIMME\_ORTHO\_CONST\_FAILURE) the provided orthogonal constraints (see `numOrthoConst`) are not full rank.
- -43: (PRIMME\_PARALLEL\_FAILURE) some process has a different value in an input option than the process zero, or it is not acting coherently; set `printLevel > 0` to see the call stack that produced the error.
- -44: (PRIMME\_FUNCTION\_UNAVAILABLE) PRIMME was not compiled with support for the requesting precision or for GPUs.
- -100 up to -199: eigensolver error from first stage; see the value plus 100 in *Error Codes*.
- -200 up to -299: eigensolver error from second stage; see the value plus 200 in *Error Codes*.

## INDICES

- `genindex`
- `search`



## BIBLIOGRAPHY

- [r1] A. Stathopoulos and J. R. McCombs *PRIMME: PReconditioned Iterative MultiMethod Eigensolver: Methods and software description*, ACM Transaction on Mathematical Software Vol. 37, No. 2, (2010), 21:1-21:30.
- [r6] L. Wu, E. Romero and A. Stathopoulos, *PRIMME\_SVDS: A High-Performance Preconditioned SVD Solver for Accurate Large-Scale Computations*, J. Sci. Comput., Vol. 39, No. 5, (2017), S248–S271.
- [r2] A. Stathopoulos, *Nearly optimal preconditioned methods for Hermitian eigenproblems under limited memory. Part I: Seeking one eigenvalue*, SIAM J. Sci. Comput., Vol. 29, No. 2, (2007), 481–514.
- [r3] A. Stathopoulos and J. R. McCombs, *Nearly optimal preconditioned methods for Hermitian eigenproblems under limited memory. Part II: Seeking many eigenvalues*, SIAM J. Sci. Comput., Vol. 29, No. 5, (2007), 2162-2188.
- [r4] J. R. McCombs and A. Stathopoulos, *Iterative Validation of Eigensolvers: A Scheme for Improving the Reliability of Hermitian Eigenvalue Solvers*, SIAM J. Sci. Comput., Vol. 28, No. 6, (2006), 2337-2358.
- [r5] A. Stathopoulos, *Locking issues for finding a large number of eigenvectors of Hermitian matrices*, Tech Report: WM-CS-2005-03, July, 2005.
- [r7] L. Wu and A. Stathopoulos, *A Preconditioned Hybrid SVD Method for Computing Accurately Singular Triplets of Large Matrices*, SIAM J. Sci. Comput. 37-5(2015), pp. S365-S388.



## C

c\_ptr (fortran type), 37  
 cprimme (C function), 18  
 cprimme\_f77 () (fortran subroutine), 26  
 cprimme\_normal (C function), 20  
 cprimme\_normal\_f77 () (fortran subroutine), 30  
 cprimme\_svds (C function), 82  
 cprimme\_svds\_f77 () (fortran subroutine), 87

## D

dprimme (C function), 18  
 dprimme\_f77 () (fortran subroutine), 27  
 dprimme\_svds (C function), 82  
 dprimme\_svds\_f77 () (fortran subroutine), 88

## E

eigsh () (in module primme), 44

## H

hprimme (C function), 18  
 hprimme\_svds (C function), 82  
 hsprimme (C function), 18  
 hsprimme\_svds (C function), 82

## I

interior problem, 58, 114

## K

kcprimme\_normal (C function), 20  
 kprimme (C function), 18  
 kprimme\_normal (C function), 20  
 kprimme\_svds (C function), 82  
 ksprimme (C function), 18  
 ksprimme\_svds (C function), 82

## M

magma\_cprimme (C function), 19  
 magma\_cprimme\_f77 () (fortran subroutine), 28  
 magma\_cprimme\_normal (C function), 21  
 magma\_cprimme\_normal\_f77 () (fortran subroutine), 31

magma\_cprimme\_svds (C function), 83  
 magma\_cprimme\_svds\_f77 () (fortran subroutine), 90  
 magma\_dprimme (C function), 19  
 magma\_dprimme\_f77 () (fortran subroutine), 29  
 magma\_dprimme\_svds (C function), 83  
 magma\_dprimme\_svds\_f77 () (fortran subroutine), 91  
 magma\_hprimme (C function), 19  
 magma\_hprimme\_svds (C function), 83  
 magma\_hsprimme (C function), 19  
 magma\_hsprimme\_svds (C function), 83  
 magma\_kcprimme\_normal (C function), 21  
 magma\_kprimme (C function), 19  
 magma\_kprimme\_normal (C function), 21  
 magma\_kprimme\_svds (C function), 83  
 magma\_ksprimme (C function), 19  
 magma\_ksprimme\_svds (C function), 83  
 magma\_sprimme (C function), 19  
 magma\_sprimme\_f77 () (fortran subroutine), 28  
 magma\_sprimme\_svds (C function), 83  
 magma\_sprimme\_svds\_f77 () (fortran subroutine), 89  
 magma\_xprimme () (fortran function), 39  
 magma\_xprimme\_normal () (fortran function), 40  
 magma\_xprimme\_svds () (fortran function), 99  
 magma\_zprimme (C function), 19  
 magma\_zprimme\_f77 () (fortran subroutine), 29  
 magma\_zprimme\_normal (C function), 21  
 magma\_zprimme\_normal\_f77 () (fortran subroutine), 31  
 magma\_zprimme\_svds (C function), 83  
 magma\_zprimme\_svds\_f77 () (fortran subroutine), 91

## P

PRIMME\_COMPLEX\_DOUBLE (C type), 52  
 PRIMME\_COMPLEX\_FLOAT (C type), 52  
 PRIMME\_COMPLEX\_HALF (C type), 52  
 primme\_display\_params (C function), 23  
 primme\_eigs\_matvec () (fortran subroutine), 37  
 primme\_free (C function), 23

primme\_free\_f77() (fortran subroutine), 26  
 primme\_get\_member() (fortran function), 43  
 primme\_get\_member\_f77() (fortran subroutine), 35  
 primme\_get\_prec\_shift\_f77() (fortran subroutine), 36  
 PRIMME\_HALF (C type), 52  
 primme\_initialize (C function), 22  
 primme\_initialize\_f77() (fortran subroutine), 25  
 PRIMME\_INT (C type), 52  
 primme\_params (C type), 52  
 primme\_params.aNorm (C member), 60  
 primme\_params.applyPreconditioner (C member), 53  
 primme\_params.applyPreconditioner\_type (C member), 54  
 primme\_params.BNorm (C member), 60  
 primme\_params.broadcastReal (C member), 57  
 primme\_params.broadcastReal\_type (C member), 57  
 primme\_params.commInfo (C member), 55  
 primme\_params.convtest (C member), 73  
 primme\_params.convTestFun (C member), 72  
 primme\_params.convTestFun\_type (C member), 73  
 primme\_params.correctionParams.convTest (C member), 66  
 primme\_params.correctionParams.maxInnerIterations (C member), 65  
 primme\_params.correctionParams.preconditioner (C member), 65  
 primme\_params.correctionParams.projectorLeft (C member), 66  
 primme\_params.correctionParams.projectorLeftType (C member), 66  
 primme\_params.correctionParams.projectorRight (C member), 66  
 primme\_params.correctionParams.projectorRightType (C member), 66  
 primme\_params.correctionParams.projectorSkewQ (C member), 66  
 primme\_params.correctionParams.projectorSkewX (C member), 66  
 primme\_params.correctionParams.relTolBasis (C member), 65  
 primme\_params.correctionParams.robustShifts (C member), 65  
 primme\_params.dynamicMethodSwitch (C member), 61  
 primme\_params.eps (C member), 61  
 primme\_params.globalSumReal (C member), 56  
 primme\_params.globalSumReal\_type (C member), 56  
 primme\_params.initBasisMode (C member), 64  
 primme\_params.initSize (C member), 62  
 primme\_params.internalPrecision (C member), 58  
 primme\_params.invBNorm (C member), 60  
 primme\_params.iseed (C member), 63  
 primme\_params.ldevecs (C member), 62  
 primme\_params.ldOPs (C member), 67  
 primme\_params.locking (C member), 62  
 primme\_params.massMatrix (C member), 64  
 primme\_params.massMatrixMatvec (C member), 54  
 primme\_params.massMatrixMatvec\_type (C member), 55  
 primme\_params.matrix (C member), 64  
 primme\_params.matrixMatvec (C member), 52  
 primme\_params.matrixMatvec\_type (C member), 53  
 primme\_params.maxBasisSize (C member), 63  
 primme\_params.maxBlockSize (C member), 63  
 primme\_params.maxMatvecs (C member), 63  
 primme\_params.maxOuterIterations (C member), 63  
 primme\_params.minRestartSize (C member), 63  
 primme\_params.monitor (C member), 69  
 primme\_params.monitorFun (C member), 67  
 primme\_params.monitorFun\_type (C member), 69  
 primme\_params.n (C member), 52  
 primme\_params.nLocal (C member), 55  
 primme\_params.numEvals (C member), 58  
 primme\_params.numOrthoConst (C member), 62  
 primme\_params.numProcs (C member), 55  
 primme\_params.numTargetShifts (C member), 58  
 primme\_params.ortho (C member), 60  
 primme\_params.outputFile (C member), 61  
 primme\_params.preconditioner (C member), 64  
 primme\_params.printLevel (C member), 59  
 primme\_params.procID (C member), 55  
 primme\_params.projectionParams.projection (C member), 64  
 primme\_params.queue (C member), 73  
 primme\_params.restartingParams.maxPrevRetain (C member), 65  
 primme\_params.ShiftsForPreconditioner (C member), 64  
 primme\_params.stats.elapsedTime (C member), 71  
 primme\_params.stats.estimateLargestSVal (C member), 72



primme\_params.stats.estimateMaxEval (C member), 72  
 primme\_params.stats.estimateMinEval (C member), 72  
 primme\_params.stats.lockingIssue (C member), 72  
 primme\_params.stats.maxConvTol (C member), 72  
 primme\_params.stats.numBroadcast (C member), 70  
 primme\_params.stats.numGlobalSum (C member), 70  
 primme\_params.stats.numMatvecs (C member), 70  
 primme\_params.stats.numOrthoInnerProds (C member), 71  
 primme\_params.stats.numOuterIterations (C member), 70  
 primme\_params.stats.numPreconds (C member), 70  
 primme\_params.stats.numRestarts (C member), 70  
 primme\_params.stats.timeBroadcast (C member), 72  
 primme\_params.stats.timeGlobalSum (C member), 71  
 primme\_params.stats.timeMatvec (C member), 71  
 primme\_params.stats.timeOrtho (C member), 71  
 primme\_params.stats.timePrecond (C member), 71  
 primme\_params.stats.volumeBroadcast (C member), 71  
 primme\_params.stats.volumeGlobalSum (C member), 70  
 primme\_params.target (C member), 58  
 primme\_params.targetShifts (C member), 58  
 primme\_params\_create (C function), 22  
 primme\_params\_create () (fortran function), 37  
 primme\_params\_destroy (C function), 24  
 primme\_params\_destroy () (fortran function), 38  
 primme\_preset\_method (C enum), 74  
 primme\_preset\_method.PRIMME\_Arnoldi (C enumerator), 74  
 primme\_preset\_method.PRIMME\_DEFAULT\_MIN\_MATRIX\_SIZE (C enumerator), 74  
 primme\_preset\_method.PRIMME\_DEFAULT\_MIN\_TIME (C enumerator), 74  
 primme\_preset\_method.PRIMME\_DYNAMIC (C enumerator), 74  
 primme\_preset\_method.PRIMME\_GD (C enumerator), 74  
 primme\_preset\_method.PRIMME\_GD\_Olsen\_plusK (C enumerator), 74  
 primme\_preset\_method.PRIMME\_GD\_plusK (C enumerator), 74  
 primme\_preset\_method.PRIMME\_JD\_Olsen\_plusK (C enumerator), 74  
 primme\_preset\_method.PRIMME\_JDQMR (C enumerator), 75  
 primme\_preset\_method.PRIMME\_JDQMR\_ETol (C enumerator), 76  
 primme\_preset\_method.PRIMME\_JDQR (C enumerator), 75  
 primme\_preset\_method.PRIMME\_LOBPCG\_OrthoBasis (C enumerator), 76  
 primme\_preset\_method.PRIMME\_LOBPCG\_OrthoBasis\_Wind (C enumerator), 76  
 primme\_preset\_method.PRIMME\_RQI (C enumerator), 75  
 primme\_preset\_method.PRIMME\_STEEPEST\_DESCENT (C enumerator), 76  
 primme\_set\_member () (fortran function), 40  
 primme\_set\_member\_f77 () (fortran subroutine), 32  
 primme\_set\_method (C function), 23  
 primme\_set\_method () (fortran function), 37  
 primme\_set\_method\_f77 () (fortran subroutine), 25  
 primme\_svds\_display\_params (C function), 85  
 primme\_svds\_display\_params\_f77 () (fortran subroutine), 93  
 primme\_svds\_free (C function), 85  
 primme\_svds\_free\_f77 () (fortran subroutine), 93  
 primme\_svds\_get\_member () (fortran function), 102  
 primme\_svds\_get\_member\_f77 () (fortran subroutine), 96  
 primme\_svds\_initialize (C function), 84  
 primme\_svds\_initialize\_f77 () (fortran subroutine), 92  
 primme\_svds\_matvec () (fortran subroutine), 97  
 primme\_svds\_params (C type), 109  
 primme\_svds\_params.aNorm (C member), 115  
 primme\_svds\_params.applyPreconditioner (C member), 110  
 primme\_svds\_params.applyPreconditioner\_type (C member), 110  
 primme\_svds\_params.broadcastReal (C member), 112  
 primme\_svds\_params.broadcastReal\_type (C member), 113  
 primme\_svds\_params.commInfo (C member), 111  
 primme\_svds\_params.convtest (C member), 119  
 primme\_svds\_params.convTestFun (C member), 119

ber), 118  
 primme\_svds\_params.convTestFun\_type (C member), 119  
 primme\_svds\_params.eps (C member), 116  
 primme\_svds\_params.globalSumReal (C member), 112  
 primme\_svds\_params.globalSumReal\_type (C member), 112  
 primme\_svds\_params.initSize (C member), 116  
 primme\_svds\_params.initSize.numOrthoCons (C member), 116  
 primme\_svds\_params.internalPrecision (C member), 113  
 primme\_svds\_params.iseed (C member), 117  
 primme\_svds\_params.locking (C member), 116  
 primme\_svds\_params.m (C member), 109  
 primme\_svds\_params.matrix (C member), 117  
 primme\_svds\_params.matrixMatvec (C member), 109  
 primme\_svds\_params.matrixMatvec\_type (C member), 109  
 primme\_svds\_params.maxBasisSize (C member), 117  
 primme\_svds\_params.maxBlockSize (C member), 117  
 primme\_svds\_params.maxMatvecs (C member), 117  
 primme\_svds\_params.method (C member), 118  
 primme\_svds\_params.methodStage2 (C member), 118  
 primme\_svds\_params.mLocal (C member), 111  
 primme\_svds\_params.monitor (C member), 121  
 primme\_svds\_params.monitorFun (C member), 119  
 primme\_svds\_params.monitorFun\_type (C member), 121  
 primme\_svds\_params.n (C member), 109  
 primme\_svds\_params.nLocal (C member), 111  
 primme\_svds\_params.numProcs (C member), 111  
 primme\_svds\_params.numSvals (C member), 113  
 primme\_svds\_params.numTargetShifts (C member), 114  
 primme\_svds\_params.outputFile (C member), 116  
 primme\_svds\_params.precondition (C member), 117  
 primme\_svds\_params.preconditioner (C member), 117  
 primme\_svds\_params.primme (C member), 118  
 primme\_svds\_params.primmeStage2 (C member), 118  
 primme\_svds\_params.printLevel (C member), 114  
 primme\_svds\_params.procID (C member), 111  
 primme\_svds\_params.queue (C member), 124  
 primme\_svds\_params.stats.elapsedTime (C member), 123  
 primme\_svds\_params.stats.lockingIssue (C member), 124  
 primme\_svds\_params.stats.numBroadcast (C member), 122  
 primme\_svds\_params.stats.numGlobalSum (C member), 122  
 primme\_svds\_params.stats.numMatvecs (C member), 122  
 primme\_svds\_params.stats.numOrthoInnerProds (C member), 123  
 primme\_svds\_params.stats.numOuterIterations (C member), 122  
 primme\_svds\_params.stats.numPreconds (C member), 122  
 primme\_svds\_params.stats.numRestarts (C member), 122  
 primme\_svds\_params.stats.timeBroadcast (C member), 124  
 primme\_svds\_params.stats.timeGlobalSum (C member), 123  
 primme\_svds\_params.stats.timeMatvec (C member), 123  
 primme\_svds\_params.stats.timeOrtho (C member), 123  
 primme\_svds\_params.stats.timePrecond (C member), 123  
 primme\_svds\_params.stats.volumeBroadcast (C member), 123  
 primme\_svds\_params.stats.volumeGlobalSum (C member), 122  
 primme\_svds\_params.target (C member), 114  
 primme\_svds\_params.targetShifts (C member), 114  
 primme\_svds\_params\_create (C function), 84  
 primme\_svds\_params\_create() (fortran function), 97  
 primme\_svds\_params\_destroy (C function), 86  
 primme\_svds\_params\_destroy() (fortran function), 99  
 primme\_svds\_preset\_method (C enum), 125  
 primme\_svds\_preset\_method.primme\_svds\_augmented (C enumerator), 125  
 primme\_svds\_preset\_method.primme\_svds\_default (C enumerator), 125  
 primme\_svds\_preset\_method.primme\_svds\_hybrid (C enumerator), 125  
 primme\_svds\_preset\_method.primme\_svds\_normalequation (C enumerator), 125

`primme_svds_set_member()` (*fortran function*),  
 100  
`primme_svds_set_member_f77()` (*fortran sub-  
 routine*), 93  
`primme_svds_set_method(C function)`, 85  
`primme_svds_set_method()` (*fortran function*),  
 97  
`primme_svds_set_method_f77()` (*fortran sub-  
 routine*), 92  
`primme_svdstop_get_member_f77()` (*fortran  
 subroutine*), 95  
`PRIMME_VERSION_MAJOR(C macro)`, 52  
`PRIMME_VERSION_MINOR(C macro)`, 52  
`primmetop_get_member_f77()` (*fortran subrou-  
 tine*), 34  
`primmetop_get_prec_shift_f77()` (*fortran  
 subroutine*), 35  
`ptr` (*fortran type*), 25

## S

`sprimme(C function)`, 18  
`sprimme_f77()` (*fortran subroutine*), 26  
`sprimme_svds(C function)`, 82  
`sprimme_svds_f77()` (*fortran subroutine*), 87  
 stopping criterion, 63, 117  
`svds()` (*in module primme*), 103

## X

`xprimme()` (*fortran function*), 38  
`xprimme_normal()` (*fortran function*), 39  
`xprimme_svds()` (*fortran function*), 98

## Z

`zprimme(C function)`, 18  
`zprimme_f77()` (*fortran subroutine*), 27  
`zprimme_normal(C function)`, 20  
`zprimme_normal_f77()` (*fortran subroutine*), 30  
`zprimme_svds(C function)`, 82  
`zprimme_svds_f77()` (*fortran subroutine*), 89