MLD2P4
User's and Reference Guide

A guide for the Multi-Level Domain Decomposition Parallel Preconditioners Package based on PSBLAS

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Abstract

MLD2P4 (Multi-Level Domain Decomposition Parallel Preconditioners Package based on PSBLAS) is a package of parallel algebraic multi-level preconditioners. It implements various versions of one-level additive and of multi-level additive and hybrid Schwarz algorithms. In the multi-level case, a purely algebraic approach is applied to generate coarse-level corrections, so that no geometric background is needed concerning the matrix to be preconditioned. The matrix is assumed to be square, real or complex, with a symmetric sparsity pattern.

MLD2P4 has been designed to provide scalable and easy-to-use preconditioners in the context of the PSBLAS (Parallel Sparse Basic Linear Algebra Subprograms) computational framework and can be used in conjuction with the Krylov solvers available in this framework. MLD2P4 enables the user to easily specify different aspects of a generic algebraic multilevel Schwarz preconditioner, thus allowing to search for the "best" preconditioner for the problem at hand.

The package employs object-oriented design techniques in Fortran 2003, with interfaces to additional third party libraries such as UMFPACK, SuperLU, SuperLU_Dist and MUMPS, that can be exploited in building multi-level preconditioners. The parallel implementation is based on a Single Program Multiple Data (SPMD) paradigm for distributed-memory architectures; the inter-process data communication is based on MPI and is managed mainly through PSBLAS.

This guide provides a brief description of the functionalities and the user interface of MLD2P4.

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1 General Overview

The Multi-Level Domain Decomposition Parallel Preconditioners Package based on PSBLAS (MLD2P4) provides *multi-level Schwarz preconditioners* [23], to be used in the iterative solutions of sparse linear systems:

$$Ax = b, \tag{1}$$

where A is a square, real or complex, sparse matrix with a symmetric sparsity pattern. These preconditioners have the following general features:

- both *additive and hybrid multilevel* variants are implemented, i.e. variants that are additive among the levels and inside each level, and variants that are multiplicative among the levels and additive inside each level; the basic Additive Schwarz (AS) preconditioners are obtained by considering only one level;
- a *purely algebraic* approach is used to generate a sequence of coarse-level corrections to a basic AS preconditioner, without explicitly using any information on the geometry of the original problem (e.g. the discretization of a PDE). The *smoothed aggregation* technique is applied as algebraic coarsening strategy [1, 27].

Version 2.1 of the package is written in *Fortran 2003*, following an *object-oriented design* through the exploitation of features such as abstract data type creation, functional overloading and dynamic memory management. The parallel implementation is based on a Single Program Multiple Data (SPMD) paradigm for distributed-memory architectures. Single and double precision implementations of MLD2P4 are available for both the real and the complex case, that can be used through a single interface.

MLD2P4 has been designed to implement scalable and easy-to-use multilevel preconditioners in the context of the *PSBLAS (Parallel Sparse BLAS) computational framework* [18, 17]. PSBLAS is a library originally developed to address the parallel implementation of iterative solvers for sparse linear system, by providing basic linear algebra operators and data management facilities for distributed sparse matrices; it also includes parallel Krylov solvers, built on the top of the basic PSBLAS kernels. The preconditioners available in MLD2P4 can be used with these Krylov solvers. The choice of PSBLAS has been mainly motivated by the need of having a portable and efficient software infrastructure implementing "de facto" standard parallel sparse linear algebra kernels, to pursue goals such as performance, portability, modularity ed extensibility in the development of the preconditioner package. On the other hand, the implementation of MLD2P4 has led to some revisions and extentions of the PSBLAS kernels, leading to the PSBLAS 2.0 version [16]. The inter-process comunication required by MLD2P4 is encapsulated into the PSBLAS routines, except few cases where MPI [24] is explicitly called. Therefore, MLD2P4 can be run on any parallel machine where PSBLAS and MPI implementations are available.

MLD2P4 has a layered and modular software architecture where three main layers can be identified. The lower layer consists of the PSBLAS kernels, the middle one implements the construction and application phases of the preconditioners, and the

upper one provides a uniform and easy-to-use interface to all the preconditioners. This architecture allows for different levels of use of the package: few black-box routines at the upper layer allow non-expert users to easily build any preconditioner available in MLD2P4 and to apply it within a PSBLAS Krylov solver. On the other hand, the routines of the middle and lower layer can be used and extended by expert users to build new versions of multi-level Schwarz preconditioners. We provide here a description of the upper-layer routines, but not of the medium-layer ones.

The user interface of version 2.1 is essentially identical (except for the support of additional solvers) to that of version 1.1. The internal implementation however has been changed significantly; as a result, it has become much easier to extend the library by adding new smoothers and/or solvers, thanks to the Fortran 2003 features exploited in the design of PSBLAS 3.

This guide is organized as follows. General information on the distribution of the source code is reported in Section 2, while details on the configuration and installation of the package are given in Section 3. A description of multi-level Schwarz preconditioners based on smoothed aggregation is provided in Section 4, to help the users in choosing among the different preconditioners implemented in MLD2P4. The basics for building and applying the preconditioners with the Krylov solvers implemented in PSBLAS are reported in Section 5, where the Fortran codes of a few sample programs are also shown. A reference guide for the upper-layer routines of MLD2P4, that are the user interface, is provided in Section 6. The error handling mechanism used by the package is briefly described in Section 7. The copyright terms concerning the distribution and modification of MLD2P4 are reported in Appendix A.

2 Code Distribution

MLD2P4 is available from the web site

`http://www.mld2p4.it`

where contact points for further information can be also found.

The software is available under a modified BSD license, as specified in Appendix A; please note that some of the optional third party libraries may be licensed under a different and more stringent license, most notably the GPL, and this should be taken into account when treating derived works.

The library defines a version string with the constant

`mld_version_string_`

whose current value is `2.1.0`

3 Configuring and Building MLD2P4

To build MLD2P4 it is necessary to set up a Makefile with appropriate values for your system; this is done by means of the `configure` script. The distribution also includes the autoconf and automake sources employed to generate the script, but usually this is not needed to build the software.

MLD2P4 is implemented almost entirely in Fortran 2003, with some interfaces to external libraries in C; the Fortran compiler must support the Fortran 2003 standard plus the extension `MOLD=` feature, which enhances the usability of `ALLOCATE`. Many compiles do this; in particular, this is supported by the GNU Fortran compiler, for which we recommend to use at least version 4.8. The software defines data types and interfaces for real and complex data, in both single and double precision.

3.1 Prerequisites

The following base libraries are needed:

BLAS [12, 13, 20] Many vendors provide optimized versions of the Basic Linear Algebra Subprograms; if no vendor version is available for a given platform, the ATLAS software (`http://math-atlas.sourceforge.net/`) may be employed. The reference BLAS from Netlib (`http://www.netlib.org/blas`) are meant to define the standard behaviour of the BLAS interface, so they are not optimized for any particular plaftorm, and should only be used as a last resort. Note that BLAS computations form a relatively small part of the MLD2P4/PSBLAS computations; they are however critical when using preconditioners based on the UMFPACK or SuperLU third party libraries.

MPI [19, 24] A version of MPI is available on most high-performance computing systems;

PSBLAS [16, 18] Parallel Sparse BLAS is available from `http://www.ce.uniroma2.it/psblas`; version 3.4.0 (or later) is required. Indeed, all the prerequisites listed so far are also prerequisites of PSBLAS.

Please note that the four previous libraries must have Fortran interfaces compatible with MLD2P4; usually this means that they should all be built with the same compiler as MLD2P4.

3.2 Optional third party libraries

We provide interfaces to the following third-party software libraries; note that these are optional, but if you enable them some defaults for multilevel preconditioners may change to reflect their presence.

UMFPACK [9] A sparse direct factorization package available from `http://www.cise.ufl.edu/research/sparse/umfpack/`; provides serial factor-

ization and triangular system solution for double precision real and complex data. We have tested versions 5.4.

SuperLU [11] A sparse direct factorization package available from `http://crd.lbl.gov/~xiaoye/SuperLU/`; provides serial factorization and triangular system solution for single and double precision, real and complex data. We have tested version 4.3 and 5.0.

SuperLU_Dist [21] A sparse direct factorization package available from the same site as SuperLU; provides parallel factorization and triangular system solution for double precision real and complex data. We have tested version 3.3 and 4.2.

MUMPS [10] MUMPS (MUltifrontal Massively Parallel Solver) is a sparse, direct factorization package available from `http://mumps.enseeiht.fr/`. It implements a direct method based on a multifrontal approach which performs a Gaussian factorization. We have tested versions 4.10.0 and version 5.0.1.

3.3 Configuration options

To build MLD2P4 the first step is to use the `configure` script in the main directory to generate the necessary makefile(s).

As a minimal example consider the following:

```
./configure --with-psblas=PSB-INSTALL-DIR
```

which assumes that the various MPI compilers and support libraries are available in the standard directories on the system, and specifies only the PSBLAS install directory (note that the latter directory must be specified with an *absolute* path). The full set of options may be looked at by issuing the command `./configure --help`, which produces:

```
‘configure’ configures MLD2P4 2.0 to adapt to many kinds of systems.

Usage: ./configure [OPTION]... [VAR=VALUE]...

To assign environment variables (e.g., CC, CFLAGS...), specify them as
VAR=VALUE.  See below for descriptions of some of the useful variables.

Defaults for the options are specified in brackets.

Configuration:
  -h, --help              display this help and exit
      --help=short        display options specific to this package
      --help=recursive    display the short help of all the included packages
  -V, --version           display version information and exit
```

```
  -q, --quiet, --silent   do not print ‘checking...’ messages
      --cache-file=FILE   cache test results in FILE [disabled]
  -C, --config-cache      alias for ‘--cache-file=config.cache’
  -n, --no-create         do not create output files
      --srcdir=DIR        find the sources in DIR [configure dir or ‘..’]

Installation directories:
  --prefix=PREFIX         install architecture-independent files in PREFIX
                          [/usr/local]
  --exec-prefix=EPREFIX   install architecture-dependent files in EPREFIX
                          [PREFIX]

By default, ‘make install’ will install all the files in
‘/usr/local/bin’, ‘/usr/local/lib’ etc.  You can specify
an installation prefix other than ‘/usr/local’ using ‘--prefix’,
for instance ‘--prefix=$HOME’.

For better control, use the options below.

Fine tuning of the installation directories:
  --bindir=DIR            user executables [EPREFIX/bin]
  --sbindir=DIR           system admin executables [EPREFIX/sbin]
  --libexecdir=DIR        program executables [EPREFIX/libexec]
  --sysconfdir=DIR        read-only single-machine data [PREFIX/etc]
  --sharedstatedir=DIR    modifiable architecture-independent data [PREFIX/com]
  --localstatedir=DIR     modifiable single-machine data [PREFIX/var]
  --libdir=DIR            object code libraries [EPREFIX/lib]
  --includedir=DIR        C header files [PREFIX/include]
  --oldincludedir=DIR     C header files for non-gcc [/usr/include]
  --datarootdir=DIR       read-only arch.-independent data root [PREFIX/share]
  --datadir=DIR           read-only architecture-independent data [DATAROOTDIR]
  --infodir=DIR           info documentation [DATAROOTDIR/info]
  --localedir=DIR         locale-dependent data [DATAROOTDIR/locale]
  --mandir=DIR            man documentation [DATAROOTDIR/man]
  --docdir=DIR            documentation root [DATAROOTDIR/doc/mld2p4]
  --htmldir=DIR           html documentation [DOCDIR]
  --dvidir=DIR            dvi documentation [DOCDIR]
  --pdfdir=DIR            pdf documentation [DOCDIR]
  --psdir=DIR             ps documentation [DOCDIR]

Optional Features:
  --disable-option-checking  ignore unrecognized --enable/--with options
  --disable-FEATURE       do not include FEATURE (same as --enable-FEATURE=no)
  --enable-FEATURE[=ARG]  include FEATURE [ARG=yes]
```

```
  --enable-serial         Specify whether to enable a fake mpi library to run
                          in serial mode.

Optional Packages:
  --with-PACKAGE[=ARG]    use PACKAGE [ARG=yes]
  --without-PACKAGE       do not use PACKAGE (same as --with-PACKAGE=no)
  --with-psblas=DIR       The install directory for PSBLAS, for example,
                          --with-psblas=/opt/packages/psblas-3.3
  --with-psblas-incdir=DIR
                          Specify the directory for PSBLAS includes.
  --with-psblas-libdir=DIR
                          Specify the directory for PSBLAS library.
  --with-extra-libs       List additional link flags here. For example,
                          --with-extra-libs=-lspecial_system_lib or
                          --with-extra-libs=-L/path/to/libs
  --with-mumps=LIBNAME    Specify the libname for MUMPS. Default: "-lsmumps
                          -ldmumps -lcmumps -lzmumps -lmumps_common -lpord"
  --with-mumpsdir=DIR     Specify the directory for MUMPS library and
                          includes. Note: you will need to add auxiliary
                          libraries with --extra-libs; this depends on how
                          MUMPS was configured and installed, at a minimum you
                          will need SCALAPACK and BLAS
  --with-mumpsincdir=DIR  Specify the directory for MUMPS includes.
  --with-mumpslibdir=DIR  Specify the directory for MUMPS library.
  --with-umfpack=LIBNAME  Specify the library name for UMFPACK and its support
                          libraries. Default: "-lumfpack -lamd"
  --with-umfpackdir=DIR   Specify the directory for UMFPACK library and
                          includes.
  --with-umfpackincdir=DIR
                          Specify the directory for UMFPACK includes.
  --with-umfpacklibdir=DIR
                          Specify the directory for UMFPACK library.
  --with-superlu=LIBNAME  Specify the library name for SUPERLU library.
                          Default: "-lsuperlu"
  --with-superludir=DIR   Specify the directory for SUPERLU library and
                          includes.
  --with-superluincdir=DIR
                          Specify the directory for SUPERLU includes.
  --with-superlulibdir=DIR
                          Specify the directory for SUPERLU library.
  --with-superludist=LIBNAME
                          Specify the libname for SUPERLUDIST library.
                          Requires you also specify SuperLU. Default:
                          "-lsuperlu_dist"
```

```
  --with-superludistdir=DIR
                          Specify the directory for SUPERLUDIST library and
                          includes.
  --with-superludistincdir=DIR
                          Specify the directory for SUPERLUDIST includes.
  --with-superludistlibdir=DIR
                          Specify the directory for SUPERLUDIST library.

Some influential environment variables:
  FC          Fortran compiler command
  FCFLAGS     Fortran compiler flags
  LDFLAGS     linker flags, e.g. -L<lib dir> if you have libraries in a
              nonstandard directory <lib dir>
  LIBS        libraries to pass to the linker, e.g. -l<library>
  CC          C compiler command
  CFLAGS      C compiler flags
  CPPFLAGS    C/C++/Objective C preprocessor flags, e.g. -I<include dir> if
              you have headers in a nonstandard directory <include dir>
  CPP         C preprocessor
  MPICC       MPI C compiler command
  F77         Fortran 77 compiler command
  FFLAGS      Fortran 77 compiler flags
  MPIF77      MPI Fortran 77 compiler command
  MPIFC       MPI Fortran compiler command

Use these variables to override the choices made by 'configure' or to help
it to find libraries and programs with nonstandard names/locations.

Report bugs to <bugreport@mld2p4.it>.
```

For instance, if a user has built and installed PSBLAS 3.4 under the `/opt` directory and is using the SuiteSparse package (which includes UMFPACK), then MLD2P4 might be configured with:

```
./configure --with-psblas=/opt/psblas-3.4/ \
--with-umfpackincdir=/usr/include/suitesparse
```

Once the configure script has completed execution, it will have generated the file `Make.inc` which will then be used by all Makefiles in the directory tree; this file will be copied in the install directory under the name `Make.inc.MLD2P4`.

To use the MUMPS solver package, the user has to add the appropriate options to the configure script; by default we are looking for the libraries `-ldmumps -lsmumps -lzmumps -lzmumps -mu` MUMPS often uses additional packages such as ScaLAPACK, ParMETIS, SCOTCH, as well as enabling OpenMP; in such cases it is necessary to add linker options with the `--with-extra-libs` configure option.

To build the library the user will now enter

```
make
```

followed (optionally) by

```
make install
```

3.4 Bug reporting

If you find any bugs in our codes, please let us know at `bugreport@mld2p4.it` ; be aware that the amount of information needed to reproduce a problem in a parallel program may vary quite a lot.

3.5 Example and test programs

The package contains the `examples` and `tests` directories; both of them are further divided into `fileread` and `pdegen` subdirectories. Their purpose is as follows:

`examples` contains a set of simple example programs with a predefined choice of preconditioners, selectable via integer values. These are intended to get an acquaintance with the multilevel preconditioners.

`tests` contains a set of more sophisticated examples that will allow the user, via the input files in the `runs` subdirectories, to experiment with the full range of preconditioners implemented in the library.

The `fileread` directories contain sample programs that read sparse matrices from files, according to the Matrix Market or the Harwell-Boeing storage format; the `pdegen` instead generate matrices in full parallel mode from the discretization of a sample PDE.

4 Multi-level Domain Decomposition Background

Domain Decomposition (DD) preconditioners, coupled with Krylov iterative solvers, are widely used in the parallel solution of large and sparse linear systems. These preconditioners are based on the divide and conquer technique: the matrix to be preconditioned is divided into submatrices, a "local" linear system involving each submatrix is (approximately) solved, and the local solutions are used to build a preconditioner for the whole original matrix. This process often corresponds to dividing a physical domain associated to the original matrix into subdomains, e.g. in a PDE discretization, to (approximately) solving the subproblems corresponding to the subdomains and to building an approximate solution of the original problem from the local solutions [6, 7, 23].

Additive Schwarz preconditioners are DD preconditioners using overlapping submatrices, i.e. with some common rows, to couple the local information related to the submatrices (see, e.g., [23]). The main motivation for choosing Additive Schwarz preconditioners is their intrinsic parallelism. A drawback of these preconditioners is that the number of iterations of the preconditioned solvers generally grows with the number of submatrices. This may be a serious limitation on parallel computers, since the number of submatrices usually matches the number of available processors. Optimal convergence rates, i.e. iteration numbers independent of the number of submatrices, can be obtained by correcting the preconditioner through a suitable approximation of the original linear system in a coarse space, which globally couples the information related to the single submatrices.

Two-level Schwarz preconditioners are obtained by combining basic (one-level) Schwarz preconditioners with a coarse-level correction. In this context, the one-level preconditioner is often called 'smoother'. Different two-level preconditioners are obtained by varying the choice of the smoother and of the coarse-level correction, and the way they are combined [23]. The same reasoning can be applied starting from the coarse-level system, i.e. a coarse-space correction can be built from this system, thus obtaining *multi-level* preconditioners.

It is worth noting that optimal preconditioners do not necessarily correspond to minimum execution times. Indeed, to obtain effective multi-level preconditioners a tradeoff between optimality of convergence and the cost of building and applying the coarse-space corrections must be achieved. The choice of the number of levels, i.e. of the coarse-space corrections, also affects the effectiveness of the preconditioners. One more goal is to get convergence rates as less sensitive as possible to variations in the matrix coefficients.

Two main approaches can be used to build coarse-space corrections. The geometric approach applies coarsening strategies based on the knowledge of some physical grid associated to the matrix and requires the user to define grid transfer operators from the fine to the coarse levels and vice versa. This may result difficult for complex geometries; furthermore, suitable one-level preconditioners may be required to get efficient interplay between fine and coarse levels, e.g. when matrices with highly varying coefficients are considered. The algebraic approach builds coarse-space corrections using only matrix information. It performs a fully automatic coarsening and enforces the

interplay between the fine and coarse levels by suitably choosing the coarse space and the coarse-to-fine interpolation [25].

MLD2P4 uses a pure algebraic approach for building the sequence of coarse matrices starting from the original matrix. The algebraic approach is based on the *smoothed aggregation* algorithm [1, 27]. A decoupled version of this algorithm is implemented, where the smoothed aggregation is applied locally to each submatrix [26]. In the next two subsections we provide a brief description of the multi-level Schwarz preconditioners and of the smoothed aggregation technique as implemented in MLD2P4. For further details the reader is referred to [2, 3, 4, 8, 23].

4.1 Multi-level Schwarz Preconditioners

The Multilevel preconditioners implemented in MLD2P4 are obtained by combining AS preconditioners with coarse-space corrections; therefore we first provide a sketch of the AS preconditioners.

Given the linear system (1), where $A = (a_{ij}) \in \Re^{n\times n}$ is a nonsingular sparse matrix with a symmetric nonzero pattern, let $G = (W, E)$ be the adjacency graph of A, where $W = \{1, 2, \ldots, n\}$ and $E = \{(i, j) : a_{ij} \neq 0\}$ are the vertex set and the edge set of G, respectively. Two vertices are called adjacent if there is an edge connecting them. For any integer $\delta > 0$, a δ-overlap partition of W can be defined recursively as follows. Given a 0-overlap (or non-overlapping) partition of W, i.e. a set of m disjoint nonempty sets $W_i^0 \subset W$ such that $\cup_{i=1}^m W_i^0 = W$, a δ-overlap partition of W is obtained by considering the sets $W_i^\delta \supset W_i^{\delta-1}$ obtained by including the vertices that are adjacent to any vertex in $W_i^{\delta-1}$.

Let n_i^δ be the size of W_i^δ and $R_i^\delta \in \Re^{n_i^\delta \times n}$ the restriction operator that maps a vector $v \in \Re^n$ onto the vector $v_i^\delta \in \Re^{n_i^\delta}$ containing the components of v corresponding to the vertices in W_i^δ. The transpose of R_i^δ is a prolongation operator from $\Re^{n_i^\delta}$ to $\Re^n$. The matrix $A_i^\delta = R_i^\delta A (R_i^\delta)^T \in \Re^{n_i^\delta \times n_i^\delta}$ can be considered as a restriction of A corresponding to the set W_i^δ.

The *classical one-level AS* preconditioner is defined by

$$M_{AS}^{-1} = \sum_{i=1}^{m} (R_i^\delta)^T (A_i^\delta)^{-1} R_i^\delta,$$

where A_i^δ is assumed to be nonsingular. Its application to a vector $v \in \Re^n$ within a Krylov solver requires the following three steps:

1. restriction of v as $v_i = R_i^\delta v$, $i = 1, \ldots, m$;
2. solution of the linear systems $A_i^\delta w_i = v_i$, $i = 1, \ldots, m$;
3. prolongation and sum of the w_i's, i.e. $w = \sum_{i=1}^m (R_i^\delta)^T w_i$.

Note that the linear systems at step 2 are usually solved approximately, e.g. using incomplete LU factorizations such as ILU(p), MILU(p) and ILU(p, t) [22, Chapter 10].

A variant of the classical AS preconditioner that outperforms it in terms of convergence rate and of computation and communication time on parallel distributed-memory computers is the so-called *Restricted AS (RAS)* preconditioner [5, 15]. It is obtained by zeroing the components of w_i corresponding to the overlapping vertices when applying the prolongation. Therefore, RAS differs from classical AS by the prolongation operators, which are substituted by $(\tilde{R}_i^0)^T \in \Re^{n_i^\delta \times n}$, where $\tilde{R}_i^0$ is obtained by zeroing the rows of R_i^δ corresponding to the vertices in $W_i^\delta \backslash W_i^0$:

$$M_{RAS}^{-1} = \sum_{i=1}^{m} (\tilde{R}_i^0)^T (A_i^\delta)^{-1} R_i^\delta.$$

Analogously, the AS variant called *AS with Harmonic extension (ASH)* is defined by

$$M_{ASH}^{-1} = \sum_{i=1}^{m} (R_i^\delta)^T (A_i^\delta)^{-1} \tilde{R}_i^0.$$

We note that for $\delta = 0$ the three variants of the AS preconditioner are all equal to the block-Jacobi preconditioner.

As already observed, the convergence rate of the one-level Schwarz preconditioned iterative solvers deteriorates as the number m of partitions of W increases [7, 23]. To reduce the dependency of the number of iterations on the degree of parallelism we may introduce a global coupling among the overlapping partitions by defining a coarse-space approximation A_C of the matrix A. In a pure algebraic setting, A_C is usually built with the Galerkin approach. Given a set W_C of *coarse vertices*, with size n_C, and a suitable restriction operator $R_C \in \Re^{n_C \times n}$, A_C is defined as

$$A_C = R_C A R_C^T$$

and the coarse-level correction matrix to be combined with a generic one-level AS preconditioner M_{1L} is obtained as

$$M_C^{-1} = R_C^T A_C^{-1} R_C,$$

where A_C is assumed to be nonsingular. The application of M_C^{-1} to a vector v corresponds to a restriction, a solution and a prolongation step; the solution step, involving the matrix A_C, may be carried out also approximately.

The combination of M_C and M_{1L} may be performed in either an additive or a multiplicative framework. In the former case, the *two-level additive* Schwarz preconditioner is obtained:

$$M_{2LA}^{-1} = M_C^{-1} + M_{1L}^{-1}.$$

Applying M_{2L-A}^{-1} to a vector v within a Krylov solver corresponds to applying M_C^{-1} and M_{1L}^{-1} to v independently and then summing up the results.

In the multiplicative case, the combination can be performed by first applying the smoother M_{1L}^{-1} and then the coarse-level correction operator M_C^{-1}:

$$\begin{aligned} w &= M_{1L}^{-1} v, \\ z &= w + M_C^{-1}(v - Aw); \end{aligned}$$

this corresponds to the following *two-level hybrid pre-smoothed* Schwarz preconditioner:

$$M_{2LH-PRE}^{-1} = M_C^{-1} + \left(I - M_C^{-1}A\right) M_{1L}^{-1}.$$

On the other hand, by applying the smoother after the coarse-level correction, i.e. by computing

$$\begin{aligned} w &= M_C^{-1}v, \\ z &= w + M_{1L}^{-1}(v - Aw), \end{aligned}$$

the *two-level hybrid post-smoothed* Schwarz preconditioner is obtained:

$$M_{2LH-POST}^{-1} = M_{1L}^{-1} + \left(I - M_{1L}^{-1}A\right) M_C^{-1}.$$

One more variant of two-level hybrid preconditioner is obtained by applying the smoother before and after the coarse-level correction. In this case, the preconditioner is symmetric if A, M_{1L} and M_C are symmetric.

As previously noted, on parallel computers the number of submatrices usually matches the number of available processors. When the size of the system to be preconditioned is very large, the use of many processors, i.e. of many small submatrices, often leads to a large coarse-level system, whose solution may be computationally expensive. On the other hand, the use of few processors often leads to local sumatrices that are too expensive to be processed on single processors, because of memory and/or computing requirements. Therefore, it seems natural to use a recursive approach, in which the coarse-level correction is re-applied starting from the current coarse-level system. The corresponding preconditioners, called *multi-level* preconditioners, can significantly reduce the computational cost of preconditioning with respect to the two-level case (see [23, Chapter 3]). Additive and hybrid multilevel preconditioners are obtained as direct extensions of the two-level counterparts. For a detailed descrition of them, the reader is referred to [23, Chapter 3]. The algorithm for the application of a multi-level hybrid post-smoothed preconditioner M to a vector v, i.e. for the computation of $w = M^{-1}v$, is reported, for example, in Figure 1. Here the number of levels is denoted by $nlev$ and the levels are numbered in increasing order starting from the finest one, i.e. the finest level is level 1; the coarse matrix and the corresponding basic preconditioner at each level l are denoted by A_l and M_l, respectively, with $A_1 = A$, while the related restriction operator is denoted by R_l.

4.2 Smoothed Aggregation

In order to define the restriction operator R_C, which is used to compute the coarse-level matrix A_C, MLD2P4 uses the *smoothed aggregation* algorithm described in [1, 27]. The basic idea of this algorithm is to build a coarse set of vertices W_C by suitably grouping the vertices of W into disjoint subsets (aggregates), and to define the coarse-to-fine space transfer operator R_C^T by applying a suitable smoother to a simple piecewise constant prolongation operator, to improve the quality of the coarse-space correction.

Three main steps can be identified in the smoothed aggregation procedure:

$v_1 = v$;
for $l = 2, nlev$ **do**
  ! transfer v_{l-1} to the next coarser level
  $v_l = R_l v_{l-1}$
endfor
! apply the coarsest-level correction
$y_{nlev} = A_{nlev}^{-1} v_{nlev}$
for $l = nlev - 1, 1, -1$ **do**
  ! transfer y_{l+1} to the next finer level
  $y_l = R_{l+1}^T y_{l+1}$;
  ! compute the residual at the current level
  $r_l = v_l - A_l^{-1} y_l$;
  ! apply the basic Schwarz preconditioner to the residual
  $r_l = M_l^{-1} r_l$
  ! update y_l
  $y_l = y_l + r_l$
endfor
$w = y_1$;

Figure 1: Application of the multi-level hybrid post-smoothed preconditioner.

1. coarsening of the vertex set W, to obtain W_C;
2. construction of the prolongator R_C^T;
3. application of R_C and R_C^T to build A_C.

To perform the coarsening step, we have implemented the aggregation algorithm sketched in [4]. According to [27], a modification of this algorithm has been actually considered, in which each aggregate N_r is made of vertices of W that are *strongly coupled* to a certain root vertex $r \in W$, i.e.

$$N_r = \left\{ s \in W : |a_{rs}| > \theta \sqrt{|a_{rr} a_{ss}|} \right\} \cup \{r\},$$

for a given $\theta \in [0, 1]$. Since this algorithm has a sequential nature, a *decoupled* version of it has been chosen, where each processor i independently applies the algorithm to the set of vertices W_i^0 assigned to it in the initial data distribution. This version is embarrassingly parallel, since it does not require any data communication. On the other hand, it may produce non-uniform aggregates near boundary vertices, i.e. near vertices adjacent to vertices in other processors, and is strongly dependent on the number of processors and on the initial partitioning of the matrix A. Nevertheless, this algorithm has been chosen for the implementation in MLD2P4, since it has been shown to produce good results in practice [3, 4, 26].

The prolongator $P_C = R_C^T$ is built starting from a *tentative prolongator* $P \in \Re^{n \times n_C}$, defined as

$$P = (p_{ij}), \quad p_{ij} = \begin{cases} 1 & \text{if } i \in V_C^j \\ 0 & \text{otherwise} \end{cases} . \tag{2}$$

P_C is obtained by applying to P a smoother $S \in \Re^{n \times n}$:

$$P_C = SP, \tag{3}$$

in order to remove oscillatory components from the range of the prolongator and hence to improve the convergence properties of the multi-level Schwarz method [1, 25]. A simple choice for S is the damped Jacobi smoother:

$$S = I - \omega D^{-1} A, \tag{4}$$

where the value of ω can be chosen using some estimate of the spectral radius of $D^{-1}A$ [1].

5 Getting Started

We describe the basics for building and applying MLD2P4 one-level and multi-level Schwarz preconditioners with the Krylov solvers included in PSBLAS [16]. The following steps are required:

1. *Declare the preconditioner data structure.* It is a derived data type, `mld_`x`prec_type`, where x may be `s`, `d`, `c` or `z`, according to the basic data type of the sparse matrix (`s` = real single precision; `d` = real double precision; `c` = complex single precision; `z` = complex double precision). This data structure is accessed by the user only through the MLD2P4 routines, following an object-oriented approach.

2. *Allocate and initialize the preconditioner data structure, according to a preconditioner type chosen by the user.* This is performed by the routine `mld_precinit`, which also sets defaults for each preconditioner type selected by the user. The defaults associated to each preconditioner type are given in Table 1, where the strings used by `mld_precinit` to identify the preconditioner types are also given. Note that these strings are valid also if uppercase letters are substituted by corresponding lowercase ones.

3. *Modify the aggregation parameters.* This is performed by the routine `mld_precset`. This routine must be called only if the user wants to modify the default values of the parameters associated to the aggregation hierarchy construction. Examples of use of `mld_precset` are given in Section 5.1; a complete list of all the preconditioner parameters and their allowed and default values is provided in Section 6, Tables 2-6.

4. *Build the aggregation hierarchy for a given matrix.* This is performed by the routine `mld_hierarchy_bld`.

5. *Modify the selected preconditioner type, by properly setting preconditioner parameters.* This is performed by the routine `mld_precset`. This routine must be called only if the user wants to modify the default values of the parameters associated to the selected preconditioner type, to obtain a variant of the preconditioner. Examples of use of `mld_precset` are given in Section 5.1; a complete list of all the preconditioner parameters and their allowed and default values is provided in Section 6, Tables 2-6.

6. *Build the preconditioner for a given matrix.* This is performed by the routine `mld_ml_prec_bld`.

7. *Apply the preconditioner at each iteration of a Krylov solver.* This is performed by the routine `mld_precaply`. When using the PSBLAS Krylov solvers, this step is completely transparent to the user, since `mld_precaply` is called by the PSBLAS routine implementing the Krylov solver (`psb_krylov`).

8. *Free the preconditioner data structure.* This is performed by the routine `mld_precfree`. This step is complementary to step 1 and should be performed when the preconditioner is no more used.

A detailed description of the above routines is given in Section 6. Examples showing the basic use of MLD2P4 are reported in Section 5.1.

Note that the Fortran 95 module `mld_prec_mod`, containing the definition of the preconditioner data type and the interfaces to the routines of MLD2P4, must be used in any program calling such routines. The modules `psb_base_mod`, for the sparse matrix and communication descriptor data types, and `psb_krylov_mod`, for interfacing with the Krylov solvers, must be also used (see Section 5.1).

Remark 1. The coarsest-level solver used by the default two-level preconditioner has been chosen by taking into account that, on parallel machines, it often leads to the smallest execution time when applied to linear systems coming from finite-difference discretizations of basic elliptic PDE problems, considered as standard tests for multi-level Schwarz preconditioners [3, 4]. However, this solver does not necessarily correspond to the smallest number of iterations of the preconditioned Krylov method, which is usually obtained by applying a direct solver to the coarsest-level system, e.g. based on the LU factorization (see Section 6 for the coarsest-level solvers available in MLD2P4).

5.1 Examples

The code reported in Figure 2 shows how to set and apply the default multi-level preconditioner available in the real double precision version of MLD2P4 (see Table 1). This preconditioner is chosen by simply specifying `'ML'` as second argument of `mld_precinit` (a call to `mld_precset` is not needed) and is applied with the BiCGSTAB solver provided by PSBLAS. As previously observed, the modules `psb_base_mod`, `mld_prec_mod` and `psb_krylov_mod` must be used by the example program.

The part of the code concerning the reading and assembling of the sparse matrix and the right-hand side vector, performed through the PSBLAS routines for sparse matrix and vector management, is not reported here for brevity; the statements concerning the deallocation of the PSBLAS data structure are neglected too. The complete code can be found in the example program file `mld_dexample_ml.f90`, in the directory `examples/fileread` of the MLD2P4 tree (see Section 3.5). For details on the use of the PSBLAS routines, see the PSBLAS User's Guide [16].

The setup and application of the default multi-level preconditioners for the real single precision and the complex, single and double precision, versions are obtained with straightforward modifications of the previous example (see Section 6 for details). If these versions are installed, the corresponding Fortran 95 codes are available in `examples/fileread/`.

Different versions of multi-level preconditioners can be obtained by changing the default values of the preconditioner parameters. The code reported in Figure 3 shows how to set a three-level hybrid Schwarz preconditioner, which uses block Jacobi with ILU(0)

```
  use psb_base_mod
  use mld_prec_mod
  use psb_krylov_mod
... ...
!
! sparse matrix
  type(psb_dspmat_type) :: A
! sparse matrix descriptor
  type(psb_desc_type)   :: desc_A
! preconditioner
  type(mld_dprec_type)  :: P
! right-hand side and solution vectors
  type(psb_d_vect_type) :: b, x
... ...
!
! initialize the parallel environment
  call psb_init(ictxt)
  call psb_info(ictxt,iam,np)
... ...
!
! read and assemble the matrix A and the right-hand side b
! using PSBLAS routines for sparse matrix / vector management
... ...
!
! initialize the default multi-level preconditioner, i.e. hybrid
! Schwarz, using RAS (with overlap 1 and ILU(0) on the blocks)
! as pre- and post-smoother and 4 block-Jacobi sweeps
! (with UMFPACK LU on the blocks) as distributed coarse-level
! solver.
  call mld_precinit(P,'ML',info)
!
! build the preconditioner
  call mld_hierarchy_bld(A,desc_A,P,info)
  call mld_ml_prec_bld(A,desc_A,P,info)

!
! set the solver parameters and the initial guess
  ... ...
!
! solve Ax=b with preconditioned BiCGSTAB
  call psb_krylov('BICGSTAB',A,P,b,x,tol,desc_A,info)
  ... ...
!
! deallocate the preconditioner
  call mld_precfree(P,info)
!
! deallocate other data structures
  ... ...
!
! exit the parallel environment
  call psb_exit(ictxt)
  stop
```

Figure 2: Setup and application of the default multi-level Schwarz preconditioner.

TYPE	STRING	DEFAULT PRECONDITIONER
No preconditioner	`'NOPREC'`	Considered only to use the PSBLAS Krylov solvers with no preconditioner.
Diagonal	`'DIAG'`	—
Block Jacobi	`'BJAC'`	Block Jacobi with ILU(0) on the local blocks.
Additive Schwarz	`'AS'`	Restricted Additive Schwarz (RAS), with overlap 1 and ILU(0) on the local blocks.
Multilevel	`'ML'`	Multi-level hybrid preconditioner (additive on the same level and multiplicative through the levels), with pre- and post-smoothing. Target aggregation size: cubic root of the size at the finest level. Smoother: RAS with overlap 1 and ILU(0) on the local blocks. Aggregation: decoupled smoothed aggregation with threshold $\theta = 0$. Coarsest matrix: distributed among the processors. Coarsest-level solver: 4 sweeps of the block-Jacobi solver, with LU or ILU factorization of the blocks (MUMPS, or UMFPACK for the double precision versions and SuperLU for the single precision ones, if the packages have been installed; ILU(0), otherwise).

Table 1: Preconditioner types, corresponding strings and default choices.

on the local blocks as post-smoother, has a coarsest matrix replicated on the processors, and solves the coarsest-level system with the LU factorization from UMFPACK [9]. Figure 4 shows how to set a three-level preconditioner similar to the one of 3, but the coarsest-level systems is solved with the multifrontal factorization from MUMPS [9]. Note that MUMPS can be used on both replicated and distributed coarsest level matrices, as a global and local solver respectively. The number of levels is specified by using `mld_precinit`; the other preconditioner parameters are set by calling `mld_precset`. Note that the type of multilevel framework (i.e. multiplicative among the levels with post-smoothing only) is not specified since it is the default set by `mld_precinit`.

Figure 5 shows how to set a three-level additive Schwarz preconditioner, which uses RAS, with overlap 1 and ILU(0) on the blocks, as pre- and post-smoother, and applies five block-Jacobi sweeps, with the UMFPACK LU factorization on the blocks, as distributed coarsest-level solver. Again, `mld_precset` is used only to set non-default values of the parameters (see Tables 2-6). In both cases, the construction and the application of the preconditioner are carried out as for the default multi-level preconditioner. The code fragments shown in in Figures 3 4-5 are included in the example program file `mld_dexample_ml.f90` too.

Finally, Figure 6 shows the setup of a one-level additive Schwarz preconditioner, i.e.

RAS with overlap 2. The corresponding example program is available in `mld_dexample_1lev.f90`.

For all the previous preconditioners, example programs where the sparse matrix and the right-hand side are generated by discretizing a PDE with Dirichlet boundary conditions are also available in the directory `examples/pdegen`.

```
... ...
! set a three-level hybrid Schwarz preconditioner, which uses
! block Jacobi (with ILU(0) on the blocks) as post-smoother,
! a coarsest matrix replicated on the processors, and the
! LU factorization from UMFPACK as coarse-level solver
  call mld_precinit(P,'ML',info)
  call mld_hierarchy_bld(A,desc_A,P,info)

  call_mld_precset(P,'SMOOTHER_TYPE','BJAC',info)
  call_mld_precset(P,'SMOOTHER_POS,'POST'w,info)
  call mld_precset(P,'COARSE_MAT','REPL',info)
  call mld_precset(P,'COARSE_SOLVE','UMF',info)
  call mld_ml_prec_bld(A,desc_A,P,info)
... ...
```

Figure 3: Setup of a hybrid three-level Schwarz preconditioner.

```
... ...
! set a three-level hybrid Schwarz preconditioner, which uses
! block Jacobi (with ILU(0) on the blocks) as post-smoother,
! a coarsest matrix replicated on the processors, and the
! multifrontal solver in MUMPS as coarse-level solver

  call mld_precinit(P,'ML',info,nlev=3)
  call mld_hierarchy_bld(A,desc_A,P,info)

  call mld_precset(P,mld_smoother_type_,'BJAC',info)
  call mld_precset(P,mld_coarse_mat_,'REPL',info)
  call mld_precset(P,mld_coarse_solve_,'MUMPS',info)
  call mld_ml_prec_bld(A,desc_A,P,info)
... ...
```

Figure 4: Setup of a hybrid three-level Schwarz preconditioner.

```
... ...
! set a three-level additive Schwarz preconditioner, which uses
! RAS (with overlap 1 and ILU(0) on the blocks) as pre- and
! post-smoother, and 5 block-Jacobi sweeps (with UMFPACK LU
! on the blocks) as distributed coarsest-level solver
  call mld_precinit(P,'ML',info,nlev=3)
  call mld_ml_prec_bld(A,desc_A,P,info)
  call mld_precset(P,'ML_TYPE','ADD',info)
  call_mld_precset(P,'SMOOTHER_POS','TWOSIDE',info)
  call mld_precset(P,'COARSE_SWEEPS',5,info)
  call mld_ml_prec_bld(A,desc_A,P,info)
... ...
```

Figure 5: Setup of an additive three-level Schwarz preconditioner.

```
... ...
! set RAS with overlap 2 and ILU(0) on the local blocks
  call mld_precinit(P,'AS',info)
  call mld_precset(P,'SUB_OVR',2,info)
  call mld_precbld(A,desc_A,P,info)
... ...
```

Figure 6: Setup of a one-level Schwarz preconditioner.

6 User Interface

The basic user interface of MLD2P4 consists of six routines. The four routines `mld_precinit`, `mld_precset`, `mld_precbld` and `mld_precaply` encapsulate all the functionalities for the setup and the application of any one-level and multi-level preconditioner implemented in the package. The routine `mld_precfree` deallocates the preconditioner data structure, while `mld_precdescr` prints a description of the preconditioner setup by the user.

For each routine, the same user interface is overloaded with respect to the real/complex case and the single/double precision; arguments with appropriate data types must be passed to the routine, i.e.

- the sparse matrix data structure, containing the matrix to be preconditioned, must be of type `psb_`x`spmat_type` with x = `s` for real single precision, x = `d` for real double precision, x = `c` for complex single precision, x = `z` for complex double precision;
- the preconditioner data structure must be of type `mld_`x`prec_type`, with x = `s`, `d`, `c`, `z`, according to the sparse matrix data structure;
- the arrays containing the vectors v and w involved in the preconditioner application $w = M^{-1}v$ must be of type `psb_`x`vect_type` with x = `s`, `d`, `c`, `z`, in a manner completely analogous to the sparse matrix type;
- real parameters defining the preconditioner must be declared according to the precision of the sparse matrix and preconditioner data structures (see Section 6.2).

A description of each routine is given in the remainder of this section.

6.1 Subroutine mld_precinit

```
mld_precinit(p,ptype,info)
mld_precinit(p,ptype,info,nlev)
```

This routine allocates and initializes the preconditioner data structure, according to the preconditioner type chosen by the user.

Arguments

`p` `type(mld_`x`prec_type), intent(inout)`.
The preconditioner data structure. Note that x must be chosen according to the real/complex, single/double precision version of MLD2P4 under use.

`ptype` `character(len=*), intent(in)`.
The type of preconditioner. Its values are specified in Table 1.
Note that the strings are case insensitive.

`info` `integer, intent(out)`.
Error code. If no error, 0 is returned. See Section 7 for details.

`nlev` `integer, optional, intent(in)`.
The number of levels of the multilevel preconditioner. This optional argument is deprecated, new codes should set the number of levels with `mld_precset`.

6.2 Subroutine mld_precset

```
call mld_precset(p,what,val,info)
```

This routine sets the parameters defining the preconditioner. More precisely, the parameter identified by `what` is assigned the value contained in `val`.

The routine may also be invoked as a method of the preconditioner object as in the following:

```
call p%set(what,val,info [,ilev, pos])
```

In this case it is also possible to specify an optional `ilev` argument that restricts the effect of the call to the specified level.

Finally, if the user has developed a new type of smoother and/or solver by extending one of the base MLD2P4 types, and has declared a variable of the new type in the main program, it is possible to pass the new smoother/solver variable to the setup routine as follows:

```
call p%set(smoother,info [,ilev ,pos])
 call p%set(solver,info [,ilev ,pos])
```

In this way, the variable will act as a *mold* to which the preconditioner will conform, even though the MLD2P4 library is not modified, and thus has no direct knowledge about the new type.

Arguments

`p` `type(mld_`*x*`prec_type), intent(inout).`
The preconditioner data structure. Note that *x* must be chosen according to the real/complex, single/double precision version of MLD2P4 under use.

`what` `integer, intent(in)` *or* `character(len=*).`
The parameter to be set. It can be specified by a predefined constant, or through its name; the string is case-insensitive. See also Tables 2-6.

`val` `integer` *or* `character(len=*)` *or* `real(psb_spk_)` *or* `real(psb_dpk_), intent(in).`
The value of the parameter to be set. The list of allowed values and the corresponding data types is given in Tables 2-6. When the value is of type `character(len=*)`, it is also treated as case insensitive.

`smootherclass(mld_x_base_smoother_type)`
The user-defined new smoother to be employed in the preconditioner.

`solver` `class(mld_x_base_solver_type)`
The user-defined new solver to be employed in the preconditioner.

`info` `integer, intent(out).`
Error code. If no error, 0 is returned. See Section 7 for details.

`pos` `charater(len=*), intent(in).`
Whether the other arguments apply to the `'PRE'` or to the `'POST'` smoothers.

A variety of (one-level and multi-level) preconditioners can be obtained by a suitable setting of the preconditioner parameters. These parameters can be logically divided into four groups, i.e. parameters defining

1. the type of multi-level preconditioner;
2. the one-level preconditioner used as smoother;
3. the aggregation algorithm;
4. the coarse-space correction at the coarsest level.

A list of the parameters that can be set, along with their allowed and default values, is given in Tables 2-6. For a detailed description of the meaning of the parameters, please refer to Section 4.

The smoother and solver objects are arranged in a hierarchical manner; when specifying a smoother object, its parameters including the contained solver are set to default values, and when a solver object is specified its defaults are also set, overriding in both cases any previous settings even if explicitly specified. Therefore if the user sets a new smoother, and wishes to use a solver different from the default one, the call to set the solver must come *after* the call to set the smoother.

The combination of a Jacobi smoother with a Diagonal Scaling local solver is equivalent to the strategy called Point Jacobi in the literature; similarly, having a Jacobi smoother with a Gauss-Seidel local solver is equivalent to a "hybrid Gauss-Seidel" solver.

Completely new smoother and/or solver class derived from the base objects in the library may be used without recompiling the library itself. Once the new smoother/solver class has been developed, the user can declare a variable of that new type in the application, and pass that variable to the `p%set(solver,info)` call; the new solver object is then dynamically included in the preconditioner structure.

The `what,val` pairs described here are those of the predefined smoother/solver objects; newly developed solvers may define new pairs according to their needs.

what	DATA TYPE	val	DEFAULT	COMMENTS
mld_ml_type_ ML_TYPE	character(len=*)	'ADD' 'MULT'	'MULT'	Basic multi-level framework: additive or multiplicative among the levels (always additive inside a level).
mld_smoother_type_ SMOOTHER_TYPE	character(len=*)	'JACOBI' 'BJAC' 'AS'	'AS'	Basic predefined one-level preconditioner (i.e. smoother): Jacobi, block Jacobi, AS.
mld_smoother_pos_ SMOOTHER_POS	character(len=*)	'PRE' 'POST' 'TWOSIDE'	'TWOSIDE'	"Position" of the smoother: pre-smoother, post-smoother, pre- and post-smoother.

Table 2: Parameters defining the type of multi-level preconditioner.

what	DATA TYPE	val	DEFAULT	COMMENTS
mld_sub_ovr_ SUB_OVR	integer	any int. num. ≥ 0	1	Number of overlap layers.
mld_sub_restr_ SUB_RESTR	character(len=*)	'HALO' 'NONE'	'HALO'	Type of restriction operator: 'HALO' for taking into account the overlap, 'NONE' for neglecting it.
mld_sub_prol_ SUB_PROL	character(len=*)	'SUM' 'NONE'	'NONE'	Type of prolongation operator: 'SUM' for adding the contributions from the overlap, 'NONE' for neglecting them.
mld_sub_solve_ SUB_SOLVE	character(len=*)	'DIAG' 'GS' 'BWGS' 'ILU' 'MILU' 'ILUT' 'UMF' 'SLU' 'MUMPS'	'ILU'	Predefined local solver: pointwise Jacobi (diagonal scaling), (forward) Gauss-Seidel, Backward Gauss-Seidel, ILU(p), MILU(p), ILU(p,t), LU from UMFPACK, LU from SuperLU (plus triangular solve), LU from MUMPS.
mld_sub_fillin_ SUB_FILLIN	integer	Any int. num. ≥ 0	0	Fill-in level p of the incomplete LU factorizations.
mld_sub_iluthrs_ SUB_ILUTHRS	real(*kind_parameter*)	Any real num. ≥ 0	0	Drop tolerance t in the ILU(p,t) factorization.
mld_sub_ren_ SUB_REN	character(len=*)	'RENUM_NONE' 'RENUM_GLOBAL'	'RENUM_NONE'	Row and column reordering of the local submatrices: no reordering, reordering according to the global numbering of the rows and columns of the whole matrix.
mld_solver_sweeps_ SOLVER_SWEEPS	integer	Any int. num. ≥ 1	1	Number of sweeps for iterative local solver (currently only Gauss-Seidel).

Table 3: Parameters defining the one-level preconditioner used as smoother.

what	DATA TYPE	val	DEFAULT	COMMENTS
mld_coarse_aggr_size_ COARSE_AGGR_SIZE	integer	A positive number	The cubic root of the matrix size at the fine level.	Coarse size threshold. Aggregation will proceed until either the global number of variables is below this threshold, or the aggregation does not reduce the size any longer, or the maximum number of levels is reached.
mld_min_aggr_ratio MIN_AGGR_RATIO	real	A number greater than one	1.5	Minimum aggregation ratio. Aggregation will stop if the ratio between the matrix sizes at two consecutive levels drops below this threshold.
mld_n_prec_levs_ N_PREC_LEVS	integer	A number greater than 1, or -1.	-1	Number of levels; if set to a positive number greater than 1, it will force the aggregation algorithm to use this many levels (unless there is no reduction in the coarse matrix size).
mld_max_prec_levs_ MAX_PREC_LEVS	integer	A positive number	20	Maximum number of levels: irrespective of the other settings, do not use more than this many levels.
mld_aggr_alg_ AGGR_ALG	character(len=*)	'DEC', 'SYMDEC'	'DEC'	Aggregation algorithm. Currently, only the decoupled aggregation is available; the SYMDEC option applies decoupled aggregation to the sparsity pattern of $A + A^T$.
mld_aggr_ord_ AGGR_ORD	character(len=*)	'NATURAL'	'DEGREE'	Initial ordering of indices for aggregation algorithm: natural ordering or sorted by descending degree of the node in the matrix graph. Since aggregation is heuristics, results will be different.

Table 4: Parameters defining the aggregation algorithm.

what	DATA TYPE	val	DEFAULT	COMMENTS
mld_aggr_kind_ AGGR_KIND	character(len=*)	'SMOOTHED' 'NONSMOOTHED'	'SMOOTHED'	Type of aggregation: smoothed, nonsmoothed (i.e. using the tentative prolongator).
mld_aggr_thresh_ AGGR_THRESH	real(*kind_parameter*)	Any real num. $\in [0,1]$	0.05	Threshold θ in the aggregation algorithm.
mld_aggr_scale_ AGGR_SCALE	real(*kind_parameter*)	Any real num. $\in [0,1]$	1.0	Scale factor applied to the threshold going from level *ilev* to level *ilev*+1.
mld_aggr_omega_alg_ AGGR_OMEGA_ALG	character(len=*)	'EIG_EST' 'USER_CHOICE'	'EIG_EST'	How the damping parameter ω in the smoothed aggregation should be computed: either via an estimate of the spectral radius of $D^{-1}A$, or explicily specified by the user.
mld_aggr_eig_ AGGR_EIG	character(len=*)	'A_NORMI'	'A_NORMI'	How to estimate the spectral radius of $D^{-1}A$. Currently only the infinity norm estimate is available.
mld_aggr_omega_val_ AGGR_OMEGA_VAL	real(*kind_parameter*)	Any nonnegative real num.	$4/(3\rho(D^{-1}A))$	Damping parameter ω in the smoothed aggregation algorithm. It must be set by the user if USER_CHOICE was specified for mld_aggr_omega_alg_, otherwise it is computed by the library, using the selected estimate of the spectral radius $\rho(D^{-1}A)$ of $D^{-1}A$.

Table 5: Parameters defining the aggregation algorithm.

what	DATA TYPE	val	DEFAULT	COMMENTS
mld_coarse_mat_ COARSE_MAT	character(len=*)	'DISTR' 'REPL'	'DISTR'	Coarsest matrix: distributed among the processors or replicated on each of them.
mld_coarse_solve_ COARSE_SOLVE	character(len=*)	'BJAC' 'UMF' 'MUMPS' 'SLU' 'SLUDIST'	'BJAC'	Solver used at the coarsest level: block Jacobi, sequential LU from UMFPACK, sequential LU from SuperLU, distributed LU from SuperLU_Dist or MUMPS. 'SLUDIST' and 'MUMPS' require the coarsest matrix to be distributed, while 'UMF' and 'SLU' require it to be replicated.
mld_coarse_subsolve_ COARSE_SUBSOLVE	character(len=*)	'ILU' 'MILU' 'ILUT' 'UMF' 'SLU' 'MUMPS'	See note	Solver for the diagonal blocks of the coarse matrix, in case the block Jacobi solver is chosen as coarsest-level solver: ILU(p), MILU(p), ILU(p,t), LU from UMFPACK, LU from SuperLU, plus triangular solve.
mld_coarse_sweeps_ COARSE_SWEEPS	integer	Any int. num. > 0	4	Number of Block-Jacobi sweeps when 'BJAC' is used as coarsest-level solver.
mld_coarse_fillin_ COARSE_FILLIN	integer	Any int. num. ≥ 0	0	Fill-in level p of the incomplete LU factorizations.
mld_coarse_iluthrs_ COARSE_ILUTHRS	real(*kind_parameter*)	Any real. num. ≥ 0	0	Drop tolerance t in the ILU(p,t) factorization.
Note: defaults for mld_coarse_subsolve_ are chosen as single precision version: 'MUMPS' if installed, 'SLU' if installed, 'ILU' otherwise double precision version: 'MUMPS' if installed, 'UMF' if installed, else 'SLU' if installed, 'ILU' otherwise				

Table 6: Parameters defining the coarse-space correction at the coarsest level.

6.3 Subroutine mld_precbld

```
mld_precbld(a,desc_a,p,info)
```

This routine builds the preconditioner according to the requirements made by the user through the routines `mld_precinit` and `mld_precset`.

For multilevel preconditioner this routine is supported for backward compatibility, but we recommend to use the routines of Sec. 6.4 and 6.5.

Arguments

`a`	`type(psb_`x`spmat_type), intent(in).` The sparse matrix structure containing the local part of the matrix to be preconditioned. Note that x must be chosen according to the real/complex, single/double precision version of MLD2P4 under use. See the PSBLAS User's Guide for details [16].
`desc_a`	`type(psb_desc_type), intent(in).` The communication descriptor of `a`. See the PSBLAS User's Guide for details [16].
`p`	`type(mld_`x`prec_type), intent(inout).` The preconditioner data structure. Note that x must be chosen according to the real/complex, single/double precision version of MLD2P4 under use.
`info`	`integer, intent(out).` Error code. If no error, 0 is returned. See Section 7 for details.

6.4 Subroutine mld_hierarchy_bld

```
mld_hierachy_bld(a,desc_a,p,info)
```

This routine builds the aggregation hierarchy according to the requirements made by the user through the routines `mld_precinit` and `mld_precset`.

Arguments

`a` `type(psb_`x`spmat_type), intent(in).`
The sparse matrix structure containing the local part of the matrix to be preconditioned. Note that x must be chosen according to the real/complex, single/double precision version of MLD2P4 under use. See the PSBLAS User's Guide for details [16].

`desc_a` `type(psb_desc_type), intent(in).`
The communication descriptor of `a`. See the PSBLAS User's Guide for details [16].

`p` `type(mld_`x`prec_type), intent(inout).`
The preconditioner data structure. Note that x must be chosen according to the real/complex, single/double precision version of MLD2P4 under use.

`info` `integer, intent(out).`
Error code. If no error, 0 is returned. See Section 7 for details.

6.5 Subroutine mld_ml_prec_bld

```
mld_ml_prec_bld(a,desc_a,p,info)
```

This routine builds the preconditioner according to the requirements made by the user through the routines `mld_precinit` and `mld_precset`, based on the aggregation hierahy produced by a previous call to `mld_hierarchy_bld` (see Sec. 6.4).

Arguments

`a` `type(psb_`x`spmat_type), intent(in).`
The sparse matrix structure containing the local part of the matrix to be preconditioned. Note that x must be chosen according to the real/complex, single/double precision version of MLD2P4 under use. See the PSBLAS User's Guide for details [16].

`desc_a` `type(psb_desc_type), intent(in).`
The communication descriptor of `a`. See the PSBLAS User's Guide for details [16].

`p` `type(mld_`x`prec_type), intent(inout).`
The preconditioner data structure. Note that x must be chosen according to the real/complex, single/double precision version of MLD2P4 under use.

`info` `integer, intent(out).`
Error code. If no error, 0 is returned. See Section 7 for details.

6.6 Subroutine mld_precaply

```
mld_precaply(p,x,y,desc_a,info)
mld_precaply(p,x,y,desc_a,info,trans,work)
```

This routine computes $y = op(M^{-1})\,x$, where M is a previously built preconditioner, stored into `p`, and op denotes the preconditioner itself or its transpose, according to the value of `trans`. Note that, when MLD2P4 is used with a Krylov solver from PSBLAS, `mld_precaply` is called within the PSBLAS routine `psb_krylov` and hence it is completely transparent to the user.

Arguments

`p` `type(mld_`x`prec_type), intent(inout).`
The preconditioner data structure, containing the local part of M. Note that x must be chosen according to the real/complex, single/double precision version of MLD2P4 under use.

`x` *type*`(`*kind_parameter*`), dimension(:), intent(in).`
The local part of the vector x. Note that *type* and *kind_parameter* must be chosen according to the real/complex, single/double precision version of MLD2P4 under use.

`y` *type*`(`*kind_parameter*`), dimension(:), intent(out).`
The local part of the vector y. Note that *type* and *kind_parameter* must be chosen according to the real/complex, single/double precision version of MLD2P4 under use.

`desc_a` `type(psb_desc_type), intent(in).`
The communication descriptor associated to the matrix to be preconditioned.

`info` `integer, intent(out).`
Error code. If no error, 0 is returned. See Section 7 for details.

`trans` `character(len=1), optional, intent(in).`
If `trans` = `'N','n'` then $op(M^{-1}) = M^{-1}$; if `trans` = `'T','t'` then $op(M^{-1}) = M^{-T}$ (transpose of M^{-1}); if `trans` = `'C','c'` then $op(M^{-1}) = M^{-C}$ (conjugate transpose of M^{-1}).

`work` *type*`(`*kind_parameter*`), dimension(:), optional, target.`
Workspace. Its size should be at least `4 * psb_cd_get_local_cols(desc_a)` (see the PSBLAS User's Guide). Note that *type* and *kind_parameter* must be chosen according to the real/complex, single/double precision version of MLD2P4 under use.

6.7 Subroutine mld_precfree

```
mld_precfree(p,info)
```

This routine deallocates the preconditioner data structure.

Arguments

`p` `type(mld_`x`prec_type), intent(inout)`.
The preconditioner data structure. Note that x must be chosen according to the real/complex, single/double precision version of MLD2P4 under use.

`info` `integer, intent(out)`.
Error code. If no error, 0 is returned. See Section 7 for details.

6.8 Subroutine mld_precdescr

```
mld_precdescr(p,info)
mld_precdescr(p,info,iout)
```

This routine prints a description of the preconditioner to the standard output or to a file. It must be called after `mld_precbld` has been called.

Arguments

`p` `type(mld_`x`prec_type), intent(in)`.
The preconditioner data structure. Note that x must be chosen according to the real/complex, single/double precision version of MLD2P4 under use.

`info` `integer, intent(out)`.
Error code. If no error, 0 is returned. See Section 7 for details.

`iout` `integer, intent(in), optional`.
The id of the file where the preconditioner description will be printed; the default is the standard output.

7 Error Handling

The error handling in MLD2P4 is based on the PSBLAS (version 2) error handling. Error conditions are signaled via an integer argument `info`; whenever an error condition is detected, an error trace stack is built by the library up to the top-level, user-callable routine. This routine will then decide, according to the user preferences, whether the error should be handled by terminating the program or by returning the error condition to the user code, which will then take action, and whether an error message should be printed. These options may be set by using the PSBLAS error handling routines; for further details see the PSBLAS User's Guide [16].

A License

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