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 required 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 has been designed employing object-oriented techniques, using Fortran 95, with interfaces to additional third party libraries such as UMFPACK, SuperLU and SuperLU Dist, 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 [\[20\]](#page-39-0), 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 [\[1,](#page-38-1) [24\]](#page-39-1).

The package is written in Fortran 95, following an object-oriented approach 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 frame-work [\[15\]](#page-39-2). 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 recent PSBLAS 2.0 version [\[14\]](#page-39-3). The inter-process comunication required by MLD2P4 is encapsulated into the PSBLAS routines, except few cases where MPI [\[21\]](#page-39-4) 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.

This guide is organized as follows. General information on the distribution of the source code is reported in Section [2,](#page-8-0) while details on the configuration and installation of the package are given in Section [3.](#page-9-0) A description of multi-level Schwarz preconditioners based on smoothed aggregation is provided in Section [4,](#page-14-0) 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,](#page-20-0) where the Fortran 95 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.](#page-25-0) The error handling mechanism used by the package is briefly described in Section [7.](#page-36-0) The copyright terms concerning the distribution and modification of MLD2P4 are reported in Appendix [A.](#page-37-0)

2 Code Distribution

MLD2P4 is available from the web site

http://www.mld2p4.it

where contact points for further information can be also found. To report bugs or ask general usage questions, please, send an email to bugreport@mld2p4.it.

The software is available under a modified BSD license, as specified in Appendix [A;](#page-37-0) 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.

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 95, with some interfaces to external libraries in C; the Fortran compiler must support the Fortran 95 standard plus the extension TR15581, which enhances the usability of ALLOCATABLE variables. Most modern Fortran compilers support this language level. In particular, this is supported by the GNU Fortran compiler as of version 4.2.0; however we recommend to use the latest available release (4.3.1 at the time of this writing). 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 The Basic Linear Algebra subprograms [\[10,](#page-38-2) [10,](#page-38-2) [17\]](#page-39-5). Many vendors provide optimized versions; 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 computation 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 A version of MPI [\[16,](#page-39-6) [21\]](#page-39-4) is available on most high performance computing system; only version 1.1 is required.
- BLACS The Basic Linear Algebra Communication Subroutines [\[12\]](#page-38-3) are available in source form from http://www.netlib.org/blacs; some vendors include them in their parallel computing support libraries.
- PSBLAS Parallel Sparse BLAS [\[14,](#page-39-3) [15\]](#page-39-2) is available from
	- http://www.ce.uniroma2.it/psblas; indeed, all the prerequisites listed so far are also prerequisites of PSBLAS. Version 2.3 (or later) is required. To build the MLD2P4 library it is necessary to get access to the source PSBLAS directory employed to build the version under use; after the MLD2P4 build process completes, only the compiled form of the PSBLAS library is necessary to build user applications.

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 [\[8\]](#page-38-4) A sparse direct factorization package available from

http://www.cise.ufl.edu/research/sparse/umfpack/; provides serial factorization and triangular system solution for double precision real and complex data. We have tested versions 4.4 and 5.1;

- SuperLU [\[9\]](#page-38-5) 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 versions 3.0 and 3.1.
- SuperLU Dist [\[18\]](#page-39-7) 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 2.1.

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=/home/user/PSBLAS/psblas-2.3
```
which assumes that the various MPI compilers and support libraries are available in the standard directories on the system, and specifies only the PSBLAS build 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 --help
'configure' configures MLD2P4 1.0 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 Packages:
 --with-PACKAGE[=ARG] use PACKAGE [ARG=yes]
 --without-PACKAGE do not use PACKAGE (same as --with-PACKAGE=no)
```
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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

add
2p4.it>.

Thus, a sample build with libraries in installation directories specifics to the GNU 4.3 compiler suite might be as follows, specifying only the UMFPACK external package:

```
./configure --with-psblas=/home/user/psblas-2.3/ \
--with-libs="-L/usr/local/BLAS/gnu43 -L/usr/local/BLACS/gnu43" \
--with-blacs=-lmpiblacs --with-umfpackdir=/usr/local/UMFPACK/gnu43
```
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.

To build the library the user will now enter

make

followed (optionally) by

make install

3.4 Example and test programs

The package contains the examples and tests directories; both of them are further divided into fileread and pargen 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.
- test 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 pargen 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 $[6, 7, 20]$ $[6, 7, 20]$ $[6, 7, 20]$ $[6, 7, 20]$ $[6, 7, 20]$.

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., $[20]$). 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 [\[20\]](#page-39-0). The same reasoning can be applied starting from the coarselevel 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 [\[22\]](#page-39-8).

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 $[1, 24]$ $[1, 24]$ $[1, 24]$. A decoupled version of this algorithm is implemented, where the smoothed aggregation is applied locally to each submatrix $[23]$. 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 user is referred to [\[2,](#page-38-8) [3,](#page-38-9) [4,](#page-38-10) [20\]](#page-39-0).

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 [\(1\)](#page-6-1), where $A = (a_{ij}) \in \mathbb{R}^{n \times n}$ 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 $v \in \mathbb{R}^n$ onto the vector $v_i^{\delta} \in \mathbb{R}^{n_i^{\delta}}$ containing the components of v corresponding to the vertices in W_i^{δ} . The transpose of R_i^{δ} is a prolongation operator from $\mathbb{R}^{n_i^{\delta}}$ to \mathbb{R}^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 $v \in \mathbb{R}^n$ 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 $ILU(p,t)$ [\[19,](#page-39-10) Chapter 10].

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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 $[5, 13]$ $[5, 13]$ $[5, 13]$. 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 $(\tilde{R}_i^0)^T \in \mathbb{R}^{n_i^{\delta} \times n}$, 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 $[7, 20]$ $[7, 20]$ $[7, 20]$. 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 a Galerkin approach. Given a set W_C of *coarse vertices*, with size n_C , and a suitable restriction operator $R_C \in \mathbb{R}^{n_C \times n}$, 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} :

$$
w = M_{1L}^{-1}v,
$$

\n
$$
z = w + M_C^{-1}(v - Aw);
$$

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

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

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

$$
w = M_C^{-1} v,
$$

\n
$$
z = w + M_{1L}^{-1} (v - Aw),
$$

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

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

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 [\[20,](#page-39-0) 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 [\[20,](#page-39-0) 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.](#page-18-0) 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 $A_1 = A$.

4.2 Smoothed Aggregation

In order to define the restriction operator R_C , which is used to compute the coarselevel matrix A_C , MLD2P4 uses the *smoothed aggregation* algorithm described in [\[1,](#page-38-1) [24\]](#page-39-1). 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 coarseto-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:

1. coarsening of the vertex set W , to obtain W_C ;

```
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_ly_l = y_l + r_lendfor
w = y_1;
```
Figure 1: Application of the multi-level hybrid post-smoothed preconditioner.

- 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 $[24]$, 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.

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

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 [\[3,](#page-38-9) [4,](#page-38-10) [23\]](#page-39-9).

The prolongator $P_C = R_C^T$ is built starting from a *tentative prolongator* $P \in \mathbb{R}^{n \times n_C}$, 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 $S \in \mathbb{R}^{n \times n}$:

$$
P_C = SP,\t\t(3)
$$

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 [\[1,](#page-38-1) [22\]](#page-39-8). 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 $D^{-1}A$ [\[1\]](#page-38-1).

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 [\[14\]](#page-39-3). The following steps are required:

- 1. Declare the preconditioner data structure. It is a derived data type, mld_xprec 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,](#page-21-0) 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 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;](#page-22-0) a complete list of all the preconditioner parameters and their allowed and default values is provided in Section [6,](#page-25-0) Tables [2-](#page-28-0)[5.](#page-31-0)
- 4. Build the preconditioner for a given matrix. This is performed by the routine mld_precbld.
- 5. 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).
- 6. 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.](#page-25-0) Examples showing the basic use of MLD2P4 are reported in Section [5.1.](#page-22-0)

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\)](#page-22-0).

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 multilevel Schwarz preconditioners [\[3,](#page-38-9) [4\]](#page-38-10). 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](#page-25-0) for the coarsest-level solvers available in MLD2P4).

Remark 2. The include path for MLD2P4 must override those for PSBLAS, e.g. the latter must come first in the sequence passed to the compiler, as the MLD2P4 version of the Krylov solver interfaces must override that of PSBLAS. This will change in the future when the support for the class statement becomes widespread in Fortran compilers.

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 (ad-
		ditive on the same level and mul-
		tiplicative through the levels), with
		post-smoothing only. Number of lev-
		Post-smoother: RAS with els: 2.
		overlap 1 and $ILU(0)$ on the local
		blocks. Aggregation: smoothed aggre-
		gation with threshold $\theta = 0$. Coarsest
		matrix: distributed among the proces-
		sors. Coarsest-level solver: 4 sweeps
		of the block-Jacobi solver, with LU
		(or ILU) factorization of the blocks
		(UMFPACK for the double precision
		versions and SuperLU for the single
		precision ones, if they have been in-
		stalled; $ILU(0)$, otherwise).

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

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5.1 Examples

The code reported in Figure [2](#page-23-0) shows how to set and apply the default multi-level preconditioner available in the real double precision version of MLD2P4 (see Table [1\)](#page-21-0). 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 [3.4\)](#page-13-0). For details on the use of the PSBLAS routines, see the PSBLAS User's Guide [\[14\]](#page-39-3).

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](#page-25-0) 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](#page-24-0) shows how to set a three-level hybrid Schwarz preconditioner, which uses block Jacobi with ILU(0) 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 [\[8\]](#page-38-4). 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 [4](#page-24-1) 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-](#page-28-0)[5\)](#page-31-0). 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-](#page-24-0)[4](#page-24-1) are included in the example program file mld_dexample_ml.f90 too.

Finally, Figure [5](#page-24-2) 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.

```
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
 real(kind(1.d0)) :: 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 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_precbld(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.

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... ...

Remark 3. Any PSBLAS-based program using the basic preconditioners implemented in PSBLAS 2.0, i.e. the diagonal and block-Jacobi ones, can use the diagonal and block-Jacobi preconditioners implemented in MLD2P4 without any change in the code. The PSBLAS-based program must be only recompiled and linked to the MLD2P4 library.

```
... ...
! 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,nlev=3)
 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_,'UMF',info)
... ...
```
Figure 3: 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_precset(P,mld_ml_type_,'ADD',info)
 call_mld_precset(P,mld_smoother_pos_,'TWOSIDE',info)
 call mld_precset(P,mld_coarse_sweeps_,5,info)
... ...
```
Figure 4: 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,mld_sub_ovr_,2,info)

Figure 5: 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 mld_xspmat_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 type (kind parameter), with type = real, complex and kind parameter = kind(1.e0), kind(1.d0), according to the sparse matrix and preconditioner data structure; note that the PSBLAS module psb_base_mod provides the constants $psb_spk = kind(1.e0)$ and $psb_dpk = kind(1.d0)$;
- real parameters defining the preconditioner must be declared according to the precision of the sparse matrix and preconditioner data structures (see Section [6.2\)](#page-27-0).

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

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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.

6.2 Subroutine mld precset

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.

Arguments

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-](#page-28-0)[5.](#page-31-0) For a detailed description of the meaning of the parameters, please refer to Section [4.](#page-14-0)

[6](#page-25-0) USER INTERFACE 25

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.

6.4 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 mld_krylov and hence it is completely transparent to the user.

6.5 Subroutine mld precfree

mld_precfree(p,info)

This routine deallocates the preconditioner data structure.

6.6 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.

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 [\[14\]](#page-39-3).

A License

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MLD2P4 version 1.0 MultiLevel Domain Decomposition Parallel Preconditioners Package based on PSBLAS (Parallel Sparse BLAS version 2.3)

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