MLD2P4 User's and Reference Guide

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

Pasqua D'Ambra ICAR-CNR, Naples, Italy

Daniela di Serafino Second University of Naples, Italy

Salvatore Filippone University of Rome "Tor Vergata", Italy

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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 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

1 General Overview

The Multi-Level Domain Decomposition Parallel Preconditioners Package based on PSBLAS (MLD2P4) provides multi-level Schwarz preconditioners [22], to be used in the iterative solutions of sparse linear systems:

$$Ax = b, (1)$$

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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, 26].

Version 2.0 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 [17, 16]. 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 [15]. The inter-process comunication required by MLD2P4 is encapsulated into the PSBLAS routines, except few cases where MPI [23] 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 2.0 is essentially identical 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 3.0.

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 3

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 2.0.0

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 4.7.2. 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 [11, 12, 19] 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 [18, 23] A version of MPI is available on most high-performance computing systems;

PSBLAS [15, 17] Parallel Sparse BLAS is available from

http://www.ce.uniroma2.it/psblas; version 3.3 (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 factorization and triangular system solution for double precision real and complex data. We have tested versions 5.4.

SuperLU [10] 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.

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
                        display the short help of all the included packages
   --help=recursive
                        display version information and exit
-V, --version
-q, --quiet, --silent
                        do not print 'checking...' messages
                        cache test results in FILE [disabled]
   --cache-file=FILE
-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-umfpack=LIBNAME Specify the library name for UMFPACK library.

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 3.3 under the /opt directory and is using the SuiteSparse package (which includes UMFPACK), then MLD2P4 might be configured with:

```
./configure --with-psblas=/opt/psblas-3.3/ \
--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 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.

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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, 22].

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., [22]). 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 [22]. 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 [24].

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, 26]. A decoupled version of this algorithm is implemented, where the smoothed aggregation is applied locally to each submatrix [25]. 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, 22].

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 $\cup_{i=1}^mW_i^0=W$, 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 $v_i = R_i^{\delta} v$, $i = 1, \dots, m$;
- 2. solution of the linear systems $A_i^{\delta} w_i = v_i, i = 1, \dots, m$;
- 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) [21, 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, 14]. 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, 22]. 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} :

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

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

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

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

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

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 [22, 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 [22, 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 coarselevel matrix A_C , MLD2P4 uses the *smoothed aggregation* algorithm described in [1, 26]. 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:

```
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 [26], 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, 4, 25].

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

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

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

$$P_C = SP, (3)$$

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, 24]. 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 [15]. 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, 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; a complete list of all the preconditioner parameters and their allowed and default values is provided in Section 6, Tables 2-5.
- 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. 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).

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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).

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 over-
		lap 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 post-smoothing only. Number of
		levels: 2. Post-smoother: RAS with overlap 1
		and ILU(0) on the local blocks. Aggregation:
		decoupled smoothed aggregation with thresh-
		old $\theta = 0$. Coarsest matrix: distributed among
		the processors. Coarsest-level solver: 4 sweeps
		of the block-Jacobi solver, with LU or ILU fac-
		torization of the blocks (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.

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 [15].

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) 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]. 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 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 2-5). 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 Figures 3-4 are included in the example program file mld_dexample_ml.f90 too.

Finally, Figure 5 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.

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```
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)
  . . . . . .
Ţ
! 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.

```
! 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.

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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_xspmat_type with x = s for real single precision, x = d for real double precision, x = c for complex single precision, x = c for complex double precision;
- the preconditioner data structure must be of type mld_xprec_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_xvect_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_xprec_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. If nlev is not present and ptype='ML', 'ml', then nlev=2 is assumed. Otherwise, nlev is ignored.

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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])
```

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

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_xprec_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 2-5.

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 2-5. 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.

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 2-5. 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. 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	DEFAULT COMMENTS
mld_ml_type_	character(len=*)	'ADD'	, MOLT,	Basic multi-level framework: additive or
ML_TYPE		, MULT,		multiplicative among the levels (always additive inside a level).
mld_smoother_type_	character(len=*)	'DIAG'	'AS'	Basic predefined one-level preconditioner
SMOOTHER_TYPE		'BJAC'		(i.e. smoother): diagonal, block Jacobi,
		'AS'		AS.
mld_smoother_pos_	character(len=*)	'PRE'	'POST'	"Position" of the smoother: pre-smoother,
SMOOTHER_POS		'POST'		post-smoother, pre- and post-smoother.
		'TWOSIDE'		

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

Row and column reordering of the local submatrices: no re- ordering, reordering according to the global numbering of the rows and columns of the whole matrix.	RENUM_NONE	RENUM_GLOBAL'	character(len=*)	mld_sub_ren_ SUB_REN
Drop tolerance t in the ILU (p,t) factorization.	0	Any real num. ≥ 0	real(kind_parameter)	mld_sub_iluthrs_ SUB_ILUTHRS
Fill-in level p of the incomplete LU factorizations.	0	Any int. num. ≥ 0	integer	mld_sub_fillin_ SUB_FILLIN
from SuperLU (plus triangular solve).		UMF'		
ILU (p) , MILU (p) , ILU (p,t) , LU from UMFPACK, LU		MILU,		SUB_SOLVE
Predefined local solver:	'ILU'	'ILU'	<pre>character(len=*)</pre>	mld_sub_solve_
tributions from the overlap, 'NONE' for neglecting them.				
Type of prolongation operator: 'SUM' for adding the con-	, NONE,	'SUM'	character(len=*)	mld_sub_prol_ SUB_PROL
neglecting it.				
		NONE		SUB_RESTR
Type of restriction operator:	'HALO'	'HALO'	<pre>character(len=*)</pre>	mld_sub_restr_
Number of overlap layers.	1	any int. num. ≥ 0	integer	mld_sub_ovr_ SUB_OVR
COMMENTS	DEFAULT	val	DATA TYPE	what

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

6	Us	ER	In	TE	RFA	ACI	3
mber	ntinue	global	r this	does		ently,	

what	DATA TYPE	val	DEFAULT	COMMENTS
mld_coarse_aggr_size_	integer	A positive	0, meaning	Coarse size threshold. Disregard
COARSE_AGGR_SIZE		number	that the size	the original specification of number
			is fixed at	of levels in precinit and continue
			precinit	aggregation until either the global
			time	number of variables is below this
				threshold, or the aggregation does
				not reduce the size any longer.
mld_aggr_alg_	character(len=*)	, DEC,	,DEC,	Aggregation algorithm. Currently,
AGGR_ALG				only the decoupled aggregation is
				available.
mld_aggr_kind_	character(len=*)	'SMOOTHED'	'SMOOTHED'	Type of aggregation: smoothed,
AGGR_KIND		'NONSMOOTHED'		nonsmoothed (i.e. using the tenta-
				tive prolongator).
mld_aggr_thresh_	real(kind_parameter)	Any real num.	0	Threshold θ in the aggregation algo-
AGGR_THRESH		$\in [0,1]$		rithm.
mld_aggr_omega_alg_	character(len=*)	'EIG_EST'	'EIG_EST'	How the damping parameter ω in
AGGR_OMEGA_ALG		'USER_CHOICE'		the smoothed aggregation should be
				computed: either via an estimate of
				the spectral radius of $D^{-1}A$, or ex-
				plicily specified by the user.
mld_aggr_eig_	character(len=*)	'A_NORMI'	'A_NORMI'	How to estimate the spectral radius
AGGR_EIG				of $D^{-1}A$. Currently only the infin-
				ity norm estimate is available.
mld_aggr_omega_val_	real(kind_parameter)	Any nonnega-	$4/(3\rho(D^{-1}A))$	Damping parameter ω in the
AGGR_OMEGA_VAL		tive real num.		smoothed aggregation algorithm.
				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 4: Parameters defining the aggregation algorithm.

		sen as	Note: defaults for mid_coarse_subsolve_ are chosen as single precision version: 'SLII' if installed 'ILII' otherwise	Note: defaults for mld single precision version
				COARSE_ILUTHRS
Drop tolerance t in	0	Any real. num. ≥ 0	_real(kind_parameter)	mld_coarse_iluthrs_
plete LU factorizations.				COARSE_FILLIN
Fill-in level p of the incom-	0	Any int. num. ≥ 0	integer	mld_coarse_fillin_
as coarsest-level solver.				COARSE_SWEEPS
whe		•	(
Number of Block-Jacobi	4	Any int. num. > 0	integer	mld_coarse_sweeps_
lar solve.				
from SuperLU, plus triangu-				
LU from UMFPACK,				
ILU(p), MILU(p), ILU(p,t),		SLU		
sen as coarsest-level solver:		'UMF'		
the block Jacobi solver is cho-		'ILUT'		COARSE_SUBSOLVE
of the coarse matrix, in case		MILU'		
Solver for the diagonal blocks	See note	'ILU'	e <u>c</u> haracter(len=*)	mld_coarse_subsolve_character(len=*)
replicated.				
and 'SLU' require it to be				
to be distributed, while 'UMF'				
requires the coarsest matrix				
perLU_Dist. 'SLUDIST'				
distributed LU from Su-				
sequential LU from SuperLU,		'SLUDIST'		
tial LU from UMFPACK,		SLU		COARSE_SOLVE
level: block Jacobi, sequen-		'UMF'		
Solver used at the coarsest	'BJAC'	'BJAC'	<pre>character(len=*)</pre>	mld_coarse_solve_
cated on each of them.				
among the processors or repli-		'REPL'		COARSE_MAT
Coarsest matrix: distributed	'DISTR'	DISTR'	<pre>character(len=*)</pre>	mld_coarse_mat_
COMMENTS	DEFAULT	Val	DATA TILE	200

Table 5: Parameters defining the coarse-space correction at the coarsest level.

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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.

Arguments

a type(psb_xspmat_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 [15].

desc_a type(psb_desc_type), intent(in).

The communication descriptor of a. See the PSBLAS User's Guide for details [15].

p type(mld_xprec_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_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_xprec_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.
- 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.

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6.5 Subroutine mld_precfree

mld_precfree(p,info)

This routine deallocates the preconditioner data structure.

Arguments

p type(mld_xprec_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_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_xprec_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 33

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 [15].

A License

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MLD2P4 version 2.0

MultiLevel Domain Decomposition Parallel Preconditioners Package based on PSBLAS (Parallel Sparse BLAS version 3.0)

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Salvatore Filippone University of Rome Tor Vergata
Alfredo Buttari CNRS-IRIT, Toulouse
Pasqua D'Ambra ICAR-CNR, Naples
Daniela di Serafino Second University of Naples

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