ML 3.0 Smoothed Aggregation User’s Guide

Marzio Sala
Computational Math & Algorithms
Sandia National Laboratories
P.O. Box 5800
Albuquerque, NM 87185-1110

Jonathan J. Hu and Ray S. Tuminaro
Computational Math & Algorithms
Sandia National Laboratories
P.O. Box 0969
Livermore, CA 94551-0969

Abstract

ML is a multigrid preconditioning package intended to solve linear systems of equations $Ax = b$ where $A$ is a user supplied $n \times n$ sparse matrix, $b$ is a user supplied vector of length $n$ and $x$ is a vector of length $n$ to be computed. ML should be used on large sparse linear systems arising from partial differential equation (PDE) discretizations. While technically any linear system can be considered, ML should be used on linear systems that correspond to things that work well with multigrid methods (e.g. elliptic PDEs). ML can be used as a stand-alone package or to generate preconditioners for a traditional iterative solver package (e.g. Krylov methods). We have supplied support for working with the Aztec 2.1 and Aztecoo iterative package [15]. However, other solvers can be used by supplying a few functions.

This document describes one specific algebraic multigrid approach: smoothed aggregation. This approach is used within several specialized multigrid methods: one for the eddy current formulation for Maxwell’s equations, and a multilevel and domain decomposition method for symmetric and nonsymmetric systems of equations (like elliptic equations, or compressible and incompressible fluid dynamics problems). Other methods exist within ML but are not described in this document. Examples are given illustrating the problem definition and exercising multigrid options.
Contents

1 Notational Conventions 8
2 Overview 8
3 Multigrid Background 8
4 Configuring and Building ML 9
  4.1 Building in Standalone Mode .......................... 10
  4.2 Building with AZTEC 2.1 Support .................. 10
  4.3 Building with TRILINOS Support (RECOMMENDED) .. 10
    4.3.1 Enabling Third Party Library Support .......... 11
    4.3.2 Enabling Profiling ............................. 12
5 ML and Epetra: Getting Started with the MultiLevelPreconditioner Class 13
  5.1 Example 1: ml_example_epetra_preconditioner.cpp .... 13
  5.2 Example 2: ml_example_epetra_preconditioner_2level.cpp 15
6 Parameters for the ML_Epetra::MultiLevelPreconditioner Class 16
  6.1 Setting Options on a Specific Level ................ 17
  6.2 General Usage of the Parameter List ................. 17
  6.3 Default Parameter Settings for Common Problem Types .. 18
  6.4 Commonly Used Parameters .......................... 20
  6.5 List of All Parameters for MultiLevelPreconditioner Class 20
    6.5.1 General Options .................................. 20
    6.5.2 Aggregation Parameters ......................... 22
    6.5.3 Smoothing Parameters ......................... 22
    6.5.4 Coarsest Grid Parameters .................... 23

7 Advanced Usage of ML 24
8 Multigrid & Smoothing Options 25
9 Smoothed Aggregation Options 27
  9.1 Aggregation Options ................................. 27
  9.2 Interpolation Options .............................. 28
10 Advanced Usage of ML and Epetra 29
11 Using ML without Epetra 30
  11.1 Creating a ML matrix: Single Processor .......... 30
  11.2 Creating a ML matrix: Multiple Processors ....... 32
12 Visualization Capabilities 35
13 ML Functions

AZ_ML_Set_Amat .................................................................................. 37
AZ_set_ML_preconditioner ................................................................ 37
ML_Aggregate_Create ........................................................................ 38
ML_Aggregate_Destroy ...................................................................... 38
ML_Aggregate_Set_CoarsenScheme_Coupled .................................... 39
ML_Aggregate_Set_CoarsenScheme_MIS ........................................... 39
ML_Aggregate_Set_CoarsenScheme_Uncoupled ................................ 40
ML_Aggregate_Set_CoarsenScheme_METIS ....................................... 40
ML_Aggregate_Set_CoarsenScheme_ParMETIS ................................. 41
ML_Aggregate_Set_DampingFactor .................................................. 41
ML_Aggregate_Set_MaxCoarseSize .................................................. 42
ML_Aggregate_Set_NullSpace ......................................................... 42
ML_Aggregate_Set_SpectralNormScheme_Calc ................................. 43
ML_Aggregate_Set_SpectralNormScheme_Anorm ............................. 43
ML_Aggregate_Set_Threshold ......................................................... 44
ML_Create ....................................................................................... 44
ML_Destroy ..................................................................................... 45
ML_Gen_Blocks_Aggregates ............................................................. 45
ML_Gen_Blocks_Metis ...................................................................... 46
ML_Gen_CoarseSolverSuperLU ....................................................... 46
ML_Gen_MGHierarchy_UsingAggregation ....................................... 47
ML_Gen_SmootherAmesos ............................................................... 48
ML_Gen_SmootherAztec .................................................................. 48
ML_Gen_Smoother_BlockGaussSeidel .............................................. 49
ML_Gen_Smoother_GaussSeidel ....................................................... 50
ML_Gen_Smoother_Jacobi ............................................................... 51
ML_Gen_Smoother_SymGaussSeidel ................................................. 52
ML_Gen_Smoother_VBlockJacobi ..................................................... 52
ML_Gen_Smoother_VBlockSymGaussSeidel .................................... 53
ML_Gen_Solver ................................................................................ 54
ML_Get_Amatrix ............................................................................... 55
ML_Get_MyGetrowData ................................................................... 55
ML_Get_MyMatvecData ................................................................... 56
ML_Get_MySmotherData .................................................................. 56
ML_Init_Amatrix .............................................................................. 57
ML_Iterate ....................................................................................... 58
ML_Operator_Apply .......................................................................... 58
ML_Operator_Get_Diag ................................................................... 59
ML_Operator_Getrow ...................................................................... 59
ML_Set_Amatrix_Getrow .................................................................. 60
ML_Set_Amatrix_Matvec ................................................................. 61
ML_Set_ResidualOutputFrequency .................................................. 61
ML_Set_Smoother ............................................................................ 62
ML_Set_Tolerance ............................................................................ 63
1 Notational Conventions

In this guide, we show typed commands in this font:

\%

a_really_long_command

The character \% indicates any shell prompt\. Function names are shown as \texttt{ML\_Gen\_Solver}. Names of packages or libraries as reported in small caps, as \texttt{EPETRA}. Mathematical entities are shown in italics.

2 Overview

This guide describes the use of an algebraic multigrid method within the \texttt{ML} package. The algebraic multigrid method can be used to solve linear system systems of type

\[
Ax = b
\]

where \(A\) is a user supplied \(n \times n\) sparse matrix, \(b\) is a user supplied vector of length \(n\) and \(x\) is a vector of length \(n\) to be computed. \texttt{ML} is intended to be used on (distributed) large sparse linear systems arising from partial differential equation (PDE) discretizations. While technically any linear system can be considered, \texttt{ML} should be used on linear systems that correspond to things that work well with multigrid methods (e.g. elliptic PDEs).

The \texttt{ML} package is used by creating a \texttt{ML} object and then associating a matrix, \(A\), and a set of multigrid parameters which describe the specifics of the solver. Once created and initialized, the \texttt{ML} object can be used to solve linear systems.

This manual is structured as follows. Multigrid and multilevel methods are briefly recalled in Section 3. The process of configuring and building \texttt{ML} is outlined in Section 4. Section 5 shows the basic usage of \texttt{ML} as a black-box preconditioner for \texttt{EPETRA} matrices. The definition of (parallel) preconditioners using \texttt{ML\_Epetra::MultiLevelPreconditioner} is detailed. This class only requires the linear system matrix, and a list of options. Available parameters for \texttt{ML\_Epetra::MultiLevelPreconditioner} are reported in Section 6. More advanced uses of \texttt{ML} are presented in Section 7. Here, we present how to define and fine-tune smoothers, coarse grid solver, and the multilevel hierarchy. Multigrid options are reported in Section 8. Smoothing options are reported in Section 9, where we also present how to construct a user’s defined smoother. Advanced usage of \texttt{ML} with \texttt{EPETRA} objects is reported in Section 10. Section 11 reports how to define matrices in \texttt{ML} format without depending on \texttt{EPETRA}. Section 12 details the (limited) visualization capabilities of \texttt{ML}.

3 Multigrid Background

A brief multigrid description is given (see \cite{1}, \cite{6}, or \cite{7} for more information). A multigrid solver tries to approximate the original PDE problem of interest on a hierarchy of grids and use ‘solutions’ from coarse grids to accelerate the convergence on the finest grid. A simple multilevel iteration is illustrated in Figure 1. In the above method, the \(S_k^1()\)'s and \(S_k^2()\)'s

\footnote{For simplicity, commands are shown as they would be issued in a Linux or Unix environment. Note, however, that \texttt{ML} has and can be built successfully in a Windows environment.}
/* Solve $A_k u = b$ (k is current grid level) */

proc multilevel($A_k$, $b$, $u$, $k$)

$u = S_1^k(A_k, b, u)$;

if ( $k \neq \text{Nlevel} - 1$ )

$P_k = \text{determine_interpolant}(A_k)$;

$\hat{r} = P_k^T(b - A_k u)$;

$A_{k+1} = P_k^T A_k P_k$; $v = 0$;

multilevel($A_{k+1}, \hat{r}, v, k + 1$);

$u = u + P_k v$;

$u = S_2^k(A_k, b, u)$;

Figure 1: High level multigrid V cycle consisting of ‘Nlevel’ grids to solve (1), with $A_0 = A$.

are approximate solvers corresponding to $k$ steps of pre and post smoothing, respectively. These smoothers are discussed in Section 8. For now, it suffices to view them as basic iterative methods (e.g. Gauss-Seidel) which effectively smooth out the error associated with the current approximate solution. The $P_k$’s (interpolation operators that transfer solutions from coarse grids to finer grids) are the key ingredient that are determined automatically by the algebraic multigrid method$^2$. For the purposes of this guide, it is important to understand that when the multigrid method is used, a hierarchy of grids, grid transfer operators ($P_k$), and coarse grid discretizations ($A_k$) are created. To complete the specification of the multigrid method, smoothers must be supplied on each level. There are several smoothers within ML or an iterative solver package can be used, or users can write their own smoother (see Section 8).

4 Configuring and Building ML

ML is configured and built using the GNU autoconf [4] and automake [5] tools. It can be configured and build as a standalone package without or with Aztec 2.1 support (as detailed in Section 4.1 and 4.2), or as a part of the Trilinos framework [8] (as described in Section 4.3). Even though ML can be compiled and used as a standalone package, the recommended approach is to build ML as part of the Trilinos framework, as a richer set of features are then available.

ML has been configured and built successfully on a wide variety of operating systems, and with a variety of compilers (as reported in Table 1).

<table>
<thead>
<tr>
<th>Operating System</th>
<th>Compilers(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Linux</td>
<td>GNU and Intel</td>
</tr>
<tr>
<td>IRIX N32, IRIX 64, HPUX, Solaris, DEC</td>
<td>Native</td>
</tr>
<tr>
<td>ASCI Red</td>
<td>Native and Portland Group</td>
</tr>
<tr>
<td>CPPlant</td>
<td>Native</td>
</tr>
<tr>
<td>Windows</td>
<td>Microsoft</td>
</tr>
</tbody>
</table>

Table 1: Main operating systems and relative compilers supported by ML.

$^2$The $P_k$’s are usually determined as a preprocessing step and not computed within the iteration.
Although it is possible to configure directly in the ML home directory, we strongly advise against this. Instead, we suggest working in an independent directory and configuring and building there.

4.1 Building in Standalone Mode

To configure and build ML as a standalone package without any Aztec support, do the following. It’s assumed that the shell variable $ML_HOME identifies the ML directory.

```bash
% cd $ML_HOME
% mkdir standalone
% cd standalone
% $ML_HOME/configure --disable-epetra --disable-aztecoo \
    --prefix=$ML_HOME/standalone
% make
% make install
```

The ML library file libml.a and the header files will be installed in the directory specified in --prefix.

4.2 Building with Aztec 2.1 Support

To enable the supports for Aztec 2.1, ML must be configured with the options reported in the previous section, plus --with-ml_aztec2_1 (defaulted to no).

All of the Aztec 2.1 functionality that ML accesses is contained in the file ml_aztec_utils.c. In principal by creating a similar file, other solver packages could work with ML in the same way. For the Aztec users there are essentially three functions that are important. The first is AZ_ML_Set_Amat which converts Aztec matrices into ML matrices by making appropriate ML calls (see Section 11.1 and Section 11.2). It is important to note that when creating ML matrices from Aztec matrices information is not copied. Instead, wrapper functions are made so that ML can access the same information as Aztec. The second is ML_Gen_SmootherAztec that is used for defining Aztec iterative methods as smoothers (discussed in Section 8 and Section 13). The third function, AZ_set_ML_preconditioner, can be invoked to set the Aztec preconditioner to use the multilevel ‘V’ cycle constructed in ML. Thus, it is possible to invoke several instances of Aztec within one solve: smoother on different multigrid levels and/or outer iterative solve.

4.3 Building with Trilinos Support (RECOMMENDED)

We recommend to configure and build ML as part of the standard Trilinos build and configure process. In fact, ML is built by default if you follow the standard Trilinos configure and build directions. Please refer to the Trilinos documentation for information about the configuration and building of other Trilinos packages.

To configure and build ML through Trilinos, you may need do the following (actual configuration options may vary depending on the specific architecture, installation, and user’s need). It’s assumed that shell variable $TRILINOS_HOME identifies the Trilinos directory, and, for example, that we are compiling under LINUX and MPI.
% cd $TRILINOS_HOME
% mkdir LINUX_MPI
% cd LINUX_MPI
% $TRILINOS_HOME/configure --with-mpi-compilers \
   --prefix=$TRILINOS_HOME/LINUX_MPI
% make
% make install

If required, other Trilinos and ML options can be specified in the configure line. A complete list of ML options is given in Section 4.3.1 and 4.3.2. You can also find a complete list and explanations by typing ./configure --help in the ML home directory.

4.3.1 Enabling Third Party Library Support

ML can be configured with the following third party libraries (TPLs): SUPERLU, SUPERLU_DIST, METIS, and PARMETIS. It can take advantage of the following Trilinos packages: Ifpack, Teuchos, Triutils, Amesos. Through Amesos, ML can interface with the direct solvers KLU, Umfpack, SuperLU, SuperLU_dist,3 Mumps. It is assumed that you have already built the appropriate libraries (e.g., libsuperlu.a) and have the header files. To configure ML with one of the above TPLs, you must enable the particular TPL interface in ML. All of the options below are disabled by default.

The same configure options that one uses to enable certain other Trilinos packages also enables the interfaces to those packages within ML:

--enable-epetra
   Enable support for the Epetra package.

--enable-aztecoo
   Enable support for the AztecOO package.

--enable-amesos
   Enables support for the Amesos package. Amesos is an interface with several direct solvers. ML supports Umfpack [2], KLU, SuperLU_dist (1.0 and 2.0), Mumps [14]. This package is used only in function ML_Gen_SmootherAmesos.

--enable-teuchos
   Enables support for the Teuchos package. This package is used only in the definition of class ML_Epetra::MultiLevelPreconditioner (see Section 5). and by the Amesos smoother

--enable-triutils
   Enables support for the Triutils package. ML uses Triutils only in some examples, to create the linear system matrix.

--enable-ifpack
   Enable support for the Ifpack package [9]. Ifpack is used only to create smoothers via ML_Gen_SmootherIfpack.

---

3Currently, ML can support SuperLU_DIST directly (without Amesos support), or through Amesos.
### --enable-anasazi
Enable support for the Anasazi package. Anasazi is a high level interface package for various eigenvalue computations.

The following configure line options enable interfaces in ML to certain TPLs.

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>--with-ml.mmetis</td>
<td>Enables interface for Metis [12].</td>
</tr>
<tr>
<td>--with-ml.parmetis2x</td>
<td>Enables interface for ParMETIS, version 2.x.</td>
</tr>
<tr>
<td>--with-ml.parmetis3x</td>
<td>Enables interface for ParMETIS [11], version 3.x.</td>
</tr>
<tr>
<td>--with-ml.superlu</td>
<td>Enables ML interface for serial SuperLU [3].</td>
</tr>
<tr>
<td>--with-ml.superlu_dist</td>
<td>Enables ML interface for SuperLU_dist [3]. The ML interface to SuperLU is deprecated in favor of the Amesos interface.</td>
</tr>
</tbody>
</table>

For Metis, ParMETIS, and the ML interface to SuperLU and SuperLU_dist, the user must specify the location of the header files, with the option

```
--with-incdirs=include-locations
```

(Header files for Trilinos libraries are automatically located if ML is built through the Trilinos configure.) In order to link the ML examples, the user must indicate the location of all the enabled packages’ libraries\(^4\), with the option

```
--with-ldflags=lib-locations
```

The user might find useful the option

```
--disable-examples
```

which turns off compilation and linking of the examples.

More details about the installation of Trilinos can be found at the Trilinos web site, http://software.sandia.gov/Trilinos and [10, Chapter 1].

### 4.3.2 Enabling Profiling

All of the options below are disabled by default.

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>--enable-ml.timing</td>
<td>This prints out timing of key ML routines.</td>
</tr>
<tr>
<td>--enable-ml.flops</td>
<td>This enables printing of flop counts.</td>
</tr>
</tbody>
</table>

Timing and flop counts are printed when the associated object is destroyed.

\(^4\)An example of configuration line that enables Metis and ParMETIS might be as follows:

```
./configure --with-mpi-compilers --enable-ml.mmetis --enable-ml.parmetis3x --with-cflags="-I$HOME/include"
--with-cppflags="-I$HOME/include" --with-ldflags="-L$HOME/lib/LINUX_MPI -lparmetis-3.1 -lmetis-4.0"
```

12
5 ML and Epetra: Getting Started with the MultiLevelPreconditioner Class

In this Section we show how to use ML as a preconditioner to Epetra and AztecOO through the MultiLevelPreconditioner class in the ML_Epetra namespace. Although limited to algebraic multilevel preconditioners, this allows the use of ML as a black-box preconditioner.

The MultiLevelPreconditioner class automatically constructs all the components of the preconditioner, using the parameters specified in a Teuchos parameter list. The constructor of this class takes as input an Epetra_RowMatrix pointer and a Teuchos parameter list.

In order to compile, it may also be necessary to include the following files: ml_config.h (as first ML include), Epetra_ConfigDefs.h (as first Epetra include), Epetra_RowMatrix.h, Epetra_MultiVector.h, Epetra_LinearProblem.h, and AztecOO.h. Check the Epetra and AztecOO documentation for more details. Additionally, the user must include the header file "ml_epetra_preconditioner.h". Also note that the macro HAVE_CONFIG_H must be defined either in the user’s code or as a compiler flag.

5.1 Example 1: ml_example_epetra_preconditioner.cpp

We now give a very simple fragment of code that uses the MultiLevelPreconditioner. For the complete code, see $ML_HOME/examples/ml_example_epetra_preconditioner.cpp. (In order to be effectively compiled, this example requires ML to be configured with option --enable-triutils; see Section 4.) The linear operator A is derived from an Epetra_RowMatrix, Solver is an AztecOO object, and Problem is an Epetra_LinearProblem object.

```cpp
#include "ml_include.h"
#include "ml_epetra_preconditioner.h"
#include "Teuchos_ParameterList.hpp"
...

Teuchos::ParameterList MList;

// set default values for smoothed aggregation in MLList
ML_Epetra::SetDefaults("SA",MList);

// overwrite with user’s defined parameters
MList.set("max levels",6);
MList.set("increasing or decreasing","decreasing");
MList.set("aggregation: type", "MIS");
MList.set("coarse: type", "Amesos-KLU");
```

---

5 The MultiLevelPreconditioner class is derived from the Epetra_RowMatrix class.
6 ML does not rely on any particular matrix format or iterative solver. Examples of using ML as a preconditioner for user-defined matrices (i.e., non-Epetra matrices) are reported in Section 11.1 and 11.2.
7 In order to use the MultiLevelPreconditioner class, ML must be configured with options --enable-epetra --enable-teuchos.
// create the preconditioner
ML_Epetra::MultiLevelPreconditioner * MLPrec =
    new ML_Epetra::MultiLevelPreconditioner(A, MLList, true);

// create an AztecOO solver
AztecOO Solver(Problem)

// set preconditioner and solve
Solver.SetPrecOperator(MLPrec);
Solver.SetAztecOption(AZ_solver, AZ_gmres);
Solver.Iterate(Niters, 1e-12);
...

delete MLPrec;

We now detail the general procedure to define the MultiLevelPreconditioner. First, the user
defines a Teuchos parameter list\(^8\). Table 2 briefly reports the most important methods of
this class.

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>set(Name,Value)</td>
<td>Add entry Name with value and type specified by Value. Any C++ type (like int, double, a pointer, etc.) is valid.</td>
</tr>
<tr>
<td>get(Name,DefValue)</td>
<td>Get value (whose type is automatically specified by DefValue). If not present, return DefValue.</td>
</tr>
<tr>
<td>subList(Name)</td>
<td>Get a reference to sublist List. If not present, create the sublist.</td>
</tr>
</tbody>
</table>

Table 2: Some methods of Teuchos::ParameterList class.

Input parameters are set via method set(Name,Value), where Name is a string defining
the parameter, and Value is the specified parameter, that can be any C++ object or pointer.
A complete list of parameters available for class MultiLevelPreconditioner is reported in
Section 6.

The parameter list is passed to the constructor, together with a pointer to the matrix,
and a boolean flag. If this flag is set to false, the constructor will not create the multilevel
hierarchy until when MLPrec->ComputePreconditioner() is called. The hierarchy can be
destroyed using MLPrec->Destroy()\(^9\). For instance, the user may define a code like:

// A is still not filled with numerical values
ML_Epetra::MultiLevelPreconditioner * MLPrec =
    new ML_Epetra::MultiLevelPreconditioner(A, MLList, false);

// compute the elements of A
...

// now compute the preconditioner

\(^8\)See the Teuchos documentation for a detailed overview of this class.

\(^9\)We suggest to create the preconditioning object with new and to free memory with delete. Some MPI calls occur in
Destroy(), so the user should not call MPI_Finalize() or delete the communicator used by ML before the preconditioning
object is destroyed.
MLPrec->ComputePreconditioner();

// solve the linear system
...
// destroy the previously define preconditioner, and build a new one
MLPrec->Destroy();

// re-compute the elements of A
// now re-compute (if required) the preconditioner
MLPrec->ComputePreconditioner();

// re-solve the linear system

In this fragment of code, the user defines the ML preconditioner, but the preconditioner is created only with the call ComputePreconditioner(). This may be useful, for example, when ML is used in conjunction with nonlinear solvers (like Nox [13]).

5.2 Example 2: ml_example_epetra_preconditioner_2level.cpp

As a second example, here we explain with some details the construction of a 2-level domain decomposition preconditioner, with a coarse space defined using aggregation.

File $ML_HOME/examples/ml_example_epetra_preconditioner_2level.cpp reports the entire code. In the example, the linear system matrix A, coded as an Epetra_CrsMatrix, corresponds to the discretization of a 2D Laplacian on a Cartesian grid. x and b are the solution vector and the right-hand side, respectively.
The AztecOO linear problem is defined as

Epetra_LinearProblem problem(&A, &x, &b);
AztecOO solver(problem);

We create the Teuchos parameter list as follows:

ParameterList MLList;
ML_Epetra::SetDefaults("DD", MLList);
MLList.set("max levels",2);
MLList.set("increasing or decreasing","increasing");

MLList.set("aggregation: type", "METIS");
MLList.set("aggregation: nodes per aggregate", 16);
MLList.set("smoother: pre or post", "both");
MLList.set("coarse: type","Amesos-KLU");
MLList.set("smoother: type", "Aztec");

The last option tells ML to use the Aztec preconditioning function as a smoother. All Aztec preconditioning options can be used as ML smoothers. Aztec requires an integer vector options and a double vector params. Those can be defined as follows:

int options[AZ_OPTIONS_SIZE];
double params[AZ_PARAMS_SIZE];
AZ_defaults(options, params);
options[AZ_precond] = AZ_dom_decomp;
options[AZ_subdomain_solve] = AZ_icc;
MLList.set("smoother: Aztec options", options);
MLList.set("smoother: Aztec params", params);

The last two commands set the pointer to options and params in the parameter list\(^{10}\).

The ML preconditioner is created as in the previous example,

\[
\text{ML_Epetra::MultiLevelPreconditioner * MLPrec =}
\]
\[
\text{new ML_Epetra::MultiLevelPreconditioner(A, MLList, true);
}
\]

and we can check that no options have been mispelled, using

\[
\text{MLPrec->PrintUnused();
}
\]

The AztecOO solver is called using, for instance,

\[
\text{solver.SetPrecOperator(MLPrec);
}
\]
\[
\text{solver.SetAztecOption(AZ_solver, AZ_cg_condnum);
}
\]
\[
\text{solver.SetAztecOption(AZ_kspace, 160);
}
\]
\[
\text{solver.Iterate(1550, 1e-12);
}
\]

Finally, some (limited) information about the preconditioning phase are obtained using

\[
\text{cout << MLPrec->GetOutputList();
}
\]

Note that the input parameter list is copied in the construction phase, hence later changes to MLList will not affect the preconditioner. Should the user need to modify parameters in the MLPrec's internally stored parameter list, he can get a reference to the internally stored list:

\[
\text{ParameterList & List = MLPrec->GetList();
}
\]

and then directly modify List.

### 6 Parameters for the ML_Epetra::MultiLevelPreconditioner Class

In this section we give general guidelines for using the MultiLevelPreconditioner class effectively. The complete list of input parameters is also reported.

\(^{10}\)Only the pointer is copied in the parameter list, not the array itself. Therefore, options and params should not go out of scope before the destruction of the preconditioner.
6.1 Setting Options on a Specific Level

Some of the parameters that affect MultiLevelPreconditioner can in principle be different from level to level. By default, the set method for the MultiLevelPreconditioner class affects all levels in the multigrid hierarchy. In order to change a setting on a particular level (say, \( d \)), the string \((\text{level } d)\) is appended to the option string (note that a space must separate the option and the level specification). For instance, assuming decreasing levels starting from 4, one could set the aggregation schemes as follows:

```plaintext
MLList.set("aggregation: type","Uncoupled");
MLList.set("aggregation: type (level 1)","METIS");
MLList.set("aggregation: type (level 3)","MIS");
```

If the finest level is 0, and one has 5 levels, the code will use \text{Uncoupled} for level 0, \text{METIS} for levels 1 and 2, then \text{MIS} for levels 3 and 4.

In §6.5, parameters that can be set differently on individual levels are denoted with the symbol \(?\) (that is not part of the parameter name). Note that some parameters (e.g., \text{Uncoupled-MIS aggregation}) correspond to quantities that must be the same at all levels.

6.2 General Usage of the Parameter List

All \text{ML} options can have a common prefix, specified by the user in the construction phase. For example, suppose that we require \text{ML:} (in this case with a trailing space) to be the prefix. The constructor will be

```plaintext
char Prefix[] = "ML: ";
ML_Epetra::MultiLevelPreconditioner * MLPrec =
    new ML_Epetra::MultiLevelPreconditioner(*A, MLList, true, Prefix);
```

A generic parameter, say \text{aggregation: type}, will now be defined as

```plaintext
MLList.set("ML: aggregation: type", "METIS");
```

It is important to point out that some options can be effectively used only if \text{ML} has been properly configured. In particular:

- **METIS** aggregation scheme requires --with-mlmetis, or otherwise the code will include all nodes in the calling processor in a unique aggregate;

- **PARMETIS** aggregation scheme required --with-mlmetis --enable-epetra and --with-mlparmetis2x or --with-mlparmetis3x.

- **AMESOS** coarse solvers require --enable-amesos. Moreover, AMESOS must have been configure to support the requested coarse solver. Please refer to the AMESOS documentation for more details;

- **IFPACK** smoother requires --enable-ifpack.
6.3 Default Parameter Settings for Common Problem Types

The MultiLevelPreconditioner class provides default values for four different preconditioner types:

1. Linear elasticity
2. Classical 2-level domain decomposition for the advection diffusion operator
3. 3-level algebraic domain decomposition for the advection diffusion operator
4. Eddy current formulation of Maxwell’s equations

Default values are listed in Table 3. In the table, SA refers to “classical” smoothed aggregation (with small aggregates and relative large number of levels), DD and DD-ML to domain decomposition methods (whose coarse matrix is defined using aggressive coarsening and limited number of levels). Maxwell refers to the solution of Maxwell’s equations.

Default values for the parameter list can be set by ML_Epetra::SetDefaults(). The user can easily put the desired default values in a given parameter list as follows:

```cpp
Teuchos::ParameterList MLList;
ML_Epetra::SetDefaults(ProblemType, MLList);
```

or as

```cpp
Teuchos::ParameterList MLList;
ML_Epetra::SetDefaults(ProblemType, MLList, Prefix);
```

**Prefix** (defaulted to an empty string) is the prefix to assign to each entry in the parameter list.

For DD and DD-ML, the default smoother is Aztec, with an incomplete factorization ILUT, and minimal overlap. Memory for the two AZTEC vectors is allocated using new, and the user is responsible to free this memory, for instance as follows:

```cpp
int * options;
options = MLList.get("smoother: Aztec options", options);
double * params;
params = MLList.get("smoother: Aztec params", params);
.
.
// Make sure solve is completed before deleting options & params!!
delete [] options;
delete [] params;
```

The rational behind this is that the parameter list stores a pointer to those vectors, not the content itself. (As a general rule, the vectors stored in the parameter list should not be prematurely destroyed or permitted to go out of scope.)
<table>
<thead>
<tr>
<th>Option Name</th>
<th>Type</th>
<th>SA</th>
<th>DD</th>
<th>DD-ML</th>
<th>maxwell</th>
</tr>
</thead>
<tbody>
<tr>
<td>max levels</td>
<td>int</td>
<td>16</td>
<td>2</td>
<td>3</td>
<td>5</td>
</tr>
<tr>
<td>output</td>
<td>int</td>
<td>8</td>
<td>8</td>
<td>8</td>
<td>10</td>
</tr>
<tr>
<td>increasing or decreasing</td>
<td>string</td>
<td>increasing</td>
<td>increasing</td>
<td>increasing</td>
<td>decreasing</td>
</tr>
<tr>
<td>PDE equations</td>
<td>int</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>-</td>
</tr>
<tr>
<td>null space dimension</td>
<td>int</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>-</td>
</tr>
<tr>
<td>null space vectors</td>
<td>double *</td>
<td>NULL</td>
<td>NULL</td>
<td>NULL</td>
<td>NULL</td>
</tr>
<tr>
<td>aggregation: type</td>
<td>string</td>
<td>Uncoupled</td>
<td>METIS</td>
<td>METIS</td>
<td>Uncoupled-MIS</td>
</tr>
<tr>
<td>aggregation: type (level 1)</td>
<td>string</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>aggregation: type (level 8)</td>
<td>string</td>
<td>MIS</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>aggregation: local aggregates</td>
<td>int</td>
<td>-</td>
<td>1</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>aggregation: nodes per aggregate</td>
<td>int</td>
<td>-</td>
<td>-</td>
<td>512</td>
<td>-</td>
</tr>
<tr>
<td>aggregation: damping factor</td>
<td>double</td>
<td>4/3</td>
<td>4/3</td>
<td>4/3</td>
<td>0.0</td>
</tr>
<tr>
<td>eigen-analysis: type</td>
<td>string</td>
<td>Anorm</td>
<td>Anorm</td>
<td>Anorm</td>
<td>Anorm</td>
</tr>
<tr>
<td>coarse: max size</td>
<td>int</td>
<td>128</td>
<td>128</td>
<td>128</td>
<td>128</td>
</tr>
<tr>
<td>aggregation: threshold</td>
<td>double</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>aggregation: next-level aggregates</td>
<td>int</td>
<td>-</td>
<td>-</td>
<td>128</td>
<td>-</td>
</tr>
<tr>
<td>per process</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>smoother: sweeps</td>
<td>int</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>smoother: damping factor</td>
<td>double</td>
<td>0.67</td>
<td>-</td>
<td>-</td>
<td>0.67</td>
</tr>
<tr>
<td>smoother: pre or post</td>
<td>string</td>
<td>both</td>
<td>both</td>
<td>both</td>
<td>both</td>
</tr>
<tr>
<td>smoother: type</td>
<td>string</td>
<td>Gauss-Seidel</td>
<td>Aztec</td>
<td>Aztec</td>
<td>-</td>
</tr>
<tr>
<td>smoother: Aztec as solver</td>
<td>bool</td>
<td>-</td>
<td>false</td>
<td>false</td>
<td>-</td>
</tr>
<tr>
<td>smoother: MLS polynomial order</td>
<td>int</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>3</td>
</tr>
<tr>
<td>smoother: MLS alpha</td>
<td>double</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>30.0</td>
</tr>
<tr>
<td>coarse: type</td>
<td>string</td>
<td>Amesos_KLU</td>
<td>Amesos_KLU</td>
<td>Amesos_KLU</td>
<td>SuperLU</td>
</tr>
<tr>
<td>coarse: sweeps</td>
<td>int</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>coarse: damping factor</td>
<td>double</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>coarse: max processes</td>
<td>int</td>
<td>16</td>
<td>16</td>
<td>16</td>
<td>-</td>
</tr>
<tr>
<td>print unused</td>
<td>int</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 3: Default values for ML_Epetra::MultiLevelPreconditioner for the 4 currently supported problem types SA, DD, DD-ML, Maxwell. "-" means not set.
### Uncoupled
Attempts to construct aggregates of optimal size ($3^d$ nodes in $d$ dimensions). Each process works independently, and aggregates cannot span processes.

### Coupled
As Uncoupled, but aggregates can span processes (deprecated).

### MIS
Uses a maximal independent set technique to define the aggregates. Aggregates can span processes. May provide better quality aggregates than either Coupled or uncoupled. Computationally more expensive than either because it requires matrix-matrix product.

### Uncoupled-MIS
Uses Uncoupled for all levels until there is 1 aggregate per processor. Then switches over to MIS. The coarsening scheme on a given level cannot be specified with this option.

### METIS
Use a graph partitioning algorithm to create the aggregates, working process-wise. The number of nodes in each aggregate is specified with the option `aggregation: nodes per aggregate`. Requires ML to be configured with `--with-mlmetis`.

### ParMETIS
As METIS, but partition the global graph. Requires `--with-mlparmetis2x` or `--with-mlparmetis3x`. Aggregates can span arbitrary number of processes. Global number of aggregates can be specified with the option `aggregation: global number`.

<table>
<thead>
<tr>
<th>Coarsening Scheme</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Uncoupled</td>
<td>Attempts to construct aggregates of optimal size ($3^d$ nodes in $d$ dimensions). Each process works independently, and aggregates cannot span processes.</td>
</tr>
<tr>
<td>Coupled</td>
<td>As Uncoupled, but aggregates can span processes (deprecated).</td>
</tr>
<tr>
<td>MIS</td>
<td>Uses a maximal independent set technique to define the aggregates. Aggregates can span processes. May provide better quality aggregates than either Coupled or uncoupled. Computationally more expensive than either because it requires matrix-matrix product.</td>
</tr>
<tr>
<td>Uncoupled-MIS</td>
<td>Uses Uncoupled for all levels until there is 1 aggregate per processor. Then switches over to MIS. The coarsening scheme on a given level cannot be specified with this option.</td>
</tr>
<tr>
<td>METIS</td>
<td>Use a graph partitioning algorithm to create the aggregates, working process-wise. The number of nodes in each aggregate is specified with the option <code>aggregation: nodes per aggregate</code>. Requires ML to be configured with <code>--with-mlmetis</code>.</td>
</tr>
<tr>
<td>ParMETIS</td>
<td>As METIS, but partition the global graph. Requires <code>--with-mlparmetis2x</code> or <code>--with-mlparmetis3x</code>. Aggregates can span arbitrary number of processes. Global number of aggregates can be specified with the option <code>aggregation: global number</code>.</td>
</tr>
</tbody>
</table>

### Table 4: ML_Epetra::MultiLevelPreconditioner: Available coarsening schemes.

#### 6.4 Commonly Used Parameters
Table 4 lists parameter for changing aggregation schemes. Table 5 lists common choices for smoothing options. Table 6 lists common choices affecting the coarse grid solve.

**Note that, in the parameters name, spaces are important:** Do not include non-required leading or trailing spaces, and separate words by just one space! Misspelled parameters will not be detected. One may find useful to print unused parameters by calling `PrintUnused()` after the construction of the multilevel hierarchy.

#### 6.5 List of All Parameters for MultiLevelPreconditioner Class

##### 6.5.1 General Options

- **output**
  Output level, from 0 to 10 (10 being verbose).

- **print unused**
  If non-negative, will print all the unused parameter on the specified processor.

- **max levels**
  Maximum number of levels.

- **increasing or decreasing**
  If set to `increasing`, level 0 will correspond to the finest level. If set to `decreasing`, max levels - 1 will correspond to the finest level.
<table>
<thead>
<tr>
<th>Smoother</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Jacobi</td>
<td>Point-Jacobi. Damping factor is specified using smoother: dampig factor, and the number of sweeps with smoother: sweeps.</td>
</tr>
<tr>
<td>Aztec</td>
<td>Use AZTECOO's built-in preconditioning functions as smoothers. Or, if smoother: Aztec as solver is true, use approximate solutions with AZTECOO(with smoothers: sweeps iterations as smoothers. The AZTECOOvectors options and params can be set using smoother: Aztec options and smoother: Aztec params.</td>
</tr>
<tr>
<td>MLS</td>
<td>Use MLS smoother. The polynomial order is specified by smoother: MLS polynomial order, and the alpha value by smoother: MLS alpha.</td>
</tr>
</tbody>
</table>

Table 5: ML_Epetra::MultiLevelPreconditioner: Commonly used smoothers.

<table>
<thead>
<tr>
<th>Smoother</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Jacobi</td>
<td>Use coarse: sweeps steps of Jacobi (with damping parameter coarse: damping parameter) as a solver.</td>
</tr>
<tr>
<td>Gauss-Seidel</td>
<td>Use coarse: sweeps steps of Gauss-Seidel(with damping parameter coarse: damping parameter) as a solver.</td>
</tr>
<tr>
<td>Amesos-KLU</td>
<td>Use KLU through AMESOS. Coarse grid problem is shipped to proc 0, solved, and solution is broadcast.</td>
</tr>
<tr>
<td>Amesos-UMFPACK</td>
<td>Use UMFPACK through AMESOS. Coarse grid problem is shipped to proc 0, solved, and solution is broadcasted.</td>
</tr>
<tr>
<td>Amesos-Superludist</td>
<td>Use SUPERLU DIST through AMESOS.</td>
</tr>
<tr>
<td>Amesos-MUMPS</td>
<td>Use double precision version of MUMPS through AMESOS.</td>
</tr>
<tr>
<td>Amesos-ScalAPACK</td>
<td>Use double precision version of SCALAPACK through AMESOS.</td>
</tr>
<tr>
<td>SuperLU</td>
<td>Use ML interface to SUPERLU.</td>
</tr>
</tbody>
</table>

Table 6: ML_Epetra::MultiLevelPreconditioner: Some of the available coarse matrix solvers. Note: Amesos solvers requires ML to be configured with with-ml_amos, and Amesos to be properly configured to support the specified solver.

PDE equations        Number of PDE equations for each grid node. This value is not considered for Epetra_VbrMatrix objects, as in this case is obtained from the block map used to construct the object. Note that only block maps with constant element size can be considered.
null space dimension Dimension of the null space.
null space vectors Pointer to the null space vectors. If NULL, ML will use the default null space.
6.5.2 Aggregation Parameters

**aggregation: type**

Define the aggregation scheme. Can be: Uncoupled, Coupled, MIS, METIS, ParMETIS. See Table 4.

**aggregation: global aggregates**

Defines the global number of aggregates (only for METIS and ParMETIS aggregation schemes).

**aggregation: local aggregates**

Defines the number of aggregates of the calling processor (only for METIS and ParMETIS aggregation schemes). Note: this value overwrites `aggregation: global aggregates`.

**aggregation: nodes per aggregate**

Defines the number of nodes to be assigned to each aggregate (only for METIS and ParMETIS aggregation schemes). Note: this value overwrites `aggregation: local aggregates`. If none among `aggregation: global aggregates`, `aggregation: local aggregates` and `aggregation: nodes per aggregate` is specified, the default value is 1 aggregate per process.

**aggregation: damping factor**

Damping factor for smoothed aggregation.

**eigen-analysis: type**

Defines the numerical scheme to be used to compute an estimation of the maximum eigenvalue of $D^{-1}A$, where $D = diag(A)$ (for smoothed aggregation only). It can be: cg (use 10 steps of conjugate gradient method), Anorm (use A-norm of matrix), Anasazi (use the ANASAZI package; the problem is supposed to be non-symmetric), or power-method.

**aggregation: threshold**

Threshold in aggregation.

**aggregation: next-level aggregates per process**

Defines the maximum number of next-level matrix rows per process (only for ParMETIS aggregation scheme).

6.5.3 Smoothing Parameters

**smoother: sweeps**

Number of sweeps of smoother.
smoother: damping factor * Smoother damping factor.

smoother: pre or post * If set to pre, only pre-smoothing will be used. If set to post, only post-smoothing will be used. If set to both, pre- and post-smoothing will be used.

smoother: type * Type of the smoother. It can be: Jacobi, Gauss-Seidel, sym Gauss-Seidel, Aztec, IFPACK. See Table 5.

smoother: Aztec options * Pointer to AZTEC’s options vector (only for aztec smoother).

smoother: Aztec params * Pointer to AZTEC’s params vector (only for aztec smoother).

smoother: Aztec as solver * If true, smoother: sweeps iterations of AZTEC solvers will be used as smoothers. If false, only the AZTEC’s preconditioner function will be used as smoother (only for aztec smoother).

smoother: MLS polynomial order * Polynomial order for MLS smoothers.

smoother: MLS alpha * Alpha value for MLS smoothers.

6.5.4 Coarsest Grid Parameters

coarse: max size Maximum dimension of the coarse grid. ML will not coarsen further is the size of the current level is less than this value.

coarse: type Coarse solver. It can be: Jacobi, Gauss-Seidel, Amesos_KLU, Amesos UMFPACK, Amesos Superludist, Amesos MUMPS. See Table 6.

coarse: sweeps (only for Jacobi and Gauss-Seidel) Number of sweeps in the coarse solver.

coarse: damping factor (only for Jacobi and Gauss-Seidel) Damping factor in the coarse solver.
7 Advanced Usage of ML

Sections 5 and 6 have detailed the use of ML as a black box preconditioner. In some cases, instead, the user may need to explicitly construct the ML hierarchy. This is reported in the following sections.

A brief sample program is given in Figure 2. The function ML_Create creates a multilevel solver object that is used to define the preconditioner. It requires the maximum number of multigrid levels be specified. In almost all cases, $N_{\text{grids}} = 20$ is more than adequate. The three ‘Amatrix’ statements are used to define the discretization matrix, $A$, that is solved. This is discussed in greater detail in Section 11.1. The multigrid hierarchy is generated via ML_Gen_MGHierarchy_UseAggregation. Controlling the behavior of this function is discussed in Section 9. For now, it is important to understand that this function takes the matrix $A$ and sets up relevant multigrid operators corresponding to the smoothed aggregation multigrid method [18] [17]. In particular, it generates a graph associated with $A$, coarsens this graph, builds functions to transfer vector data between the original graph and the coarsened graph, and then builds an approximation to $A$ on the coarser graph. Once this second multigrid level is completed, the same operations are repeated to the second level approximation to $A$ generating a third level. This process continues until the current graph is sufficiently coarse. The function ML_Gen_Smoother_Jacobi indicates that a Jacobi smoother should be used on all levels. Smoothers are discussed further in Section 8. Finally, ML_Gen_Solver is invoked when the multigrid preconditioner is fully specified. This function performs any needed initialization and checks for inconsistent options. After ML_Gen_Solver completes ML_Iterate can be used to solve the problem with an initial guess.
of sol (which will be overwritten with the solution) and a right hand side of rhs. At the present time, the external interface to vectors are just arrays. That is, rhs and sol are simple one-dimensional arrays of the same length as the number of rows in A. In addition to ML_Iterate, the function ML_Solve_MGV can be used to perform one multigrid ‘V’ cycle as a preconditioner.

8 Multigrid & Smoothing Options

Several options can be set to tune the multigrid behavior. In this section, smoothing and high level multigrid choices are discussed. In the next section, the more specialized topic of the grid transfer operator is considered. The details of the functions described in these next two sections are given in Section 13.

For most applications, smoothing choices are important to the overall performance of the multigrid method. Unfortunately, there is no simple advice as to what smoother will be best and systematic experimentation is often necessary. ML offers a variety of standard smoothers. Additionally, user-defined smoothers can be supplied and it is possible to use Aztec as a smoother. A list of ML functions that can be invoked to use built-in smoothers are given below along with a few general comments.

ML_Gen_Smoother_Jacobi
Typically, not the fastest smoother. Should be used with damping. For Poisson problems, the recommended damping values are \( \frac{2}{3} \) (1D), \( \frac{4}{5} \) (2D), and \( \frac{5}{7} \) (3D). In general, smaller damping numbers are more conservative.

ML_Gen_Smoother_GaussSeidel
Probably the most popular smoother. Typically, faster than Jacobi and damping is often not necessary nor advantageous.

ML_Gen_Smoother_SymGaussSeidel
Symmetric version of Gauss Seidel. When using multigrid preconditioned conjugate gradient, the multigrid operator must be symmetrizable. This can be achieved by using a symmetric smoother with the same number of pre and post sweeps on each level.

ML_Gen_Smoother_BlockGaussSeidel
Block Gauss-Seidel with a fixed block size. Often used for PDE systems where the block size is the number of degrees of freedom (DOFs) per grid point.

ML_Gen_Smoother_VBlockJacobi
Variable block Jacobi smoother. This allows users to specify unknowns to be grouped into different blocks when doing block Jacobi.
ML_Gen_Smoother_VBlockSymGaussSeidel Symmetric variable block Gauss-Seidel smoothing. This allows users to specify unknowns to be grouped into different blocks when doing symmetric block Gauss-Seidel.

It should be noted that the parallel Gauss-Seidel smoothers are not true Gauss-Seidel. In particular, each processor does a Gauss-Seidel iteration using off-processor information from the previous iteration.

AZTEC user's [15] can invoke ML_Gen_SmootherAztec to use either Aztec solvers or Aztec preconditioners as smoothers on any grid level. Thus, for example, it is possible to use preconditioned conjugate-gradient (where the preconditioner might be an incomplete Cholesky factorization) as a smoother within the multigrid method. Using Krylov smoothers as a preconditioner could potentially be more robust than using the simpler schemes provided directly by ML. However, one must be careful when multigrid is a preconditioner to an outer Krylov iteration. Embedding an inner Krylov method within a preconditioner to an outer Krylov method may not converge due to the fact that the preconditioner can no longer be represented by a simple matrix. Finally, it is possible to pass user-defined smoothing functions into ML via ML_Set_Smoother. The signature of the user defined smoother function is

```c
int user_smoothing(ML_Smoother *smoother, int x_length, double x[], int rhs_length, double rhs[])
```

where smoother is an internal ML object, x is a vector (of length x_length) that corresponds to the initial guess on input and is the improved solution estimate on output, and rhs is the right hand side vector of length rhs_length. The function ML_Get_MySmootherData(smoother) can be used to get a pointer back to the user’s data (i.e. the data pointer given with the ML_Set_Smoother invocation). A simple (and suboptimal) damped Jacobi smoother for the finest grid of our example is given below:

```c
int user_smoothing(ML_Smoother *smoother, int x_length, double x[], int rhs_length, double rhs[])
{
    int i;
    double ap[5], omega = .5; /* temp vector and damping factor */

    Poisson_matvec(ML_Get_MySmootherData(smoother), x_length, x, rhs_length, ap);
    for (i = 0; i < x_length; i++) x[i] = x[i] + omega*(rhs[i] - ap[i])/2.;

    return 0;
}
```

A more complete smoothing example that operates on all multigrid levels is given in the file mlguide.c. This routine uses the functions ML_Operator_Apply, ML_Operator_Get_Diag, and ML_Get_Amatrix to access coarse grid matrices constructed during the algebraic multigrid process. By writing these user-defined smoothers, it is possible to tailor smoothers to a particular application or to use methods provided by other packages. In fact, the AZTEC methods within ML have been implemented by writing wrappers to existing AZTEC functions and passing them into ML via ML_Set_Smoother.

At the present time there are only a few supported general parameters that may be altered by users. However, we expect that this list will grow in the future. When using ML_Iterate, the convergence tolerance (ML_Set_Tolerance) and the frequency with which
9 Smoothed Aggregation Options

When performing smooth aggregation, the matrix graph is first coarsened (actually vertices are aggregated together) and then a grid transfer operator is constructed. A number of parameters can be altered to change the behavior of these phases.

9.1 Aggregation Options

A graph of the matrix is usually constructed by associating a vertex with each equation and adding an edge between two vertices $i$ and $j$ if there is a nonzero in the $(i, j)^{th}$ or $(j, i)^{th}$ entry. It is this matrix graph whose vertices are aggregated together that effectively determines the next coarser mesh. The above graph generation procedure can be altered in two ways. First, a block matrix graph can be constructed instead of a point matrix graph. In particular, all the degrees of freedom (DOFs) at a grid point can be collapsed into a single vertex of the matrix graph. This situation arises when a PDE system is being solved where each grid point has the same number of DOFs. The resulting block matrix graph is significantly smaller than the point matrix graph and by aggregating the block matrix graph, all unknowns at a grid point are kept together. This usually results in better convergence rates (and the coarsening is actually less expensive to compute). To indicate the number of DOFs per node, the function `MLAggregate_Set_NullSpace` is used. The second way in which the graph matrix can be altered is by ignoring small values. In particular, it is often preferential to ignore weak coupling during coarsening. The error between weakly coupled points is generally hard to smooth and so it is best not to coarsen in this direction. For example, when applying a Gauss-Seidel smoother to a standard discretization of

$$u_{xx} + \epsilon u_{yy} = f$$

(with $0 \leq \epsilon \leq 10^{-6}$), there is almost no coupling in the $y$ direction. Consequently, simple smoothers like Gauss-Seidel do not effectively smooth the error in this direction. If we apply a standard coarsening algorithm, convergence rates suffer due to this lack of $y$-direction smoothing. There are two principal ways to fix this: use a more sophisticated smoother or coarsen the graph only in the $x$ direction. By ignoring the $y$-direction coupling in the matrix graph, the aggregation phase effectively coarsens in only the $x$-direction (the direction for which the errors are smooth) yielding significantly better multigrid convergence rates. In general, a drop tolerance, $tol_d$, can be set such that an individual matrix entry, $A(i, j)$ is dropped in the coarsening phase if

$$|A(i, j)| \leq tol_d \sqrt{|A(i, i)A(j, j)|}.$$ 

This drop tolerance (whose default value is zero) is set by `MLAggregate_Set_Threshold`. There are two different groups of graph coarsening algorithms in ML:
• schemes with fixed ratio of coarsening between levels: uncoupled aggregation, coupled aggregation, and MIS aggregation. A description of those three schemes along with some numerical results are given in [16]. As the default, the Uncoupled-MIS scheme is used which does uncoupled aggregation on finer grids and switches to the more expensive MIS aggregation on coarser grids;

• schemes with variable ratio of coarsening between levels: METIS and PARMETIS aggregation. Those schemes use the graph decomposition algorithms provided by METIS and PARMETIS, to create the aggregates.

Poorly done aggregation can adversely affect the multigrid convergence and the time per iteration. In particular, if the scheme coarsens too rapidly multigrid convergence may suffer. However, if coarsening is too slow, the number of multigrid levels increases and the number of nonzeros per row in the coarse grid discretization matrix may grow rapidly. We refer the reader to the above paper and indicate that users might try experimenting with the different schemes via ML_Aggregate_Set_CoarsenScheme_Uncoupled, ML_Aggregate_Set_CoarsenScheme_Coupled, ML_Aggregate_Set_CoarsenScheme_MIS, ML_Aggregate_Set_CoarsenScheme_METIS, and ML_Aggregate_Set_CoarsenScheme_ParMETIS.

9.2 Interpolation Options

An interpolation operator is built using coarsening information, seed vectors, and a damping factor. We refer the reader to [17] for details on the algorithm and the theory. In this section, we explain a few essential features to help users direct the interpolation process.

Coarsening or aggregation information is first used to create a tentative interpolation operator. This process takes a seed vector or seed vectors and builds a grid transfer operator. The details of this process are not discussed in this document. It is, however, important to understand that only a few seed vectors are needed (often but not always equal to the number of DOFs at each grid point) and that these seed vectors should correspond to components that are difficult to smooth. The tentative interpolation that results from these seed vectors will interpolate the seed vectors perfectly. It does this by ensuring that all seed vectors are in the range of the interpolation operator. This means that each seed vector can be recovered by interpolating the appropriate coarse grid vector. The general idea of smoothed aggregation (actually all multigrid methods) is that errors not eliminated by the smoother must be removed by the coarse grid solution process. If the error after several smoothing iterations was known, it would be possible to pick this error vector as the seed vector. However, since this is not the case, we look at vectors associated with small eigenvalues (or singular values in the nonsymmetric case) of the discretization operator. Errors in the direction of these eigenvectors are typically difficult to smooth as they appear much smaller in the residual ($r = Ae$ where $r$ is the residual, $A$ is discretization matrix, and $e$ is the error). For most scalar PDEs, a single seed vector is sufficient and so we seek some approximation to the eigenvector associated with the lowest eigenvalue. It is well known that a scalar Poisson operator with Neumann boundary conditions is singular and that the null space is the constant vector. Thus, when applying smoothed aggregation to Poisson operators, it is quite natural to choose the constant vector as the seed vector. In many cases, this constant vector is a good choice as all spatial derivatives within the operator are zero and so it is often associated with small singular values. Within ML the default is to choose...
the number of seed vectors to be equal to the number of DOFs at each node (given via `ML_Aggregate_Set_NullSpace`). Each seed vector corresponds to a constant vector for that DOF component. Specifically, if we have a PDE system with two DOFs per node. Then one seed vector is one at the first DOF and zero at the other DOF throughout the graph. The second seed vector is zero at the first DOF and one at the other DOF throughout the graph. In some cases, however, information is known as to what components will be difficult for the smoother or what null space is associated with an operator. In elasticity, for example, it is well known that a floating structure has six rigid body modes (three translational vectors and three rotation vectors) that correspond to the null space of the operator. In this case, the logical choice is to take these six vectors as the seed vectors in smoothed aggregation. When this type of information is known, it should be given to ML via the command `ML_Agggregate_Set_NullSpace`.

Once the tentative prolongator is created, it is smoothed via a damped Jacobi iteration. The reasons for this smoothing are related to the theory where the interpolation basis functions must have a certain degree of smoothness (see [17]). However, the smoothing stage can be omitted by setting the damping to zero using the function `ML_Agggregate_Set_DampingFactor`. Though theoretically poorer, unsmoothed aggregation can have considerably less set up time and less cost per iteration than smoothed aggregation. When smoothing, ML has two ways to determine the Jacobi damping parameter and each require some estimate of the largest eigenvalue of the discretization operator. The current default is to use a few iterations of a conjugate-gradient method to estimate this value. However, if the matrix is nonsymmetric, the infinity norm of the matrix should be used instead via `ML_Agggregate_Set_SpectralNormScheme_Anorm`. There are several other internal parameters that have not been discussed in this document. In the future, it is anticipated that some of these will be made available to users.

10 Advanced Usage of ML and Epetra

Class `ML_Epetra::MultiLevelOperator` is defined in a header file, that must be included as

```
#include "ml_epetra_operator.h"
```

Users may also need to include `ml_config.h`, `Epetra_Operator.h`, `Epetra_MultiVector.h`, `Epetra_LinearProblem.h`, `AztecOO.h`. Check the Epetra and AztecOO documentation for more details.

Let \( A \) be an Epetra_RowMatrix for which we aim to construct a preconditioner, and let `ml_handle` be the structure ML requires to store internal data (see Section 7), created with the instruction

```
ML_Create(&ml_handle, N_levels);
```

where `N_levels` is the specified (maximum) number of levels. As already pointed out, ML can accept in input very general matrices. Basically, the user has to specify the number of local rows, and provide a function to update the ghost nodes (that is, nodes requires in the matrix-vector product, but assigned to another process). For Epetra matrices, this is done by the following function

```
EpetraMatrix2MLMatrix(ml_handle, 0, &A);
```
and it is important to note that $A$ is not converted to ML format. Instead, EpetraMatrix2MLMatrix defines a suitable getrow function (and other minor data structures) that allows ML to work with $A$.

Let `agg_object` a ML_Aggregate pointer, created using

```c
ML_Aggregate_Create(&agg_object);
```

At this point, users have to create the multilevel hierarchy, define the aggregation schemes, the smoothers, the coarse solver, and create the solver. Then, we can finally create the ML_Epetra::MultiLevelOperator object

```c
ML_Epetra::MultiLevelOperator MLop(ml_handle,comm,map,map);
```

(map being the Epetra_Map used to create the matrix) and set the preconditioning operator of our AZTEC00 solver,

```c
epetra_linearProblem Problem(A,&x,&b);
Aztec00 Solver(Problem);
solver.SetPrecOperator(&MLop);
```

where $x$ and $b$ are Epetra_MultiVector's defining solution and right-hand side. The linear problem can now be solved as, for instance,

```c
Solver.SetAztecOption( AZ_solver, AZ_gmres );
solver.Iterate(Niters, 1e-12);
```

## Using ML without Epetra

### Creating a ML matrix: Single Processor

Matrices are created by defining some size information, a matrix-vector product and a getrow function (which is used to extract matrix information). We note that EPETRA and AZTEC users do not need to read this (or the next) section as there are special functions to convert EPETRA objects and AZTEC matrices to ML matrices (see Section 4.2). Further, functions for some common matrix storage formats (CSR & MSR) already exist within ML and do not need to be rewritten\(^{11}\).

Size information is indicated via `ML_Init_Amatrix`. The third parameter in the Figure 2 invocation indicates that a matrix with `nlocal` rows is being defined. The fourth parameter gives the vector length of vectors that can be multiplied with this matrix. Additionally, a data pointer, `A_data`, is associated with the matrix. This pointer is passed back into the matrix-vector product and getrow functions that are supplied by the user. Finally, the number `0` indicates at what level within the multigrid hierarchy the matrix is to be stored. For discussions within this document, this is always `0`. It should be noted that there appears to be some redundant information. In particular, the number of rows and the vector length in `ML_Init_Amatrix` should be the same number as the discretization matrices are square. Cases where these `apparently` redundant parameters might be set differently are not discussed in this document.

\(^{11}\)The functions `CSR_matvec`, `CSR_getrows`, `MSR_matvec` and `MSR_getrows` can be used.
The function \texttt{ML\_Set\_Amatrix\_Matvec} associates a matrix-vector product with the discretization matrix. The invocation in Figure 2 indicates that the matrix-vector product function \texttt{user\_matvec} is associated with the matrix located at level ‘0’ of the multigrid hierarchy. The signature of \texttt{user\_matvec} is

\begin{verbatim}
int user\_matvec(ML\_Operator *Amat, int in\_length, double p[], int out\_length, double ap[])
\end{verbatim}

where \texttt{A\_mat} is an internal \texttt{ML} object, \texttt{p} is the vector to apply to the matrix, \texttt{in\_length} is the length of this vector, and \texttt{ap} is the result after multiplying the discretization matrix by the vector \texttt{p} and \texttt{out\_length} is the length of \texttt{ap}. The function \texttt{ML\_Get\_MyMatvecData(Amat)} can be used to get a pointer back to the user’s data (i.e. the data pointer given with the \texttt{ML\_Init\_Amatrix} invocation).

Finally, \texttt{ML\_Set\_Amatrix\_Getrow} associates a getrow function with the discretization matrix. This getrow function returns nonzero information corresponding to specific rows. The invocation in Figure 2 indicates that a user supplied function \texttt{user\_getrow} is associated with the matrix located at level ‘0’ of the multigrid hierarchy and that this matrix contains \texttt{nlocal\_allcolumns} columns and that no communication (\texttt{NULL}) is used (discussed in the next section). It again appears that some redundant information is being asked as the number of columns was already given. However, when running in parallel this number will include ghost node information and is usually different from the number of rows. The signature of \texttt{user\_getrow} is

\begin{verbatim}
int user\_getrow(ML\_Operator *Amat, int N\_requested\_rows, int requested\_rows[], int allocated\_space, int columns[], double values[], int row\_lengths[])
\end{verbatim}

where \texttt{Amat} is an internal \texttt{ML} object, \texttt{N\_requested\_rows} is the number of matrix rows for which information is returned, \texttt{requested\_rows} are the specific rows for which information will be returned, \texttt{allocated\_space} indicates how much space has been allocated in \texttt{columns} and \texttt{values} for nonzero information. The function \texttt{ML\_Get\_MyGetrowData(Amat)} can be used to get a pointer back to the user’s data (i.e. the data pointer given with the \texttt{ML\_Init\_Amatrix} invocation). On return, the user’s function should take each row in order within \texttt{requested\_rows} and place the column numbers and the values corresponding to nonzeros in the arrays \texttt{columns} and \texttt{values}. The length of the \texttt{i}th requested row should appear in \texttt{row\_lengths[i]}. If there is not enough allocated space in \texttt{columns} or \texttt{values}, this routine simply returns a ‘0’, otherwise it returns a ‘1’.

To clarify, these functions, one concrete example is given corresponding to the matrix:

\[
\begin{pmatrix}
2 & -1 \\
-1 & 2 & -1 \\
-1 & 2 & -1 \\
-1 & 2 & -1 \\
-1 & 2 & -1
\end{pmatrix}
\]  

(2)

To implement this matrix, the following functions are defined:

\begin{verbatim}
int Poisson\_getrow(ML\_Operator *Amat, int N\_requested\_rows, int requested\_rows[], int allocated\_space, int columns[], double values[], int row\_lengths[])
{
    int count = 0, i, start, row;
}
\end{verbatim}
for (i = 0; i < N_requested_rows; i++) {
    if (allocated_space < count+3) return(0);
    start = count;
    row = requested_rows[i];
    if ( (row >= 0) || (row <= 4) ) {
        columns[count] = row; values[count++] = 2.;
        if (row != 0) { columns[count] = row-1; values[count++] = -1.; }
        if (row != 4) { columns[count] = row+1; values[count++] = -1.; }
    }
    row_lengths[i]= count - start;
}
return(1);

and

int Poisson_matvec(ML_Operator *Amat, int in_length, double p[], int out_length,
                  double ap[])
{
    int i;

    for (i = 0; i < 5; i++ ) {
        ap[i] = 2*p[i];
        if (i != 0) ap[i] -= p[i-1];
        if (i != 4) ap[i] -= p[i+1];
    }
    return 0;
}

Finally, these matrix functions along with size information are associated with the fine grid
discretization matrix via

    ML_Init_Amatrix (ml_object, 0, 5, 5, NULL);
    ML_Set_Amatrix_Getrow(ml_object, 0, Poisson_getrow, NULL, 5);
    ML_Set_Amatrix_Matvec(ml_object, 0, Poisson_matvec);

Notice that in these simple examples Amat was not used. In the next section we give a
parallel example which makes use of Amat. The complete sample program can be found in
the file mlguide.c within the ML code distribution.

11.2 Creating a ML matrix: Multiple Processors

Creating matrices in parallel requires a bit more work. In this section local versus global
indexing as well as communication are discussed. In the description, we reconsider the
previous example (2) partitioned over two processors. The matrix row indices (ranging from
0 to 4) are referred to as global indices and are independent of the number of processors
being used. On distributed memory machines, the matrix is subdivided into pieces that are
assigned to individual processors. ML requires matrices be partitioned by rows (i.e. each
row is assigned to a processor which holds the entire data for that row). These matrix pieces
are stored on each processor as smaller local matrices. Thus, global indices in the original
matrix get mapped to local indices on each processor. In our example, we will assign global
rows 0 and 4 to processor 0 and store them locally as rows 1 and 0 respectively. Global
columns 0, 1, 3, and 4 are stored locally as columns 1, 3, 2, and 0. This induces the local matrix
\[
\begin{pmatrix}
2 & -1 \\
2 & -1
\end{pmatrix}.
\]
Likewise, processor 1 is assigned global rows 1, 2, and 3 which are stored locally as rows 0, 1, and 2 respectively. Global columns 0 - 4 are stored locally as columns 3, 0, 1, 2, and 4 inducing the local matrix
\[
\begin{pmatrix}
2 & -1 & -1 \\
-1 & 2 & -1 \\
-1 & 2 & -1
\end{pmatrix}.
\]
At the present time, there are some restrictions as to what type of mappings can be used. In particular, all global rows stored on a processor must be mapped from 0 to \(k - 1\) where \(k\) is the number of rows assigned to this processor. This row mapping induces a partial column mapping. Any additional columns must be mapped with consecutive increasing numbers starting from \(k\).

**ML** has no notion of global indices and uses only the local indices. In most cases, another package or application already mapped the global indices to local indices and so **ML** works with the existing local indices. Specifically, the parallel version of **user_getrow** and **user_matvec** should correspond to each processor’s local matrix. This means that when giving the column information with **ML_Set_Amatrix_Getrow**, the total number of columns in the local matrix should be given and that when row \(k\) is requested, **user_getrow** should return the \(k^{th}\) local row using local column indices. Likewise, the matrix-vector product takes a local input vector and multiplies it by the local matrix. It is important to note that this local input vector does not contain ghost node data (i.e. the input vector is of length \(n_{\text{local}}\) where \(n_{\text{local}}\) is the number of matrix rows). Thus, **user_matvec** must perform the necessary communication to update ghost variables. When invoking **ML_Init_Amatrix**, the local number of rows should be given for the number of rows and the vector length\(^{12}\). A specific communication function must also be passed into **ML** when supplying the getrow function so that **ML** can determine how local matrices on different processors are ‘glued’ together. The signature of the communication function is

\[
\text{int} \ \text{user}_\text{comm}(\text{double} \ x[], \ \text{void} \ *\text{Adata})
\]

where \(A_{\text{data}}\) is the user-defined data pointer specified in the **ML_Init_Amatrix** and \(x\) is a vector of length \(n_{\text{local}}\_\text{allcolumns}\) specified in **ML_Set_Amatrix_Getrow**. This parameter should be set to the total number of matrix columns stored on this processor. On input, only the first \(n_{\text{local}}\) elements of \(x\) are filled with data where \(n_{\text{local}}\) is the number of rows/columns specified in **ML_Init_Amatrix**. On output, the ghost elements are updated to their current values (defined on other processors). Thus, after this function a local matrix-vector product could be properly performed using \(x\). To make all this clear, we give the new functions corresponding to our two processor example.

\[
\text{int} \ \text{Poisson_getrow}(\text{ML}_\text{Operator} \ *\text{Amat}, \ \text{int} \ N\_\text{requested_rows}, \ \text{int} \ \text{requested_rows}[],
\quad \text{int} \ \text{allocated_space}, \ \text{int} \ \text{cols}[][], \ \text{double} \ \text{values}[][], \ \text{int} \ \text{row_lengths}[])
\]

\(^{12}\)In contrast to **ML_Set_Amatrix_Getrow** in which the number of local columns are given (including those that correspond to ghost variables), **ML_Init_Amatrix** does not include ghost variables and so both size parameters should be the number of local rows.


```c
{ int m = 0, i, row, proc, *itemp, start;

itemp = (int *) ML_Get_MyGetrowData(Amat);
proc = *itemp;

for (i = 0; i < N_requested_rows; i++) {
    row = requested_rows[i];
    if (allocated_space < m+3) return(0);
    values[m] = 2; values[m+1] = -1; values[m+2] = -1;
    start = m;
    if (proc == 0) {
        if (row == 0) {cols[m++] = 0; cols[m++] = 2; }
        if (row == 1) {cols[m++] = 1; cols[m++] = 3;}
    }
    if (proc == 1) {
        if (row == 0) {cols[m++] = 0; cols[m++] = 1; cols[m++] = 4;}
        if (row == 1) {cols[m++] = 1; cols[m++] = 0; cols[m++] = 2;}
        if (row == 2) {cols[m++] = 2; cols[m++] = 1; cols[m++] = 3;}
    }
    row_lengths[i] = m - start;
}
return(1);
}

int Poisson_matvec(ML_Operator *Amat, int in_length, double p[], int out_length,
        double ap[])
{
    int i, proc, *itemp;
    double new_p[5];

    itemp = (int *) ML_Get_MyMatvecData(Amat);
    proc = *itemp;

    for (i = 0; i < in_length; i++) new_p[i] = p[i];
    Poisson_comm(new_p, A_data);

    for (i = 0; i < out_length; i++) ap[i] = 2.*new_p[i];
    if (proc == 0) {
    }
    if (proc == 1) {
        ap[0] -= new_p[1]; ap[0] -= new_p[4];
    }
    return 0;
}

and

int Poisson_comm(double x[], void *A_data)
{
    int proc, neighbor, length, *itemp;
    double send_buffer[2], recv_buffer[2];

    int m = 0, i, row, proc, *itemp, start;

    itemp = (int *) ML_Get_MyGetrowData(Amat);
    proc = *itemp;

    for (i = 0; i < N_requested_rows; i++) {
        row = requested_rows[i];
        if (allocated_space < m+3) return(0);
        values[m] = 2; values[m+1] = -1; values[m+2] = -1;
        start = m;
        if (proc == 0) {
            if (row == 0) {cols[m++] = 0; cols[m++] = 2; }
            if (row == 1) {cols[m++] = 1; cols[m++] = 3;}
        }
        if (proc == 1) {
            if (row == 0) {cols[m++] = 0; cols[m++] = 1; cols[m++] = 4;}
            if (row == 1) {cols[m++] = 1; cols[m++] = 0; cols[m++] = 2;}
            if (row == 2) {cols[m++] = 2; cols[m++] = 1; cols[m++] = 3;}
        }
        row_lengths[i] = m - start;
    }
    return(1);
}
```

```c
itemp = (int *) A_data;
proc = *itemp;

length = 2;
if (proc == 0) {
    neighbor = 1;
    send_buffer[0] = x[0]; send_buffer[1] = x[1];
    send_msg(send_buffer, length, neighbor);
    recv_msg(recv_buffer, length, neighbor);
    x[2] = recv_buffer[1]; x[3] = recv_buffer[0];
} else {
    neighbor = 0;
    send_buffer[0] = x[0]; send_buffer[1] = x[2];
    send_msg(send_buffer, length, neighbor);
    recv_msg(recv_buffer, length, neighbor);
    x[3] = recv_buffer[1]; x[4] = recv_buffer[0];
}
return 0;
```

Finally, these matrix functions along with size information are associated with the fine grid discretization matrix via

```c
if (proc == 0) {nlocal = 2; nlocal_allcolumns = 4;}
else if (proc == 1) {nlocal = 3; nlocal_allcolumns = 5;}
else {nlocal = 0; nlocal_allcolumns = 0;}
ML_Init_Amatrix (ml_object, 0, nlocal, nlocal, &proc);
ML_Set_Amatrix_Getrow(ml_object, 0, Poisson_getrow, Poisson_comm,
                      nlocal_allcolumns);
ML_Set_Amatrix_Matvec(ml_object, 0, Poisson_matvec);
```

### 12 Visualization Capabilities

**ML** supports limited capabilities for the visualization of and statistical information for aggregates, with an interface to OpenDX. Currently, only Uncoupled, METIS and ParMETIS aggregation routines can dump files in OpenDX format.

The procedure to create the OpenDX input files is as follows:

1. Add the following line after the creation of the ML_Aggregate object

   ```c
   ML_Aggregate_VizAndStats_Setup( ag, MaxMgLevels);
   ```

   where MaxMgLevels is the maximum number of levels (this is the same value used to create the ML object).

2. Create the multilevel hierarchy;

3. Write OpenDX file using the instruction

   ```c
   ML_Aggregate_VizAndStats_Compute( ml, ag, MaxMgLevels, x, y, z,
                                    option, filename);
   ```
where \texttt{ml} is the \texttt{ML} object, \texttt{ag} the \texttt{MLAggregation} object, and \texttt{x,y,z} are double vectors, whose size equals the number of local nodes in the fine grid, containing the coordinates of fine grids nodes. \texttt{option} is an integer value defined so that:

- option = 1 : solution of 1D problem (\texttt{y} and \texttt{z} can be \texttt{NULL});
- option = 2 : solution of 2D problems (\texttt{z} can be \texttt{NULL});
- option = 3 : solution of 3D problems.

Processor X will write its own file, \texttt{filename\_level\_Y\_proc\_X}, where \texttt{Y} is the level. \texttt{filename} can be set to \texttt{NULL} (default value of .\texttt{graph} will be used in this case).

Note that in AMG there is no mesh associated with coarser levels. Therefore \texttt{ML\_Aggregate\_VizAndStats\_Compute} needs to assign a set of coordinates to each aggregate. This is done by computing the center of gravity of each aggregate (starting from the fine grid and finishing at the coarsest level).

\texttt{ML\_Aggregate\_VizAndStats\_Compute} will also write statistical information to the screen.

4. Deallocate memory using

\begin{verbatim}
ML\_Aggregate\_VizAndStats\_Clean( ag, MaxMgLevels ).
\end{verbatim}

At this point, one should copy file \texttt{viz\_aggre\_net} and \texttt{viz\_aggre\_cfg} (located in \$\texttt{ML\_HOME/util/}) in the directory where the output files are located, and run OpenDX with the instruction

\begin{verbatim}
% dx -edit viz\_aggre\_net
\end{verbatim}

Other instructions are reported in file \$\texttt{ML\_HOME/util/viz\_aggre\_README}. An example of code can be found in file \$\texttt{ML\_HOME/examples/ml\_aztec\_simple\_METIS.c}. 

13 ML Functions

Prototype

```c
int AZ_ML_Set_Amat(ML *ml_object, int k, int isize, int osize, AZ_MATRIX *Amat,
                   int *proc_config)
```

Description

Create an ML matrix view of an existing Aztec matrix and store it within the ‘ml_object’ context.

Parameters

- **ml_object**: On input, ML object pointer (see ML_Create). On output, the discretization matrix of level k is the same as given by Amat.
- **k**: On input, indicates level within ml_object hierarchy (should be between 0 and Nlevels†-1).
- **isize**: On input, the number of local rows in the submatrix stored on this processor.
- **osize**: On input, the number of columns in the local submatrix stored on this processor not including any columns associated with ghost unknowns.
- **Amat**: On input, an Aztec data structure representing a matrix. See the AztecUser’s Guide.
- **proc_config**: On input, an Aztec data structure representing processor information. See the AztecUser’s Guide.

Prototype

```c
void AZ_set_ML_preconditioner(AZ_PRECOND **Precond, AZ_MATRIX *Amat,
                               ML *ml_object, int options[])
```
Description

Associate the multigrid V cycle method defined in ml_object with an Aztec preconditioner. Thus, when Precond and options are passed into the Aztec iterative solver, it will invoke the V cycle multigrid algorithm described by ml_object.

Parameters

Precond On input, an Aztec data structure representing a preconditioner. On output, the multigrid V cycle method described by ml_object will be associated with this preconditioner. See the AztecUser’s Guide.

Amat On input, an Aztec data structure representing a matrix. See the AztecUser’s Guide.

ml_object On input, ML object pointer (see ML_Create) representing a V cycle multigrid method.

options On input, an Aztec data structure representing user chosen options. On output, set appropriately for multigrid V cycle preconditioner.

Prototype

```c
int ML_Aggregate_Create(ML_Aggregate **agg_object)
```

Description

Create an aggregate context (or handle). This instance will be used in all subsequent function invocations that set aggregation options.

Parameters

agg_object On input, a pointer to a noninitialized ML_Aggregate object pointer. On output, points to an initialized ML_Aggregate object pointer.
Prototype

```c
int ML_Aggregate_Destroy(ML_Aggregate **agg_object)
```

Description

Destroy the aggregate context, `agg_object`, and delete all memory allocated by ML in building and setting the aggregation options.

Parameters

- `agg_object` On input, aggregate object pointer (see ML_Aggregate_Create). On output, all memory allocated by ML and associated with this context is freed.

Prototype

```c
int ML_Aggregate_Set_CoarsenScheme_Coupled(ML_Aggregate *agg_object)
```

Description

Set the aggregate coarsening scheme to be used as ‘coupled’ (see Section 9).

Parameters

- `agg_object` On input, aggregate object pointer (see ML_Aggregate_Create). On output, the ‘coupled’ aggregation will be used for automatic coarsening.

Prototype

```c
int ML_Aggregate_Set_CoarsenScheme_MIS(ML_Aggregate *agg_object)
```
Set the aggregate coarsening scheme to be used as ‘MIS’ (see Section 9).

**Parameters**

\[ agg\_object \]

On input, aggregate object pointer (see ML\_Aggregate\_Create). On output, the ‘MIS’ aggregation will be used for automatic coarsening.

**Prototype**

```
int ML\_Aggregate\_Set\_CoarsenScheme\_Uncoupled(ML\_Aggregate *agg\_object)
```

Set the aggregate coarsening scheme to be used as ‘uncoupled’ (see Section 9).

**Parameters**

\[ agg\_object \]

On input, aggregate object pointer (see ML\_Aggregate\_Create). On output, the ‘uncoupled’ aggregation will be used for automatic coarsening.

**Prototype**

```
int ML\_Aggregate\_Set\_CoarsenScheme\_METIS(ML\_Aggregate *agg\_object)
```

Set the aggregate coarsening scheme to be used as ‘METIS (see Section 9).
Parameters

\texttt{agg\_object} \\
On input, aggregate object pointer (see ML\_Aggregate\_Create). On output, the ‘METIS’ aggregation will be used for automatic coarsening.

Prototype

\begin{verbatim}
int ML\_Aggregate\_Set\_CoarsenScheme\_ParMETIS(ML\_Aggregate *agg\_object)
\end{verbatim}

Description

Set the aggregate coarsening scheme to be used as ‘ParMETIS (see Section 9).

Parameters

\texttt{agg\_object} \\
On input, aggregate object pointer (see ML\_Aggregate\_Create). On output, the ‘ParMETIS’ aggregation will be used for automatic coarsening.

Prototype

\begin{verbatim}
int ML\_Aggregate\_Set\_DampingFactor( ML\_Aggregate *ag, double factor)
\end{verbatim}

Description

Set the damping factor used within smoothed aggregation. In particular, the interpolation operator will be generated by

$$P = (I - \frac{\omega}{\rho} A)P_t$$

where \(A\) is the discretation matrix, \(\omega\) is the damping factor (default is \(\frac{4}{3}\)), \(\rho\) is an estimate of the spectral radius of \(A\), and \(P_t\) are the seed vectors (tentative prolongator).
Parameters

\textit{agg\_object} \hspace{1cm} On input, aggregate object pointer (see ML\_Aggregate\_Create). On output, the damping factor is set to \textit{factor}.

\textit{factor} \hspace{1cm} On input, damping factor that will be associated with this aggregation object.

Prototype

\begin{verbatim}
int ML_Aggregate_Set_MaxCoarseSize( ML_Aggregate *agg\_object, int size )
\end{verbatim}

Description

Set the maximum coarsest mesh to \textit{size}. No further coarsening is performed if the total number of matrix equations is less than this \textit{size} (see Section 8).

Parameters

\textit{agg\_object} \hspace{1cm} On input, aggregate object pointer (see ML\_Aggregate\_Create). On output, the coarsest mesh size will be set.

\textit{size} \hspace{1cm} On input, size indicating the maximum coarsest mesh size.

Prototype

\begin{verbatim}
int ML_Aggregate_Set_NullSpace(ML_Aggregate *agg\_object, int num_PDE\_eqns, int null\_dim,
                                double *null\_vect, int leng)
\end{verbatim}

Description

Set the seed vectors (rigid body mode vectors) to be used in smoothed aggregation. Also indicate the number of degrees of freedom (DOF) per node so that the aggregation algorithm can group them together.
Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>agg_object</td>
<td>On input, an ML_Aggregate object pointer created by invoking ML_Aggregate_Create. On output, the seed vectors and DOFs per node are set to null_vect and num_PDE_eqns respectively.</td>
</tr>
<tr>
<td>num_PDE_eqns</td>
<td>On input, indicates number of equations that should be grouped in blocks when performing the aggregation. This guarantees that different DOFs at a grid point remain within the same aggregate.</td>
</tr>
<tr>
<td>null_dim</td>
<td>On input, number of seed vectors that will be used when creating the smoothed aggregation grid transfer operator.</td>
</tr>
<tr>
<td>null_vect</td>
<td>On input, the seed vectors are given in sequence. Each processor gives only the local components residing on the processor. If null, default seed vectors are used.</td>
</tr>
<tr>
<td>leng</td>
<td>On input, the length of each seed vector.</td>
</tr>
</tbody>
</table>

Prototype

```c
int ML_Aggregate_Set_SpectralNormScheme_Calc( ML_Aggregate *ag )
```

Description

Set the method to be used for estimating the spectral radius of $A$ (the discretization matrix) to be conjugate gradient. This spectral radius estimate is used when smoothing the initial prolongation operator (see ML_Aggregate_Set_DampingFactor).

Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>agg_object</td>
<td>On input, aggregate object pointer (see ML_Aggregate_Create). On output, the spectral radius estimate will be determined by a conjugate gradient routine.</td>
</tr>
</tbody>
</table>

Prototype

```c
int ML_Aggregate_Set_SpectralNormScheme_Anorm( ML_Aggregate *ag)
```
Set the method to be used for estimating the spectral radius of $A$ (the discretization matrix) to be the infinity norm. This spectral radius estimate is used when smoothing the initial prolongation operator (see ML_Agggregate_Set_DampingFactor).

**Parameters**

agg_object  
On input, aggregate object pointer (see ML_Agggregate_Create). On output, the spectral radius estimate will be taken as the infinity norm of the matrix.

**Prototype**

```c
int ML_Agggregate_Set_Threshold(ML_Agggregate *agg_object, double tolerance)
```

Set the drop tolerance used when creating the matrix graph for aggregation. Entries in the matrix $A$ are dropped when $|A(i, j)| \leq tol \cdot d \cdot \sqrt{|A(i, i)A(j, j)|}$. See Section 9 for more details.

**Parameters**

agg_object  
On input, an ML_Agggregate object pointer created by invoking ML_Agggregate_Create. On output, drop tolerance for creating the matrix graph is set.

tolerance  
On input, value to be used for dropping matrix entries.

**Prototype**

```c
int ML_Create(ML **ml_object, int Nlevels)
```
Create an ML solver context (or handle). This ML instance will be used in all subsequent ML function invocations. The ML object has a notation of levels where different multigrid operators corresponding to different grid levels are stored.

**Parameters**

- **ml_object**
  - On input, a pointer to a noninitialized ML object pointer. On output, points to an initialized ML object pointer.
- **Nlevels**
  - Maximum number of multigrid levels within this ML object.

**Prototype**

```
int ML_Destroy(ML **ml_object)
```

Destroy the ML solver context, ml_object, and delete all memory allocated by ML in building and setting options.

**Parameters**

- **ml_object**
  - On input, ML object pointer (see ML_Create). On output, all memory allocated by ML and associated with this context is freed.

**Prototype**

```
int ML_Gen_Blocks_Aggregates(ML_Aggregate *agg_object, int k, int *nblocks, int **block_list)
```
Use aggregates to partition submatrix residing on local processor into blocks. These blocks can then be used within smoothers (see for example ML_Gen_Smoother_VBlockJacobi or ML_Gen_Smoother_VBlockSymGaussSeidel).

**Parameters**

- **ml_object**
  On input, ML object pointer (see ML_Create).

- **k**
  On input, indicates level within ml_object hierarchy where the aggregate information is found that defines partitioning.

- **nbblocks**
  On input, indicates number of partitions desired on each processor. On output, indicates the number of partitions obtained.

- **block_list**
  On output, equation i resides in the block_list[i]th partition.

**Prototype**

```
int ML_Gen_Blocks_Metis(ML *ml_object, int k, int *nbblocks, int **block_list)
```

Use Metis to partition submatrix residing on local processor into blocks. These blocks can then be used within smoothers (see for example ML_Gen_Smoother_VBlockJacobi or ML_Gen_Smoother_VBlockSymGaussSeidel).

**Parameters**

- **ml_object**
  On input, ML object pointer (see ML_Create).

- **k**
  On input, indicates level within ml_object hierarchy where the discretization matrix is found that will be partitioned.

- **nbblocks**
  On input, indicates number of partitions desired on each processor. On output, indicates the number of partitions obtained.

- **block_list**
  On output, equation i resides in the block_list[i]th partition.
Prototype

\( \text{int ML\_Gen\_CoarseSolverSuperLU(ML\,*ml\_object,\,int\,k)} \)

Description

Use SuperLU for the multigrid coarse grid solver on level k within ml\_object and perform any initialization that is necessary.

Parameters

\( ml\_object \)  
On input, ML object pointer (see ML\_Create). On output, the coarse grid solver of level k is set to use SuperLU.

\( k \)  
On input, indicates level within ml\_object hierarchy (must be the coarsest level in the multigrid hierarchy).

Prototype

\( \text{int ML\_Gen\_MGHierarchy\_UsingAggregation(ML\,*ml\_object,\,int\,start,\,int\,inc\_or\_dec,\,ML\_Aggregate\,*agg\_object)} \)

Description

Generate a multigrid hierarchy via the method of smoothed aggregation. This hierarchy includes a series of grid transfer operators as well as coarse grid approximations to the fine grid discretization operator. On completion, return the total number of multigrid levels in the newly created hierarchy.

Parameters

\( ml\_object \)  
On input, ML object pointer (see ML\_Create). On output, coarse levels are filled with grid transfer operators and coarse grid discretizations corresponding to a multigrid hierarchy.
**start**  
On input, indicates multigrid level within ml_object where the fine grid discretization is stored.

**inc_or_dec**  
On input, ML_INCREMENT or ML_DECREMENT. Normally, set to ML_INCREMENT meaning that the newly created multigrid operators should be stored in the multigrid levels: start, start+1, start+2, start+3, etc. If set to ML_DECREMENT, multigrid operators are stored in start, start-1, start-2, etc.

**agg_object**  
On input, an initialized aggregation object defining options to the generation of grid transfer operators. If set to NULL, default values are used for all aggregation options. See ML_Agggregate_Create.

**Prototype**

```c
int ML_Gen_SmootherAmesos(ML *ml_object, int k, int AmesosSolver,  
                           int MaxProcs)
```

**Description**

Use Amesos interface to direct solvers for the multigrid coarse grid solver on level k within ml_object and perform any initialization that is necessary.

**Parameters**

- **ml_object**  
  On input, ML object pointer (see ML_Create). On output, the coarse grid solver of level k is set to use Amesos.

- **k**  
  On input, indicates level within ml_object hierarchy (must be the coarsest level in the multigrid hierarchy).

- **AmesosSolver**  
  On input, indicates the direct solver library to use in the coarse solution. It can be: ML Amesos UMFPACK, ML Amesos KLU, ML Amesos Superludist, ML Amesos MUMPS, ML Amesos Scalapack.

- **MaxProcs**  
  On input, indicates maximum number of processors to use in the coarse solution (only for ML Amesos Superludist).
Prototype

```c
void ML_Gen_SmootherAztec(ML *ml_object, int k, int options[], double params[],
                          int proc_config[], double status[], int N_iterations,
                          int pre_or_post, void (*prec_fun)(double *, int *, int *,
                          double *, AZ_MATRIX *, AZ_PRECOND *))
```

Description

Set the smoother (either pre or post as indicated by pre_or_post) at level k within the multigrid solver context to invoke Aztec. The specific Aztec scheme is given by the Aztec arrays: options, params, proc_config, and status and Aztec preconditioning function: prec_function.

Parameters

- **ml_object**: On input, ML object pointer (see ML_Create). On output, a smoother function is associated within ml_object at level k.
- **k**: On input, indicates where the smoother function pointer will be stored within the multigrid hierarchy.
- **options, params, proc_config, status**: On input, Aztec arrays that determine the Aztec scheme and are used for Aztec to return information. See the Aztec User’s Guide.
- **N_iterations**: On input, maximum Aztec iterations within a single smoother invocation. When set to AZ_ONLY_PRECONDITIONER, only one iteration of the preconditioner is used without an outer Krylov method.
- **pre_or_post**: On input, ML_PRESMOOTHER or ML_POSTSMOOTHER indicating whether the smoother should be performed before or after the coarse grid correction.
- **prec_fun**: On input, Aztec preconditioning function indicating what preconditioner will be used within Aztec. Normally, this is set to AZ_precondition. See the Aztec User’s Guide.
int ML_Gen_Smoother_BlockGaussSeidel(ML *ml_object, int k, int pre_or_post, int ntimes, double omega, int blocksize)

Description

Set the multigrid smoother for level k of ml_object and perform any initialization that is necessary. When using block Gauss Seidel, the total number of equations must be a multiple of blocksize. Each consecutive group of blocksize unknowns is grouped into a block and a block Gauss Seidel algorithm is applied.

Parameters

- **ml_object**: On input, ML object pointer (see ML_Create). On output, the pre or post smoother of level k is set to block Gauss Seidel.
- **k**: On input, indicates level within ml_object hierarchy (should be between 0 and Nlevels-1). ML_ALL_LEVELS sets the smoothing on all levels in ml_object.
- **pre_or_post**: On input, ML_PRESMOOTHER or ML_POSTSMOOTHER indicating whether the pre or post smoother is to be set.
- **ntimes**: On input, sets the number of block Gauss Seidel iterations that will be performed.
- **omega**: On input, sets the damping parameter to be used during this block Gauss Seidel smoothing.
- **blocksize**: On input, sets the size of the blocks to be used during block Gauss Seidel smoothing.

Prototype

int ML_Gen_Smoother_GaussSeidel(ML *ml_object, int k, int pre_or_post, int ntimes, double omega)
Description

Set the multigrid smoother for level k of ml_object and perform any initialization that is necessary.

Parameters

- **ml_object**: On input, ML object pointer (see ML_Create). On output, the pre or post smoother of level k is set to Gauss Seidel.

- **k**: On input, indicates level within ml_object hierarchy (should be between 0 and Nlevels^{t-1}). ML_ALL_LEVELS sets the smoothing on all levels in ml_object.

- **pre_or_post**: On input, ML_PRESMOOTHER or ML_POSTSMOOTHER indicating whether the pre or post smoother is to be set.

- **ntimes**: On input, sets the number of Gauss Seidel iterations that will be performed.

- **omega**: On input, sets the damping parameter to be used during this Gauss Seidel smoothing.

Prototype

```c
int ML_Gen_Smoother_Jacobi(ML *ml_object, int k, int pre_or_post, int ntimes, double omega)
```

Description

Set the multigrid smoother for level k of ml_object and perform any initialization that is necessary.

Parameters

- **ml_object**: On input, ML object pointer (see ML_Create). On output, the pre or post smoother of level k is set to Jacobi.

- **k**: On input, indicates level within ml_object hierarchy (should be between 0 and Nlevels^{t-1}). ML_ALL_LEVELS sets the smoothing on all levels in ml_object.
**pre_or_post**
On input, ML_PRESMOOTHER or ML_POSTSMOOTHER indicating whether the pre or post smoother is to be set.

**ntimes**
On input, sets the number of Jacobi iterations that will be performed.

**omega**
On input, sets the damping parameter to be used during this Jacobi smoothing. ML_DEFAULT sets it to .5

Prototype

```c
int ML_Gen_Smooth_SymGaussSeidel(ML *ml_object, int k, int pre_or_post, int ntimes, double omega)
```

Description

Set the multigrid smoother for level k of ml_object and perform any initialization that is necessary.

Parameters

**ml_object**
On input, ML object pointer (see ML_Create). On output, the pre or post smoother of level k is set to symmetric Gauss Seidel.

**k**
On input, indicates level within ml_object hierarchy (should be between 0 and Nlevels-1). ML_ALL_LEVELS sets the smoothing on all levels in ml_object.

**pre_or_post**
On input, ML_PRESMOOTHER or ML_POSTSMOOTHER indicating whether the pre or post smoother is to be set.

**ntimes**
On input, sets the number of symmetric Gauss Seidel iterations that will be performed.

**omega**
On input, sets the damping parameter to be used during this symmetric Gauss Seidel smoothing.

Prototype
int ML_Gen_Smoother_VBlockJacobi(ML *ml_object, int k, int pre_or_post, int ntimes, double omega, int nBlocks, int *blockIndices)

Description

Set the multigrid smoother for level k of ml_object and perform any initialization that is necessary. A block Jacobi smoothing algorithm will be used where the size of the blocks can vary and is given by nBlocks and blockIndices (see ML_Gen_Blocks_Aggregates and ML_Gen_Blocks_Metis).

Parameters

- **ml_object**: On input, ML object pointer (see ML_Create). On output, the pre or post smoother of level k is set to variable block Jacobi.
- **k**: On input, indicates level within ml_object hierarchy (should be between 0 and Nlevels-1). ML_ALL_LEVELS sets the smoothing on all levels in ml_object.
- **pre_or_post**: On input, ML_PRESMOOTHER or ML_POSTSMOOTHER indicating whether the pre or post smoother is to be set.
- **ntimes**: On input, sets the number of block Jacobi iterations that will be performed.
- **omega**: On input, sets the damping parameter to be used during this block Jacobi smoothing.
- **nBlocks**: On input, indicates the total number of block equations in matrix.
- **blockIndices**: On input, blockIndices[i] indicates block to which ith element belongs.

Prototype

int ML_Gen_Smoother_VBlockSymGaussSeidel(ML *ml_object, int k, int pre_or_post, int ntimes, double omega, int nBlocks, int *blockIndices)
Set the multigrid smoother for level k of ml_object and perform any initialization that is necessary. A block Gauss Seidel smoothing algorithm will be used where the size of the blocks can vary and is given by nBlocks and blockIndices (see ML_Gen_Blocks_Aggregates and ML_Gen_Blocks_Metis).

**Parameters**

- **ml_object**: On input, ML object pointer (see ML_Create). On output, the pre or post smoother of level k is set to variable block symmetric Gauss Seidel.
- **k**: On input, indicates level within ml_object hierarchy (should be between 0 and Nlevels†-1). ML_ALL_LEVELS sets the smoothing on all levels in ml_object.
- **pre_or_post**: On input, ML_PRESMOOTHER or ML_POSTSMOOTHER indicating whether the pre or post smoother is to be set.
- **ntimes**: On input, sets the number of block symmetric Gauss Seidel iterations that will be performed.
- **omega**: On input, sets the damping parameter to be used during this block symmetric Gauss Seidel smoothing.
- **nBlocks**: On input, indicates the total number of block equations in matrix.
- **blockIndices**: On input, blockIndices[i] indicates block to which ith element belongs.

**Prototype**

```c
int ML_Gen_Solver(ML *ml_object, int scheme, int finest_level, int coarsest_level)
```

**Description**

Initialize the ML solver context, ml_object, so that it is ready to be used in a solve. ML_Gen_Solver should be called after the multigrid cycle is fully specified but before ML_Iterate or ML_Solve_MGV is invoked.
Parameters

ml_object  
On input, ML object pointer (see ML_Create). On output, all necessary initialization is completed.

scheme  
On input, must be set to ML_MGV indicating a multigrid V cycle is used.

finest_level  
On input, indicates the location within ml_object where the finest level is stored. Normally, this is ‘0’.

coarsest_level  
On input, indicates location within ml_object where the coarsest grid is stored. When doing smoothed aggregation, this can be determined using the total number of multigrid levels returned by ML_Gen_MGHierarchy_UsingAggregation.

Prototype

| int ML_Get_Amatrix(ML *ml_object, int k, ML_Operator **matrix) |

Description

Set *matrix to point to the discretization matrix associated at level k within the multigrid solver context ml_object. This pointer can then be passed into functions like: ML_Operator_Apply, ML_Operator_Get_Diag, and ML_Operator_Getrow.

Parameters

ml_object  
On input, ML object pointer (see ML_Create).

k  
On input, indicates which level within the multigrid hierarchy should be accessed.

matrix  
On output, *matrix points to the discretization matrix at level k within the multigrid hierarchy. This pointer can then be passed into the functions ML_Operator_Apply, ML_Operator_Get_Diag, and ML_Operator_Getrow.

Prototype
void * ML_Get_MyGetrowData(ML_Operator *Amat)

Description

Returns the user specific data pointer associated with the ML_Operator given by Amat. This function is normally employed when users write their own matrix getrow function and they need to get back the pointer that was given with ML_Init_Amatrix.

Parameters

Amat On input, points to matrix for which we seek the internal data pointer.

Prototype

void * ML_Get_MyMatvecData(ML_Operator *Amat)

Description

Returns the user specific data pointer associated with the ML_Operator given by Amat. This function is normally employed when users write their own matrix-vector product function and they need to get back the pointer that was given with ML_Init_Amatrix.

Parameters

Amat On input, points to matrix for which we seek the internal data pointer.

Prototype

void * ML_Get_MySmootherData(ML_Smoother *Smoother)
Description

Returns the user specific data pointer associated with the ML_Smoother object given by Smoother. This function is normally employed when users write their own smoother function and they need to get back the pointer that was given with ML_Set_Smoother.

Parameters

- **Smoother**: On input, points to the smoother for which we seek the internal data pointer.

Prototype

```c
int ML_Init_Amatrix(ML *ml_object, int k, int ilen, int olen, void *data)
```

Description

Set the size information for the discretization matrix associated at level k within ml_object. Additionally, associate a data pointer that can be used when writing matrix-vector product and matrix getrow functions.

Parameters

- **ml_object**: On input, ML object pointer (see ML_Create). On output, size information is associated with the discretization matrix at level k.
- **k**: On input, indicates where discretization size information will be stored within the multigrid hierarchy.
- **ilen**: On input, the number of local rows in the submatrix stored on this processor.
- **olen**: On input, the number of columns in the local submatrix stored on this processor not including any columns associated with ghost unknowns.
- **data**: On input, a data pointer that will be associated with the discretization matrix and could be used for matrix-vector product and matrix getrow functions.
Prototype

```c
int ML_Iterate(ML *ml_object, double *sol, double *rhs)
```

Description

Iterate until convergence to solve the linear system using the multigrid V cycle defined within `ml_object`.

Parameters

- **ml_object**: On input, `ML` object pointer (see `ML_Create`).
- **sol**: On input, a vector containing the initial guess for the linear system contained in `ml_object`. On output, the solution obtained by performing repeated multigrid V cycles.
- **rhs**: On input, a vector containing the right hand side for the linear system contained in `ml_object`.

Prototype

```c
int ML_Operator_Apply(ML_Operator *A, int in_length, double p[], int out_length, double ap[])
```

Description

Invoke a matrix-vector product using the `ML_Operator A`. That is perform \( ap = A \cdot p \). Any communication or ghost variables work needed for this operation is also performed.

Parameters

- **A**: On input, an `ML_Operator` (see `ML_Get_Amatrix`).
- **in_length**: On input, length of vector \( p \) (not including ghost variable space).
\( p \)  
On input, vector which will be multiplied by \( A \).

\( \text{out\_length} \)  
On input, length of vector \( ap \).

\( ap \)  
On output, vector containing result of \( A \times p \).

Prototype

```c
int ML_Operator_Get_Diag(ML_Operator *A, int length, double **diag)
```

Description

Get the diagonal of the ML_Operator \( A \) (which is assumed to be square).

Parameters

- \( A \)  
  On input, an ML_Operator (see ML_Get_Amatrix).

- \( \text{length} \)  
  On input, number of diagonal elements wanted.

- \( \text{diag} \)  
  On output, sets a pointer to an array containing the diagonal elements.  
  NOTE: this is not a copy but in fact a pointer into an ML data structure. Thus,  
  this array should not be freed.

Prototype

```c
int ML_Operator_Getrow(ML_Operator *A, int N_requested_rows, int requested_rows[],
                        int allocated_space, int columns[], double values[],
                        int row_lengths[])
```

Description

Get a row (or several rows) from the ML_Operator \( A \). If there is not enough space in  
\text{columns} and \text{values} to hold the nonzero information, this routine returns a ‘0’.  
Otherwise, a ‘1’ is returned.
**Parameters**

\(A\)

On input, an ML Operator (see ML_Get_Amatrix).

\(N_{\text{requested rows}}\)

On input, number of matrix rows for which information is returned.

\(\text{requested rows}\)

On input, specific rows for which information will be returned.

\(\text{allocated space}\)

On input, length of columns and values.

\(\text{columns}\)

On output, the column numbers of each nonzero within each row requested in \(\text{requested rows}\) (where column numbers associated with \(\text{requested rows}[i]\) appear before column numbers associated with \(\text{requested rows}[j]\) with \(i < j\)).

\(\text{values}\)

On output, the nonzero values of each nonzero within each row requested in \(\text{requested rows}\) (where nonzero values associated with \(\text{requested rows}[i]\) appear before nonzero values associated with \(\text{requested rows}[j]\) with \(i < j\)).

\(\text{row lengths}\)

On output, \(\text{row lengths}[i]\) indicates the number of nonzeros in row \(i\).

**Prototype**

```
int ML_Set_Amatrix_Getrow(ML *ml_object, int k, int (*getrow)(ML_Operator *, int ,
int*, int,
int*, double*, int*), int (*comm )(double *vec, void *data),
int comm_vec_leng)
```

**Description**

Set the matrix getrow function for the discretization matrix associated at level \(k\) within the multigrid solver context \(ml\_object\).

**Parameters**

\(ml\_object\)

On input, ML object pointer (see ML_Create). On output, matrix getrow function is associated with the discretization matrix at level \(k\).
$k$ On input, indicates where the matrix getrow function pointer will be stored within the multigrid hierarchy.

$getrow$ On input, a function pointer to the user-defined matrix getrow function. See Section 11.1.

$comm$ On input, a function pointer to the user-defined communication function. See Section 11.2.

Prototype

```c
int ML_Set_Amatrix_Matvec(ML *ml_object, int k, int (*matvec)(ML_Operator *, int, double *,
                           int, double *))
```

Description

Set the matrix-vector product function for the discretization matrix associated at level $k$ within the multigrid solver context $ml_object$.

Parameters

$ml_object$ On input, ML object pointer (see ML_Create). On output, matrix-vector product function is associated with the discretization matrix at level $k$.

$k$ On input, indicates where the matrix-vector product function pointer is stored within the multigrid hierarchy.

$matvec$ On input, a function pointer to the user-defined matrix-vector product function. See Section 11.1.

Prototype

```c
int ML_Set_ResidualOutputFrequency(ML *ml_object, int output_freq)
```
Description

Set the output frequency of residual information. ML_Iterate prints the two norm of the residual every output_freq iterations.

Parameters

- **ml_object**: On input, ML object pointer (see ML_Create). On output, residual printing frequency is set.
- **output_freq**: On input, value to use for printing frequency.

Prototype

```c
int ML_Set_Smoother(ML *ml_object, int k, int pre_or_post, void *data,
                    int (*func)(ML_Smoother *, int, double *, int, double *),
                    char *label)
```

Description

Set the smoother (either pre or post as indicated by pre_or_post) at level k within the multigrid solver context to invoke the user-defined function ‘func’ and pass in the data pointer ‘data’ via ML_Get_MySmotherData.

Parameters

- **ml_object**: On input, ML object pointer (see ML_Create). On output, a smoother function is associated within ml_object at level k.
- **k**: On input, indicates where the smoother function pointer will be stored within the multigrid hierarchy.
- **pre_or_post**: On input, ML_PRESMOOTHER or ML_POSTSMOOTHER indicating whether the smoother should be performed before or after the coarse grid correction.
- **data**: On input, a data pointer that will be passed into the user-defined function ‘func’.

62
**func**

On input, smoothing function to be used at level k when performing a multigrid V cycle. The specific signature and details of this function are given in Section 8.

**label**

On input, a character string to be associated with Smoother. This string is printed by some routines when identifying the method.

---

**Prototype**

```c
int ML_Set_Tolerance(ML *ml_object, double tolerance)
```

**Description**

Set the convergence criteria for ML_Iterate. Convergence is declared when the 2-norm of the residual is reduced by ‘tolerance’ over the initial residual. This means that if the initial residual is quite small (i.e. the initial guess corresponds quite closely with the true solution), ML_Iterate might continue to iterate without recognizing that the solution cannot be improved due to round-off error. Note: the residual is always computed after performing presmoothing on the finest level (as opposed to at the beginning or end of the iteration). Thus, the true residual should be a little bit better than the one used by ML.

**Parameters**

- **ml_object**
  On input, ML object pointer (see ML_Create). On output, tolerance is set for convergence of ML_Iterate.

- **tolerance**
  On input, value to use for convergence tolerance.

---

**Prototype**

```c
int ML_Solve_MGV(ML *ml_object, double *din, double *dout)
```

**Description**

Perform one multigrid V cycle iteration to the solve linear system defined within ml_object.
## Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>ml_object</code></td>
<td>On input, ML object pointer (see ML_Create).</td>
</tr>
<tr>
<td><code>din</code></td>
<td>On input, the right hand side vector to be used when performing multigrid.</td>
</tr>
<tr>
<td><code>dout</code></td>
<td>On output, an approximate solution obtained after one multigrid V cycle.</td>
</tr>
</tbody>
</table>

\[\text{Nlevels refers to the argument given with ML_Create.}\]
References


