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## ML 3.0 Smoothed Aggregation User's Guide

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#### Abstract

 $\mathbf{ML}$  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.  $\mathbf{ML}$  should be used on large sparse linear systems arising from partial differential equation (PDE) discretizations. While technically any linear system can be considered,  $\mathbf{ML}$  should be used on linear systems that correspond to things that work well with multigrid methods (e.g. elliptic PDEs).  $\mathbf{ML}$  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 non-symmetric 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.

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#### 1 Notational Conventions

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

#### % a\_really\_long\_command

The character % indicates any shell prompt<sup>1</sup>. Function names are shown as ML\_Gen\_Solver. Names of packages or libraries as reported in small caps, as EPETRA. Mathematical entities are shown in italics.

#### 2 Overview

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

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

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.  $\mathbf{ML}$  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,  $\mathbf{ML}$  should be used on linear systems that correspond to things that work well with multigrid methods (e.g. elliptic PDEs).

The ML package is used by creating a 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 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 ML is outlined in Section 4. Section 5 shows the basic usage of ML as a black-box preconditioner for EPETRA matrices. The definition of (parallel) preconditioners using ML\_Epetra::MultiLevelPreconditioner is detailed. This class only requires the linear system matrix, and a list of options. Available parameters for ML\_Epetra::MultiLevelPreconditioner are reported in Section 6. More advanced uses of 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 ML with EPETRA objects is reported in Section 10. Section 11 reports how to define matrices in ML format without depending on EPETRA. Section 12 detailes the (limited) visualization capabilities of ML.

## 3 Multigrid Background

A brief multigrid description is given (see [1], [6], or [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

<sup>&</sup>lt;sup>1</sup>For simplicity, commands are shown as they would be issued in a Linux or Unix environment. Note, however, that **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_k^1(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);
\hat{A}_{k+1} = P_k^T A_k P_k; \quad \mathbf{v} = 0;
multilevel(\hat{A}_{k+1}, \hat{r}, v, k+1);
u = u + P_k \text{ v};
u = S_k^2(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<sup>2</sup>. 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 Trillinos 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 Trillinos 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).

Operating System	Compilers(s)
Linux	GNU and Intel
IRIX N32, IRIX 64, HPUX, Solaris, DEC	Native
ASCI Red	Native and Portland Group
CPlant	Native
Windows	Microsoft

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

<sup>&</sup>lt;sup>2</sup>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.

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<sup>3</sup>, 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 UMF-PACK [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. <b>ML</b> 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.

<sup>&</sup>lt;sup>3</sup>Currently, 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.

--with-ml\_metis Enables interface for Metis [12].

--with-ml\_parmetis2x Enables interface for PARMETIS, version 2.x.

--with-ml\_parmetis3x Enables interface for PARMETIS [11], version

3.x.

--with-ml\_superlu Enables ML interface for serial SUPERLU [3].

The ML interface to SuperLU is deprecated

in favor of the AMESOS interface.

--with-ml\_superlu\_dist Enables ML interface for SUPERLU\_DIST [3].

The  $\mathbf{ML}$  interface to  $\mathbf{SUPERLU\_DIST}$  is depre-

cated in favor of the AMESOS interface.

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  $\mathbf{ML}$  is built through the Trilinos configure.) In order to link the  $\mathbf{ML}$  examples, the user must indicate the location of all the enabled packages' libraries<sup>4</sup>, 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.

--enable-ml\_timing

This prints out timing of key ML routines.

--enable-ml\_flops

This enables printing of flop counts.

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

<sup>&</sup>lt;sup>4</sup>An example of configuration line that enables Metis and Parmetis might be as follows: ./configure --with-mpi-compilers --enable-ml\_metis --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".

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

In this Section we show how to use  $\mathbf{ML}$  as a preconditioner to EPETRA and AZTECOO through the MultiLevelPreconditioner class<sup>5</sup> in the ML\_Epetra namespace.<sup>6</sup> Although limited to algebraic multilevel preconditioners, this allows the use of  $\mathbf{ML}$  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<sup>7</sup>.

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.

```
#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",MLList);

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

<sup>&</sup>lt;sup>5</sup>The MultiLevelPreconditioner class is derived from the Epetra\_RowMatrix class.

 $<sup>^6</sup>$ ML does not rely on any particular matrix format or iterative solver. Examples of using of ML as a preconditioner for user-defined matrices (i.e., non-Epetra matrices) are reported in Section 11.1 and 11.2.

 $<sup>^7</sup>$ In order to use the MultiLevelPreconditioner class,  $\mathbf{ML}$  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<sup>8</sup>. Table 2 briefly reports the most important methods of this class.

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

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()<sup>9</sup>. 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
```

<sup>&</sup>lt;sup>8</sup>See the Teuchos documentation for a detailed overview of this class.

<sup>&</sup>lt;sup>9</sup>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<sup>10</sup>.
  The ML preconditioner is created as in the previous example,
  ML_Epetra::MultiLevelPreconditioner * MLPrec =
    new ML_Epetra::MultiLevelPreconditioner(A, MLList, true);
and we can check that no options have been mispelled, using
  MLPrec->PrintUnused();
The AztecOO solver is called using, for instance,
  solver.SetPrecOperator(MLPrec);
  solver.SetAztecOption(AZ_solver, AZ_cg_condnum);
  solver.SetAztecOption(AZ_kspace, 160);
  solver.Iterate(1550, 1e-12);
Finally, some (limited) information about the preconditioning phase are obtained using
  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:

```
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.

<sup>&</sup>lt;sup>10</sup>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 "(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:

```
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 Uncoupled for level 0, METIS for levels 1 and 2, then MIS for levels 3 and 4.

In  $\S6.5$ , parameters that can be set differently on individual levels are denoted with the symbol  $\star$  (that is not part of the parameter name). Note that some parameters (e.g., Uncoupled-MIS aggregation) correspond to quantities that must be the same at all levels.

#### 6.2 General Usage of the Parameter List

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

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

A generic parameter, say aggregation: type, will now be defined as

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

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

- Metis aggregation scheme requires --with-ml\_metis, or otherwise the code will include all nodes in the calling processor in a unique aggregate;
- ParMetis aggregation scheme required --with-ml\_metis --enable-epetra and --with-ml\_parmetis2x or --with-ml\_parmetis3x.
- 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:

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

```
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.)

Option Name	Type	SA	DD	DD-ML	maxwell
max levels	int	16	2	3	5
output	int	8	8	8	10
increasing or decreasing	string	increasing	increasing	increasing	decreasing
PDE equations	int	1	1	1	_
null space dimension	int	1	1	1	_
null space vectors	double *	NULL	NULL	NULL	NULL
aggregation: type	string	Uncoupled	METIS	METIS	Uncoupled-MIS
aggregation: type (level 1)	string	_	_	ParMETIS	_
aggregation: type (level 8)	string	MIS	_	_	_
aggregation: local aggregates	int	_	1	_	_
aggregation: nodes per aggregate	int	_	_	512	_
aggregation: damping factor	double	4/3	4/3	4/3	0.0
eigen-analysis: type	string	Anorm	Anorm	Anorm	Anorm
coarse: max size	int	128	128	128	128
aggregation: threshold	double	0.0	0.0	0.0	0.0
aggregation: next-level aggregates	int	_	_	128	_
per process					
smoother: sweeps	int	2	2	2	2
smoother: damping factor	double	0.67	_	_	0.67
smoother: pre or post	string	both	both	both	both
smoother: type	string	Gauss-Seidel	Aztec	Aztec	_
smoother: Aztec as solver	bool	_	false	false	_
smoother: MLS polynomial order	int	_	_	_	3
smoother: MLS alpha	double	_	_	_	30.0
coarse: type	string	Amesos_KLU	Amesos_KLU	Amesos_KLU	SuperLU
coarse: sweeps	int	1	1	1	1
coarse: damping factor	double	1.0	1.0	1.0	1.0
coarse: max processes	int	16	16	16	_
print unused	int	0	0	0	0

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 $(3^d \text{ nodes in } d)$
	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 aggre-
	gates. Aggregates can span processes. May provide better qual-
	ity aggregates than either Coupled or uncoupled. Computation-
	ally more expensive than either because it requires matrix-matrix
	product.
Uncoupled-MIS	Uses Uncoupled for all levels until there is 1 aggregate per pro-
	cessor. 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 creates 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 withwith-ml_metis.
ParMETIS	As METIS, but partition the global graph. Requires
	with-ml_parmetis2x orwith-ml_parmetis3x. Aggregates
	can span arbitrary number of processes. Global number of ag-
	gregates can be specified with the option aggregation: global
	number.

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! Mispelled 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.

Jacobi	Point-Jacobi. Damping factor is specified using smoother:			
	dampig factor, and the number of sweeps with smoother:			
	sweeps			
Gauss-Seidel	Point Gauss-Seidel. Damping factor is specified using smoother:			
	dampig factor, and the number of sweeps with smoother:			
	sweeps			
Aztec	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.			
MLS	Use MLS smoother. The polynomial order is specified by			
	smoother: MLS polynomial order, and the alpha value by			
	smoother: MLS alpha.			

 ${\it Table 5: ML\_Epetra::} MultiLevel Preconditioner: Commonly used smoothers.$ 

Jacobi	Use coarse: sweeps steps of Jacobi (with damping parameter		
Jacobi	1 1 1		
	coarse: damping parameter) as a solver.		
Gauss-Seidel	Use coarse: sweeps steps of Gauss-Seidel(with damping pa-		
	rameter coarse: damping parameter) as a solver.		
Amesos-KLU	Use Kluthrough Amesos. Coarse grid problem is shipped to proc		
	0, solved, and solution is broadcast		
Amesos-UMFPACK Use Umfpack through Amesos. Coarse grid problem is shipped to the coarse grid problem in the coarse grid problem is shipped to the coarse grid problem in the coarse grid problem is shipped to the coarse grid problem in the coarse grid problem is shipped to the coarse grid problem in the c			
to proc 0, solved, and solution is broadcasted.			
Amesos-Superludist	rludist Use SuperLU_distthrough Amesos.		
Amesos-MUMPS	Use double precision version of Mumps through Amesos.		
Amesos-ScaLAPACK	Use double precision version of Scalapack through Amesos.		
SuperLU	Use ML interface to SuperLU.		

Table 6: ML\_Epetra::MultiLevelPreconditioner: Some of the available coarse matrix solvers. Note: Amesos solvers requires **ML** to be configured with with-ml\_amesos, 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 ob-
	tained from the block map used to construct the
	object. Note that only block maps with con-
	stant element size can be considered.
	stant clement size can be considered.
null space dimension	Dimension of the null space.
1	<b>.</b>
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  $\star$  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  $\star$  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 as-

signed 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 com-

pute 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 Anorm 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 Defines the maximum number of next-level ma-

per process \* trix rows per process (only for ParMETIS aggre-

gation scheme).

#### 6.5.3 Smoothing Parameters

 $smoother: sweeps \star Number of sweeps of smoother.$ 

smoother: damping factor  $\star$  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  $\star$  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  $\star$  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  $\star$  Polynomial order for MLS smoothers.

smoother: MLS alpha  $\star$  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.

coarse: max processes

Maximum number of processes to be used in the coarse grid solution (only for Amesos-Superludist, Amesos-MUMPS, Amesos-Scalapack).

## 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 mul-

Figure 2: High level multigrid sample code.

tilevel solver object that is used to define the preconditioner. It requires the maximum number of multigrid levels be specified. In almost all cases, N\_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\_UsingAggregation. 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

ML\_Gen\_Smoother\_VBlockJacobi

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 AZTECas 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.

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

```
int user_smoothing(void *data, int x_length, double x[],
                   int rhs_length, double rhs[])
```

where data is a pointer given with the ML\_Set\_Smoother invocation, 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. A simple (and suboptimal) damped Jacobi smoother for the finest grid of our example is given below:

```
int user_smoothing(void *data, int x_length, double x[], int rhs_length, double rhs[])
{
   double ap[5], omega = .5; /* temp vector and damping factor */
   Poisson_matvec(data, 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 residual information is output (ML\_Set\_ResidualOutputFrequency) can both be set. Additionally, the level of diagnostic output from either ML\_Iterate or ML\_Solve\_MGV can be set via ML\_Set\_OutputLevel. The maximum number of multigrid levels can be set via ML\_Create or ML\_Set\_MaxLevels. Otherwise, ML continues coarsening until the coarsest grid is less than or equal to a specified size (by default 10 degrees of freedom). This size can be set via ML\_Aggregate\_Set\_MaxCoarseSize.

## 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 ML\_Aggregate\_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  $0 \le \epsilon \le 10^{-6}$ ), 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

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

This drop tolerance (whose default value is zero) is set by ML\_Aggregate\_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 PARMETISaggregation. 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\_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\_Aggregate\_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\_Aggregate\_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\_Aggregate\_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

```
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

```
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 AZTECOO solver,

```
Epetra_LinearProblem Problem(A,&x,&b);
AztecOO 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,

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

## 11 Using ML without Epetra

#### 11.1 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<sup>11</sup>.

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.

<sup>&</sup>lt;sup>11</sup>The functions CSR\_matvec, CSR\_getrows, MSR\_matvec and MSR\_getrows can be used.

The function 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 user\_matvec is associated with the matrix located at level '0' of the multigrid hierarchy. The signature of user\_matvec is

where A\_data is the user-defined data pointer specified in the ML\_Init\_Amatrix, p is the vector to apply to the matrix, in\_length is the length of this vector, and ap is the result after multiplying the discretization matrix by the vector p and out\_length is the length of ap.

Finally, 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 user\_getrow is associated with the matrix located at level '0' of the multigrid hierarchy and that this matrix contains nlocal\_allcolumns columns and that no communication (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 user\_getrow is

```
int user_getrow(void *A_data, int N_requested_rows, int requested_rows[],
  int allocated_space, int columns[], double values[], int row_lengths[])
```

where A\_data is the user-defined data pointer in ML\_Init\_Amatrix, N\_requested\_rows is the number of matrix rows for which information is returned, requested\_rows are the specific rows for which information will be returned, allocated\_space indicates how much space has been allocated in columns and values for nonzero information. On return, the user's function should take each row in order within requested\_rows and place the column numbers and the values corresponding to nonzeros in the arrays columns and values. The length of the ith requested row should appear in row\_lengths[i]. If there is not enough allocated space in columns or 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:

$$\begin{pmatrix}
2 & -1 & & & & \\
-1 & 2 & -1 & & & & \\
& -1 & 2 & -1 & & & \\
& & -1 & 2 & -1 & & \\
& & & -1 & 2
\end{pmatrix}.$$
(2)

To implement this matrix, the following functions are defined:

```
int Poisson_getrow(void *A_data, int N_requested_rows, int requested_rows[],
   int allocated_space, int columns[], double values[], int row_lengths[])
{
   int count = 0, i, start, row;

   for (i = 0; i < N_requested_rows; i++) {
      if (allocated_space < count+3) return(0);
}</pre>
```

```
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(void *A_data, 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 A\_data was not used. In the next section we give a parallel example which makes use of A\_data. 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 nlocal where nlocal 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

```
int user_comm(double x[], void *Adata)
```

where A\_data is the user-defined data pointer specified in the ML\_Init\_Amatrix and x is a vector of length nlocal\_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 nlocal elements of x are filled with data where nlocal 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.

```
int Poisson_getrow(void *A_data, int N_requested_rows, int requested_rows[],
   int allocated_space, int cols[], double values[], int row_lengths[])
{
   int m = 0, i, row, proc, *itemp, start;

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

 $<sup>^{12}</sup>$ 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

```
for (i = 0; i < N_requested_rows; i++) {</pre>
      row = requested_rows[i];
      if (allocated_space < m+3) return(0);</pre>
      values[m] = 2; values[m+1] = -1; values[m+2] = -1;
      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(void *A_data, int in_length, double p[], int out_length,
                   double ap[])
{
   int i, proc, *itemp;
   double new_p[5];
   itemp = (int *) A_data;
   proc = *itemp;
   for (i = 0; i < in_length; i++) new_p[i] = p[i];</pre>
   Poisson_comm(new_p, A_data);
   for (i = 0; i < out_length; i++) ap[i] = 2.*new_p[i];
   if (proc == 0) {
      ap[0] -= new_p[2];
      ap[1] -= new_p[3];
   if (proc == 1) {
      ap[0] -= new_p[1]; ap[0] -= new_p[4];
      ap[1] -= new_p[2]; ap[1] -= new_p[0];
      ap[2] -= new_p[3]; ap[2] -= new_p[1];
   return 0;
}
   and
int Poisson_comm(double x[], void *A_data)
{
          proc, neighbor, length, *itemp;
   double send_buffer[2], recv_buffer[2];
   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

## 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

```
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

where ml is the ML object, ag the ML-Aggregation object, and 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. option is an integer value defined so that:

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

Processor X will write its own file, filename\_levelY\_procX, where Y is the level. filename can be set to NULL (default value of .graph will be used in this case).

Note that in AMG there is no mesh associated with coarser levels. Therefore 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).

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

#### 4. Deallocate memory using

```
ML_Aggregate_VizAndStats_Clean( ag, MaxMgLevels ).
```

At this point, one should copy file viz\_aggre.net and viz\_aggre.cfg (located in \$ML\_HOME/util/) in the directory where the output files are located, and run OpendDX with the instruction

#### % dx -edit viz\_aggre.net

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

## 13 ML Functions

# Prototype \_\_\_\_\_

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 AZTECmatrix and store it within the 'ml\_object' context.

#### Parameters \_\_\_\_\_

$ml\_object$	On input, <b>ML</b> 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 $^\dagger$ -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 un- knowns.
Amat	On input, an Aztecdata structure representing a matrix. See the AztecUser's Guide.
$proc\_config$	On input, an AZTECdata structure representing processor information. See the AZTECUser's Guide.

## Prototype \_\_\_\_\_

#### 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 AZTECdata 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 AZTECdata structure representing a matrix. See the AZTECUser's Guide.
$ml\_object$	On input, $\mathbf{ML}$ object pointer (see ML_Create) representing a V cycle multigrid method.
options	On input, an Aztecdata structure representing user chosen options. On output, set appropriately for multigrid V cycle preconditioner.

Prototype \_\_\_\_\_

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	
int ML_Aggregat	e_Destroy(ML_Aggregate **agg_object)
Description	
Destroy the aggr	egate context, agg_object, and delete all memory allocated by <b>ML</b> in sing the aggregation options.
Parameters	
$agg\_object$	On input, aggregate object pointer (see ML_Aggregate_Create). On output, all memory allocated by <b>ML</b> and associated with this context is freed.
Prototype	
int ML_Aggregat	e_Set_CoarsenScheme_Coupled(ML_Aggregate *agg_object)
Description	
Set the aggregate	e 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	
int ML_Aggregat	e_Set_CoarsenScheme_MIS(ML_Aggregate *agg_object)

Description			
Set the aggregate	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_Aggregat	e_Set_CoarsenScheme_Uncoupled(ML_Aggregate *agg_object)		
Description			
Set the aggregate	e 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_Aggregat	e_Set_CoarsenScheme_METIS(ML_Aggregate *agg_object)		
Description			
Set the aggregate	e coarsening scheme to be used as 'METIS (see Section 9).		

# Parameters \_ On input, aggregate object pointer (see ML\_Aggregate\_Create). On agg\_object output, the 'METIS' aggregation will be used for automatic coarsening. Prototype \_\_\_\_\_ int ML\_Aggregate\_Set\_CoarsenScheme\_ParMETIS(ML\_Aggregate \*agg\_object) Description \_\_\_\_\_ Set the aggregate coarsening scheme to be used as 'ParMETIS (see Section 9). Parameters \_\_\_\_\_ On input, aggregate object pointer (see ML\_Aggregate\_Create). On $agg\_object$ output, the 'ParMETIS' aggregation will be used for automatic coarsening. Prototype \_\_\_\_\_ int ML\_Aggregate\_Set\_DampingFactor( ML\_Aggregate \*ag, double factor) Description \_\_\_\_\_

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

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

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 \_

agg\_object On input, aggregate object pointer (see ML\_Aggregate\_Create). On

output, the damping factor is set to factor.

factor On input, damping factor that will be associated with this aggrega-

tion object.

### Prototype \_\_\_\_\_

int ML\_Aggregate\_Set\_MaxCoarseSize( ML\_Aggregate \*agg\_object, int size )

### Description \_\_\_\_\_

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

#### Parameters \_\_\_\_\_

agg\_object On input, aggregate object pointer (see ML\_Aggregate\_Create). On

output, the coarsest mesh size will be set.

size On input, size indicating the maximum coarsest mesh size.

### Prototype \_\_\_\_\_

int ML\_Aggregate\_Set\_NullSpace(ML\_Aggregate \*agg\_object, int num\_PDE\_eqns, int null\_dim,

double \*null\_vect, int leng)

#### 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	
$agg\_object$	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.
$num\_PDE\_eqns$	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.
$null\_dim$	On input, number of seed vectors that will be used when creating the smoothed aggregation grid transfer operator.
$null\_vect$	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.
leng	On input, the length of each seed vector.

Prototype _		
- I - I		

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	
$agg\_object$	On input, aggregate object pointer (see ML_Aggregate_Create). On output, the spectral radius estimate will be determined by a conjugate gradient routine.

Prototype			
<i>J</i> 1			

int ML\_Aggregate\_Set\_SpectralNormScheme\_Anorm( ML\_Aggregate \*ag)

Description	
Set the method to be matrix) to be the infi	used for estimating the spectral radius of $A$ (the discretization nity norm. This spectral radius estimate is used when smoothing the perator (see ML_Aggregate_Set_DampingFactor).
Parameters	
$agg\_object$	On input, aggregate object pointer (see ML_Aggregate_Create). On output, the spectral radius estimate will be taken as the infinity norm of the matrix.
Prototype	
int ML_Aggregate_Set	z_Threshold(ML_Aggregate *agg_object, double tolerance)
Description	
Set the drop tolerance matrix $A$ are dropped details.	e used when creating the matrix graph for aggregation. Entries in the d when $ A(i,j)  \leq tol_{-}d * \sqrt{ A(i,i)A(j,j) }$ . See Section 9 for more
Parameters	
agg_object	On input, an ML_Aggregate object pointer created by invoking ML_Aggregate_Create. On output, drop tolerance for creating the matrix graph is set.
tolerance	On input, value to be used for dropping matrix entries.

int ML\_Create(ML \*\*ml\_object, int Nlevels)

Prototype \_\_\_\_\_

	vocations. The <b>ML</b> object has a notation of levels where different ors corresponding to different grid levels are stored.
Parameters	
$ml\_object$	On input, a pointer to a noninitialized $\mathbf{ML}$ object pointer. On output, points to an initialized $\mathbf{ML}$ object pointer.
Nlevels	Maximum number of multigrid levels within this $\mathbf{ML}$ object.
Prototype	
int ML_Destroy(	ML **ml_object)
Description	
Destroy the ML building and set	solver context, ml_object, and delete all memory allocated by <b>ML</b> in ting options.
Parameters	
$ml\_object$	On input, $\mathbf{ML}$ object pointer (see ML_Create). On output, all memory allocated by $\mathbf{ML}$ and associated with this context is freed.
Prototype	
int ML_Gen_Blo **block_list)	ocks_Aggregates(ML_Aggregate *agg_object, int k, int *nblocks, int

Create an  $\mathbf{ML}$  solver context (or handle). This  $\mathbf{ML}$  instance will be used in all subsequent

Description \_\_\_\_\_

#### Description \_

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, $\mathbf{ML}$ object pointer (see ML_Create).
k	On input, indicates level within ml_object hierarchy where the aggregate information is found that defines partitioning.
nblocks	On output, indicates the number of partitions.
$block\_list$	On output, equation i resides in the block_list[i]th partition.

#### ${f Prototype}$

int ML\_Gen\_Blocks\_Metis(ML \*ml\_object, int k, int \*nblocks, int \*\*block\_list)

#### Description \_

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, <b>ML</b> object pointer (see ML_Create).
k	On input, indicates level within ml_object hierarchy where the discretization matrix is found that will be partitioned.
nblocks	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.

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 \_\_\_\_\_

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_Aggregate_Create.

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).
Amesos Solver	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).

#### 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 AZTECscheme is given by the AZTECarrays: options, params, proc\_config, and status and AZTECpreconditioning function: prec\_function.

Parameters	
$ml\_object$	On input, <b>ML</b> 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, AZTECarrays that determine the AZTECscheme and are used for AZTECto return information. See the AZTECUser's Guide.
$N\_iterations$	On input, maximum AZTECiterations 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, AzteCpreconditioning function indicating what preconditioner will be used within Aztec. Normally, this is set to Az-precondition. See the AztecUser's Guide.

#### Prototype \_\_\_\_

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, $\mathbf{ML}$ 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 $^{\dagger}$ -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.
block size	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, <b>ML</b> 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 $^{\dagger}$ -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 \_\_\_\_\_

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, $\mathbf{ML}$ 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 $^{\dagger}$ -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 $$

int ML\_Gen\_Smoother\_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 $^{\dagger}$ -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, $\mathbf{ML}$ 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.
block Indices	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)

#### Description \_

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, $\mathbf{ML}$ 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 $^{\dagger}$ -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.
block Indices	On input, blockIndices[i] indicates block to which ith element belongs.

#### Prototype \_\_\_\_\_

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, $\mathbf{ML}$ 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.

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, <b>ML</b> 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 \_\_\_\_\_

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 writting matrix-vector product and matrix getrow functions.

Parameters	
$ml\_object$	On input, <b>ML</b> 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 un- knowns.
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

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 contain the right hand side for the linear system contained in ml_object.

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 \* 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 $A$ .
$out\_length$	On input, length of vector $ap$ .
ap	On output, vector containing result of $A * p$ .

## Prototype \_\_\_\_\_

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).

length On input, number of diagonal elements wanted.

On output, sets a pointer to an array containing the diagonal ele-

ments. NOTE: this is not a copy but in fact a pointer into an ML

data structure. Thus, this array should not be freed.

#### Prototype \_\_

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 columns and values to hold the nonzero information, this routine returns a '0'. Otherwise, a '1' is returned.

A On input, an ML\_Operator (see ML\_Get\_Amatrix).

N\_requested\_rows On input, number of matrix rows for which information is returned.

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

allocated\_space On input, length of columns and values.

columns On output, the column numbers of each nonzero within each row re-

quested in requested\_rows (where column numbers associated with requested\_rows[i] appear before column numbers associated with

requested\_rows[j] with i < j).

values On output, the nonzero values of each nonzero within each row re-

quested in requested\_rows (where nonzero values associated with requested\_rows[i] appear before nonzero values associated with

requested\_rows[j] with i < j).

row\_lengths On output, row\_lengths[i] indicates the number of nonzeros in row

i.

## Prototype \_\_\_\_\_

int ML\_Set\_Amatrix\_Getrow(ML \*ml\_object, int k, int (\*getrow)(void \*, 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, <b>ML</b> 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 \_\_\_\_\_

### 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, <b>ML</b> 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

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, $\mathbf{ML}$ object pointer (see ML_Create). On output, residual printing frequency is set.
$output\_freq$	On input, value to use for printing frequency.

## Prototype \_\_\_\_\_

## 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'.

Parameters		
$ml\_object$	On input, <b>ML</b> 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'.	
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	
V <del>-</del>	
nt 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 can not 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, $\mathbf{ML}$ 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 \_\_\_\_

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	
$ml\_object$	On input, <b>ML</b> object pointer (see ML_Create).
din	On input, the right hand side vector to be used when performing multigrid.
dout	On output, an approximate solution obtained after one multigrid V cycle.

 $<sup>^\</sup>dagger \text{Nlevels}$  refers to the argument given with ML\_Create.

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