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ML 4.0 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 packages [19]. 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 prompt¹. 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. A quick start is reported in Section 4. The process of configuring and building ML is outlined in Section 5. Section 6 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 6.4. Section 7 reports how to use the Maxwell solvers of ML. More advanced uses of ML are presented in Section 8. Here, we present how to define and fine-tune smoothers, coarse grid solver, and the multilevel hierarchy. Multigrid options are reported in Section 9. Smoothing options are reported in Section 10, where we also present how to construct a user's defined smoother. Advanced usage of ML with EPETRA objects is reported in Section 11. Section 12 reports how to define matrices in ML format without depending on EPETRA.

3 Multigrid Background

A brief multigrid description is given (see [3], [9], or [10] 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

 $^{^1}$ 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 \mathbf{Nlevel} - \mathbf{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 \mathbf{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 9. 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 method². 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 9).

4 Quick Start

This section is intended for the impatient user. It's assumed that you've already have a local copy of Trilinos³. Using the instructions here, your build of Trilinos will have the following libraries: Aztecoo, Epetra, EpetraExt, Ifpack, Loca, ML, New_Package, NOX, Amesos and Teuchos.

- 1. cd into the Trillinos directory.
- 2. Make a build directory, e.g., mkdir sandbox.
- 3. cd sandbox.
- 4. Configure Trillings:
 - (a) ../configure --enable-teuchos --enable-amesos if you do not want to use MPI.
 - (b) ../configure --enable-teuchos
 --enable-amesos --with-mpi-compilers=/usr/local/mpich/bin (or wherever your MPI compilers are located) to use MPI.

 $^{^{2}}$ The P_{k} 's are usually determined as a preprocessing step and not computed within the iteration.

³Please refer to the web page http://software.sandia.gov/trilinos to know how to obtain a copy of TRILINOS.

- 5. Build TRILINOS: make.⁴
- 6. If your build finished without errors, you should see the directory Trilinos/sandbox/packages/, with subdirectories below that for each individual library. ML's subdirectory, ml, should contain files config.log, config.status, Makefile, and Makefile.export, and directories src and examples. Directory src contains object files and libml.a. Directory examples contains executables with extension .exe, symbolic links to the corresponding source code, and object files. Directory test is intended primarily for developers and can be ignored.
- 7. Look in Trilinos/sandbox/packages/ml/examples for examples of how to use ML. File Trilinos/packages/ml/examples/README suggests how to use the examples.

5 Configuring and Building ML

ML is configured and built using the GNU autoconf [7] and automake [8] tools. It can be configured and build as a standalone package without or with AZTEC 2.1 support (as detailed in Section 5.1 and 5.2), or as a part of the TRILINOS framework [11] (as described in Section 5.3). Even though ML can be compiled and used as a standalone package, the recommended approach is to build ML as part of the TRILINOS framework, as a richer set of features are then available.

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

Operating System	Compilers(s)
Linux	GNU and Intel
MAC OS X	GNU
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.

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.

5.1 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.

```
% cd $ML_HOME
% mkdir standalone
% cd standalone
```

⁴If you are using GNU's make on a machine with more than one processor, then you can speed up the build with make -j XX, where XX is the number of processors.

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

5.2 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 12.1 and Section 12.2). 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 9. 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.

5.3 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 (here introduced for the sake of simplicity only) identifies the Trilinos directory, and, for example, that we are compiling under LINUX and MPI.

```
% cd $TRILINOS_HOME
% mkdir LINUX_MPI
% cd LINUX_MPI
% $TRILINOS_HOME/configure \
     --enable-teuchos \
     --enable-amesos \
     --with-mpi-compilers \
     --prefix=$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 5.3.1 and 5.3.2. You can also find a complete list and explanations by typing ./configure --help in the ML home directory.

5.3.1 Enabling Third Party Library Support

ML can be configured with the following third party libraries (TPLs): SUPERLU, SUPERLU_DIST, PARASAILS, ZOLTAN, METIS, and PARMETIS. It can take advantage of the following Trilinos packages: IFPACK, TEUCHOS, TRIUTILS, AMESOS, EPETRAEXT. Through AMESOS, ML can interface with the direct solvers Klu, UMFPACK, SUPERLU, SUPERLU_DIST⁵, 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.

The same configure options that enable certain other Trilinos packages also enable the interfaces to those packages within ML.

enable-epetra	Enable support for the EPETRA package.
enable-epetraext	Enable support for the EPETRAEXT package.
enable-aztecoo	Enable support for the AZTECOO package.
enable-amesos	Enables support for the AMESOS package. AMESOS is an interface with several direct solvers. ML supports UMFPACK [5], KLU, SUPERLU_DIST (1.0 and 2.0), MUMPS [1]. This package is necessary to use the AMESOS interface to direct solvers.
enable-teuchos	Enables support for the Teuchos package. This package is necessary to use the ML_Epetra::MultiLevelPreconditioner class.
enable-triutils	Enables support for the Triutils package. ML uses Triutils only in some examples, to create the linear system matrix.
enable-ifpack	Enable support for the Ifpack package [12], to use Ifpack factorizations as smoothers for ML.
enable-anasazi	Enable support for the Anasazi package. Anasazi can be used by ML for eigenvalue computations.

To know whether the **--enable-**package options below reported are enabled or disabled by default⁶, please consult the configure at the Trilinos level by typing

 $^{^5\}mathrm{Currently},\,\mathbf{ML}$ can support SuperLU_dist directly (without Amesos support), or through Amesos.

⁶This refers to configurations from the Trilinos top level (that is, using \$TRILINOS.HOME/configure). If ML if configured from the ML level (that is, the user directly calls \$ML.HOME/configure), then all the --enable-package are off by default.

\$TRILINOS_HOME/configure --help

The following configure line options enable interfaces in ML to certain TPLs. By default, all the --with-ml_TPL options are disabled. For the most up-to-date list, please type configure --help at the ML package level.

with-ml_parasails	Enables interface for Parasails [4].
with-ml_metis	Enables interface for Metis [16].
with-ml_parmetis2x	Enables interface for PARMETIS, version $2.x$.
with-ml_parmetis3x	Enables interface for PARMETIS [15], version $3.x.$
with-ml_superlu	Enables ML's direct interface for serial SU-PERLU [6] 1.0. This interface is deprecated in favor of the AMESOS interface. Note: you cannot configure ML with both this option andenable-amesos.
with-ml_superlu2	Enables ML's direct interface for serial SU-PERLU [6] 2.0. This interface is deprecated in favor of the AMESOS interface. Note: you cannot configure ML with both this option andenable-amesos.
with-ml_superlu_dist	Enables ML interface for SUPERLU_DIST [6]. This interface is deprecated in favor of the AME-SOS interface. Note: you cannot configure ML with both this option andenable-amesos.

If one of the above options is enabled, then the user must specify the location of the header files, with the option

--with-incdirs=<include-locations>

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

```
--with-ldflags="<lib-locations>"
--with-libs="<lib-list>"
```

The user might find useful the option

--disable-examples

which turns off compilation and linking of all Trilinos examples, or

--disable-ml-examples

which turns off compilation and linking of ML examples.

Here is an example configure line, where Metis, Parmetis, Zoltan, and Superlu are all used:

```
./configure --with-mpi-compilers="/usr/local/mpich/bin" CXXFLAGS="-03" CFLAGS="-03" FFLAGS="-03" --cache-file=config.cache --with-gnumake --with-ml_metis --with-ml_zoltan --with-ml_parmetis3x --with-ldflags="-L/usr/local/superlu-3.0/lib -L/usr/local/parmetis -L/usr/local/zoltan/lib" --with-libs="-lsuperlu -lparmetis -lmetis -lzoltan" --with-incdirs="-I/usr/local/superlu-3.0/SRC -I/usr/local/parmetis-3.1 -I/usr/local/parmetis-3.1/ParMETISLib -I/usr/local/zoltan/include"
```

More details about the installation of Trilinos can be found at the Trilinos web site,

http://software.sandia.gov/Trilinos

and [18, Chapter 1].

5.3.2 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.

6 ML and Epetra: Getting Started with the MultiLevelPreconditioner Class

In this Section we show how to use **ML** as a preconditioner to EPETRA and AZTECOO through the MultiLevelPreconditioner class. This class is derived from the Epetra_RowMatrix class, and is defined in the ML_Epetra namespace.

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 pointer⁷ and a Teuchos parameter list⁸.

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_MultiLevelPreconditioner.h". Also note that the macro HAVE_CONFIG_H must be defined either in the user's code or as a compiler flag.

6.1 Example 1: ml_preconditioner.cpp

We now give a very simple fragment of code that uses the MultiLevelPreconditioner. For the complete code, see \$ML_HOME/examples/BasicExamples/ml_preconditioner.cpp. 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_MultiLevelPreconditioner.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");

// create the preconditioner
```

⁷Note that not all Epetra matrices can be used with ML. Clearly, the input matrix must be a square matrix. Besides, it is supposed that the OperatorDomainMap(), the OperatorRangeMap() and the RowMatrixRowMap() of the matrix all coincide, and that each row is assigned to exactly one process.

⁸In order to use the MultiLevelPreconditioner class, **ML** must be configured with options -enable-epetra --enable-teuchos.

```
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;
```

A MultiLavelDresconditioner may be defined as fello

A MultiLevelPreconditioner may be defined as follows. First, the user defines a Teu-CHOS parameter list⁹. 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.
get(Name,DefValue)	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 containing the parameter name, and Value is the specified parameter value, whose type can be any C++ object or pointer. A complete list of parameters available for class MultiLevelPreconditioner is reported in Section 6.4.

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->DestroyPreconditioner()¹⁰. 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
MLPrec->ComputePreconditioner();
```

⁹See the Teuchos documentation for a detailed overview of this class.

¹⁰We suggest to always create the preconditioning object with new and to delete it using delete. Some MPI calls occur in DestroyPreconditioner(), so the user should not call MPI_Finalize() or delete the communicator used by ML before the preconditioning object is destroyed.

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

// re-compute the elements of A
// now re-compute the preconditioner, using either
MLPrec->ComputePreconditioner();
// or
MLPrec->ReComputePreconditioner();

// re-solve the linear system

// .. finally destroy the object
delete MLPrec;
```

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 [17]). Method ReComputePreconditioner() can be used to recompute the preconditioner using already available information about the aggregates. ReComputePreconditioner() reuses the already computed tentative prolongator, then recomputes the smoothed prolongators and the other components of the hierarchy, like smoothers and coarse solver¹¹.

6.2 Example 2: ml_2level_DD.cpp

In the second example, a two level domain decomposition preconditioner is constructed. The coarse space is defined using aggregation. It is worthwhile to compare the parameters selected here to the default parameters stated in Table 6.

File \$ML_HOME/examples/TwoLevelDD/ml_2level_DD.cpp reports the entire code. In the example, the linear system matrix A, is an Epetra_CrsMatrix corresponding to the discretization of a Laplacian on a 2D Cartesian grid. The solution vector and right-hand side are x and b respectively.

The AztecOO linear problem is defined as

```
Epetra_LinearProblem problem(&A, &x, &b);
Aztec00 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");
```

¹¹Note that the hierarchy produced by ReComputePreconditioner() can differ from that produced by ComputePreconditioner() for non-zero threshold values.

```
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>12</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);
```

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

```
cout << MLPrec->GetOutputList();
```

solver.Iterate(1550, 1e-12);

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 or she can get a reference to the internally stored list:

```
ParameterList& List = MLPrec->GetList();
```

and then directly modify List. Method GetList() should be used carefully, as a change to List may modify the behavior of MLPrec.

6.3 Parallel Performance

This section gives a few tips on tuning ML's parallel performance.

¹²Only 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.

Uncoupled	Attempts to construct aggregates of optimal size $(3^d \text{ nodes in } d)$
oncoupied	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 proces-
	sor, 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 3: ML_Epetra::MultiLevelPreconditioner: Available coarsening schemes.

6.3.1 Dynamic Load-balancing

ML supports dynamic load-balancing of coarse-level matrices in the multigrid preconditioner. This is extremely important for two reasons. First, it is not unusual for the message-passing latency on a coarse level to be roughly equivalent to the latency of the fine level, even though the number of matrix unknowns on the coarse level is much smaller than on the fine level. Second, as the number of unknowns per processor becomes small, ML's aggregation methods become less effective. The coarsening rate may drop, thus leading to more multigrid levels than one might observe in serial.

We now give two code fragments to demonstrate how to use the repartitioning options. The complete description of options that control repartitioning is given in §6.4.6. The following code demonstrates repartitioning for a matrix with unknowns that are node-based.

```
Teuchos::ParameterList MLList;
MLList.set("repartition: enable",1);
MLList.set("repartition: max min ratio",1.3);
MLList.set("repartition: min per proc",500);
MLList.set("repartition: partitioner","Zoltan");
MLList.set("repartition: Zoltan dimensions",2);

// Zoltan requires coordinates
double *xcoord, *ycoord, *zcoord;

// user must load the coordinates, of coarse ...
```

Jacobi	Point-Jacobi. Damping factor is specified using smoother:				
	damping factor, and the number of sweeps with smoother:				
	sweeps				
Gauss-Seidel	Point Gauss-Seidel. Damping factor is specified using smoother:				
	damping factor, and the number of sweeps with smoother:				
	sweeps				
symmetric Gauss-Seidel	Point symmetric Gauss-Seidel. Damping factor is specified us-				
	ing smoother: damping 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 AZTECOO vectors 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.				
user-defined	User-defined smoothing function. The function must conform				
	to the prototype int (*)(ML_Smoother *, int inLength,				
	double *invec, int outLength, double *outvec). The				
	number of sweeps is controlled via smoother: sweeps. See				
	ml/examples/BasicExamples/ml_user_smoothing.cpp.				

Table 4: ML_Epetra::MultiLevelPreconditioner: Commonly used smoothers.

```
MLList.set("x-coordinates", xcoord);
MLList.set("y-coordinates", xcoord);
```

The following code demonstrates repartitioning for a matrix with unknowns that are edgebased.

```
Teuchos::ParameterList MLList;

// these correspond to the main edge matrix

MLList.set("repartition: enable",1);

MLList.set("repartition: max min ratio",1.3);

MLList.set("repartition: min per proc",1000);

MLList.set("repartition: partitioner","Zoltan");

// Zoltan requires coordinates

double *xcoord, *ycoord, *zcoord;

// user must load the coordinates, of coarse ...

MLList.set("x-coordinates", xcoord);

MLList.set("y-coordinates", ycoord);

MLList.set("z-coordinates", zcoord);

// these correspond to the auxiliary node matrix
```

Jacobi	Use coarse: sweeps steps of Jacobi (with damping parameter
	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.
MLS	Use degree coarse: MLS polynomial order Chebychev poly-
	nomial as a solver.
Hiptmair	Use coarse: sweeps steps of two-stage Hiptmair smoothing,
	with subsmoother coarse: subsmoother type, as a solver.
Amesos-KLU	Use Klu through Amesos. Coarse grid problem is shipped to
	proc 0, solved, and solution is broadcast
Amesos-Superlu	Use SuperLU, version 3.0, through Amesos.
Amesos-UMFPACK	Use Umfpack through Amesos. Coarse grid problem is shipped
	to proc 0, solved, and solution is broadcasted.
Amesos-Superludist	Use SuperLU_dist through Amesos.
Amesos-MUMPS	Use double precision version of Mumps through Amesos.
SuperLU	Use ML interface to SuperLU(depreacated).

Table 5: 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.

```
MLList.set("repartition: node max min ratio",1.5);
MLList.set("repartition: node min per proc",300);
MLList.set("repartition: node partitioner","Zoltan");
MLList.set("repartition: Zoltan dimensions",3);

double *node_xcoord, *node_ycoord, *node_zcoord;

// user must load the coordinates, of coarse ...

MLList.set("x-coordinates", node_xcoord);
MLList.set("y-coordinates", node_ycoord);
MLList.set("z-coordinates", node_zcoord);
```

6.4 List of All Parameters for MultiLevelPreconditioner Class

In this section we give general guidelines for using the MultiLevelPreconditioner class effectively. The complete list of input parameters is also reported. 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 requires --with-ml_metis --enable-epetra and --with-ml_parmetis2x or --with-ml_parmetis3x.

- AMESOS coarse solvers require --enable-amesos --enable-epetra --enable-teuchos. Moreover, AMESOS must have been configure to support the requested coarse solver. Please refer to the AMESOS documentation for more details.
- IFPACK smoothers require --enable-ifpack --enable-epetra --enable-teuchos.
- PARASAILS smoother requires --with-ml_parasails.

Note that, in the parameters name, spaces are important: Do not include non-required leading or trailing spaces, and do 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.

Some of the parameters that affect the MultiLevelPreconditioner class 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. Parameters that can be set differently on individual levels are denoted with the symbol \star (this symbol is not part of the parameter name).

6.4.1 General Options

output

[int] Controls the amount of information printed to the screen. Ranges from 0 to 10 (0 is no output, and 10 is incredibly detailed output). Default: 10.

print unused

[int] If non-negative, will print all the unused parameters on the specified processor. If -1, the unused parameters will be printed on all processes. If -2, nothing will be printed. Default: -2.

PDE equations

[int] Number of PDE equations for each grid node. This value is not considered for Epetra_VbrMatrix objects, as in this case is obtained from the block map used to construct the object. Note that only block maps with constant element size can be considered. Default:

6.4.2 Multigrid Cycle Options

cycle applications [int] Number of applications of the multilevel

V-cycle. Default: 1.

max levels [int] Maximum number of levels. Default: 10.

increasing or decreasing [string] If set to increasing, level 0 will corre-

spond to the finest level. If set to decreasing, max levels - 1 will correspond to the finest

level. Default: increasing.

prec type [string] Multigrid cycle type.

Possible values: MGV, MGW, full-MGV, one-level-postsmoothing, two-level-additive, two-level-hybrid, two-level-hybrid2, projected MGV. Default:

MGV.

projected modes [double**] Array of double vectors containing

modes that should be projected out before and after the AMG V-cycle is applied. For use with

the projected MGV option. Default: NULL.

number of projected modes [int] Number of modes that are to be projected

out before and after the AMG V-cycle is applied. For use with the projected MGV option.

Possible values: 1,2, or 3. Default: 0.

6.4.3 Aggregation Parameters

aggregation: type * [string] Define the aggregation scheme. See

Table 3. Default: Uncoupled.

aggregation: threshold [double] Dropping threshold in aggregation.

Default: 0.0.

aggregation: damping factor [double] Damping factor for smoothed aggrega-

tion. Default: 4/3.

aggregation: smoothing sweeps

[int] Number of smoothing sweeps to use in the prolongator smoother. This should be used in conjunction with larger aggregates, from using either METIS or ParMETIS aggregation schemes. If sweeps is equal to 1, then the value of aggregation: damping factor is used. sweeps is greater than 1, the damping factors are calculated automatically. Default: 1.

aggregation: global aggregates *

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

aggregation: local aggregates *

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

eigen-analysis: type

[string] Defines the numerical scheme to be used to compute an estimation of the maximum eigenvalue of $D^{-1}A$, where D = diag(A)(for smoothed aggregation only). Choices are: cg (10 steps of conjugate gradient method), Anomr (the A-norm of the matrix), Anasazi (use the Arnoldi method), power-method. Default: Anorm.

aggregation: next-level aggregates[int] Defines the maximum number of nextper process * level matrix rows per process (only for ParMETIS aggregation scheme). Default: 128.

aggregation: use tentative

restriction

[bool] If true, then the final restriction operator at level ℓ is computed as $R_{\ell} = P_{\ell,0}^T$, where $P_{\ell,0}$ is the tentative prolongator. Note that the final prolongator is still computed as specified by parameter aggregation: damping factor. Default: false.

aggregation: symmetrize

[bool] If true, then the final prolongator for level ℓ is computed as $P_{\ell} = (I - \omega/\lambda_{max}(A + A^T))P_{0,\ell}$, where ω is the damping parameter specified using aggregation: damping factor, λ_{max} is the maximum eigenvalue of $D^{-1}A$, and $P_{0,\ell}$ is the tentative prolongator at level ℓ . The restriction is defined as $R_{\ell} = P_{\ell}^T$. Default: false.

6.4.4 Smoothing Parameters

smoother: sweeps ★

[int] Number of sweeps of smoother. Default:

1.

smoother: damping factor \star

[double] Smoother damping factor. Default:

0.67.

smoother: pre or post *

[string] It can assume on the following values:

pre, post, both. Default: both.

smoother: type \star

[string] Type of the smoother. See Table 4.

Default: symmetric Gauss-Seidel.

smoother: Aztec options *

[int*] Pointer to AZTEC's options vector (only

for Aztec smoother).

smoother: Aztec params \star

[double*] Pointer to Aztec's params vector

(only for Aztec smoother).

smoother: Aztec as solver \star

[bool] 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). Default: false.

smoother: MLS polynomial order \star

[int] Polynomial order for MLS smoothers. De-

fault: 3.

smoother: MLS alpha *

[double] Alpha value for MLS smoothers. De-

fault: 30.0.

smoother: user-defined function [int (*)(ML_Smoother *, int inLength,

double *invec, int outLength, double
*outvec) Pointer to user-defined smoothing

function. Default: NULL.

smoother: user-defined name [string] Label for user-defined smoother. De-

fault: "User-defined".

smoother: Hiptmair sweeps ★ [int] Number of Hiptmair iterations to perform.

Default: 1.

smoother: Hiptmair efficient

symmetric

[boo1] Reduce the preconditioner computational work while maintaining symmetry by doing edge-node relaxation on the first leg of the V-cycle, and node-edge relaxation on the second

leg. Default: true.

subsmoother: type * [string] Smoother to be used as a subsmoother

at each step of Hiptmair smoothing. It can assume on the following values: MLS, symmetric

Gauss-Seidel. Default: MLS.

subsmoother: MLS polynomial order [int] Polynomial order for Hiptmair MLS sub-

smoother. Default: 3.

subsmoother: MLS alpha * [int] Polynomial coefficient for Hiptmair MLS

sub-smoother. Default: 3.

subsmoother: SGS damping factor * [double] Damping factor for Hiptmair sub-

smoother symmetric Gauss-Seidel. Auto-

matically calculated in the range (0, 2).

subsmoother: SGS edge sweeps * | int | Number of iterations of Hiptmair sub-

smoother SGS to perform on edge problem. De-

fault: 1.

subsmoother: SGS node sweeps * [int] Number of iterations of Hiptmair sub-

smoother SGS to perform on nodal projection

problem. Default: 1.

6.4.5 Coarsest Grid Parameters

coarse: max size [int] Maximum dimension of the coarse grid.

ML will not coarsen further if current levels size

is less than this value. Default: 128.

coarse: type [string] Coarse solver. See Table 5. Default:

Amesos_KLU.

coarse: sweeps [int] (Only for Jacobi, Gauss-Seidel,

symmetric Gauss-Seidel, and Hiptmair.)
Number of sweeps in the coarse solver. Default:

1.

coarse: damping factor [double] (Only for Jacobi and Gauss-Seidel.)

Damping factor in the coarse solver. Default:

0.67.

coarse: max processes [int] Maximum number of processes to be

used in the coarse grid solution (only for Amesos-Superludist, Amesos-MUMPS). If -1, AMESOS will decide the optimal number of pro-

cessors to be used. Default: -1.

6.4.6 Load-balancing Options

repartition: enable [int] Enable/disable repartitioning. Default: 0

(off).

repartition: partitioner [string] Partitioning package to use. Can as-

sume the following values: Zoltan, ParMETIS.

Default: Zoltan.

repartition: max min ratio [double] Specifies desired ratio of g_{max}/g_{min} ,

where g_{max} is the maximum number rows over all processors, and g_{min} is the minimum number of rows over all processors. If the actual ratio is larger, then repartitioning occurs. Default: 1.1.

repartition: min per proc [int] Specifies desired minimum number of rows

per processor. If the actual number is greater,

then repartitioning occurs. Default: 20.

nodal hierarchy. Specifies desired ratio of g_{max}/g_{min} , where g_{max} is the maximum number rows over all processors, and g_{min} is the minimum number of rows over all processors. If the actual ratio is larger, then repartitioning occurs.

Default: 1.1.

repartition: node min per proc [int] Maxwell-specific option for auxiliary nodal

hierarchy. Specifies desired minimum number of rows per processor. If the actual number is greater, then repartitioning occurs. Default: 20.

repartition: Zoltan dimensions [int] Dimension of the problem. Can assume

the following values: $\{2,3\}$.

6.4.7 Visualization

viz: enable [bool] Enable/disable visualization. Default:

false.

viz: output format [string] The format of the visualization files.

Can assume the following values: vtk, xyz,

openx. Default: vtk.

viz: print starting solution [bool] Enable/disable printing of initial starting

solution.

viz: equation to plot [bool] In the case of systems of PDEs, the equa-

tion number to print. Default: all equations.

6.4.8 Miscellaneous

x-coordinates [double*] Pointer to array of x-coordinates of

mesh nodes (edges, in the case of Maxwell).

y-coordinates [double*] Pointer to array of y-coordinates of

mesh nodes (edges, in the case of Maxwell).

z-coordinates [double*] Pointer to array of z-coordinates of

mesh nodes (edges, in the case of Maxwell).

node: x-coordinates [double*] Pointer to array of x-coordinates of

mesh nodes. (Maxwell only)

node: y-coordinates [double*] Pointer to array of y-coordinates of

mesh nodes. (Maxwell only)

node: z-coordinates [double*] Pointer to array of z-coordinates of

mesh nodes. (Maxwell only)

6.4.9 Null Space Detection

If used in conjunction with Anasazi, ML can compute an approximate null space of the linear operator to precondition. This can be done using the following options:

null space: type

[string] If default vectors, the default null space are used (no computation required).

If pre-computed, a pointer to the already-computed null is obtained from option null space: vectors. If enriched, ML will compute, using ANASAZI, an approximation of the null space of the operator. Default: default

vectors.

null space: vectors [double*]. Pointer to user-supplied null space

vectors.

null space: vectors to compute [int]. If null space: type is set to

enriched, this option indicates the number of

eigenvectors to compute. Default: 1.

null space: add default vectors [bool]. If true, the default null space (one con-

stant vector for each unknown) will be added to

the computed null space. Default: true.

eigen-analysis: restart [int] Number of restarts for Anasazi. Default:

2.

6.4.10 Aggregation Strategies

In some case, it is preferable to generate the aggregates using a matrix defined as follows:

$$L_{i,j} = (\mathbf{x}_i - \mathbf{x}_j)^{-2}, \quad i \neq j, \qquad L_{i,i} = -\sum_{i \neq j} L_{i,j},$$
(2)

(where \mathbf{x}_i represents the coordinates of node i) in conjunction with a given nonzero dropping threshold. This may happen, for instance, when working with bilinear finite elements on strecthed grids. \mathbf{ML} can be instructed to generate the aggregates using matrix (2), then build the preconditioner using the actual linear system matrix, as done in the following code fragment:

```
double* x_coord;
double* y_coord; // set to to 0 for 1D problems
double* z_coord; // set to to 0 for 2D problems
// here we define the nodal coordinates...
```

```
MLList.set("x-coordinates", x_coord );
MLList.set("y-coordinates", y_coord );
MLList.set("z-coordinates", z_coord );
```

The double vectors y_coord and/or z_coord can be set to 0. x_coord (and y_coord if 2D, and z_coord if 3D) must be allocated to contain the coordinates for all nodes assigned to the calling processor, plus that of the ghost nodes. For systems of PDE equations, the coordinates must refer to the block nodes (that is, x-coordinate of local row i will be reported in x_coord[i/NumPDEEqns].

The following option can be used:

```
aggregation: aux: enable [bool]. Enable/disable the use of matrix (2). Default: false.
```

6.5 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 6. 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);
```

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);
```

Option Name	Type	SA	DD	DD-ML	maxwell
max levels	int	16	2	3	10
output	int	∞	~	∞	10
increasing or decreasing	string	increasing	increasing	increasing	decreasing
PDE equations	int	1			1
print unused	int	0	0	0	0
aggregation: type	string	Uncoupled-MIS	METIS	METIS	Uncoupled-MIS
aggregation: local aggregates	int	1	1	1	1
	int	ı	ı	512	ı
aggregation: damping factor	double	4/3	4/3	4/3	4/3
eigen-analysis: type	string	Anorm	Anorm	Anorm	Anorm
aggregation: threshold	double	0.0	0.0	0.0	0.0
aggregation: next-level aggregates	int	ı	1	128	1
per process					
smoother: sweeps	int	2	2	2	1
smoother: damping factor	double	29.0	ı	I	1.0
smoother: pre or post	string	both	both	both	both
smoother: type	string	Gauss-Seidel	Aztec	Aztec	Hiptmair/MLS
smoother: Aztec as solver	bool	1	false	false	false
smoother: MLS polynomial order	int	1	1	ı	3
smoother: MLS alpha	double		_	1	27.0
coarse: type	string	Amesos_KLU	Amesos_KLU	Amesos_KLU	Amesos_KLU
coarse: max size	int	128	128	128	75
coarse: sweeps	int				
coarse: damping factor	double	1.0	1.0	1.0	1.0
coarse: max processes	int	16	16	16	ı

Table 6: Default values for ML_Epetra::MultiLevelPreconditioner for the 4 currently supported problem types SA, DD, DD-ML, Maxwell. "-" means not set.

.
// 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.)

6.6 Analyzing the ML preconditioner

A successful multilevel preconditioner require the careful choice of a large variety of parameters, for instance each level's smoother, the aggregation schemes, or the coarse solver. Often, for non-standard problems, there is no theory to support these choices. Also, sometimes it is difficult to understand which component of the multilevel cycle is not properly working. To help to set the multilevel components, **ML** offers a set of tools, to (empirically) analyze several components of the multilevel cycles, and the finest-level matrix.

Two examples are included in the **ML** distribution:

- File examples/Visualization/ml_viz.cpp shows how to visualize the effect of the ML cycle and each level's smoother on a random vector;
- File examples/Advanced/ml_analyze.cpp shows who to get some quantitative information about each level's matrix, and multilevel preconditioner.

In the following subsections, we suppose that a MultiLevelPreconditioner object has already be defined, and the preconditioned computed.

6.6.1 Cheap Analysis of All Level Matrices

Method AnalyzeMatrixCheap() will report on standard output general information about each level's matrix. An example of output is as reported below. (Here, we report only the part of output related to the finest level.)

*** Analysis of ML_Operator 'A matrix level 0' ***

```
Number of global rows
                                                    = 256
                                                    = 1
Number of equations
Number of stored elements
                                                    = 1216
Number of nonzero elements
                                                    = 1216
Mininum number of nonzero elements/row
                                                    = 3
Maximum number of nonzero elements/row
                                                    = 5
Average number of nonzero elements/rows
                                                    = 4.750000
Nonzero elements in strict lower part
                                                    = 480
Nonzero elements in strict upper part
                                                    = 480
\max |i-j|, a(i,j) != 0
                                                    = 16
Number of diagonally dominant rows
                                                    = 86 (= 33.59%)
Number of weakly diagonally dominant rows
                                                    = 67 (= 26.17\%)
```

```
Number of Dirichlet rows
                                                   = 0 (= 0.00\%)
                                                   = 244.066240
||A||_F
Min_{i,j} ( a(i,j) )
                                                    = -14.950987
Max_{i,j} ( a(i,j) )
                                                   = 15.208792
Min_{i,j} (abs(a(i,j)))
                                                    = 0.002890
Max_{i,j} (abs(a(i,j)))
                                                    = 15.208792
Min_i ( abs(a(i,i)) )
                                                   = 2.004640
Max_i ( abs(a(i,i)) )
                                                   = 15.208792
Min_i (\sum_{j=i} abs(a(i,j)))
                                                    = 2.004640
Max_i (\sum_{j=i} abs(a(i,j)))
                                                   = 15.205902
max eig(A) (using power method)
                                                   = 27.645954
\max eig(D^{-1}A) (using power method)
                                                   = 1.878674
```

Total time for analysis = 3.147979e-03 (s)

This analysis is "cheap" in the sense that it involves only element-by-element comparison, plus the computation of the largest-magnitude eigenvalue (which requires some matrix-vector products). AnalyzeMatrixCheap() can be used for both serial and parallel runs.

6.6.2 Analyze the Effect of Smoothers

For each level, method AnalyzeSmoothers() computes the eigenvectors of the matrix (say, A). Then, for each eigenvector (say, v) of A, the smoother is applied to the solution of the homogeneous system

$$Ae = 0$$

with starting solution $e_0 = v$. The code reports on file the real and imaginary values of the eigenvalue corresponding to eigenvector v, and the $||e||/||e_0||$.

The syntax is AnalyzeSmoothers(NumPre, NumPost). NumPre is the number of presmoother applications, and NumPost the number of post-smoother applications. This method reports on the standard output the following information:

Solving Ae = 0, with a random initial guess

- number of pre-smoother cycle(s) = 5
- number of post-smoother cycle(s) = 5
- all reported data are scaled with their values
 before the application of the solver
 (0 == perfect solution, 1 == no effect)
- SF is the smoothness factor

Solver					Linf	L2	SF
Presmoother	(level	Ο,	eq	0)	0.827193	0.804528	0.313705
Postsmoother	(level	Ο,	eq	0)	0.822015	0.810521	0.342827
Presmoother	(level	1,	eq	0)	0.972593	0.908874	2.51318
Postsmoother	(level	1,	ea	0)	0.982529	0.922668	2.53639

6.6.3 Analyze the effect of the ML cycle on a random vector

Method AnalyzeCycle(NumCycles), where NumCycles is the number of multilevel cycles to apply, applies the already computed ML preconditioner to a random vector, and reports on standard output the following information:

Solving Ae = 0, with a random initial guess using 5 ML cycle(s).

- (eq 0) scaled Linf norm after application(s) = 0.0224609
 (eq 0) scaled L2 norm after application(s) = 0.000249379
- (eq 0) scaled smoothness factor = 10.6517

6.6.4 Test different smoothers

The MultiLevelPreconditioner class offers a very easy way to test the effect of a variety of smoothers on the problem at hand. Once the preconditioning object has been created, a call to TestSmoothers() performs the following operations:

- 1. Creates a new linear system, whose matrix is the one used to construct the MultiLevel-Preconditioner object;
- 2. Defines a random solution, and the corresponding right-hand side;
- 3. Defines a zero starting vector for the Krylov solver;
- 4. Creates a new preconditioning object, with the same options as in the current preconditioner, except for the choice of the smoothers;
- 5. Solve the linear system with the newly created preconditioner;
- 6. Reports in a table the iterations to converge and the corresponding CPU time.

The following options, to be set *before* calling ComputePreconditioner(), can be used to tune the test session:

test: max iters [int] Maximum number of iterations for the

Krylov solver. Default: 500.

test: tolerance [double] Tolerance for the Krylov solver. De-

fault: 1e-5.

test: Jacobi [bool] Enable/disable test with Jacobi

smoother. Default: true.

test: Gauss-Seidel [bool] Enable/disable test with Gauss-Seidel

smoother. Default: true.

test: symmetric Gauss-Seidel [bool] Enable/disable test with symmetric

Gauss-Seidel smoother. Default: true.

test: block Gauss-Seidel [bool] Enable/disable test with block Gauss-

Seidel smoother. Default: true.

test: Aztec [bool] Enable/disable test with AZTECOO

smoother. Default: true.

test: Aztec as solver [bool] Enable/disable test with AZTECOO as a

solver smoother. Default: true.

test: ParaSails [bool] Enable/disable test with PARA-

Sailssmoother. Default: true.

test: IFPACK [bool] Enable/disable test with IF-

PACKsmoother. Default: true.

An example of output is reported below. Note that some smoothers (PARASAILS, IF-PACK) will be tested only if **ML** has been properly configured. Note also that TestSmoothers() requires **ML** to be configured with option --enable-aztecoo.

```
*** *************************
*** Analysis of ML parameters (smoothers) ***
*** *************************
*** maximum iterations = 500
                     = 1e-05
*** tolerance
*** All options as in the input parameter list, except that
*** all levels have the same smoother
*** M: maximum iterations exceeded without convergence
*** N: normal exit status (convergence achieved)
*** B: breakdown occurred
*** I: matrix is ill-conditioned
*** L: numerical loss of precision occurred
      smoother type.....its.....||r||/||r_0||..time (s)......
- Jacobi
#0.....n=5, omega=2.50e-01...........12.......2.97314e-06....0.0839319......N
#1.....n=5, omega=5.00e-01......12......6.21844e-06....0.0820519......N
#2.....n=5, omega=7.50e-01.......12.......7.52614e-06....0.082267.......N
#3.....n=5, omega=1.00e+00......12.......3.80406e-06....0.082956.......N
#4.....n=5, omega=1.25e+00.......12......2.15858e-06....0.0824361......N
- Gauss-Seidel
#5.....n=5, omega=2.50e-01......7......2.20736e-06....0.0857691......N
#6.....n=5, omega=5.00e-01..........7........1.91864e-06....0.0789189......N
#7.....n=5, omega=7.50e-01.........6.......8.40948e-06....0.076307.......N
#8.....n=5, omega=1.00e+00......7......1.36415e-06....0.0792729.....N
```

```
#9.....n=5, omega=1.25e+00......7......1.4833e-06.....0.0790809......N
- Gauss-Seidel (sym)
#10....n=5, omega=2.50e-01.........4........2.32835e-06....0.149586.......N
#11....n=5, omega=5.00e-01......4........2.68576e-06....0.092068......N
#12....n=5, omega=7.50e-01..........4.........8.51966e-07....0.0793679......N
#13....n=5, omega=1.00e+00......4......1.34439e-06....0.0787291.....N
#14....n=5, omega=1.25e+00......4.......5.09185e-06....0.0790669.....N
- Gauss-Seidel (block)
#15....n=5, omega=2.50e-01.........6........6.56673e-06....0.0920131......N
#16....n=5, omega=5.00e-01......7......1.77309e-06....0.0881529.....N
#17....n=5, omega=7.50e-01.........6.......8.53488e-06....0.0846661......N
#18....n=5, omega=1.00e+00.......6......2.66381e-06....0.0839909......N
#19....n=5, omega=1.25e+00.......6......4.87356e-06....0.083786......N
- Aztec preconditioner
#20....ILU(fill=0)............7.........4.93736e-06....0.0712331......N
#21....ILU(fill=1)...............6........3.54992e-06....0.0647091......N
- Aztec as solver
#23....iterations=1......7.......1.94081e-06....0.140772......N
#24....iterations=3......4......8.90029e-08....0.0687031.....N
#25....iterations=5............3.........1.00778e-07....0.069193.......N
- ParaSails
*** The best iteration count was obtain in test 25
*** The best CPU-time was obtain in test 21
*** Total time = 2.43798(s)
```

6.7 Visualization Capabilities

6.7.1 Visualizing the Aggregates

ML offers the possibility to visualize the aggregates for all levels. Aggregates generated by Uncoupled and METIS aggregation schemes can be visualized for serial and parallel runs, while aggregates generated using MIS and ParMETIS can be visualized only for serial runs.

Data can be stored in the "xyz" format, readable by packages such as XD3D [?]. For each aggregate, the file contains a line of type

x-coord y-coord <z-coord> aggregate-number

(z-coord is present only for 3D computations.) XD3D can be used to visualize files in this format, but only for 2D problems. Results are reported in Figure 2.

Data can also be stored in the "vtk legacy" format, readable by packages such as Paraview [?]. Paraview allows for 2D and 3D point clouds visualization. It is also possible to visualize sections of 3D data via cutting planes. In order to use this format, fine level coordinates must be supplied. Coarse level coordinates are derived from the fine level coordinates via the multigrid restriction operators. Data is stored as follows. The first section begins with the header

POINTS XX float

where XX is the total number of points. For each point, the coordinates are given as

x-coord y-coord <z-coord>

Next, connectivity information is given in a pair-wise fashion. For example, if the (i, j) entry of matrix A is nonzero, then there is a line in the data file of the form

2 i j

where the first entry specifies the number of points that follow. (This first entry will always be 2 because the connectivity is pair-wise.) The next data section specifies the aggregate to which each point belongs. It begins with the header

POINT_DATA XX SCALARS aggregate_number int 1 LOOKUP_TABLE default

The section then has a line for each point of the form

aggregate_number

The final section specifies the solution (residual) at each point. The section begins with the header

SCALARS solution float 1 LOOKUP_TABLE default

and then has a line for each point of the form

solution_value

With the exception of connectivity, all information is given in the same order. Hence, all information for the jth unknown can be found at the jth line of each section.

6.7.2 Visualizing the effect of the ML Preconditioner and Smoothers

In some cases, it may be useful to visualize the effect of the **ML** preconditioner, or of each level's smoother, on a random vector (whose components are contained in the interval [0.5, 1]), to understand if there are zones or directions that are not affected by the current multilevel preconditioner. This can be easily done with the following code fragment:

```
double* x_coord;
double* y_coord;
// here we define the nodal coordinates...
MLList.set("viz: enable", true);
//you can also specify "xyz" on the line below
MLList.set("viz: output format", "vtk");
MLList.set("viz: x-coordinates", x_coord);
MLList.set("viz: y-coordinates", y_coord);
// by default the starting solution is not printed
MLList.set("viz: print starting solution", true);
// create the preconditioner
ML_Epetra::MultiLevelPreconditioner * MLPrec =
 new ML_Epetra::MultiLevelPreconditioner(*A, MLList, true);
// visualize the effect of the ML preconditioner on a
// random vector. We ask for 10 multilevel cycles
MLPrec->VisualizeCycle(10);
// visualize the effect of each level's smoother on a
// random vector. We ask for 5 steps of presmoothers,
// and 1 step of postsmoother
MLPrec->VisualizeSmoothers(5,1);
```

(File ml_viz.cpp contains the compilable code.) We note that the parameters must be set before calling ComputePreconditioner(). See also Section 6.4.10 for the requirements on the coordinates vectors. Results will be written in the following files:

- before-presmoother-eqX-levelY.vtk contains the random vector before the application of the presmoother, for equation X at level Y;
- after-presmoother-eqX-levelY.vtk contains the random vector after the application of the presmoother, for equation X at level Y;
- before-postsmoother-eqX-levelY.vtk contains the random vector before the application of the postsmoother, for equation X at level Y;
- after-postsmoother-eqX-levelY.vtk contains the random vector after the application of the postsmoother, for equation X at level Y;
- before-cycle-eqX-levelY.vtk contains the random vector before the application of the MLcycle, for equation X at the finest level;
- after-cycle-eqX-levelY.vtk contains the random vector after the application of the ML cycle, for equation X at finest level.

6.8 Print the Computational Stencil for a 2D Cartesian Grid

Method PrintStencil2D() can be used to print out the computational stencil for problems defined on 2D Cartesian grids, if the nodes numbering follows the x-axis. The following fragment of code shows the use of this method:

```
int Nx = 16; // nodes along the x-axis
int Ny = 32; // nodes along the y-axis
int NodeID = -1; // print the stencil for this node
int EquationID = 0; // equation 0, useful for vector problems

// MLPrec is a pointer to an already created

// ML_Epetra::MultiLevelPreconditioner

MLPrec->PrintStencil2D(Nx,Ny,NodeID, EquationID);

// also valid in this case

MLPrec->PrintStencil2D(Nx,Ny);
```

If NodeID == -1, the code considers a node in the center of the computational domain. The result can be something as follows:

2D computational stencil for equation 0 at node 136 (grid is 16 x 16)

0	-1	0
-1	4	-1
0	-1	0

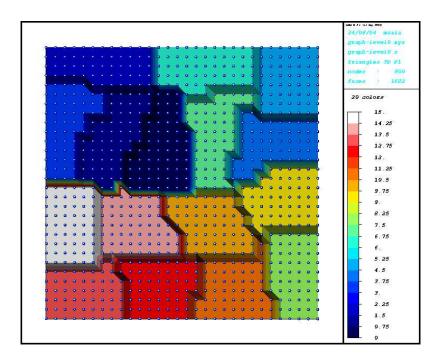
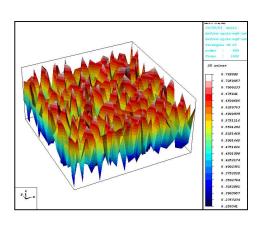


Figure 2: Decomposition into aggregates. Uniform colors between blue spheres represent the interior of aggregates. Visualization was done with $\rm XD3D$.



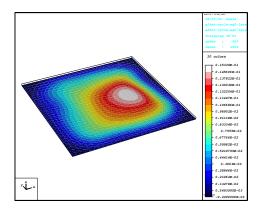


Figure 3: Starting solution (left) and solution after 10 \mathbf{ML} cycles (right). Visualization was done using XD3D.

7 Using the Maxwell Solver in ML

This section gives a brief overview of how to ML's AMG preconditioner for the eddy current formulation of Maxwell's equations. The solver is intended only for equations in the time domain (real-valued), not the frequency domain (complex-valued).

7.1 Background

The eddy current formulation of Maxwell's equations can be written as

$$\nabla \times \nabla \times \vec{E} + \sigma \vec{E} = \vec{f},\tag{3}$$

where \vec{E} is the unknown electric field to be computed, σ is the spatially-varying electrical conductivity, and \vec{f} is the known right-hand side. Neumann, Dirichlet, and/or periodic boundary conditions are supported.

Although we assume that (3) is discretized with first-order edge elements, it is possible to use this preconditioner for higher-order discretizations, as long as the user provides the sub-matrix that corresponds to just the first-order discretization. For more theoretical background and algorithm descriptions, please see [14, 2].

7.2 Notational conventions

For the remainder of the discussion, $K^{(e)}$ denotes the matrix corresponding to the first-order element discretization of (3). $K^{(e)}$ can be written as

$$K^{(e)} = S + M,$$

where S is the stiffness matrix corresponding to the $\nabla \times \nabla \times$ term in (3), and M is the mass matrix corresponding to the $\sigma \vec{E}$ term in (3). The null-space of S is given by the discrete gradient matrix, T. T corresponds to the null space of the $\nabla \times \nabla \times$ term in (3). $K^{(n)}$ is an auxiliary nodal matrix that is described in §7.3.1.

7.3 Operators that the user must supply

The user must provide three matrices:

- 1. the first-order edge element matrix $K^{(e)}$.
- 2. the auxiliary nodal matrix $K^{(n)}$.
- 3. the discrete gradient matrix T.

7.3.1 Description of the auxiliary nodal matrix $K^{(n)}$

 $K^{(n)}$ is a square, $N_n \times N_n$ matrix, where N_n is the number of nodes in the mesh. There are two ways to construct $K^{(n)}$. The first method is to discretize the PDE

$$\int_{\Omega} \sigma u \cdot v + \int_{\Omega} \nabla u \cdot \nabla v,\tag{4}$$

using nodal linear finite elements on the same mesh as (3). The second method assumes that you already have T available. $K^{(n)}$ can be formed via the triple-matrix product

$$T^{\mathrm{T}}K^{(e)}T = T^{\mathrm{T}}MT.$$

where we have used the fact that ST = 0.

7.3.2 Description of the discrete gradient matrix T

T is a rectangular, $N_e \times N_n$ matrix, where N_e is the number of edges in the mesh (rows in $K^{(e)}$) and N_n is the number of nodes in the mesh (rows in $K^{(n)}$). Each row of T has at most two entries, a +1 and/or a -1. There are two ways to construct T. In the first method, it's assumed that the mesh topology is available. T can be viewed as a node-edge incidence matrix of the mesh as a directed graph. As such, each row of T corresponds to an edge, and the +1/-1 entries in the row are the head/tail of the edge, respectively. Hence, T can be built one row at a time by visiting each edge and inserting +1/-1 in the appropriate columns. The second method assumes that $K^{(n)}$ is already constructed. Each off-diagonal nonzero entry, (i,j), in the upper triangular portion of $K^{(n)}$ corresponds to a row in T containing a 1 and a -1 in columns i and j.

7.4 Smoother options

The default smoother for Maxwell's equations is a two-stage smoother that we call Hiptmair smoothing [13]. This smoother consists of three steps: one step of a smoother S on the entire system Kx = f; one step of a smoother S on the projected system $T^TMTe = T^Tr$, where r = f - Kx; and finally one step of a smoother S on the entire system with initial guess x + e.

In serial, the default sub-smoother \mathcal{S} is symmetric Gauss-Seidel (SGS). In parallel, the default sub-smoother \mathcal{S} a degree 3 Chebyshev polynomial. The coefficients of this polynomial are calculated automatically based on the coarsening rate of the multigrid hierarchy. The Chebyshev degree can be changed with the option

smoother: Hiptmair MLS polynomial order

8 Advanced Usage of ML

Sections 6 and 6.4 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 4. The function ML_Create creates a multilevel

Figure 4: High level multigrid sample code.

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 12.1. The multigrid hierarchy is generated via ML_Gen_MGHierarchy_UsingAggregation. Controlling the behavior of this function is discussed in Section 10. 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 [22] [21]. 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 9. 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.

9 Multigrid & Smoothing Options

Several options can be set to tune the multigrid behavior. In this section, smoothing and high level multigrid choices are discussed. In the next section, the more specialized topic of the grid transfer operator is considered.

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.

the given below along with a few general comments.	
ML_Gen_Smoother_Jacobi	Typically, not the fastest smoother. Should be used with damping. For Poisson problems, the recommended damping values are $\frac{2}{3}$ (1D), $\frac{4}{5}$ (2D), and $\frac{5}{7}$ (3D). In general, smaller damping numbers are more conservative.
$ML_Gen_Smoother_GaussSeidel$	Probably the most popular smoother. Typically, faster than Jacobi and damping is often not necessary nor advantageous.
$ML_Gen_Smoother_SymGaussSeidel$	Symmetric version of Gauss Seidel. When using multigrid preconditioned conjugate gradient, the multigrid operator must be symmetrizable. This can be achieved by using a symmetric smoother with the same number of pre and post sweeps on each level.
$ML_Gen_Smoother_BlockGaussSeidel$	Block Gauss-Seidel with a fixed block size. Often used for PDE systems where the block size is the number of degrees of freedom (DOFs) per grid point.
$ML_Gen_Smoother_VBlockJacobi$	Variable block Jacobi smoother. This allows users to specify unknowns to be grouped into different blocks when doing block Jacobi.

ML_Gen_Smoother_VBlockSymGaussSeidel Symmetric variable block Gauss-Seidel smoothing. This allows users to specify unknowns to be

grouped into different blocks when doing sym-

metric 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 [19] 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

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

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

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

   return 0;
}</pre>
```

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.

10 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.

10.1 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 $(i,i)^{th}$ 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 [20]. As the default, the Uncoupled-MIS scheme is used which does uncoupled aggregation on finer grids and switches to the more expensive MIS aggregation on coarser grids;

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

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

10.2 Interpolation Options

An interpolation operator is built using coarsening information, seed vectors, and a damping factor. We refer the reader to [21] 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 [21]). 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.

11 Advanced Usage of ML and Epetra

Class ML_Epetra::MultiLevelOperator is defined in a header file, that must be included as #include "ml_MultiLevelOperator.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 8), 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);
```

12 Using ML without Epetra

12.1 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 5.2). Further, functions for some common matrix storage formats (CSR & MSR) already exist within ML and do not need to be rewritten¹³.

Size information is indicated via ML_Init_Amatrix. The third parameter in the Figure 4 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.

The function ML_Set_Amatrix_Matvec associates a matrix-vector product with the discretization matrix. The invocation in Figure 4 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

 $^{^{13}}$ The functions CSR_matvec, CSR_getrows, MSR_matvec and MSR_getrows can be used.

where A_mat is an internal ML object, 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. The function ML_Get_MyMatvecData(Amat) can be used to get a pointer back to the user's data (i.e. the data pointer given with the ML_Init_Amatrix invocation).

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 4 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(ML_Operator *Amat, int N_requested_rows, int requested_rows[],
   int allocated_space, int columns[], double values[], int row_lengths[])
```

where Amat is an internal ML object, 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. The function ML_Get_MyGetrowData(Amat) can be used to get a pointer back to the user's data (i.e. the data pointer given with the ML_Init_Amatrix invocation). 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:

$$\begin{pmatrix}
2 & -1 & & & & \\
-1 & 2 & -1 & & & & \\
& -1 & 2 & -1 & & & \\
& & -1 & 2 & -1 & & \\
& & & -1 & 2
\end{pmatrix}.$$
(5)

To implement this matrix, the following functions are defined:

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

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

```
row = requested_rows[i];
      if ( (row >= 0) || (row <= 4) ) {
         columns[count] = row; values[count++] = 2.;
         if (row != 0) { columns[count] = row-1; values[count++] = -1.; }
         if (row != 4) { columns[count] = row+1; values[count++] = -1.; }
      row_lengths[i] = count - start;
   }
   return(1);
}
and
int Poisson_matvec(ML_Operator *Amat, int in_length, double p[], int out_length,
                   double ap[])
   int i;
   for (i = 0; i < 5; i++) {
      ap[i] = 2*p[i];
      if (i != 0) ap[i] -= p[i-1];
      if (i != 4) ap[i] -= p[i+1];
   return 0;
```

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

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

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

12.2 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 (5) 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 14 . 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(ML_Operator *Amat, 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 *) ML_Get_MyGetrowData(Amat);
   proc = *itemp;
```

¹⁴In 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;
      start = m;
      if (proc == 0) {
         if (row == 0) \{cols[m++] = 0; cols[m++] = 2;
                                                                      }
         if (row == 1) \{cols[m++] = 1; cols[m++] = 3;\}
      }
      if (proc == 1) {
         if (row == 0) \{cols[m++] = 0; cols[m++] = 1; cols[m++] = 4;\}
         if (row == 1) \{cols[m++] = 1; cols[m++] = 0; cols[m++] = 2;\}
         if (row == 2) \{cols[m++] = 2; cols[m++] = 1; cols[m++] = 3;\}
      row_lengths[i] = m - start;
   }
   return(1);
}
int Poisson_matvec(ML_Operator *Amat, int in_length, double p[], int out_length,
                   double ap[])
   int i, proc, *itemp;
   double new_p[5];
   itemp = (int *) ML_Get_MyMatvecData(Amat);
   proc = *itemp;
   for (i = 0; i < in_length; i++) new_p[i] = p[i];</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

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