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Amesos Reference Guide

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Amesos Reference Guide

Abstract

This document described the main functinalities of the Amesos package (part of Trilinos). Amesos provides an object-oriented interface to several direct sparse solvers. Amesos will solve (using a direct serial or parallel factorization method) the linear systems of equations

$$AX = B \tag{1}$$

where A is an Epetra_RowMatrix object, and X and B are Epetra_MultiVector objects.

The Amesos package has been designed to face some of the challenges of direct solution of linear systems in parallel environments. In fact, many solvers have been proposed in the last years, and often each of them requires different input formats for the linear system matrix. Moreover, it is not uncommon that the interface changes between revisions. Amesos aims to solve those problems, furnishing a clean, consistent interface to many direct solvers.

Amesos Reference Guide

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1 Introduction

Aim of the Amesos package is to provide an object-oriented interface to several direct sparse solvers. All the interfaces will have the same look-and-feel, so that the user can easily switch from one package to another. Using Amesos, users can interface their codes with a (large) variety of direct linear solvers, sequential or parallel, simply by a code instruction of type

```
AmesosObject.Solve();
or, more generally, by
AmesosObject.SymbolicFactorization();
AmesosObject.NumericFactorization();
AmesosObject.Solve();
```

Amesos will take care of redistributing data among the processors, if necessary.

Amesos is an interface to other packages, mainly developed outside the Trilinos framework¹. In order to use those packages, the user should carefully check copyright and licensing of those third party codes. Please refer to the web page or the documentation of each particular package for details.

Amesos contains several classes. The classes covered in this guide are:

- Amesos_KLU: Interface to Amesos's internal solver KLU, described in Section 4.
- Amesos_Umfpack: Interface to Tim Davis's UMFPACK [4], version 4.3. Section 5 presents the basic functionalities of this class.
- Amesos_Superludist: Interface to Xiaoye S. Li's distributed SuperLU [10]. The SuperLU_dist interface is presented in Section 6.
- Amesos_Mumps: Interface to MUMPS 4.3.1 [1], see Section 7.

All the Amesos classes are derived from a base class mode, Amesos_BaseSolver. This abstract interface provides the basic functionalities for all Amesos solvers, and allows users to choose different direct solvers very easily – by changing an input scalar parameter. See Section 3 for more details.

In this document, we will suppose that matrix A in equation (1) is defined as an Epetra_RowMatrix, possibly with nonzero entries on all the processes defined in the Epetra_Comm communicator in use. X and B, instead, are Epetra_MultiVector, defined on the same communicator. Some of the supported packages are serial solvers: in this case, if solving with more than one processor, the linear problem is shipped to processor 0, solved, then the solution is broadcasted in the solution vector X. For parallel solvers, instead, the user may decide to use all the available processes, or a subset of them.

¹Currently, serial SuperLU is included in the Trilinos framework.

2 Configuring and Installation Amesos

Amesos is distributed through the Trilinos project, and can be downloaded from the web site

```
http://software.sandia.gov/Trilinos
```

Each of the Amesos classes provides an interface to a third party direct sparse solver code². In order to install a particular class, you must first install the underlying direct sparse solver code. Generally, the Amesos installation requires four steps:

- 1. Finding MPI for your machine;
- 2. Finding optimized BLAS for your machine³;
- 3. Installing the third party code needed by the Amesos class that you intend to use;
- 4. Configuring Trilinos with Amesos.

Amesos is configured and built using the GNU auatoconf [6] and automake [7] tools. This should help for the first two points. As regards the third point, we refer to the documentation of each package. The fourth point is addresses here.

Let \$TRILINOS_HOME be a shell variable representing the location of the Trilinos source directory, and % the shell prompt sign. In order to configure Trilinos with Amesos, for instance on a LINUX machine with MPI, one may do the following:

Here, FLAGS represents the set of configure options for other Trilinos packages, and AMESOS_FLAGS the configure options specific to Amesos.

The configure options required to enable a specific interface are reported in each 3-part package's section. A complete list of them can be obtained by typing

\$TRILINOS_HOME/packages/amesos/configure --help

²Exception to this rule is KLU, which is distributed within Amesos.

³Some libraries may require CBLAS, LAPACK, BLACS, ScaLAPACK.

Architecture	Communicator	KLU	UMFPACK	SuperLU_DIST 2.0	MUMPS 4.3.1
LINUX	SERIAL	•	•	_	_
LINUX, GNU	LAM/MPI	•	•	•	_
LINUX, Intel	MPICH	•	•	_	•
SGI 64	MPI	•	•	•	•
DEC/Alpha	MPI	•	•	_	_
ASCI Red	MPI	_	_	_	•

Table 1. Supported architectures for various interfaces. '●' means that the interface can successfully compiled, '–' means that it cannot, or may require specific tweaks.

3 Amesos_BaseSolver: A Generic Interface to Direct Solvers

All Amesos objects are constructed from the function class Amesos. Amesos allows a code to delay the decision about which concrete class to use to implement the Amesos_BaseSolver interface. The main goal of this class is to allow the user to select any supported (and enabled at configuration time) direct solver, simply changing an input parameter. Another remarkable advantage of Amesos_BaseSolver is that, using this class, users does not have to include the header files of the 3-part libraries in their code⁴.

An example of use of this class is as follows. First, the following header files must be included:

#include "Amesos.h"

Then, let A be an Epetra_RowMatrix object (for instance, and Epetra_CrsMatrix). Some solvers can take advantage if the matrix is an Epetra_CrsMatrix or an Epetra_VbrMatrix; this is reported in Table 2.

Class	Epetra_RowMatrix	Epetra_CrsMatrix	Epetra_VrbMatrix
Amesos_Klu	•	•	_
Amesos_Umfpack	•	•	_
Amesos_Superlu	•	•	_
Amesos_Superludist	•	•	_
Amesos_Mumps	•	•	•
Amesos_Scalapack	•	•	_

Table 2. Supported matrix formats. '•' means that the interface can take advantage of the given matrix format, '-' means that it doesn't.

We need to define a linear problem,

⁴Using Amesos_BaseSolver, 3-part libraries header fi les are required in the compilation of Amesos only.

Now, let Choice be a char array variable, with one of the following values:

- Amesos_Klu:
- Amesos_Umfpack;
- Amesos_Mumps;
- Amesos_Superlu;
- Amesos_Superludist;
- Amesos_Scalapack.
- Amesos_Dscpack.

We can construct an Amesos_BaseSolver object as follows:

```
Amesos_BaseSolver * A_Base;
Amesos Amesos_Factory;

A_Base = Amesos_Factory.Create(Choice, *Amesos_LinearProblem);
assert(A Base!=0);
```

If the class requested by Choice is not avaiable (because is not installed, or Choice is mispelled), Create() returns 0. Specific parameters can be set using a Teuchos parameters' list (which can be empty), as

```
Teuchos::ParameterList AmesosList ;
```

Parameters are set (before a call to SymbolicFactorization()) as

```
A_Base.SetParameters(AmesosList);
```

Symbolic and numeric factorizations are computed using methods

```
A_Base->SymbolicFactorization();
A_Base->NumericFactorization();
```

The numeric factorization phase will check whether a symbolic factorization exists or not. If not, method SymbolicFactorization() is invoked. Solution is computed (after setting of LHS and RHS in the linear problem), using

```
A_Base->Solve();
```

The solution phase will check whether a numeric factorization exists or not. If not, method NumericFactorization() is called.

Users must provide the nonzero structure of the matrix for the symbolic phase, and the actual nonzero values for the numeric factorization. Right-hand side and solution vectors must be set before the solution phase, for instance using

```
Amesos_LinearProblem->SetLHS(x);
Amesos_LinearProblem->SetRHS(b);
```

A common ingredient to all the Amesos classes is the Teuchos parameters' list. This object, whose definition requires the input file Teuchos_ParameterList.hpp, is used to specify the parameters that affect the 3-part libraries. For a detailed presentation of Teuchos, we refer to the Teuchos documentation. Table 3 briefly reports the most important methods of this class.

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

Table 3. Some methods of Teuchos::ParameterList class.

Here, we simply recall that the parameters' list can be created as

```
Teuchos::ParameterList AmesosList;
and parameters can be set as
AmesosList.set(ParameterName, ParameterValue);
```

Here, ParameterName is a string containing the parameter name, and ParameterValue is any valid C++ object that specifies the parameter value (for instance, an integer, a pointer to an array or to an object).

Amesos has to level of parameters:

- 1. a first level refers to parameters that affect all solvers;
- 2. a second level refers to parameters that are specific to a particular solver.

We now list all the parameters that may affect all the Amesos solvers. To know whether a specific interface supports a given parameter, we refer to table 4.

UseTranspose	If false, solve linear system (1). Otherwise, solve the linear system with the transpose matrix A^T .
Threshold	Drop all elements whose absolute value is below the specified threshold.

AddZeroToDiag If true, a zero element will be added to the diagonal if

not present.

PrintTiming Print some timing information.

PrintStatus Print some information about the solver.

Compute Vector Norms After solution, compute the 2-norm of each vector of B

and X.

ComputeTrueResidual After solution, compute the real residual $||B - AX||_2$

for vector in Epetra_MultiVector.

MaxProcs The linear system matrix will be distributed on the spec-

ified number of processes only (if this number is available to the system). If MaxProcs=-1, Amesos will estimate using internal heuristics how many processes are required to efficiently solve the linear system. If MaxProcs=-2, Amesos will use the square root of the number of processes. A new communicator will be created and used by Amesos. If MaxProcs=-3, all available processes will be used. This option may require the conversion of a C++ MPI communicator to a FORTRAN MPI communicator. On some systems, this is not possible. In this case, the specified value of MaxProcs will be ignored, and all the processes in

MPI_COMM_WORLD will be used.

MaxProcsMatrix The linear system matrix will be distributed over the

specified number of processes. This number must be

less or equal to MaxProcs. See Maxprocs.

OutpuLevel If 0, no output is printed on the screen. If 1,

output is reported as specified by other parameters. If 2, all output is printed (this is equivalent to PrintTiming == true, PrintStatus == true, ComputeVectorNorms == true,

ComputeTrueResidual == true).

DebugLevel If 1, some debugging information are printed on the

screen.

-	-	۰
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option	type	default value	KLU	UMFPACK	SuperLU_dist	MUMPS	ScaLAPACK
UseTranspose	bool	false	•	•	_	•	_
Threshold	double	0.0	_	_	_	•	_
AddZeroToDiag	bool	false	_	_	•	•	_
PrintTiming	bool	false	_	_	_	•	_
PrintStatus	bool	false	_	_	•	•	_
MaxProcs	int	-1	_	_	•	•	•
MaxProcsMatrix	int	-1	_	_	_	•	_
ComputeVectorNorms	bool	false	_	_	•	•	_
ComputeTrueResidual	bool	false	_	_	•	•	_
OutputLevel	int	1	_	_	•	•	_
DebugLevel	int	0	_	_	•	•	_

Table 4. Supported options. '•' means that the interface supports the options, '-' means that it doesn't.

Solver-specific parameters are reported in each package's subsection. The general procedure is as follows: the user creates a sublist with a given name (for instance, the sublist for MUMPS is "mumps"), then sticks all the solver's specific parameters in this sublist. An example is as follows:

```
int ictnl[40];
// defines here the entries of ictnl
Teuchos::ParameterList & AmesosMumpsList =
   AmesosList.sublist("mumps");
AmesosMumpsList.set("ICTNL", ictnl);
```

Parameters and sublists not recognized are simply ignored. Recall that spaces are important, and that parameters' list is case sensitive!

4 Amesos Interface to KLU

KLU is a serial, unblocked code ideal for getting started and for very sparse matrices, such as circuit matrces.

KLU is Tim Davis' implementation of Gilbert-Peierl's left-looking sparse partial pivoting algorithm, with Eisenstat and Liu's symmetric pruning. It doesn't exploit dense matrix kernels, but it is the only sparse LU factorization algorithm known to be asymptotically optimal, in the sense that it takes time proportional to the number of floating-point operations. It is the precursor to SuperLU, thus the name ("Clark Kent LU"). For very sparse matrices that do not suffer much fill-in (such as most circuit matrices when permuted properly) dense matrix kernels do not help, and the asymptotic run-time is of practical importance.

In order to use KLU, Amesos must be configured with the options

```
--enable-amesos-klu
```

(KLU is not an external solver.)

KLU is a serial solver. Amesos will take care of moving matrix, solution and right-hand side to processor 0 (using Epetra_Import objects), solve the linear system on processor 0, them broadcast the solution as required.

5 Amesos Interface to UMFPACK 4.3

UMFPACK is a C package copyrighted by Timothy A. Davis. More information can be obtained at the web page

```
http://www.cise.ufl.edu/research/sparse/umfpack
```

In order to use UMFPACK, Amesos must be configured with the options

```
--enable-amesos-umfpack
--with-amesos-umfpacklib=<UMFPACK library>
--with-amesos-umfpackincdir=<UMFPACK include files>
--with-amesos-umfpackamdlib=<AMD library>
--with-amesos-umfpackamdincdir=<AMD include files>
```

UMFPACK is a serial solver. Amesos will take care of moving matrix, solution and right-hand side to processor 0 (using Epetra_Import objects), solve the linear system on processor 0, them broadcast the solution as required.

6 Amesos Interface to SuperLU_dist 2.0

SuperLU_DIST, written by Xiaoye S. Li, is a parallel extension to the serial SuperLU library. SuperLU_DIST is written in ANSI C, using MPI for communication, and it is targeted for the distributed memory parallel machines. It is copyrighted by The Regents of the University of California, through Lawrence Berkeley National Laboratory. We refer to the web site

```
http://www.nersc.gov/~xiaoye/SuperLU
```

and to the SuperLU_DIST manual [5] for more information.

SuperLU_DIST includes routines to handle both real and complex matrices in double precision. However, as Amesos is currently based on the Epetra package (that does not handle complex matrices), only double precision matrices can be considered.

SuperLU_DIST provides two input interfaces for matrices A and B in equation (1). Both A and B will not be modifies by Amesos_Superludist. The solution of the linear system is copied in the distributed Epetra_MultiVector X.

Amesos_Superludist can solve the linear system on a subset of the processes, as specified in the parameters' list. This is done by creating a new process group derived from the MPI group of the Epetra_Comm object, with function superlu_gridinit(). Users can specify rows and columns of the grid (see later description of SuperLU_dist input parameters). This can be useful to obtain better scalability. Amesos_Superludist insultates the users from the creation of new MPI groups.

In order to interface with SuperLU_dist 2.0, Amesos must be configured with the options

```
--enable-amesos-superludist
--with-amesos-superludistlib=<SuperLU_dist library>
--with-amesos-superludistincdir=<SuperLUdist include files>
```

The SuperLU_dist constructor will look for a sublist, called Superludist. The following parameters reflect the behavior of SuperLU_dist options argument, as specified in the SuperLU_dist manual [5, pages 55–56]. The user is referred to this manual for a detailed explanation of the reported parameters. Default values are taken as reported in the SuperLU_dist manual.

Fact	(string) Specifies whether or not the factored form of the matrix \boldsymbol{A} is supplied onen-
	try and, if not, how the matrix will be fac-
	tored. It can be: DOFACT, SamePattern,
	SmapPattern_SameRowPerm, FACTORED.
	Default: SamePattern_SameRowPerm.
Equil)bool) Specifies whether to equilibrate the system of

)bool) Specifies whether to equilibrate the system of not. Default: true.

ColPerm (string) Specifies whether to column ordering. It

can be: NATURAL, MMD_AT_PLUS_A, MMD_ATA, COLAMD, MY_PERMC. Default: MMD_AT_PLUS_A.

perm_c (int *) Specifies the ordering to use when ColPerm

= MY_PERMC.

RowPerm (string) Specifies whether to row ordering. It can

be: NATURAL, LargeDiag, MY_PERMR. Default:

LargeDiag.

perm_r (int *) Specifies the ordering to use when RowPerm

= MY_PERMR.

ReplaceTinyPivot (bool) Specifies whether to replace the tiny diagonals

with $\varepsilon ||A||$ during LU factorization. Default: true.

IterRefine (string) Specifies how to perform iterative refine-

ment. It can be: NO, DOUBLE, EXTRA. Default: NO.

7 Amesos Interface to MUMPS 4.3.1

MUMPS ("MUltifrontal Massively Parallel Solver") is a parallel direct solver, written in FOR-TRAN 90 with C interface, copyrighted by P. R. Amestoy, I. S. Duff, J. Koster, J.-Y. L'Excellent. Up-to-date copies of the MUMPS package can be obtained from the Web page

http://www.enseeiht.fr/apo/MUMPS/

Here, for the sake of completeness, we briefly present a broad view of the MUMPS package, so that the reader can better understand the Amesos_Mumps interface. For details about the algorithms and the implementation, as well as of the input parameters, we refer to [2]

MUMPS can solve the original system (1), as well as the transposed system, given an assembled or elemental matrix. Note that only the assembled format is supported by Amesos_Mumps. Mumps offers, among other features, error analysis, iterative refinement, scaling of the original matrix, Schur complement with respect to a prescribed subset of rows. Reordering techniques can take advantage of PORD (distributed within MUMPS), or METIS [9].

Amesos_Mumps is based on the distributed double-precision version of MUMPS (which requires MPI, BLAS, BLACS and ScaLAPACK [3]). Complex linear system are not supported, and linear system in single precision are under development.

The default implementation of Amesos_Mumps handles distributed matrices. It is also possible to ask Amesos_Mumps to move the matrix to processor 0.

In order to interface with MUMPS 4.3.1, Amesos must be configured with the options

```
--enable-amesos-mumps
--with-amesos-mumpslib=<MUMPS library>
--with-amesos-mumpsincdir=<MUMPS include files>
```

The MUMPS constructor will look for a sublist, called mumps. The user can set all the MUMPS's parameters, by sticking pointers to the integer array ICNTL and the double array CNTL to the parameters' list, or by using the functions reported at the end of this section.

ICTNL	(int[40]) Pointer to an integer array, containing the integer parameters (see [2, pages 13–17]).
CTNL	(double[5]) Pointer to an double array, containing the double parameters (see [2, page 17]).
PermIn	(int *) Use integer vectors of size NumGlobalElements (global dimension of the matrix) as given ordering. PermIn must be defined on the host only, and allocated by the user, if the user sets $ICNTL(7) = 1$.
Maxis	(int) Sets Maxis value.
Maxs	(int) Sets Maxis value.
ColPrecScaling	(double *) Uses double precision vectors of size NumGlobalElements (global dimension of the matrix) as scaling for columns and rows. The double vector must be defined on the host only, and allocated by the user, if the user sets ICNTL(8) = -1.
RowPrecScaling	(double *) Uses double precision vectors of size NumGlobalElements (global dimension of the matrix) as scaling for columns and rows. The double vector must be defined on the host only, and allocated by the user, if the user sets ICNTL(8) = -1.

Other functions are avaiable to retrive the output values. The following Amesos_Mumps methods are *not* supported by the Amesos_BaseSolver class; hence, the user must create an Amesos_Mumps object in order to take advantage of them.

```
double * GetRINFO()
```

Gets the pointer to the RINFO array (defined on all processes).

```
int * GetINFO()
```

Gets the pointer to the INFO array (defined on all processes).

```
double * GetRINFOG()
```

Gets the pointer to the RINFOG array (defined on host only).

```
int * GetINFOG()
```

Gets the pointer to the INFOG array (defined on host only).

A functionality that is peculiar to MUMPS, is the ability to return the Schur complement matrix, with respect to a specified set of nodes.

This method computes (if flag is true) the Schue complement with respect to the set of indices included in the integer array SchurComplementRows, of size NumSchurComplementRows. This is a *global* Schur complement, and it is formed (as a dense matrix) on processor 0 only.

```
Epetra_CrsMatrix * GetCrsSchurComplement();
```

This method returns the Schur complement in an Epetra_CrsMatrix, on host only. No checks are performed to see whether this action is legal or not (that is, if the call comes after the solver has been invocated). The returned Epetra_CrsMatrix must be freed by the user.

```
Epetra_SerialDenseMatrix * GetDenseSchurComplement();
```

This method returns the Schur complement as a Epetra_SerialDenseMatrix (on host only).

As an example, the following frament of code shows how to use MUMPS to obtain the Schur complement matrix with respect to a given subsets of nodes. First, we need to create an parameter list, and an Amesos_Mumps object.

```
Teuchos:::ParameterList params;
Amesos_Mumps * Solver;
Solver = new Amesos_Mumps(*Problem,params);
```

Then, we define the set of nodes that will constitute the Schur complement matrix. This must be defined on processor 0 only. For instance, one may have:

```
int NumSchurComplementRows = 0;
int * SchurComplementRows = NULL;
if( Comm.MyPID() == 0 ) {
   NumSchurComplementRows = 4;
   SchurComplementRows = new int[NumSchurComplementRows];
   SchurComplementRows[0] = 0;
   SchurComplementRows[1] = 1;
   SchurComplementRows[2] = 2;
   SchurComplementRows[3] = 3;
}
```

Now, we can ask for the Schur complement using

The Schur complement matrix can be obtain after the solver phase:

```
Solver->Solve();
Epetra_CrsMatrix * SC;
SC = Solver->GetCrsSchurComplement();
Epetra_SerialDenseMatrix * SC_Dense;
SC_Dense = Solver->GetDenseSchurComplement();
```

8 Example Code

In this section we report a complete code, whose aim is to compare the performances of various direct solvers, using the Amesos_BaseSolver interface.

The source of the entire code is reported below. Several comments are reported to detail all phase. The source file is

```
$TRILINOS_HOME/packages/amesos/examples/Amesos_ReferenceGuide.cpp
```

First, we need to include the appropriate headers. The variable HAVE_CONFIG_H must have been defined – in the file, or at compilation time.

```
#ifndef HAVE_CONFIG_H
#define HAVE_CONFIG_H
#endif
#include "Epetra_config.h"
#ifdef HAVE_MPI
#include "mpi.h"
#include "Epetra_MpiComm.h"
#else
#include "Epetra_SerialComm.h"
#endif
```

```
#include "Epetra_Vector.h"
#include "Epetra_Time.h"
#include "Amesos_config.h"
#include "Teuchos_ParameterList.hpp"
#include "Amesos.h"
#include "Trilinos_Util_CrsMatrixGallery.h"
```

The code can be run with or without MPI; however, the supported versions of MUMPS and SuperLU_dist requires MPI.

```
int main(int argc, char *argv[]) {

#ifdef HAVE_MPI
    MPI_Init(&argc, &argv);
    Epetra_MpiComm Comm(MPI_COMM_WORLD);

#else
    Epetra_SerialComm Comm;

#endif
```

Here we use the class Trilinos_Util::CrsMatrixGallery to read and Harwell/Boeing matrix from file, whose name is hardwired in the code for simplicity. The name can be read from the input line using class Trilinos_Util_ShellOptions (see [8]), or the Teuchos package.

```
Trilinos_Util::CrsMatrixGallery G("hb", Comm);
G.Set("matrix_name","662_bus.rsa");
```

Class Trilinos_Util::CrsMatrixGallery automatically defines an Epetra_LinearProblem, that can be obtained as follows:

```
Epetra_LinearProblem * Problem = G.GetLinearProblem();
```

Now, we define a Teuchos parameters' list, together with sublists for SuperLU_dist and MUMPS. We set some parameters.

```
Teuchos::ParameterList params;
Teuchos::ParameterList & SluParamList=params.sublist("Superludist");
Teuchos::ParameterList & MumpsParamList=params.sublist("mumps");
params.set("Redistribute",true);
SluParamList.set("MaxProcs",8);
```

At this point, we can create an Amesos_BaseSolver object, depending on the run-time choice (here hardcoded for the sake of simplicity as a string):

```
Solver = Amesos_Factory.Create(SolutionLib, *Problem, params );
if( Solver == 0 ) cerr << "library not available" << endl;</pre>
```

We can solve the linear problem, taking some timing:

```
Epetra_Time Time(Comm);
  Solver->SymbolicFactorization();
  double TimeForSymbolicFactorization = Time.ElapsedTime();
  Time.ResetStartTime();
  Solver->NumericFactorization();
  double TimeForNumericFactorization = Time.ElapsedTime();
  Time.ResetStartTime();
  Solver->Solve();
  Solver->Solve();
  Solver->Solve();
  double TimeForSolve = Time.ElapsedTime();
and finally delete the Amesos_BaseSolver object, and exit the code.
  delete Solver;
#ifdef HAVE_MPI
 MPI_Finalize();
#endif
 return( EXIT_SUCCESS );
```

References

}

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