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# Ifpack2 User's Guide 1.0 (Trilinos version 12.6)

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#### **Abstract**

This is the definitive user manual for the IFPACK2 package in the Trilinos project. IFPACK2 provides implementations of iterative algorithms (e.g., Jacobi, SOR, additive Schwarz) and processor-based incomplete factorizations. IFPACK2 is part of the Trilinos TPETRA solver stack, is templated on index, scalar, and node types, and leverages node-level parallelism indirectly through its use of TPETRA kernels. IFPACK2 can be used to solve to matrix systems with greater than 2 billion rows (using 64-bit indices). Any options not documented in this manual should be considered strictly experimental.

# Acknowledgment

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# **Chapter 1**

# **Getting Started**

This section is meant to get you using IFPACK2 as quickly as possible. §1.1 gives a brief overview of IFPACK2. §1.2 lists IFPACK2's dependencies on other TRILINOS libraries and provides a sample cmake configuration line. Finally, some examples of code are given in §1.4.

### 1.1 Overview of IFPACK2

IFPACK2 is a C++ linear solver library in the TRILINOS project [6]. It originally began as a migration of IFPACK package capabilities to a new linear algebra stack. While it retains some commonalities with the original package, it has since diverged significantly from it and should be treated as completely independent package.

IFPACK2 only works with TPETRA [8] matrix, vector, and map types. Like TPETRA, it allows for different ordinal (index) and scalar types. IFPACK2 was designed to be efficient on a wide range of computer architectures, from workstations to supercomputers [10]. It relies on the "MPI+X" principle, where "X" can be threading or CUDA. The "X" portion, node-level parallelism, is controlled by a node template type. Users should refer to TPETRA's documentation for information about node and device types.

IFPACK2 provides a number of different solvers, including

- Jacobi, Gauss-Seidel, polynomial, distributed relaxation;
- domain decomposition solvers;
- incomplete factorizations.

This list of solvers is not exhaustive. Instead, references for further information are provided throughout the text. There are many excellent references for iterative methods, including [14].

Complete information on available capabilities and options can be found in §2.

### 1.2 Configuration and Build

IFPACK2 requires a C++11 compatible compiler for compilation. The minimum required version of compilers are GCC (4.7.2 and later), Intel (13 and later), and clang (3.5 and later).

### 1.2.1 Dependencies

Table 1.1 enumerates the dependencies of IFPACK2. Certain dependencies are optional, whereas others are required. Furthermore, IFPACK2's tests depend on certain libraries that are not required if you only want to link against the IFPACK2 library and do not want to compile its tests. Additionally, some functionality in IFPACK2 may depend on other Trilinos packages (for instance, AMESOS2) that may require additional dependencies. We refer to the documentation of those packages for a full list of dependencies.

Dependency	Library		Testing	
Bependency	Required	Optional	Required	Optional
TEUCHOS	×		×	
TPETRA	×		×	
<b>TPETRAKERNELS</b>	×			
AMESOS2		×		×
Galeri				×
XPETRA		×		×
ZOLTAN2		×		×
THYRATPETRAADAI	PTERS	×		
SHYLUHTS		×		×
MPI		×		×

**Table 1.1.** IFPACK2's required and optional dependencies, subdivided by whether a dependency is that of the IFPACK2 library itself (*Library*), or of some IFPACK2 test (*Testing*).

AMESOS2 and SUPERLU are necessary if you want to use either a sparse direct solve or ILUTP as a subdomain solve in processor-based domain decomposition. ZOLTAN2 and XPETRA are necessary if you want to reorder a matrix (e.g., reverse Cuthill McKee).

### 1.2.2 Configuration

The preferred way to configure and build IFPACK2 is to do that outside of the source directory. Here we provide a sample configure script that will enable IFPACK2 and all of its optional

#### dependencies:

```
export TRILINOS_HOME=/path/to/your/Trilinos/source/directory
cmake -D BUILD_SHARED_LIBS:BOOL=ON \
    -D CMAKE_BUILD_TYPE:STRING="RELEASE" \
    -D CMAKE_CXX_FLAGS:STRING="-g" \
    -D Trilinos_ENABLE_EXPLICIT_INSTANTIATION:BOOL=ON \
    -D Trilinos_ENABLE_TESTS:BOOL=OFF \
    -D Trilinos_ENABLE_EXAMPLES:BOOL=OFF \
    -D Trilinos_ENABLE_Ifpack2:BOOL=ON \
    -D Ifpack2_ENABLE_TESTS:STRING=ON \
    -D Ifpack2_ENABLE_EXAMPLES:STRING=ON \
    -D TPL_ENABLE_BLAS:BOOL=ON \
    -D TPL_ENABLE_BLAS:BOOL=ON \
    -D TPL_ENABLE_MPI:BOOL=ON \
    -D TPL_ENABLE_MPI:BOOL=ON
```

More configure examples can be found in Trilinos/sampleScripts. For more information on configuring, see the TRILINOS Cmake Quickstart guide [1].

### 1.3 Interface to IFPACK2 methods

All IFPACK2 operators inherit from the base class Ifpack2::Preconditioner. This in turn inherits from Tpetra::Operator. Thus, you may use an IFPACK2 operator anywhere that a Tpetra::Operator works. For example, you may use IFPACK2 operators directly as preconditioners in TRILINOS' BELOS package of iterative solvers.

You may either create an IFPACK2 operator directly, by using the class and options that you want, or by using Ifpack2::Factory. Some of IFPACK2 preconditioners only accept a Tpetra::CrsMatrix instance as input, while others also may accept a Tpetra::RowMatrix (the base class of Tpetra::CrsMatrix). They will decide at run time whether the input Tpetra::RowMatrix is an instance of the right subclass.

Ifpack2::Preconditioner includes the following methods:

• initialize()

Performs all operations based on the graph of the matrix (without considering the numerical values).

• compute()

Computes everything required to apply the preconditioner, using the matrix's values.

• apply()

Applies or "solves with" the preconditioner.

Every time that initialize() is called, the object destroys all the previously allocated information, and reinitializes the preconditioner. Every time compute() is called, the object recomputes the actual values of the preconditioner.

An IFPACK2 preconditioner may also inherit from Ifpack2::CanChangeMatrix class in order to express that users can change its matrix (the matrix that it preconditions) after construction using a setMatrix method. Changing the matrix puts the preconditioner back in an "pre-initialized" state. You must first call initialize(), then compute(), before you may call apply() on this preconditioner. Depending on the implementation, it may be legal to set the matrix to null. In that case, you may not call initialize() or compute() until you have subsequently set a nonnull matrix.

**Warning.** If you are familiar with the IFPACK package [16], please be aware that the behaviour of the IFPACK2 preconditioner is different from IFPACK. In IFPACK, the ApplyInverse() method applies or "solves with" the preconditioner  $M^{-1}$ , and the Apply() method "applies" the preconditioner M. In IFPACK2, the apply() method applies or "solves with" the preconditioner  $M^{-1}$ . IFPACK2 has no method comparable to IFPACK's Apply().

### 1.4 Example: IFPACK2 preconditioner within Belos

The most commonly used scenario involving IFPACK2 is using one of its preconditioners preconditioners inside an iterative linear solver. In TRILINOS, the BELOS package provides important Krylov subspace methods (such as preconditioned CG and GMRES).

At this point, we assume that the reader is comfortable with TEUCHOS referenced-counted pointers (RCPs) for memory management (an introduction to RCPs can be found in [3]) and the Teuchos::ParameterList class [17].

First, we create an IFPACK2 preconditioner using a provided Teuchos::ParameterList

```
typedef Tpetra::CrsMatrix<Scalar, LocalOrdinal, GlobalOrdinal, Node>
    Tpetra_Operator;

Teuchos::RCP<Tpetra_Operator> A;
// create A here ...
Teuchos::ParameterList paramList;
paramList.set( "chebyshev: degree", 1 );
paramList.set( "chebyshev: min eigenvalue", 0.5 );
paramList.set( "chebyshev: max eigenvalue", 2.0 );
// ...
Ifpack2::Factory factory;
RCP<Ifpack2::Ifpack2Preconditioner<>> ifpack2Preconditioner;
ifpack2Preconditioner = factory.create( "CHEBYSHEV", A )
ifpack2Preconditioner->setParameters( paramList );
ifpack2Preconditioner->initialize();
```

```
ifpack2Preconditioner->compute();
```

Besides the linear operator A, we also need an initial guess vector for the solution X and a right hand side vector B for solving a linear system.

```
typedef Tpetra::Map<LocalOrdinal, GlobalOrdinal, Node> Tpetra_Map;
typedef Tpetra::MultiVector<Scalar, LocalOrdinal, GlobalOrdinal, Node>
    Tpetra_MultiVector;

Teuchos::RCP<const Tpetra_Map> map = A->getDomainMap();

// create initial vector
Teuchos::RCP<Tpetra_MultiVector> X =
    Teuchos::rcp( new Tpetra_MultiVector(map, numrhs) );

// create right-hand side
X->randomize();
Teuchos::RCP<Tpetra_MultiVector> B =
    Teuchos::rcp( new Tpetra_MultiVector(map, numrhs) );
A->apply( *X, *B );
X->putScalar( 0.0 );
```

To generate a dummy example, the above code first declares two vectors. Then, a right hand side vector is calculated as the matrix-vector product of a random vector with the operator A. Finally, an initial guess is initialized with zeros.

Then, one can define a Belos::LinearProblem object where the ifpack2Preconditioner is used for left preconditioning.

```
typedef Belos::LinearProblem<Scalar, Tpetra_MultiVector, Tpetra_Operator>
    Belos_LinearProblem;

Teuchos::RCP<Belos_LinearProblem> problem =
    Teuchos::rcp( new Belos_LinearProblem( A, X, B ) );
problem->setLeftPrec( ifpack2Preconditioner );
bool set = problem.setProblem();
```

Next, we set up a Belos solver using some basic parameters.

```
Teuchos::RCP<Teuchos::ParameterList> belosList =
   Teuchos::rcp(new Teuchos::ParameterList);
belosList->set( "Block Size", 1 );
belosList->set( "Maximum Iterations", 100 );
belosList->set( "Convergence Tolerance", 1e-10 );
belosList->set( "Output Frequency", 1 );
belosList->set( "Verbosity", Belos::TimingDetails + Belos::FinalSummary );

Belos::SolverFactory<Scalar, Tpetra_MultiVector, Tpetra_Operator> solverFactory;
```

```
Teuchos::RCP<Belos::SolverManager<Scalar, Tpetra_MultiVector, Tpetra_Operator> >
   solver = solverFactory.create( "Block CG", belosList );
solver->setProblem( problem );
```

Finally, we solve the system.

```
Belos::ReturnType ret = solver.solve();
```

It is often more convenient to specify the parameters as part of an XML-formatted options file. Look in the subdirectory Trilinos/packages/ifpack2/test/belos for examples of this.

This section is only meant to give a brief introduction on how to use IFPACK2 as a preconditioner within the TRILINOS packages for iterative solvers. There are other, more complicated, ways to use to work with IFPACK2. For more information on these topics, the reader may refer to the examples and tests in the IFPACK2 source directory (Trilinos/packages/ifpack2).

## Chapter 2

# **IFPACK2 options**

In this section, we report the complete list of input parameters. Input parameters are passed to IFPACK2 in a single Teuchos::ParameterList.

In some cases, the parameter types may depend on runtime template parameters. In such cases, we will follow the conventions in Table 2.1.

MatrixType::local_ordinal_type	local_ordinal
<pre>MatrixType::global_ordinal_type</pre>	global_ordinal
MatrixType::scalar_type	scalar
MatrixType::node_type	node
<pre>Tpetra::Vector<scalar,local_ordinal,global_ordinal,node></scalar,local_ordinal,global_ordinal,node></pre>	vector
<pre>Tpetra::MultiVector<scalar,local_ordinal,global_ordinal,node></scalar,local_ordinal,global_ordinal,node></pre>	multi_vector
vector::mag_type	magnitude

**Table 2.1.** Conventions for option types that depend on templates.

**Note:** if scalar is double, then magnitude is also double.

### 2.1 Point relaxation

**Preconditioner type:** "RELAXATION".

IFPACK2 implements the following classical relaxation methods: Jacobi (with optional damping), Gauss-Seidel, Successive Over-Relaxation (SOR), symmetric version of Gauss-Seidel and SOR. IFPACK2 calls both Gauss-Seidel and SOR "Gauss-Seidel". The algorithmic details can be found in [14].

Besides the classical relaxation methods, IFPACK2 also implements  $l_1$  variants of Jacobi and Gauss-Seidel methods proposed in [2], which lead to a better performance in parallel applications.

**Note:** if a user provides a Tpetra::BlockCrsMatrix, the point relaxation methods become block

relaxation methods, such as block Jacobi or block Gauss-Seidel.

The following parameters are used in the point relaxation methods:

"relaxation: type" [string] Relaxation method to use. Accepted val-

ues: "Jacobi", "Gauss-Seidel", "Symmetric Gauss-

Seidel". Default: "Jacobi".

"relaxation: sweeps" [int] Number of sweeps of the relaxation. De-

fault: 1.

"relaxation: damping factor" [scalar] The value of the damping factor  $\omega$  for the

relaxation. **Default:** 1.0.

"relaxation: backward mode" [bool] Governs whether Gauss-Seidel is done in

forward-mode (false) or backward-mode (true). Only valid for "Gauss-Seidel" type. **Default:** false.

"relaxation: use 11" [bool] Use the  $l_1$  variant of Jacobi or Gauss-Seidel.

Default: false.

"relaxation: 11 eta" [magnitude]  $\eta$  parameter for  $l_1$  variant of Gauss-

Seidel. Only used if "relaxation: use 11" is

true. Default: 1.5.

"relaxation: zero starting

solution"

[boo1] Governs whether or not IFPACK2 uses existing values in the left hand side vector. If true, IFPACK2 fill it with zeros before applying relaxation sweeps

which may make the first sweep more efficient. **De-**

fault: true.

"relaxation: fix tiny

diagonal entries"

[bool] If true, the compute() method will do extra work (computation only, no MPI communication) to

fix diagonal entries. Specifically, the diagonal values with a magnitude smaller than the magnitude of the threshold relaxation: min diagonal value are increased to threshold for the diagonal inversion. The matrix is not modified, instead the updated diagonal values are stored. If the threshold is zero, only the diagonal entries that are exactly zero are replaced

with a small nonzero value (machine precision). **De-**

fault: false.

"relaxation: min diagonal

value"

[scalar] The threshold value used in "relaxation: fix tiny diagonal entries". Only used if

"relaxation: fix tiny diagonal entries"

is true. **Default:** 0.0.

"relaxation: check diagonal

entries"

"relaxation: mtgs cluster

size"

"relaxation: mtgs coloring

algorithm"

"relaxation: local smoothing indices"

[bool] If true, the compute() method will do extra work (both computation and communication) to count diagonal entries that are zero, have negative real part, or are small in magnitude. This information can be later shown in the description. Default: false.

[int] Only has an effect if "relaxation: type" "MT Gauss-Seidel" or "MT Symmetric Gauss-Seidel". If equal to 1 (default), point coloring parallel Gauss-Seidel is used. This has a faster compute() but may cause the preconditioned solver to converge more slowly. If set to k > 1, then multicolor block Gauss-Seidel is used with blocks of size k (see [15]). In the apply () there is significantly less error due to parallel updates of the LHS vector. Default: 1.

[string] Only has an effect if "relaxation: type" is "MT Gauss-Seidel" or "MT Symmetric Gauss-Seidel". Selects which graph coloring algorithm from Kokkos Kernels will be used to find sets of independent rows. "Default" selects the algorithm based on the Node type. "Serial" is sequential and greedy. "VB", "VBBIT" and "VBCS" are parallel vertex-based (out of these, "VBBIT" is recommended). "EB" is parallel edge-based (faster than "VBBIT" on GPUs for irregular graphs). "VBD" and "VBDBIT" are parallel and deterministic. Default: "Default".

[Teuchos::ArrayRCP<local\_ordinal>]

De-

fault: empty.

A given method will only relax on the local indices listed in the ArrayRCP, in the order that they are listed. This can be used to reorder the relaxation, or to only relax on a subset of ids.

### **Block relaxation**

**Preconditioner type:** "BLOCK\_RELAXATION".

IFPACK2 supports block relaxation methods. Each block corresponds to a set of degrees of freedom within a local subdomain. The blocks can be non-overlapping or overlapping. Block relaxation can be considered as domain decomposition within an MPI process, and should not be confused with additive Schwarz preconditioners (see 2.5) which implement domain decomposition

across MPI processes.

There are several ways the blocks are constructed:

#### • Linear partitioning of unknowns

The unknowns are divided equally among a specified number of partitions L defined by "partitioner: local parts". In other words, assuming number of unknowns n is divisible by L, unknown i will belong to block number |iL/n|.

#### • Line partitioning of unknowns

The unknowns are grouped based on a geometric criteria which tries to identify degrees of freedom that form an approximate geometric line. Current approach uses a local line detection inspired by the work of Mavriplis [11] for convection-diffusion. IFPACK2 uses coordinate information provided by "partitioner: coordinates" to pick "close" points if they are sufficiently far away from the "far" points. It also makes sure the line can never double back on itself.

These "line" partitions were found to be very beneficent to problems on highly anisotropic geometries such as ice-sheet simulations.

#### • User partitioning of unknowns

The unknowns are grouped according to a user provided partition. A user may provide a non-overlapping partition "partitioner: map" or an overlapping one "partitioner: parts".

A particular example of a smoother using this approach is a Vanka smoother [18], where a user may in "partition: parts" pressure degrees of freedom, and request a overlap of one thus constructing Vanka blocks.

The original partitioning may be further modified with "partitioner: overlap" parameter which will use the local matrix graph to construct overlapping partitions.

The blocks are applied in the order they were constructed. This means that in the case of overlap the entries in the solution vector relaxed by one block may later be overwritten by relaxing another block.

The following parameters are used in the block relaxation methods:

"relaxation: type" See 2.1.

"relaxation: container" string

"TriDi" Containers are used to store and solve block matrices. These container types are always available: "Dense", "TriDi" (equivalent to "Tridiagonal"), "Banded" and "SparseILUT". "Dense", "TriDi" and "Banded" block matrices are solved exactly LAPACK routines, and "SparseILUT" blocks are solved approximately using an incomplete LU factorization with thresholding.

If Amesos2 is enabled, "SparseAmesos" (equivalent to "SparseAmesos2") is available. The default Amesos2 sparse solver is KLU2, but this can be configured by setting "Amesos2 solver name" (see the Amesos2 documentation for all available solvers).

If experimental kokkos-kernels features are enabled (true by default), the "BlockTriDi" container (equivalent to "Block Tridiagonal") is available. This container's solver is the damped Jacobi method, using block tridiagonal matrices as the diagonal D. For a block size of 1, this is equivalent to standard damped Jacobi. This container is designed for high performance on KNL and GPU.

"relaxation: sweeps" See 2.1.

"relaxation: damping factor" See 2.1.

"relaxation: zero starting See 2.1.

solution"

"relaxation: backward mode" See 2.1. Currently has no effect.

"block relaxation: decouple

dofs"

[boo1] Whether to separate blocks according to the different degrees of freedom (PDEs) at each node. This assumes that dofs/node is constant throughout the matrix. Each block will have the same sparsity pattern as the mesh graph's corresponding diagonal block. For example, when using a line partitioner this enables the use of the tridiagonal container even if the matrix's bandwidth is greater than 3. Decoupling matches the behavior of line smoothing in ML. **De**-

fault: false.

"partitioner: type" [string] The partitioner to use for defining the

blocks. This can be either "linear", "line" or "user".

Default: "linear".

"partitioner: overlap" [int] The amount of overlap between partitions (0

corresponds to no overlap). Only valid for "Jacobi"

relaxation. **Default:** 0.

"partitioner: local parts" [int] Number of local partitions (1 corresponds to

one local partition, which means "do not partition locally"). Only valid for "linear" partitioner type. **De-**

fault: 1.

"partitioner: map" [Teuchos::ArrayRCP<local\_ordinal>] An array

containing the partition number for each element. The *i*th entry in the ArrayRCP is the part (block) number that row *i* belongs to. Use this option if the parts (blocks) do not overlap. Only valid for "user" par-

titioner type. **Default:** empty.

"partitioner: parts" [Teuchos::Array<Teuchos::ArrayRCP

<local\_ordinal>>] Use this option if the parts
(blocks) overlap. The ith entry in the Array is an
ArrayRCP that contains all the rows in part (block)
i. Only valid for "user" partitioner type. De-

fault: empty.

"partitioner: line detection [magnitude] Threshold used in line detection. If

threshold"

the distance between two connected points i and j is within the threshold times maximum distance of all points connected to i, then point j is considered close enough to line smooth. Only valid for "line" partition

type. **Default:** 0.0.

"partitioner: PDE equations" [int] Number of equations per node. Only used for

"line" partitioning, and decoupled BlockRelaxation.

Default: 1.

"partitioner: coordinates" [Teuchos::RCP<multi\_vector>] Coordinates of lo-

cal nodes. Only valid for "line" partitioner type. De-

fault: null.

"partitioner: maintain [bool] For Overlapping Partitioner, whether to sort the

sparsity" entries in each partition. **Default:** false.

### 2.3 Chebyshev

**Preconditioner type:** "CHEBYSHEV".

IFPACK2 implements a variant of Chebyshev iterative method following IFPACK's implementation. IFPACK has a special-case modification of the eigenvalue bounds for the case where the maximum eigenvalue estimate is close to one. Experiments show that the IFPACK imitation is much less sensitive to the eigenvalue bounds than the textbook version.

IFPACK2 uses the diagonal of the matrix to precondition the linear system on the left. Diagonal elements less than machine precision are replaced with machine precision.

IFPACK2 requires can take any matrix A but can only guarantee convergence for real valued symmetric positive definite matrices.

The following parameters are used in the Chebyshev method:

"chebyshev: degree"

[int] Degree of the Chebyshev polynomial, or the number of iterations. This overrides parameters "relaxation: sweeps" and "smoother: sweeps". **Default:** 1.

"relaxation: sweeps"

Same as "chebyshev: degree", for compatibility with IFPACK.

"smoother: sweeps"

Same as "chebyshev: degree", for compatibility with ML.

"chebyshev: max eigenvalue"

[scalar|double] An upper bound of the matrix eigenvalues. If not provided, the value will be computed by power method (see parameters "eigen-analysis: type" and "chebyshev: eigenvalue max iterations"). **Default:** computed.

"chebyshev: min eigenvalue"

[scalar|double] A lower bound of the matrix eigenvalues. If not provided, IFPACK2 will provide an estimate based on the maximum eigenvalue and the ratio. **Default:** computed.

"chebyshev: ratio eigenvalue"

[scalar|double] The ratio of the maximum and minimum estimates of the matrix eigenvalues. **Default:** 30.0.

"smoother: Chebyshev alpha"

Same as "chebyshev: ratio eigenvalue", for compatibility with ML.

"chebyshev: compute max residual norm"

[bool] The apply call will optionally return the norm of the residual. **Default:** false.

"eigen-analysis: type"

[string] The algorithm for estimating the max eigenvalue. Currently only supports power method ("power-method" or "power method"). The cost of the procedure is roughly equal to several matrix-vector multiplications. **Default:** "power-method".

"chebyshev: eigenvalue max iterations"

[int] Number of iterations to be used in calculating the estimate for the maximum eigenvalue, if it is not provided by the user. **Default:** 10.

"eigen-analysis: iterations"

Same as "chebyshev: eigenvalue max iterations", for compatibility with ML.

"chebyshev: min diagonal value"

[scalar] Values on the diagonal smaller than this value are increased to this value for the diagonal inversion. **Default:** 0.0.

"chebyshev: boost factor"

[double] Factor used to increase the estimate of matrix maximum eigenvalue to ensure the high-energy modes are not magnified by a smoother. **Default:** 1.1.

"chebyshev: assume matrix

does not change"

[bool] Whether compute() should assume that the matrix has not changed since the last call to compute(). If true, compute() will not recompute inverse diagonal or eigenvalue estimates. **De-**

fault: false.

"chebyshev: operator inv

diagonal"

[Teuchos::RCP<const vector>|

Teuchos::RCP<vector>|const vector\*|

vector] If nonnull, a deep copy of this vector will be used as the inverse diagonal of the matrix, instead of computing it. Expert use only. **Default:** Teu-

chos::null.

"chebyshev: min diagonal

value"

[scalar] If any entry of the matrix diagonal is less that this in magnitude, it will be replaced with this value in the inverse diagonal used for left scaling. **De-**

fault: machine precision.

"chebyshev: zero starting

solution"

See "relaxation: zero starting solution".

### 2.4 Incomplete factorizations

### **2.4.1** ILU(*k*)

**Preconditioner type:** "RILUK".

IFPACK2 implements a standard and modified (MILU) variants of the ILU(k) factorization [14]. In addition, it also provides an optional *a priori* modification of the diagonal entries of a matrix to improve the stability of the factorization.

The following parameters are used in the ILU(k) method:

"fact: iluk level-of-fill" [int|global\_ordinal|magnitude|double] Level-

of-fill of the factorization. **Default:** 0.

"fact: relax value" [magnitude|double] MILU diagonal compensation

value. Entries dropped during factorization times this factor are added to diagonal entries. **Default:** 0.0.

"fact: absolute threshold" [magnitude|double] Prior to the factorization, each

diagonal entry is updated by adding this value (with the sign of the actual diagonal entry). Can be combined with "fact: relative threshold". The

matrix remains unchanged. **Default:** 0.0.

"fact: relative threshold" [magnitude|double] Prior to the factorization, each

diagonal element is scaled by this factor (not including contribution specified by "fact: absolute threshold"). Can be combined with "fact: absolute threshold". The matrix remains un-

changed. **Default:** 1.0.

#### 2.4.2 ILUT

#### Preconditioner type: "ILUT".

IFPACK2 implements a slightly modified variant of the standard ILU factorization with specified fill and drop tolerance ILUT $(p, \tau)$  [13]. The modifications follow the AZTECOO implementation. The main difference between the IFPACK2 implementation and the algorithm in [13] is the definition of fact: ilut level-of-fill.

The following parameters are used in the ILUT method:

"fact: ilut level-of-fill" [int|magnitude|double] Maximum number of en-

tries to keep in each row of L and U. Each row of L (U) will have at most  $\lceil \frac{(\text{level-of-fill-1})nnz(A)}{2n} \rceil$  nonzero entries, where nnz(A) is the number of

nonzero entries in the matrix, and n is the number of rows. ILUT always keeps the diagonal entry in the current row, regardless of the drop tolerance or fill level. **Note:** This is different from the p in the classic

algorithm in [13]. **Default:** 1.

"fact: drop tolerance" [magnitude|double] A threshold for dropping en-

tries ( $\tau$  in [13]). **Default:** 0.0.

"fact: absolute threshold" See 2.4.1.

"fact: relative threshold" See 2.4.1.

"fact: relax value" Currently has no effect. For backwards compatibility

only.

#### **2.4.3** ILUTP

**Preconditioner type:** "AMESOS2".

IFPACK2 implements a standard ILUTP factorization [14]. This is done through is through the AMESOS2 interface to SuperLU [9]. We reproduce the AMESOS2 options here for convenience. *You should consider the* AMESOS2 *documentation to be the final authority.* 

The following parameters are used in the ILUTP method:

"ILU_DropTol"	[double] ILUT drop tolerance. <b>Default:</b> 1e-4.
"ILU_FillFactor"	[double] ILUT fill factor. <b>Default:</b> 10.0.
"ILU_Norm"	[string] Norm to be used in factorization. Accepted values: "ONE_NORM", "TWO_NORM", or "INF_NORM". <b>Default:</b> "INF_NORM".
"ILU_MILU"	[string] Type of modified ILU to use. Ac-

[string] Type of modified ILU to use. Accepted values: "SILU", "SMILU\_1", "SMILU\_2", or

"SMILU\_3". Default: "SILU".

### 2.4.4 ShyLU FastILU

IFPACK2 provides an interface to the FastILU family of factorizations provided by ShyLU. They are available if Trilinos was configured with the

-D Trilinos\_ENABLE\_ShyLU\_Node=ON

option. There are three values of "Preconditioner type:" that use the FastILU subpackage:

"Preconditioner type:"	Factorization
FAST_ILU	Incomplete LU
FAST_IC	Incomplete Cholesky
FAST_ILDL	Incomplete LDL*

FAST\_ILU, FAST\_IC, and FAST\_ILDL all use iterative factorization algorithms in compute(). "sweeps" controls this iteration count. A higher number of sweeps improves the quality of the factorization. All three preconditioners also use an triangular block Jacobi solver in apply(). The Jacobi iteration count is controlled by "triangular solve iterations". The valid set of parameters is the same for FAST\_ILU, FAST\_IC, and FAST\_ILDL:

"sweeps" [int] Number of iterations of ILU/IC/ILDL factorization algorithm. **Default:** 5.

"triangular solve iterations"	[int] Number of iterations of the block Jacobi trian-
	gular solver. <b>Default:</b> 1.

"level" [int] Level of fill. **Default:** 0.

"damping factor" [double] Damping factor  $\omega$  for the Jacobi triangular

solver.  $0 < \omega \le 1$ . A lower  $\omega$  slows convergence but

improves stability. **Default:** 0.5.

"shift" [double] Manteuffel shifting parameter  $\alpha$ . **De-**

fault: 0.

"guess" [bool] Whether to run another instance of

FastILU/IC/ILDL (but with a lower level of fill) to compute the initial guess (only has an effect if

level of fill > 0). **Default:** true.

"block size" [int] Block size for the block Jacobi solver. **De-**

fault: 1.

### 2.5 Additive Schwarz

**Preconditioner type:** "SCHWARZ".

IFPACK2 implements additive Schwarz domain decomposition with optional overlap. Each subdomain corresponds to exactly one MPI process in the given matrix's MPI communication. For domain decomposition within an MPI process see 2.2.

One-level overlapping domain decomposition preconditioners use local solvers of Dirichlet type. This means that the inverse of the local matrix (possibly with overlap) is applied to the residual to be preconditioned. The preconditioner can be written as:

$$P_{AS}^{-1} = \sum_{i=1}^{M} P_i A_i^{-1} R_i,$$

where M is the number of subdomains (in this case, the number of (MPI) processes in the computation),  $R_i$  is an operator that restricts the global vector to the vector lying on subdomain i,  $P_i$  is the prolongator operator, and  $A_i = R_i A P_i$ .

Constructing a Schwarz preconditioner requires defining two components.

**Definition of the restriction and prolongation operators.** Users may control how the data is combined with existing data by setting "combine mode" parameter. Table 2.2 contains a list of modes to combine overlapped entries. The default mode is "ZERO" which is equivalent to using a restricted additive Schwarz [5] method.

Combine name	mode	Description
"ADD" "ZERO" "INSERT" "REPLACE" "ABSMAX"		Sum values into existing values Replace old values with zero Insert new values that don't currently exist Replace existing values with new values Replace old values with maximum of magnitudes of old and new values

**Table 2.2.** Combine mode descriptions.

**Definition of a solver for subdomain linear system.** Some preconditioners may benefit from local modifications to the subdomain matrix. It can be filtered to eliminate singletons and/or reordered. Reordering will often improve performance during incomplete factorization setup, and improve the convergence. The matrix reordering algorithms specified in "schwarz: reordering list" are provided by ZOLTAN2. At the present time, the only available reordering algorithm is RCM (reverse Cuthill-McKee). Other orderings will be supported by the Zoltan2 package in the future.

To solve linear systems involving  $A_i$  on each subdomain, a user can specify the inner solver by setting "inner preconditioner name" parameter (or any of its aliases) which allows to use any IFPACK2 preconditioner. These include but are not necessarily limited to the preconditioners in Table 2.3.

Inner solver type	Description
"DIAGONAL"	Diagonal scaling
"RELAXATION"	Point relaxation (see 2.1)
"BLOCK_RELAXATION"	Block relaxation (see 2.2)
"CHEBYSHEV"	Chebyshev iteration (see 2.3)
"RILUK"	ILU(k) (see 2.4.1)
"ILUT"	ILUT (see 2.4.2)
"FAST_ILU"	FastILU (see 2.4.4)
"FAST_IC"	FastIC (see 2.4.4)
"FAST_ILDL"	FastILDL(see 2.4.4)
"AMESOS2"	AMESOS2's interface to sparse direct solvers
"DENSE" or "LAPACK"	LAPACK's LU factorization for a dense representation of a
	subdomain matrix
"CUSTOM"	User provided inner solver

**Table 2.3.** Additive Schwarz solver preconditioner types.

The following parameters are used in the Schwarz method:

[string] The name of the subdomain solver. De-"schwarz: inner fault: none. preconditioner name" "inner preconditioner name" Same inner preconditioner as "schwarz: name". "schwarz: subdomain solver Same "schwarz: inner preconditioner as name" name". "subdomain solver name" Same inner preconditioner as "schwarz: name". "schwarz: [Teuchos::ParameterList] Parameters for the subinner preconditioner parameters" If not provided, the subdomain domain solver. solver will use its specific default parameters. Default: empty. "inner preconditioner Same as "schwarz: inner preconditioner parameters" parameters". "schwarz: subdomain solver Same as "schwarz: inner preconditioner parameters" parameters". "subdomain solver parameters" Same as "schwarz: inner preconditioner parameters". "schwarz: combine mode" [string] The rule for combining incoming data with existing data in overlap regions. Accepted values: see Table 2.2. **Default:** "ZERO". overlap level" [int] The level of overlap (0 corresponds to no over-"schwarz: lap). **Default:** 0. "schwarz: num iterations" [int] Number of iterations to perform. **Default:** 1. [bool] If true, local matrix is reordered before com-"schwarz: use reordering" puting subdomain solver. TRILINOS must have been built with ZOLTAN2 and XPETRA enabled. fault: false. "schwarz: reordering list" [Teuchos::ParameterList] Specify options for a ZOLTAN2 reordering algorithm to use. See "order\_method". You should consider the ZOLTAN2 documentation to be the final authority. Default: empty. "order\_method" [string] Reordering algorithm. Accepted values: "rcm", "minimum\_degree", "natural", "random", or "sorted\_degree". Only used in "schwarz: reordering list" sublist. Default: "rcm". See "relaxation: zero starting solution". "schwarz: zero starting

solution"

```
"schwarz: filter singletons" [bool] If true, exclude rows with just a single entry
on the calling process. Default: false.

"schwarz: subdomain id" Currently has no effect.

"schwarz: compute condest" Currently has no effect. For backwards compatibility
only.

"schwarz: update damping" [double] The amount by which to damp the updates
from the Schwarz solve (1.0 is no damping). Default: 1.0.
```

### 2.6 Hiptmair

IFPACK2 implements Hiptmair algorithm of [7]. The method operates on two spaces: a primary space and an auxiliary space. This situation arises, for instance, when preconditioning Maxwell's equations discretized by edge elements. It is used in MUELU [12] "RefMaxwell" solver [4].

Hiptmair's algorithm does not use Ifpack2::Factory interface for construction. Instead, a user must explicitly call the constructor

```
Teuchos::RCP<Tpetra::CrsMatrix<> > A, Aaux, P;
// create A, Aaux, P here ...
Teuchos::ParameterList paramList;
paramList.set("hiptmair: smoother type 1", "CHEBYSHEV");
// ...
RCP<Ifpack2::Ifpack2Preconditioner<> > ifpack2Preconditioner =
   Teuchos::rcp(new Ifpack2::Hiptmair(A, Aaux, P);
ifpack2Preconditioner->setParameters(paramList);
```

Here, A is a matrix in the primary space, Aaux is a matrix in auxiliary space, and P is a prolongator/restrictor between the two spaces.

The following parameters are used in the Hiptmair method:

"hiptmair:	smoother type 1"	[string] Smoother type for smoothing the primary space. <b>Default:</b> "CHEBYSHEV".
"hiptmair:	smoother list 1"	[Teuchos::ParameterList] Smoother parameters for smoothing the primary space. <b>Default:</b> empty.
"hiptmair:	smoother type 2"	[string] Smoother type for smoothing the auxiliary space. <b>Default:</b> "CHEBYSHEV".
"hiptmair:	smoother list 2"	[Teuchos::ParameterList] Smoother parameters for smoothing the auxiliary space. <b>Default:</b> empty.

"hiptmair: pre or post"

[string] IFPACK2 always relaxes on the auxiliary space. "pre" ("post") means that it relaxes on the primary space before (after) the relaxation on the auxiliary space. "both" means that we do both "pre" and "post". **Default:** "both".

"hiptmair: zero starting

solution"

See "relaxation: zero starting solution".

### References

- [1] Trilinos CMake Quickstart. http://trilinos.org/build\_instructions.html, 2014.
- [2] Allison H Baker, Robert D Falgout, Tzanio V Kolev, and Ulrike Meier Yang. Multigrid smoothers for ultraparallel computing. *SIAM Journal on Scientific Computing*, 33(5):2864–2887, 2011.
- [3] Roscoe A. Bartlett. Teuchos::RCP beginner's guide. Technical Report SAND2004-3268, Sandia National Labs, 2010.
- [4] Pavel B Bochev, Jonathan J Hu, Christopher M Siefert, and Raymond S Tuminaro. An algebraic multigrid approach based on a compatible gauge reformulation of Maxwell's equations. *SIAM Journal on Scientific Computing*, 31(1):557–583, 2008.
- [5] Xiao-Chuan Cai and Marcus Sarkis. A restricted additive Schwarz preconditioner for general sparse linear systems. *SIAM Journal on Scientific Computing*, 21(2):792–797, 1999.
- [6] Michael A. Heroux and James M. Willenbring. A new overview of the Trilinos project. *Scientific Programming*, 20(2):83–88, 2012.
- [7] Ralf Hiptmair. Multigrid method for H(div) in three dimensions. *Electron. Trans. Numer. Anal*, 6:133–152, 1997.
- [8] Mark Hoemmen, Heidi Thornquist, Michael Heroux, and Michael Parks. Tpetra: next-generation distributed linear algebra. http://trilinos.org/packages/tpetra, 2014.
- [9] Xiaoye S. Li, James W. Demmel, John R. Gilbert, Laura Grigori, Meiyue Shao, and Ichitaro Yamazaki. SuperLU Users' Guide. 2011.
- [10] Paul Lin, Matthew Bettencourt, Stefan Domino, Travis Fisher, Mark Hoemmen, Jonathan Hu, Eric Phipps, Andrey Prokopenko, Sivasankaran Rajamanickam, Christopher Siefert, and Stephen Kennon. Towards extreme-scale simulations for low Mach fluids with second-generation Trilinos. *Parallel Processing Letters*, 24(04):1442005, 2014.
- [11] Dimitri J Mavriplis. Directional agglomeration multigrid techniques for high-Reynolds-number viscous flows. *AIAA journal*, 37(10):1222–1230, 1999.
- [12] Andrey Prokopenko, Jonathan J. Hu, Tobias A. Wiesner, Christopher M. Siefert, and Raymond S. Tuminaro. MueLu User's Guide 1.0. Technical Report SAND2014-18874, Sandia National Labs, 2014.
- [13] Yousef Saad. ILUT: A dual threshold incomplete LU factorization. *Numerical Linear Algebra with Applications*, 1(4):387–402, 1994.

- [14] Yousef Saad. Iterative methods for sparse linear systems. SIAM, 2nd edition, 2003.
- [15] Yousef Saad and Masha Sosonkina. Enhanced parallel multicolor preconditioning techniques for linear systems. In *PPSC*, 1999.
- [16] M. Sala and M. Heroux. Robust algebraic preconditioners with IFPACK 3.0. Technical Report SAND-0662, Sandia National Laboratories, 2005.
- [17] Heidi Thornquist, Roscoe A. Bartlett, Mark Hoemmen, Christopher Baker, and Michael Heroux. Teuchos: Trilinos tools library. http://trilinos.org/packages/teuchos, 2014.
- [18] S Pratap Vanka. Block-implicit multigrid solution of Navier-Stokes equations in primitive variables. *Journal of Computational Physics*, 65(1):138–158, 1986.

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