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Supporting 64-bit global indices in Epetra and other Trilinos packages – Techniques used and lessons learned

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Abstract

The Trilinos Project is an effort to facilitate the design, development, integration and on-going support of mathematical software libraries within an object-oriented framework. It is intended for large-scale, complex multiphysics engineering and scientific applications [2, 4, 3]. Epetra is one of its basic packages. It provides serial and parallel linear algebra capabilities. Before Trilinos version 11.0, released in 2012, Epetra used the C++ int data-type for storing global and local indices for degrees of freedom (DOFs). Since int is typically 32-bit, this limited the largest problem size to be smaller than approximately two billion DOFs. This was true even if a distributed memory machine could handle larger problems. We have added optional support for C++ long long data-type, which is at least 64-bit wide, for global indices. To save memory, maintain the speed of memory-bound operations, and reduce further changes to the code, the local indices are still 32-bit. We document the changes required to achieve this feature and how the new functionality can be used. We also report on the lessons learned in modifying a mature and popular package from various perspectives – design goals, backward compatibility, engineering decisions, C++ language features, effects on existing users and other packages, and build integration.

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1 Introduction

Large scientific and engineering simulations are typically run in parallel on machines with distributed memory. Recent progress in distributed hardware has made it possible to run simulations with number of degrees of freedom (DOFs) that cannot fit the C++ int data-type. Thus, it becomes necessary to modify existing codes or create new ones so that hardware can be utilized fully for more accurate and reliable simulations.

Trilinos [2, 4, 3] is a popular and mature software library that serves as a foundation of various applications. It provides linear algebra data structures like vectors, matrices, maps, and also algorithms that act on them. Till recently, the only way of using 64-bit global indices in Trilinos was to use its newer package Tpetra, which is C++ template based. This allowed applications to break the barrier of 2 billion DOFs (or $2^{31} - 1$ DOFs to be precise). However, many Trilinos packages and end-user codes depend on the older Epetra package that till recently did not have 64-bit support.

We have added support for C++ long long data-type which is at least 64-bit wide (and typically is exactly 64-bit wide). It can be used for storing global indices in Epetra. To save memory, maintain the speed of memory-bound operations, and reduce further changes to the code, the local indices are still int-based, typically 32-bit. Before our modifications, Epetra used int data-type for both global and local indices, without any typedefs, and this design assumption was deeply ingrained. The type int was also used for data that is not a global or local index, and thus it is not possible to easily search and replace with a typedef. Even if this was possible within Epetra, such a change would imply that a lot of user code would also have to use a typedef for compatibility. Instead of typedef or template mechanisms, which are completely compile-time features, we have used the following combination of C++ language [7] features and preprocessor and build tool features to retrofit Epetra.

- C++ function-overloading
- type-conversion for function return values so as to implicitly convert a long long to int where it can fit without loss of data.
- C++ exceptions when a “wrong” function is called for a data-type
- Preprocessor and CMake [6] flags to enforce correctness at compile-time
- A judicious and minimal use of C++ templates internally to avoid code duplication

There are significant differences between how we added this 64-bit support to Epetra (and some other dependent Trilinos packages), and how such a feature is made available in Tpetra and PETSc [1]. Although much of this article is on Epetra and dependent packages, we briefly mention how this support is present in other packages. Tpetra relies on C++ templates and compile-time specification of both local and global index types. A user can choose the desired index type when constructing and using Tpetra objects. Different objects in the same application can have different index types at the same time. PETSc uses the typedef feature to handle types of indices.

When building PETSc, one specifies whether a PetscInt typedef should be 64-bit using the option `--with-64-bit-indices`. By default it is 32-bit. Since PETSc consistently uses PetscInt for indices, and expects users to do the same, changing the typedef meaning in just one location leads to a different type everywhere. A drawback is that an application can only use a single index type unless both PETSc and the application are recompiled for a different type. Both these techniques are common in other softwares and have advantages and disadvantages. However, our goals, listed ahead, are different and both these techniques are not suitable for modifying Epetra.

We document the changes required to achieve 64-bit compatible Epetra. Rather than just produce only a list of what changed and how to use the new functionality, we also present lessons learned in modifying a mature and popular package from various perspectives – design goals, backward compatibility, engineering decisions, compile-time and run-time issues, C++ language features, effects on existing users and other packages, and build integration.

Users who wish to convert their existing Epetra-based source to take advantage of 64-bit functionality should go through Sections 5, 7, and 10 at least.

Here is an outline of the sections ahead. We briefly mention the basic Epetra data structures for new users in Section 2. Section 3 lists our design goal for this task. Section 4 reports the high-level progress and future tasks. In Section 5, we describe the changes in detail and this will be useful for users who wish to use the 64-bit functionality. Section 6 contains information for developers. Section 7 shows how to switch off selected functionality (32-bit or 64-bit) at compile-time. This is useful for debugging and initial porting. Existing users should pay attention to backward compatibility issues we describe in Section 8. In Section 9, we describe the changes made to two other Trilinos packages – AztecOO and TriUtils. Section 10 shows how we test the new functionality. Finally, in Section 11 we list a few facts that might help people who may want to retrofit a software package for different data types.

2 Basic Epetra data structures

Many linear algebra Epetra classes, serial and distributed, use one or more instances of the `Epetra_BlockMap` class directly or indirectly. This class manages the global sizes and layouts of the objects with global indices. Since this class is limited by the size of C++ `int`, other Epetra classes, for example for graphs, matrices, vectors, and Epetra-dependent Trilinos packages also have this limitation. The goal is to modify basic Epetra classes like `Epetra_BlockMap`, `Epetra_CrsGraph`, `Epetra_CrsMatrix`, `Epetra_Vector`, and many other classes so they contain data structures and member functions that provide them with 64-bit capability.

3 Design goals

Here are our design goals in removing the 32-bit global index limitation. This was not our full list of goals when we started the project in late 2011. But as we experimented and learned more over time, this detailed list came into existence.

1. Remove the size limitation by using long long for global sizes in appropriate locations.
2. Preserve int for local sizes and local indices so that any increase in the storage and run-time for memory-bound routines is minimal.
3. Trilinos packages that depend on Epetra should not be heavily affected.
4. Ideally, the code of existing users should compile without making any changes. A few harmless warnings are all right.
5. There should be little to no effect on run-time performance for existing (32-bit) users.
6. Users who wish to use the 64-bit functionality would have to make very small changes to their existing int based code. Ideally it should be possible to find a large fraction of changes at compile-time.
7. Very little code should be duplicated for the two distinct data types, using C++ templates locally for example.
8. C++ templates are not to be exposed in any publicly visible function and only be used internally.
9. New testing code should be created to test the long long functionality.
10. It should be possible to “switch off” 64-bit functionality so that complete backward compatibility is maintained
11. It should be possible to “switch off” 32-bit functionality so that new users can find locations where their code is not 64-bit compatible.

Achieving the last two goals would allow users to check at compile-time whether their code is incompatible with 32-bit Epetra or 64-bit Epetra or both. We will show ahead how all these goals are achieved.

4 Status of the transition

The 64-bit addition to Epetra and dependent packages is an ongoing effort. We have modified Epetra nearly completely except for a few classes that are not used very often. We mention their names for the sake of completeness. They are CrsSingletonFilter, FEVbrMatrix, LinearProblemRedistor, MapColoring, RowMatrixTransposer, and VbrMatrix each with the prefix Epetra_.

Many other packages in Trilinos depend on Epetra. We have currently modified TriUtils (utilities for other Trilinos packages) and AztecOO (preconditioned Krylov methods) so they are 64-bit compatible. We are working on Ifpack (algebraic preconditioners) and EpetraExt (construction and service functions for linear algebra).

5 Using the 64-bit functionality

We now describe how to use the 64-bit functionality starting from map construction and then moving on to member functions of other important classes for vectors, graphs, and matrices. The starting point in using the 64-bit support is that the user should construct 64-bit maps using the long long based constructors. Such maps in turn lead vectors, graphs, and matrices that are 64-bit enabled. The user can then call new functions in these data structure classes that support 64-bit input and output. We will list the specific functions.

5.1 Map construction

The code below shows a common way of creating a 32-bit map with a given number of global indices. The constructor then divides the elements evenly across all processors in the communicator.

```
Epetra_MpiComm Comm(MPI_COMM_WORLD);
int NumGlobalElements = 10;
int IndexBase = 0;
Epetra_Map Map(NumGlobalElements, IndexBase, Comm);
```

Another way is to create a map that puts NumMyElements global indices on the calling processor. The array MyGlobalElements, which passes the global indices, is also provided. If NumGlobalElements is -1, the number of global elements are computed by the constructor. Here is its signature.

```
Epetra_Map(int NumGlobalElements, int NumMyElements,
           const int *MyGlobalElements,
           int IndexBase, const Epetra_Comm& Comm);
```

To use 64-bit functionality, the caller must use long long data-type for certain arguments. We provide extra constructors for that. For example, the first constructor call becomes

```
long long NumGlobalElements = 10;
int IndexBase = 0; // IndexBase can be int or long long
Epetra_Map Map(NumGlobalElements, IndexBase, Comm);
```

Similarly, the long long version of the second constructor is

```
Epetra_Map(long long NumGlobalElements, int NumMyElements,
           const long long *MyGlobalElements,
           int IndexBase, const Epetra_Comm& Comm);
```

As before, `IndexBase` can be `long long` or `int` for this constructor.

Note that `NumMyElements` is still an `int`, which means the number of local indices (indices on a single processor) is still limited by 32-bit integer type. This is so that one does not increase local index storage and reduce performance of memory-bound operations just because global indices are 64-bit. This is a design assumption keeping in mind the typical use-case and typical local memory sizes. Even if one were to change local index type to `long long`, the number of changes would be much higher.

In summary, every map constructor has overloads for two different integral types. Similar changes are present in the low-level class `Epetra_BlockMap`. A map then has the knowledge of which kind of map it is – 32-bit or 64-bit. This construction process also allows user to choose the data-type at run-time. No change is required to function signatures that may have (previously constructed) maps as arguments.

When passing a literal `-1` for the first argument (`NumGlobalElements`), one should do it like `(long long)-1` or `-1LL` or explicitly use a named `long long` variable. This holds for other function calls also where a literal is passed without a named variable and remaining arguments are not sufficient to deduce that a `long long` based function should be called. Otherwise, the `int` overload will be called.

5.2 32-bit and 64-bit state of maps

Maps can be in either of two states – 32-bit or 64-bit – or none of them in case they were default constructed. Thus, it is important to query the state. The following new functions are added to `Epetra_BlockMap` for this requirement.

```
// Returns true if map created with int
bool GlobalIndicesInt() const;

// Returns true if map create with long long
bool GlobalIndicesLongLong() const;

// Returns true if map index type is of type int_type
// Useful to get type at compile-time via templates
template<typename int_type>
bool GlobalIndicesIsType() const;

// Returns true if the global index type is valid
bool GlobalIndicesTypeValid() const;

// Returns true if the global index types match
bool GlobalIndicesTypeMatch(
    const Epetra_BlockMap& other) const;
```

This is a good place to mention another important design assumption. We expect that objects with identical global index type will interact with each other. For example, we do not allow a matrix with int based row map and long long based column map. Such conditions can be enforced at run-time only and we throw an exception whenever we encounter mixing of int and long long based objects. We use GlobalIndicesTypeMatch function shown above for checking this.

5.3 GID related map member functions

GID (global index) related functions in map classes typically have an int return type. Since C++ does not have overloading by return type, we cannot create functions of the same name and just change the return type. To maintain backward compatibility, new functions have been added with a suffix “64”. The functions that could be differentiated based on argument data type were not given a suffix. For example, we have

```
// Return GID for int based maps
// Exception for long long based maps
int GID(int LID) const;

// Return GID for int or long long based maps
long long GID64(int LID) const;
```

The idea is that any old user code that used GID(...) will continue to work as usual but a new code that is forward-looking will use GID64(...) since it works for both kinds of maps. Since GID(...) might lead to overflow in case of long long map we are extra cautious and throw an exception in all cases, even if the return value might fit an int.

Similar changes are made to other int returning functions. Here is the list of the new suffixed functions.

```
long long MinAllGID64() const;
long long MaxAllGID64() const;
long long MinMyGID64() const;
long long MaxMyGID64() const;
long long NumGlobalElements64() const;
long long IndexBase64() const;
long long NumGlobalPoints64() const;
```

There are other functions that do not return values but return pointers instead. In these cases, the long long one cannot work correctly for int based maps and is a mistake. Thus the right way is to throw an exception.

```
// Old function. Exception for long long based maps.
```

```
int* MyGlobalElements() const;

// Additional function. Exception for int based maps.
long long* MyGlobalElements64() const;
```

There also exists code that did not receive global indices by a returned pointer but it copied the indices to a user provided pointer. This is easily handled by overloading and there is no need for a suffix.

```
int MyGlobalElements(int * MyGlobalElementList) const;
int MyGlobalElements(long long * MyGlobalElementList) const;
```

Sometimes, however, it is easier to not worry about separate calls (MyGlobalElements and MyGlobalElements64) when returning pointers. It is easier to get two pointers and pick the one that is non-zero. This also simplifies switching-off 32-bit or 64-bit functions as will show in Section 7.1. The following two functions are added for this purpose. One of the pointers in the arguments will be zero after calling the function.

```
void MyGlobalElements(const int*& IntGIDs,
                     const long long*& LLGIDs) const;

void MyGlobalElements(int*& IntGIDs,
                     long long*& LLGIDs);
```

Computing an LID (local index) for a given GID is done by the LID function. We overload it for long long.

```
// Exception for long long based map
int LID(int GID_in) const;

// Works for int and long long based maps.
int LID(long long GID_in) const;
```

Similarly, checking if a given GID is local is done by the MyGID function. We overload it for long long.

```
// Exception for long long based map
bool MyGID(int GID_in) const;

// Works for int and long long based maps.
bool MyGID(long long GID_in) const;
```

5.4 Additions to the row matrix interface

The `Epetra_RowMatrix` is an abstract class with all pure virtual functions. The interface is intended for real-valued double-precision row-oriented sparse matrices. It is implemented by `Epetra_CrsMatrix` and many classes in other packages such as `Ifpack`, `ML`, `EpetraExt`, and `AztecOO`. Since it specifies some functions that return `int` for GIDs, the return type should be `long long` for long long based matrices. As before we add new functions with suffix 64 to the interface. Since they are pure virtual functions, they have to be implemented by all deriving concrete classes. We have added such implementations for classes in `Trilinos`.

Here are the original four functions.

```
virtual int NumGlobalNonzeros() const = 0;
virtual int NumGlobalRows() const = 0;
virtual int NumGlobalCols() const = 0;
virtual int NumGlobalDiagonals() const = 0;
```

The added functions are

```
virtual long long NumGlobalNonzeros64() const = 0;
virtual long long NumGlobalRows64() const = 0;
virtual long long NumGlobalCols64() const = 0;
virtual long long NumGlobalDiagonals64() const = 0;
```

The logic remains the same. Any old user code that used the non-suffixed version will continue to work as usual but a new code that is forward-looking will use the suffixed version. A user implementing this abstract class should implement these functions so that the new functions work for both kinds of maps and the non-suffixed version should throw an exception if called for long long based matrix.

5.5 New classes for long long global indices

For brevity, we ignore the `Epetra_` prefix in class names here. `Epetra` contains these three classes that store `int` data – `IntVector`, `IntSerialDenseVector`, and `IntSerialDenseMatrix`. They are also used for storing global indices. Introduction of long long global indices required objects that can store long long data. This facility is provided by the following three new classes – `LongLongVector`, `LongLongSerialDenseVector`, and `LongLongSerialDenseMatrix`. The interface is identical up to the change that in certain locations the `int` keyword has been replaced with `long long`.

`IntSerialDenseVector` is used as function argument in `FECrsMatrix` class. The corresponding overloaded functions for long long use `LongLongSerialDenseVector`. This pattern can be used in other such situations.

Additionally, to allow compile-time polymorphism using templates, two new classes have been added – `GIDTypeVector` and `GIDTypeSerialDenseVector`. `GIDTypeVector<int>::impl` is a typedef for `IntVector` and `GIDTypeVector<long long>::impl` is a typedef for `LongLongVector`. Hence, inside template functions, one can write code that works for both `int` and `long long`.

5.6 Vector, Graph, and Matrix construction

The classes `Epetra_MultiVector`, `Epetra_Vector`, `Epetra_CrsGraph`, and `Epetra_CrsMatrix` are a few of the basic and most important in `Epetra`. All of them take an `Epetra_BlockMap` or `Epetra_Map` argument in their constructors. This keeps the 32-bit or 64-bit issue hidden and thus their construction process does not have to change. The additions are only for some of the member functions. They are those that have global indices as arguments or return types. We describe this ahead.

Just like for maps, a suffixed function returns a `long long` and thus it can meaningfully return an `int` value. It will work for both 32-bit and 64-bit objects. The corresponding non-suffixed function will throw an exception if called for 32-bit objects.

5.7 MultiVector and Vector member functions

We show the new functions added to the class `Epetra_MultiVector` and `Epetra_Vector`, its derived class. Similar changes have been made to `Epetra_FEVector`, the derived class for Finite Elements, but we do not show them here to reduce duplication. In `Epetra_MultiVector`, the functions `ReplaceGlobalValue` and `SumIntoGlobalValue` are overloaded so that the new functions take a `long long` global row index. To return the global length we need a new function with the suffix `64`, as explained in Section 5.3. Its signature follows.

```
long long GlobalLength64() const;
```

`Epetra_Vector` has two new overloaded member functions for working with 64-bit indices – `ReplaceGlobalValues` and `ChangeValues`. Both the new functions take pointers to `long long` instead of pointers to `int`.

5.8 Graph and Matrix member functions

There are many additional member functions in `Epetra_CrsGraph` and `Epetra_CrsMatrix` to support `long long` functionality. Rather than show their new signatures, we just list the names of overloaded or suffixed functions. As before, the functions with suffix `64` are new functions that return a `long long` and those without the suffix are overloads with `long long` arguments instead of `int`.

Both classes implement the four functions of `Epetra_RowMatrix` mentioned earlier. These are `NumGlobalNonzeros64`, `NumGlobalRows64`, `NumGlobalCols64`, and `NumGlobalDiagonals64`.

See Section 5.4 for further details. They also implement `IndexBase64`, `GRID64`, `GCID64`, `MyGRID`, `MyGCID`, `LRID`, `LCID`, and `MyGlobalRow`.

In addition to these, the following new functions in `Epetra_CrsGraph` return long long and thus need the 64 suffix. They are `NumGlobalBlockRows64`, `NumGlobalBlockCols64`, `NumGlobalBlockDiagonals64`, and `NumGlobalEntries64`.

We have also added the overloaded counterparts for `InsertGlobalIndices`, `RemoveGlobalIndices`, `ExtractGlobalRowCopy`, `ExtractGlobalRowView`, `RemoveGlobalIndices`, `NumGlobalIndices`, `NumAllocatedGlobalIndices` in `Epetra_CrsGraph`. Their global index related arguments are long long instead of int.

`Epetra_CrsMatrix` class overloads these functions for long long instead of int – `InsertGlobalValues`, `InsertGlobalValues`, `ReplaceGlobalValues`, `SumIntoGlobalValues`, `ExtractGlobalRowCopy`, `ExtractGlobalRowView`, and `NumGlobalEntries`.

Similar additions have been made to `Epetra_FE_CrsGraph` and `Epetra_FE_CrsMatrix`, the derived classes for Finite Elements, but we do not show them here to reduce duplication.

6 Information for developers

This section briefly describes internal implementation details. Trilinos users can skip this part.

6.1 Changes to CrsGraphData

We have changed the struct `EntriesInOneRow` nested in the class `Epetra_CrsGraphData` to be dependent on a template argument `int_type`. The class is instantiated with an `int` and a `long long`. This is done because a user who fills in the `CrsGraph` objects can do it using global indices (`int` or `long long`) or local indices (always `int`). Since this is a run-time decision by caller and not a compile time decision, `Epetra_CrsGraphData` uses instantiation with both types but populates the one that is necessary.

We have also defined a new nested struct `IndexData` in `Epetra_CrsGraphData`. It is dependent on a template parameter `int_type` and contains all the index related data. One can get the reference to the appropriate data with the functions

```
Epetra_CrsGraphData::IndexData<long long>&  
    Epetra_CrsGraphData::Data<long long>();
```

and

```
Epetra_CrsGraphData::IndexData<int>&  
    Epetra_CrsGraphData::Data<int>();
```

The first function will work only if the map's global indices are `long long` based and indices have not been made local (by a call to `MakeIndicesLocal`, for example). The second function will work if the map's global indices are `int` based or they are `long long` based but have been made local. If the conditions are not satisfied, we throw an exception.

6.2 Wrappers over MPI collectives

We have added the `long long` versions of the following MPI collective functions – `GatherAll`, `SumAll`, `MaxAll`, `MinAll`, `ScanSum`. They have been added to the classes `Epetra_Comm`, `Epetra_SerialComm`, and `Epetra_MpiComm`.

6.3 Companion arrays in sorting

The function `Epetra_Util::Sort` is overloaded for `long long` in two ways. One addition takes `long long` companion arrays for simultaneous sorting. Another addition allows for `long long` keys. We

show both of them. Just like for other companion arrays, if there is no long long companion, one can pass zero for number of companions and a null pointer.

```
void Sort(  
    bool SortAscending, int NumKeys, int* Keys,  
    int NumDoubleCompanions, double ** DoubleCompanions,  
    int NumIntCompanions, int ** IntCompanions,  
    int NumLongLongCompanions, long long ** LongLongCompanions);
```

```
void Sort(  
    bool SortAscending, int NumKeys, long long* Keys,  
    int NumDoubleCompanions, double ** DoubleCompanions,  
    int NumIntCompanions, int ** IntCompanions,  
    int NumLongLongCompanions, long long ** LongLongCompanions);
```

6.4 Additions to Distributor and Directory classes

The `Epetra_Distributor` class is an interface that encapsulates gather and scatter operations on parallel hardware. It has two implementations – `Epetra_SerialDistributor` and `Epetra_MpiDistributor`. All these now have an additional member function overloaded for long long data.

```
int CreateFromRecv(  
    const int & NumRemoteIDs, const long long * RemoteGIDs,  
    const int * RemotePIDs, bool Deterministic,  
    int & NumExportIDs, long long *& ExportGIDs,  
    int *& ExportPIDs);
```

The `Epetra_Directory` class is an abstract base class to reference non-local elements. `Epetra_BasicDirectory` is its implementation. Both classes now have the following new overloaded function.

```
int GetDirectoryEntries(  
    const Epetra_BlockMap& Map, const int NumEntries,  
    const long long * GlobalEntries, int * Procs,  
    int * LocalEntries, int * EntrySizes,  
    bool high_rank_sharing_procs=false) const;
```

7 Multiple compilation modes

Trilinos now has three distinct modes of compilation for global index types that can be chosen using compile time flags. See Section 7.1 for how these can be specified in CMake. The three modes are as follows.

1. 32-bit and 64-bit. This is the default mode. In this mode both 32-bit and 64-bit global index code coexist so the user can choose the best data size for global indices at run-time.
2. 32-bit. This mode hides all the new 64-bit interfaces and implementation. The objective is to give users the old interface for full compatibility.
3. 64-bit. This mode hides the old 32-bit interfaces and implementations that are counterparts to the new 64-bit interfaces. The objective is to ensure that new 64-bit code is not relying on any 32-bit code internally. This helps in debugging and porting code that desires new functionality.

The dual mode is backward compatible up to the extent that user code does not rely on automatic type conversion (see Section 8.1) and user had not implemented `Epetra_RowMatrix` interface (see Section 5.4). If the user had implemented it, four additional functions must be implemented so that the class is not abstract.

Here is an example from `Epetra_BlockMap` header of the two kinds of functions and how they exist in different modes.

```
#ifndef EPETRA_NO_32BIT_GLOBAL_INDICES
    int LID(int GID) const;
#endif
#ifndef EPETRA_NO_64BIT_GLOBAL_INDICES
    int LID(long long GID) const;
#endif

#ifndef EPETRA_NO_32BIT_GLOBAL_INDICES
    int GID(int LID) const;
#endif
    long long GID64(int LID) const;
```

Note that `GID64` is present in all modes and its return value does not depend on the run-time chosen object mode. This makes it simple to use in downstream packages irrespective of the compile-time mode. See Section 5.3 for further details.

The preprocessor macros don't have to be defined by the user but are supplied (if at all) by the CMake build system. In the dual mode both

- EPETRA_NO_32BIT_GLOBAL_INDICES and
- EPETRA_NO_64BIT_GLOBAL_INDICES

are left undefined. The first one is defined in pure 64-bit mode and the second one is defined in pure 32-bit mode. A code that wishes to use these macros must include the Epetra_ConfigDefs.h header file.

Any user code for the new 64-bit functionality should ideally compile for all three modes preferably with few or no conversion warnings. This ensures that a large fraction of porting effort is complete.

7.1 Integration with CMake

The preprocessor macros discussed earlier can be controlled via options given to CMake at configuration time. The corresponding CMake macros are

- Trilinos_NO_32BIT_GLOBAL_INDICES and
- Trilinos_NO_64BIT_GLOBAL_INDICES

7.2 Multiple mode design pattern

We describe a design pattern so that one can write code appropriate for multiple modes and one that has minimal run-time overhead. Consider a function that wishes to use an Epetra_Map, which may be 32-bit or 64-bit. It can be written like this and it works for all three compilation modes. Typically such a code is needed only in a few critical locations.

```
void func(const Epetra_Map& Map)
{
#ifdef EPETRA_NO_32BIT_GLOBAL_INDICES
    if(Map.GlobalIndicesInt()) {
        const int* gids = Map.MyGlobalElements();
        // Use gids now
    }
    else
#endif
#ifdef EPETRA_NO_64BIT_GLOBAL_INDICES
    if(Map.GlobalIndicesLongLong()) {
        const long long* gids = Map.MyGlobalElements64();
        // Use gids now
    }
}
```

```
    else
#endif
    throw "func: GlobalIndices type unknown";
}
```

Note that instead of duplicating code manually after “Use gids now”, one may also call a C++ template function with template arguments long long or int.

Since these specific functions (MyGlobalElements and its 64-bit version) are very common, we have provided a new function specifically for them so that such verbosity and use of macros can be avoided. See Section 5.3 for details. However, in other cases, this pattern is very useful.

8 Backward compatibility

We mention two cases where existing user code (written for older 32-bit Epetra) can fail to compile when 64-bit additions are also present.

8.1 Ambiguity in type conversion

The addition of new constructors and other functions uses the C++ function overloading mechanism. This is backward compatible to the extent that automatic type conversion are not expected. For example, before we added the new constructors, any user code that relied on conversion from types other than int, say unsigned int or short or size_t relied on type conversion in passing by value. Such code will not compile when both int and long long versions are present because of the resulting ambiguity. The best way is to not rely on type conversion. However, in the short term, one may switch-off the 64-bit functionality using CMake flags discussed in Section 7.1. This will remove the ambiguity and the errors due to it.

8.2 New pure virtual functions

We have added new pure virtual functions to Epetra_RowMatrix interface for 64-bit functionality. The interface is intended for real-valued double-precision row-oriented sparse matrices. Any user code that implemented this interface will now require four simple additional functions. See Section 5.4 for details. Of course, if the user never intends to use the interface for 64-bit functionality, a simple implementation that throws an exception unconditionally will suffice.

9 Changes to other Trilinos packages

We have modified the packages TriUtils (utilities for other Trilinos packages) and AztecOO (pre-conditioned Krylov methods) so they are 64-bit compatible. AztecOO does not have any publicly visible changes for 64-bit compatibility.

Triutils now has the following new 64-bit global functions. The ones with suffix 64 are those that cannot be distinguished by C++ overloading since they construct maps rather than use any pre-existing input maps.

- `Trilinos_Util_CountTriples`
- `Trilinos_Util_CountMatrixMarket`
- `Trilinos_Util_ReadMatrixMarket2Epetra64`
- `Trilinos_Util_ReadHb2Epetra64`
- `Trilinos_Util_ReadHpc2Epetra64`
- `Trilinos_Util_GenerateCrsProblem64`
- `Trilinos_Util_ReadTriples2Epetra64`

We don't expect that users will read really large matrices (that require 64-bit GIDs) from a file. Still, it is useful for testing to read a small matrix as if it required 64-bit.

Additionally, the class `CrsMatrixGallery` in namespace `Trilinos_Util` has a new argument "`bool UseLongLong`". A true value can be supplied to create a 64-bit compatible matrix.

10 Test suite

We have added around 20 new tests to Epetra by modifying the existing test suite so that the long long functionality can be tested. They are present in “epetra/test” directory and are suffixed with “_LL”. Most of the changes are local one-line changes. It is instructive to compare the new tests with the original code to see how to convert an application from int to long long. Similar new tests have been added to AztecOO and TriUtils.

These tests run regularly and help in catching regressions. The older tests use 32-bit maps and work whether the CMake flag

`Trilinos_NO_64BIT_GLOBAL_INDICES`

is enabled or not. Similarly, the new `_LL` tests work whether CMake flag

`Trilinos_NO_32BIT_GLOBAL_INDICES`

is enabled or not and use 64-bit maps. See Section 7 for a discussion of these flags.

11 Lessons learned and guidelines

We list some lessons learned in carrying out the task of retrofitting Epetra with 64-bit support. The purpose of listing the lessons is two-fold. Firstly, it might be useful for someone carrying out such a task to other old or popular software packages with minimal disturbance to backward compatibility. Presumably, there would be quite a few older packages written in days when C or C++ int was of sufficient size and retrofitting them for a different size might be attractive. It could also be that one may want to go from double precision to single precision floating point data. Secondly, it might help someone writing new software in understanding the effort and tools required to retrofit. This way, perhaps, the decision of future-proofing the data types or providing tools to choose them can be made with better information.

11.1 Effort estimate

Although it is hard to predict or even precisely measure how long a task like this takes. This is true partly because it is not done in isolation. Still, it is useful to know a rough estimate. We estimate that it took approximately 7 person-months spread over 15 calendar months and distributed amongst a team of 4 people (the authors) and a few other team members who helped in testing and discussion of issues. Specifically for Epetra, it required changing its library source in around 800 different locations in around 70 files. Changes to tests, examples, and other packages are not mentioned.

11.2 Language and compiler facilities

As mentioned previously, we have heavily made use of function overloading, C++ templates for internal implementation, implicit type conversion when it does not truncate, and exceptions to prevent execution of functions (when the wrong type function is called). These facilities made it possible to achieve usable 64-bit functionality. However, the two features with greatest impact on reliability and speed of retrofitting were creating compilation modes using the preprocessor and conversion warnings.

The first task, where low-level Epetra functions were enclosed by `#ifdef` macros (see Section 7), was time-consuming and repetitive but it paid off. It helped in pointing out, via compilation errors, higher-level code that had to be changed. Once such locations were found, it became a matter of intelligently choosing which language feature was appropriate to add 64-bit functionality. Once any new functionality was added, the older and new code was again enclosed in `#ifdef` macros. This process was repeated with higher-level code till the end. Compilation modes helped initially in retrofitting but later helped in finding out bugs that can be found only by running a program.

Simultaneously, it was important to watch for type conversion warnings within Trilinos. The `-Wall` option in GCC (GNU Compiler Collection) does not include the `-Wconversion` warning.

However, it is crucial for our task and had to be enabled. See [5] for a rationale of why it is not included in `-Wall` and examples.

An issue which we had not anticipated was ambiguity due to multiple types (see Section 8. This would not be an issue if users passed the exact type (int in our case). However, many users rely on implicit conversion usually from unsigned int. This issue is preventable if users have removed sign conversion warnings.

11.3 Return type

Returning a computed value in a function using the return mechanism is quite natural. However, C++ does not have overloading by return type [7]. This led to addition of extra functions with a different suffix. This made the code work, but it was not a very clean method.

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