# PyTrilinos Developers Guide

# Bill Spotz wfspotz@sandia.gov Sandia National Laboratories

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#### **Abstract**

PyTrilinos is a python interface to selected Trilinos packages. The Trilinos Project is a collection of over 30 software packages written primarily in C++ that provide linear-, nonlinear-, and eigen-solvers, along with preconditioners and supporting utilities, that are object-oriented, parallel and serial, for sparse and dense problems. PyTrilinos is one of those packages, and provides python interfaces to the most popular and important Trilinos packages. This Guide provides information, both necessary and recommended, for developing PyTrilinos packages.

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# **Introduction to PyTrilinos Development**

The purpose of PyTrilinos is to provide a high-level, dynamic and interactive interface to selected Trilinos packages. Being a PyTrilinos developer requires that you are, or will become, an expert in the following areas:

- C++. The vast majority of Trilinos development is in C++, and much of that development takes advantage of advanced C++ or object-oriented techniques such as polymorphism, templating and reference-counted memory management. A high level of comfort with C++ is required.
- **Python.** Obviously, PyTrilinos is a package of python modules, so familiarity with the language is a must. Beyond that, however, it is important to understand the philosophical underpinnings of the language (which are very different from C++) in order to develop interfaces that are "pythonic", i.e. that are consistent with the many conventions of the language.
- Trilinos. At a bare minimum, a PyTrilinos developer should have a decent level of expertise regarding the Trilinos package that is to be wrapped, as well as those packages that the package interacts with. This expertise would include related development tools such as the CMake build system and the GIT version control system.
- **SWIG.** SWIG is the Simple Wrapper and Interface Gernerator, and is the workhorse for generating the code that gets compiled to become python extension modules. The 'S' in SWIG comes from the fact that SWIG can read and parse a header file and generate code that will compile, can be imported into a python shell, and mimics the C/C++ interface (within the constraints of the language). However, SWIG is very powerful, and almost all of its provisions can be overwritten by the python interface developer. Trilinos is sufficiently complex that such overrides are commonplace, and the PyTrilinos developer must have a high degree of comfort doing this.
- The Python C/API. When such overrides are necessary, it usually involves writing code that is compliant with the Python C/API. In addition to the structs and function prototypes provided by the Python C/API, this means a thorough understanding of python exception handling (essential for a dynamic language) and reference counting (which requires more programmer intervention in C than in C++).

• NumPy. NumPy is the accepted standard python package for handling arrays of contiguous (or strided) homogeneous data. Any PyTrilinos classes or arguments that involve arrays of data should provide an interface that is highly compatible with NumPy.

Each of these languages, libraries, tools and interfaces have extensive documentation available on-line, and should be accessed frequently by the PyTrilinos developer. The purpose of this Developers Guide is detail how these tools are used together to generate PyTrilinos, and to document certain conventions that have been adopted for all PyTrilinos packages.

# **Adding New Modules to PyTrilinos**

If you want to add a Trilinos package as a new module in PyTrilinos, here are the necessary steps.

- 1. Add the package name to the <code>cmake/Dependencies.cmake</code> file, where variable <code>LIB\_OPTIONAL\_DEP\_PACKAGES</code> is set. It is important that packages be listed in build order.
- 2. If your package uses nested namespaces, then the python interface should use corresponding nested modules. To partially facilitate this, within the src/PyTrilinos directory, make a directory with your package name.
  Repeat for nested namespaces.

In src/PyTrilinos/CMakeLists.txt, you will find logic such as:

```
# The NOX module employs namespaces, so include the NOX directory
IF(${PACKAGE_NAME}_ENABLE_NOX)
   ADD_SUBDIRECTORY(NOX)
ENDIF(${PACKAGE_NAME}_ENABLE_NOX)
```

Add similar logic for your code. In each nested directory, create a new CMakeLists.txt file and provide similar logic.

3. In the top-level CMakeLists.txt file, you will find a series of if-blocks that look like this:

```
IF(PyTrilinos_ENABLE_Teuchos)
   APPEND_SET(${PACKAGE_NAME}_PACKAGES Teuchos)
   APPEND_SET(${PACKAGE_NAME}_MODULES Teuchos)
ENDIF(PyTrilinos_ENABLE_Teuchos)
```

Add a similar if-block for your new package, making sure it is placed in build-order relative to the other packages. See the logic for the  ${\tt NOX}$  package if your package supports nested namespaces (sub-modules).

- 4. If your package will require compiled code that will be archived in the pytrilinos shared library, add the headers and sources to src/CMakeLists.txt, using the existing if-blocks as a guide.
- 5. If your package supports nested namespaces (sub-modules), then in src/CMakeLists.txt, find the loop prefaced with the comment:

```
# Loop over the PyTrilinos-enabled Trilinos modules and define the
# swig-generated PyTrilinos extension modules
```

Use the existing if-blocks to add logic to support your sub-modules.

6. Add your package by writing the required SWIG interface files. For a standard PACKAGE, it will be in the file

```
PACKAGE.i
```

For a package that supports nested namespaces, the primary SWIG interface file will be named:

```
''PACKAGE init .i''
```

In both cases, of course, PACKAGE will be replaced with your package name.

# The PyTrilinos Build System

The move by Trilinos to the CMake build system has had many advantages for PyTrilinos. The two primary advantages being that shared libraries and python extension libraries can now both be built automatically by the host build system. Previously, shared libraries were built by the PyTrilinos package in an ad-hoc manner, and the python extension libraries were built using the python distutils module, which has some reports of portability issues. The move to CMake has improved the reliability and robustness of the PyTrilinos build system.

From a build-system point of view, there are two types of Trilinos packages that are supported by PyTrilinos: those that are contained within a single namespace, like Teuchos, Epetra and AztecOO; and those that are contained within nested namespaces, such as NOX. These two types are detailed below, in addition to the pytrilinos library and package-specific configuration options.

#### **Single Namespace Packages**

All supported packages must be listed in the LIB\_OPTIONAL\_DEP\_PACKAGES variable in the cmake/Dependencies.cmake file, and they should be listed in build order.

The PyTrilinos build system maintains two variables, PyTrilnos\_PACKAGES and PyTrilinos\_MODULES, both set in the top-level CMakeLists.txt file, to keep track of what to build. (Note that these variables are referenced as \${PACKAGE\_NAME}\_PACKAGES and \${PACKAGE\_NAME}\_MODULES within CMakeLists.txt.) For single namespace packages, the entries in these two variables is the same. For example,

```
IF(PyTrilinos_ENABLE_Teuchos)
   APPEND_SET(${PACKAGE_NAME}_PACKAGES Teuchos)
   APPEND_SET(${PACKAGE_NAME}_MODULES Teuchos)
ENDIF(PyTrilinos_ENABLE_Teuchos)
```

In this instance, the build system now expects to find a SWIG interface file in the source directory src/Teuchos.i that defines module PyTrilinos.Teuchos. The end products will be placed in the build directory src/PyTrilinos:

```
src/PyTrilinos/Teuchos.py
src/PyTrilinos/Teuchos.pyc
src/PyTrilinos/_Teuchos.so
```

### **Nested Namespace Packages**

Using NOX as an example, the LIB\_OPTIONAL\_DEP\_PACKAGES variable in the cmake/Dependencies.cmake file should contain the entry NOX and it should be listed in build order.

In the top-level CMakeLists.txt file, the variable PyTrilinos\_PACKAGES should be appended as before, with a single entry. But PyTrilinos\_MODULES should contain an entry for each nested namespace:

```
IF (PyTrilinos_ENABLE_NOX)
   APPEND_SET(${PACKAGE_NAME}_PACKAGES NOX)
   APPEND_SET(${PACKAGE_NAME}_MODULES NOX.__init__ )
   APPEND_SET(${PACKAGE_NAME}_MODULES NOX.Abstract )
   APPEND_SET(${PACKAGE_NAME}_MODULES NOX.StatusTest)
   APPEND_SET(${PACKAGE_NAME}_MODULES NOX.Solver )
   IF (NOX_ENABLE_Epetra)
   APPEND_SET(${PACKAGE_NAME}_MODULES NOX.Epetra.__init__ )
   APPEND_SET(${PACKAGE_NAME}_MODULES NOX.Epetra.Interface)
   ENDIF(NOX_ENABLE_Epetra)
ENDIF(PyTrilinos ENABLE NOX)
```

For every entry in PyTrilnos\_MODULES, there should be a corresponding SWIG file in the source directory:

```
src/NOX.__init__.i
src/NOX.Abstract.i
src/NOX.StatusTest.i
src/NOX.Solver.i
src/NOX.Epetra.__init__.i
src/NOX.Epetra.Interface.i
```

#### which will produce the following build products:

```
src/PyTrilinos/NOX/__init__.py
src/PyTrilinos/NOX/__init__.pyc
src/PyTrilinos/NOX/__init__.so
src/PyTrilinos/NOX/Abstract.py
src/PyTrilinos/NOX/Abstract.pyc
src/PyTrilinos/NOX/_Abstract.so
src/PyTrilinos/NOX/_StatusTest.py
src/PyTrilinos/NOX/StatusTest.pyc
src/PyTrilinos/NOX/_StatusTest.so
src/PyTrilinos/NOX/_StatusTest.so
src/PyTrilinos/NOX/_Solver.pyc
src/PyTrilinos/NOX/Solver.pyc
src/PyTrilinos/NOX/_Solver.so
src/PyTrilinos/NOX/_Solver.so
src/PyTrilinos/NOX/Epetra/__init__.pyc
src/PyTrilinos/NOX/Epetra/__init__.pyc
src/PyTrilinos/NOX/Epetra/__init__.so
```

```
src/PyTrilinos/NOX/Epetra/Interface.py
src/PyTrilinos/NOX/Epetra/Interface.pyc
src/PyTrilinos/NOX/Epetra/_Interface.so
```

### The pytrilinos Library

If you develop a module that requires compiled code not generated by SWIG, it should be put in the pytrilinos library. Simply append entries the the HEADERS and SOURCES variables in src/CMakeLists.txt file.

### **Package-Specific Configuration Options**

If you need package-specific configuration options set, they should be done so in <code>src/CMakeLists.txt</code> prior to the call to <code>PACKAGE\_CONFIGURE\_FILE()</code> and in <code>cmake/PyTrilinos\_config.h.in</code>. Currently, the following variables are set depending upon the top-level Trilinos configuration:

```
HAVE_EPETRA
HAVE_TEUCHOS
HAVE_NOX_EPETRA
HAVE_NOX_EPETRAEXT
HAVE MPI
```

# **PyTrilinos Documentation System**

## **Python Docstrings**

Python has an effective interactive documentation system, utilizing what are known as "docstrings". If the first statement of a python module, a python function or a python class is a string constant, then that string becomes the documentation string, or "docstring", for the given module, function or class. For example,

```
def func(arg):
    "Docstring for function func"
    return "Hello, world!"
```

Docstrings are fundamentally different from python comments, because of their position relative to the code they describe and because they are used by the python help facility and other documentation tools, such as pydoc:

```
>>> help(func)
Help on function func in module __main__:
func(arg)
    Docstring for function func
>>>
```

### **PyTrilinos Docstring Policy**

It is the policy of PyTrilinos that python docstrings should be maintained to provide useful, current and accurate information to PyTrilinos users that

- correctly reflect the calling arguments of PyTrilinos methods and functions.
- match the coresponding doxygen documentation provided by Trilinos developers when appropriate, and
- supercede the doxygen documentation when the python interface and/or implementation is different from the C++ interface and/or implementation.

The difficulty in adhering to these policies is that the python code (and therefore the python docstrings) that makes up PyTrilinos is automatically generated by swig. Fortunately, there are several tools available that allow these policies to be met.

### **Module docstrings**

Every PyTrilinos module should contain a module docstring. This is typically implemented in the package interface file as follows:

```
%define %my_package_docstring
"
Multi-line documentation string for
My_Package
"
%enddef
%module (docstring = %my_package_docstring) My_Package
```

SWIG does not require that SWIG macro names begin with "%", but it is allowed and it is the convention for PyTrilinos SWIG macros. Further, PyTrilinos module docstrings follow a set format:

```
PyTrilinos.My_Package is the python interface to the Trilinos such-and-such package My_Package:

http://trilinos.sandia.gov/packages/my_package

The purpose of My_Package is to . . . The python version of the My_Package package supports the following classes:

* Class1 - Short description 1

* Class2 - Short description 2

* . . .

Any other notes about the package as a whole. . . .
```

### **Function and Method Docstrings**

Docstrings for functions and methods are partially implemented by the SWIG %feature called autodoc. Before any code is directed to be wrapped within an interface file (by the first %include directive), the following feature should be activated:

```
%feature("autodoc", "1");
```

This automatically adds docstrings to each function and class method showing the function name, argument list, and return type. The argument list contains both type and name information (as per the "1" option). If a function or method is overloaded, each valid calling signature is listed.

### **Appending Doxygen Documentation to Docstrings**

A system is in place for automatically extracting Doxygen documentation from a Trilinos package source code and inserting it into the package's python module. First, Doxygen is used to extract the documentation and save it in XML format. Second, a python script is run to read this XML data and convert it to a series of valid SWIG statements of the form::

```
%feature("docstring") <symbol-name> <docstring>
```

Third, each package interface file implements an %include statement to read these documentation directives. This adds the Doxygen documentation string to the end of the string created by %feature("autodoc", "1").

All of this infrastructure is contained within the PyTrilinos subdirectory:

```
doc/Doxygen
```

Within this subdirectory are a series of Doxygen control files, one for each package: Doxyfile\_Teuchos, Doxyfile\_Epetra, etc. These Doxyfiles have certain features in common: they all generate XML output:

```
GENERATE\_XML = YES
```

while suppressing all other forms of output. They all direct output to their own subdirectory:

```
OUTPUT_DIRECTORY = Teuchos
XML_OUTPUT = .
```

If you add documentation for a new package, then add the package name to the PyTrilinos/doc/Doxygen/Makefile variable PACKAGES. When you run make from the shell, this will cause doxygen to be run on the Doxyfile and the script doxy2swig.py (generously provided by Prabhu Ramachandran) to be run on the resulting output. This produces a file with a \_dox.i suffix, e.g. Teuchos\_dox.i, intended to be included into the package interface file src/Teuchos.i. To facilitate this inclusion, SWIG is invoked with -I\$ (top\_srcdir)/doc/Doxygen.

#### **Overriding Doxygen Documentation**

Sometimes the Doxygen documentation is not appropriate for a given python function or method. This is often the case when <code>%typemap-s</code> are employed or when the python implementation replaces the C++ interface by using <code>%ignore</code>, <code>%extend</code> and/or <code>%inline</code>. This requires that the automatically created docstrings be overridden or appended, and can be accomplished by providing a SWIG documentation directive <code>after</code> the <code>%include "Teuchos\_dox.i"</code> (for example) and that redefines the docstring for a specified symbol. These directives should be placed directly in the appropriate interface file. By convention, all directives pertaining to the symbols within

a single %include file are grouped together. The documentation directives should be at the top of these groupings.

There are two SWIG documentation directives that can be employed to override or append docstrings. If you wish to append documentation to what is already present, use:

```
%feature("docstring")
<symbol-name>
"
<docstring>
";
```

If you wish to replace the existant docstring completely, use the directive:

```
%feature("autodoc",
"<docstring>")
<symbol-name>;
```

The formatting given here tends to be the most readable for the widest range of situations, both for the interface files and for the resulting docstrings.

# **Exception Handling in PyTrilinos**

All C++ exceptions raised by Trilinos should be caught by PyTrilinos and converted to python exceptions. Fortunately, there is a relatively straightforward SWIG facility for doing this. Each SWIG interface file shall include an %exception directive prior to any Trilinos header file %include directives:

```
%include "exception.i"
%exception
{
  try
  {
    $action
  }
  catch(...)
  {
    SWIG_exception(SWIG_UnknownError, "Unknown C++ exception");
  }
}
```

It is possible to implement an %exception directive that includes a symbol name, prior to the first "{", that is specific to a function or method. By omitting this symbol name, we are applying this %exception to *all* functions and methods that get wrapped. Here, \$action is a SWIG macro that is replaced by the generated code for calling the wrapped function or method. The catch(...) syntax ensures that *every* exception that might be thrown gets caught.

 ${\tt SWIG\_exception}\ is\ a\ C\ macro\ \#define-ed\ at\ the\ top\ of\ the\ generated\ source\ file.\ {\tt SWIG\_UnknownError}\ is\ also\ a\ macro\ that\ evaluates\ to\ an\ integer.\ See\ the\ SWIG\ documentation\ for\ valid\ SWIG\ error\ macro\ names.$ 

The directive given above is useful, but all exceptions will get converted to type UnknownError with a nearly meaningless error message. Realistically, we need

to convert a wider range of exceptions to more meaningful python exception types, and produce more useful error messages. SWIG also provides a macro for treating most standard C++ exceptions, converting them to appropriate python exceptions and extracting their error message from their what () method. Simply change the %exception directive to:

```
%exception
{
    try
    {
        $action
    }
    SWIG_CATCH_STDEXCEPT
    catch(...)
    {
        SWIG_exception(SWIG_UnknownError, "Unknown C++ exception");
    }
}
```

and this will convert the vast majority of standard exceptions to appropriate python exceptions with useful error messages.

There are Trilnios packages that throw exceptions other than those found in the standard library. These can be caught anywhere prior to the <code>catch(...)</code> syntax, although in general, it is best to put them before the <code>SWIG\_CATCH\_STDEXCEPT</code> macro, especially if the package exceptions inherit from the standard exceptions. Here is the current Teuchos exception handler:

```
%exception
{
 try
  {
   $action
   if (PyErr_Occurred()) SWIG_fail;
  }
 catch(Teuchos::Exceptions::InvalidParameterType & e)
  {
   SWIG_exception(SWIG_TypeError, e.what());
  }
 catch(Teuchos::Exceptions::InvalidParameter & e)
   PyErr_SetString(PyExc_KeyError, e.what());
   SWIG_fail;
 SWIG_CATCH_STDEXCEPT
 catch(...)
   SWIG_exception(SWIG_UnknownError, "Unknown C++ exception");
  }
}
```

A few notes: (1) After the  $action\ macro$ , there is a call to  $PyErr\_Occurred$ (). This is because the Teuchos wrappers  $extend\ certain\ classes$  and those new meth-

ods can set python errors. Alternatively, you could raise C++ exceptions in all of these extensions, and then skip the PyErr\_Occurred() check. (2) SWIG\_fail is a C macro provided by SWIG that evaluates to goto fail, where fail is a label that exists within all wrapper functions. (3) The Teuchos::Exceptions::InvalidParameter exception is most closely related to the python KeyError exception, but SWIG does not have a corresponding SWIG error for this. Therefore, I use the PyErr\_SetString() function and SWIG\_fail macro.

#### **Practical Considerations**

Most PyTrilinos packages will need to %import "Teuchos.i" and/or %import "Epetra.i". Both of these interface files implement their own %exception directive, but both of them "turn off" exception handling by including a:

```
%exception;
```

at the end of the file. This is considered good practice and should be followed in *all* PyTrilinos SWIG interface files.

Nevertheless, experience shows that the following represents the best order for %include-s and %import-s when dealing with exceptions in PyTrilinos:

```
%include "exception.i"
%import "Teuchos.i"
%import "Epetra.i"
%exception
{
    ...
}
```

Putting the %include "exception.i" after the %import directives can result in undefined symbols when you compile the generated wrapper code.

Finally, every effort should be made to prevent users from getting an Unknown C++ exception error message. Study the package to determine as many of the possible exceptions that might be thrown as you can, and explicitly include them in the %exception directive. Whenever testing or use of PyTrilinos results in an Unknown C++ exception error message, track it down and then explicitly allow for it within the appropriate SWIG interface file. There is no excuse for a meaningless error message.

# **Handling C-Array Arguments**

Trilinos defines a number of high-level array-like objects that store contiguous, homogenous data. Nevertheless, there are instances when Trilinos objects pass low-level C-arrays as input or return arguments.

SWIG does not handle this case automatically in the manner we would like. However, PyTrilinos has adopted a set of interface conventions for dealing with them and simple methods for achieving those interfaces.

Built-in python containers, such as list, are discontiguous and heterogeneous, which makes them unsuitable for efficiently handling C-array type data. Fortunately, there is a third party module named NumPy that has been adopted by the python community for just this purpose. (This adoption has been hard won -- NumPy brought together two

divergent efforts named Numeric and NumArray.) Included in the NumPy distribution is a file named numpy.i, which is a SWIG interface file that provides typemaps and other tools. This file has been copied to the PyTrilinos/src directory and is used by PyTrilinos SWIG interface files for handling C-array arguments.

To learn how to use numpy.i, its documentation is online.

Code that needs to interface with NumPy should call the function <code>import\_array()</code>, but only once. To avoid the possibility of two unrelated python modules both calling <code>import\_array()</code> in a conflicting way, NumPy requires that you define a macro <code>PY\_ARRAY\_UNIQUE\_SYMBOL</code>. In PyTrilinos, we do:

```
#define PY_ARRAY_UNIQUE_SYMBOL PyTrilinos
```

However, we must also guard against two or more PyTrilinos modules calling import\_array(). To do this, we define a singleton class NumPyImporter that calls import\_array() and lives in the pytrilinos shared library. All PyTrilinos extension modules link against this library and so the first one to be imported will instantiate the NumPyImporter object, which calls import\_array() in its constructor

For this reason, the initialization instructions in the numpy.i instructions should be ignored, as they are for a single python module environment. Instead, all a PyTrilinos developer has to do is add:

```
%{
#include "numpy_include.h"
%}
%include "numpy.i"
```

to his SWIG interface file, and then start using the <code>%apply</code> directive as described in the <code>numpy.i</code> documentation.

#### **Reference Counted Pointers**

Reference counting is a memory management technique whereby dynamically allocated objects can be tracked, and can be guaranteed to exist as long as any other entity (such as a class or the local scope of a function) needs it to. Such entities can "take a reference" to the dynamically-allocated reference-counted object, and the technique works by ensuring that the object is never destroyed until its reference count falls to zero.

A reference counted pointer is a data structure for implementing such a memory management technique. It consists of a raw pointer to an object and an integer count of the number of entities that have taken a reference to the object. It also consists of methods for increasing and decreasing the reference count as needed, and a destructor that waits until the reference count is zero before destroying the object. These are also called shared pointers.

### **PyTrilinos and RCPs**

Python implements just such a reference counting scheme for every python object that is constructed. It occurs "behind the scenes" and "just works", like python is famous for. The only people who ever have to worry about python reference counting are

programmers who write code using the Python/C API -- which does include PyTrilinos developers.

C++ does not have a standard reference counting system, although several reference counting classes have been developed, which are much more powerful than can be developed in C (such as the Python/C API uses) and much less prone to error. There is the boost::shared\_ptr<> class, which is planned to be moved to the std namespace at some point in the future. Trilinos could not wait for this standardization process, and thus was born the Teuchos::RCP<>, which of course stands for "reference counted pointer".

Several Trilinos packages use RCPs, and so PyTrilinos has a policy for dealing with them. First, if any package anywhere stores instances of a class using an RCP, then PyTrilinos will always store instances of that class internally using an RCP. This ensures that all reference counts remain accurate under all use cases. Second, python programmers should never have to deal with Teuchos::RCP<>. That is to say, there is no Teuchos.RCP class in PyTrilinos. If a C++ method requires a Teuchos::RCP<> of some class, the python interface will take an unadorned instance of that class. The conversion to an RCP will happen behind the scenes. And the python programmer, who has always benefitted from reference counts without ever exerting any effort, will continue in this happy state.

By default, SWIG generates code that stores dynamically allocated objects using a raw pointer. With SWIG 2.0.0, the python code generator in SWIG has a (relatively?) bug free implementation of using reference counted pointers instead of raw pointers. This is coupled with a large set of typemaps that alter the conversion code between C++ and python, taking the new storage method into account. This is implemented for boost::shared\_ptr<> and std::shared\_ptr<>. It provides a %shared\_ptr() SWIG macro that the user invokes on a class that should be stored as a shared pointer.

The Teuchos\_RCP.i file leverages the SWIG-provided boost\_shared\_ptr.i file by using #define statements to make all of the provided logic work with Teuchos::RCP<>. It also provides replacement typemaps for when the Teuchos::RCP<> interface is different from the boost::shared\_ptr<> interface and additional typemaps for directors, which boost\_shared\_ptr.i does not provide. This new logic is accessed by using a %teuchos\_rcp() SWIG macro on a class.

#### When to Store PyTrilinos Classes as RCPs

When do you use the <code>%teuchos\_rcp()</code> macro? First, whenever you encounter a class that is wrapped in <code>Teuchos::RCP<></code> as an input or output argument in a class method or function, then that class needs to be stored internally as as an RCP by using <code>%teuchos\_rcp()</code>.

Second, if B is a base class and D derives from it, then <code>%teuchos\_rcp(B)</code> requires that <code>%teuchos\_rcp(D)</code> also be invoked. Failure to do so will result in an extension module that will fail to compile. The reason is due to how type checking is performed for these RCP classes and the need for derived classes to be recognized as proper instances of base classes.

Third, using B and D as before, if %teuchos\_rcp(D) is invoked, then %teuchos\_rcp(B) almost certainly should be as well. The extension module will compile even if this rule is not followed, but type checking will fail under certain circumstances. This rule can be ignored if B is an implementation-only base class, but this is rare.

#### **Usage Details**

If a class is defined in Package 1, but not used as an RCP in Package 1, and is then used as an RCP in Package 2, the <code>%teuchos\_rcp()</code> macro should be invoked in the SWIG interface file for Package 1. This way, when <code>%import</code> is used on Package 1 from other package SWIG interface files, the storage method remains constant among all the packages.

If you are (in effect) wrapping Package 2, and Package 1 is Epetra, then there are some additional SWIG macros you should know. If the Epetra class is an array storage class implemented as a hybrid numpy array, then you should use the <code>%teuchos\_rcp\_epetra\_numpy()</code> macro. This should never be necessary, however, because all of these classes have already been treated.

### **Testing**

There are two directories in the PyTrilinos package that provide python scripts for testing PyTrilinos, example and test. Generally speaking, unit tests go in the test directory and descriptive or demonstrative example scripts go in example.

### **Naming Conventions**

Unit tests scripts shall begin with test, followed by the package name and an underscore, followed by a short description of the test, typically the class name being tested. For example:

```
testTeuchos_ParameterList
testEpetra_MultiVector
```

are the base names of the unit tests for <code>Teuchos.ParameterList</code> and <code>Epetra.MultiVector</code>, respectively. In certain situations, the underscore and test description can be omitted.

Example scripts shall begin with ex, followed by the name of the primary package being demonstrated, followed by an underscore and a short description of the test. For example:

```
exEpetra_Comm
exAztec00_Operator
```

are the base names for example scripts demonstrating the Epetra.Comm class and an AztecOO solver that uses an Epetra.Operator, respectively. In certain situations, the underscore and test description can be omitted.

### **Build System**

Running make in either the top, example or test build directories copies the test scripts from the source directory to the build directory while performing certain text substitutions. Similar to the configuration file naming convention, the source files have the suffix .py.in and the build files have the suffix .py. The reason for this is that CMake variable values can be substituted during the copy procedure. For example, the first line of each test script source file is now:

```
#! ${PYTHON_EXECUTABLE}
```

which means that the python executable that is recognized (and compiled against) by the CMake build system will also be the python executable invoked by the PyTrilinos test scripts. Note that this substitution is available to the test developers for any variable that is defined in the CMakeCache.txt file found in the top build directory.

The CMakeLists.txt files in the test and example directories control which scripts get copied to the build directory. Each test script, or group of related test scripts, should be protected with IF() statements, depending on which PyTrilinos modules need to be present for the script to run.

#### **Running All Tests**

To run all of the enabled tests, first make sure PyTrilinos and all tests and examples are up-to-date:

```
$ cd BUILD/packages/PyTrilinos
S make
```

Then you can use the CMake ctest program to run all of the tests:

```
$ ctest -W 10
```

The results of all of the tests can be found in the Testing directory, present in the directory from which ctest was run.

### **Test Script Conventions**

All test scripts shall use the optparse module to parse command line options and support the following options:

The -t option is to force use of the locally-built PyTrilinos, preventing the importing of any installed PyTrilinos modules. The verbosity option is used in all test scripts and optionally in any example scripts where it makes sense.

Tests scripts use the from PyTrilinosImport function in the testutil module, local to both test and example directories, to control where the PyTrilinos modules are imported from. The user controls this import location from the command line: -t or --testharness indicates that the build directory should be used; otherwise an import from standard locations will be attempted.

This policy is enabled by code in each test/example script like the following:

If the user specifies -t or --testharness then options.testharness will be True, else it will be False. When fromPyTrilinosImport() is called, the options.testharness argument will determine where the import is read from.

Test scripts shall run in both serial or parallel. You may use either:

```
comm = Teuchos.DefaultComm.getComm()
or:
    comm = Epetra.PyComm()
```

to obtain an appropriate communicator object for the test scripts. By convention, set the variable <code>iAmRoot</code> to either <code>True</code> or <code>False</code> depending on whether the communicator's rank is 0.

The test script shall output End Result: TEST PASSED if the test passes correctly. This helps the Trilinos test harness determine which tests pass and which do not, especially in parallel.

#### **Unit Tests**

Unit tests are based on the unittest python library module. Test case classes inherit from unittest. TestCase. Individual tests are implemented as methods of these classes that begin with test. See the python documentation (http://www.python.org) for details.

Each unit test script can have one or more TestCase classes. In main(), each test case class should be added to a unittest. TestSuite object named suite.

Unit tests shall print, from processor 0, a header with a message such as "Testing Epetra.Object" with a line of asterisks above and below the message:

The suite of tests should be run with:

```
verbosity = options.verbosity * int(iAmRoot)
result = unittest.TextTestRunner(verbosity=verbosity).run(suite)
```

and the success should be determined and output via (for the case of an Epetra communicator):

```
errsPlusFails = comm.SumAll(len(result.errors) + len(result.failures))
if errsPlusFails == 0 and iAmRoot: print "End Result: TEST PASSED"
sys.exit(errsPlusFails)
```

If there are no errors and no failures on any processors, then the test will pass.

#### **Example Scripts**

Example scripts are more free-form and should be written for readability, to make for clear demonstrations of PyTrilinos usage. However, it is encouraged that example script output be consistent with unit test output whenever possible.