

Francesc Alted

PyTables User's Guide

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*La sabiduría no vale la pena si no es
posible servirse de ella para inventar una
nueva manera de preparar los garbanzos.*

—Un sabio catalán
in "Cien años de soledad"
Gabriel García Márquez

Chapter 1

Introduction

The goal of `PyTables` is to enable the end user to manipulate easily scientific data **tables** and *Numerical Python* objects in a hierarchical structure. The foundation of the underlying hierarchical data organization is the excellent HDF5 library (<http://hdf.ncsa.uiuc.edu/HDF5>). Right now, `PyTables` provides limited support of all the HDF5 functions, but I hope to add the more interesting ones (for `PyTables` needs) in the near future. Nonetheless, this package is not intended to serve as a complete wrapper for the entire HDF5 API.

A table is defined as a collection of records whose values are stored in *fixed-length* fields. All records have the same structure and all values in each field have the same *data type*. The terms *fixed-length* and *strict data types* seems to be quite a strange requirement for an interpreted language like Python, but they serve a useful function if the goal is to save very large quantities of data (such as is generated by many scientific applications, for example) in an efficient manner that reduces demand on CPU time and I/O.

In order to emulate records (that will be mapped to C structs in HDF5) in Python `PyTables` implements a special *metaclass* object with the capability to detect errors in field assignments as well as type and range overflows. `PyTables` also provides a powerful interface to process table data. Records in tables are also known, in the HDF5 naming scheme, as *compound* data types.

For example, you can define arbitrary records in Python simply by declaring a class with the name field and types information, like in:

```
class Particle(IsRecord):
    name          = '16s'   # 16-character String
    idnumber      = 'Q'     # unsigned long long (i.e. 64-bit integer)
    TDCcount      = 'B'     # unsigned byte
    ADCcount      = 'H'     # unsigned short integer
    grid_i        = 'i'     # integer
    grid_j        = 'i'     # integer
    pressure      = 'f'     # float (single-precision)
    energy        = 'd'     # double (double-precision)
```

then, you will normally instantiate that class, fill the instance with your values, and save (arbitrary large) collections of them in a file for persistent storage. After that, this data can be retrieved and post-processed quite easily with `PyTables` or even with another HDF5 application.

Next section describes the most interesting capabilities of `PyTables`.

1.1 Main Features

`PyTables` has the next capabilities:

- *Support of table entities:* Allows working with a large number of records, i.e. that don't fit in memory.

- *Support of Numerical Python arrays:* Numeric arrays are a very useful complement of tables to keep homogeneous table slices (like selections of table columns).
- *Supports a hierarchical data model:* That way, you can structure very clearly all your data. PyTables builds up an *object tree* in memory that replicates the underlying file data structure. Access to the file objects is achieved by walking throughout this object tree, and manipulating it.
- *Appendable tables:* It supports adding records to already created tables. This can be done without copying the dataset or redefining its structure, even between different Python sessions.
- *Automatically check for correct field name, data type and data range:* That reduces programmer mistakes and if PyTables does not report an error, you can be more confident that your data is probably ok.
- *Support of files bigger than 2 GB:* The underlying HDF5 library already can do that (if your platform supports the C long long integer, or, on Windows, `__int64`), and PyTables automatically inherits this capability.
- *Data compression:* It supports data compression (through the use of the `zlib` library) out of the box. This become important when you have repetitive data patterns and don't want to loose your time searching for an optimized way to save them (i.e. it saves you data organization analysis time). This feature is also inherited from HDF5.
- *Architecture-independent:* PyTables has been carefully coded (as HDF5 itself) with little-endian/big-endian byte orderings issues in mind . So, in principle, you can write a file in a big-endian machine (like a Sparc or MIPS) and read it in other little-endian (like Intel or Alpha) without problems¹.

It should noted that PyTables is not intended to merely be a high level wrapper of selected HDF5 functionality (for this, have a look at HL-HDF5, the Swedish Meteorological and Hydrological Institute effort to provide another Python interface to HDF5; see reference 5), but to provide a flexible, *very Pythonic* tool to deal with (arbitrary) large amounts of data (typically bigger than available memory) in tables and arrays organized in a hierarchical, persistent disk storage.

PyTables take advantage of the powerful object orientation and introspection capabilities offered by Python to bring all those exposed features to the user in a friendly manner.

1.2 The Object Tree

The hierarchical model of the underlying HDF5 library allows PyTables to manage tables and arrays in a tree-like structure. In order to achieve this, an *object tree* entity is *dynamically* created imitating the HDF5 structure on disk. That way, the access to the HDF5 objects is made by walking throughout this object tree, and, by looking at their *metadata* nodes, you can get a nice picture of what kind data is kept there.

The different nodes in the object tree are instances of PyTables classes. There are several types of those classes, but the most important ones are the `Group` and the `Leaf`. `Group` instances (that we will be calling *groups* from now on) are a grouping structure containing instances of zero or more groups or leaves, together with supporting metadata. `Leaf` instances (that will be called *leaves*) are containers for actual data and cannot contain any other instances². The `Table` and `Array` classes are descendants of `Leaf`, and inherits all its properties.

Working with groups and leaves is similar in many ways to working with directories and files, respectively, in a Unix filesystem. As with Unix directories and files, objects in the object tree are often described by giving their full (or absolute) path names. In PyTables this full path can be specified either as string (like in `' / subgroup2 / table3 '`) or as a complete object path written in a certain way known as *natural name* schema (like in `file.root.subgroup2.table3`).

¹ I do actually tested that between a Sparc machine (big-endian) and an Intel machine (little-endian) and it works only for tables but not for arrays!. This flaw will hopefully be addressed in next release.

² Except `Attribute` instances in the short future

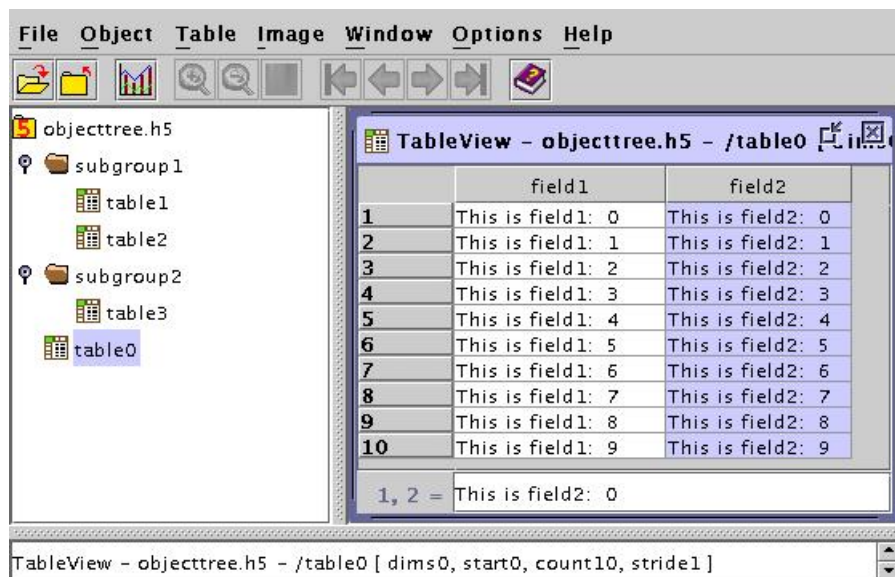


Figure 1.1: An HDF5 example with 2 subgroups and 3 tables.

The support for *natural naming* is a key aspect of PyTables and means that the names of instance variables of the node objects are the same as the names of the element's children³. This is very *Pythonic* and comfortable in many cases, as you can check in the tutorial section 3.1.6.

You should also note that not all the data present on file is loaded in the object tree, but only the *metadata* (i.e. special data that describes the structure of the actual data). The actual data is not read until you ask for it (by calling a method in a particular node). By making use of the object tree (the metadata) you can get information on the objects on disk such as table names, title, name fields, data types in fields, number of records, or, in the case of arrays, shapes, typecode, and so on. You can also traverse the tree in order to search for something and when you find the data you are interested in you can read it and process it. In some sense, you can think of PyTables as a tool that provide the same introspection capabilities of Python objects, but applied to the persistent storage of large amounts of data.

To better understand the dynamic nature of this object tree entity, imagine that we have made a script (in fact, this script actually exists and you can find it in `examples/objecttree.py`; check it out!) that creates a simple PyTables file, with the structure that appears in figure 1.1. During creation time, metadata in the object tree is updated in memory while the actual data is being saved on disk and when you close the file the object tree becomes unavailable. But, when you will open again this file the object tree will be re-constructed in memory from the metadata existent on disk, so that you can work with it exactly in the same way than during the original creation process.

In figure 1.2 you can see an example of the object tree created by reading a PyTables file (in fact, this file is the same as that of the figure 1.1). If you are going to become a PyTables user, take your time to understand it⁴. That will also make you more proactive by avoiding programming mistakes.

³ I have got this simple but powerful idea from the excellent `Objectify` module by David Mertz (see references 7 and 8)

⁴ Bear in mind, however, that this diagram is **not** a standard UML class diagram; I've used an UML tool to draw it, that's all.

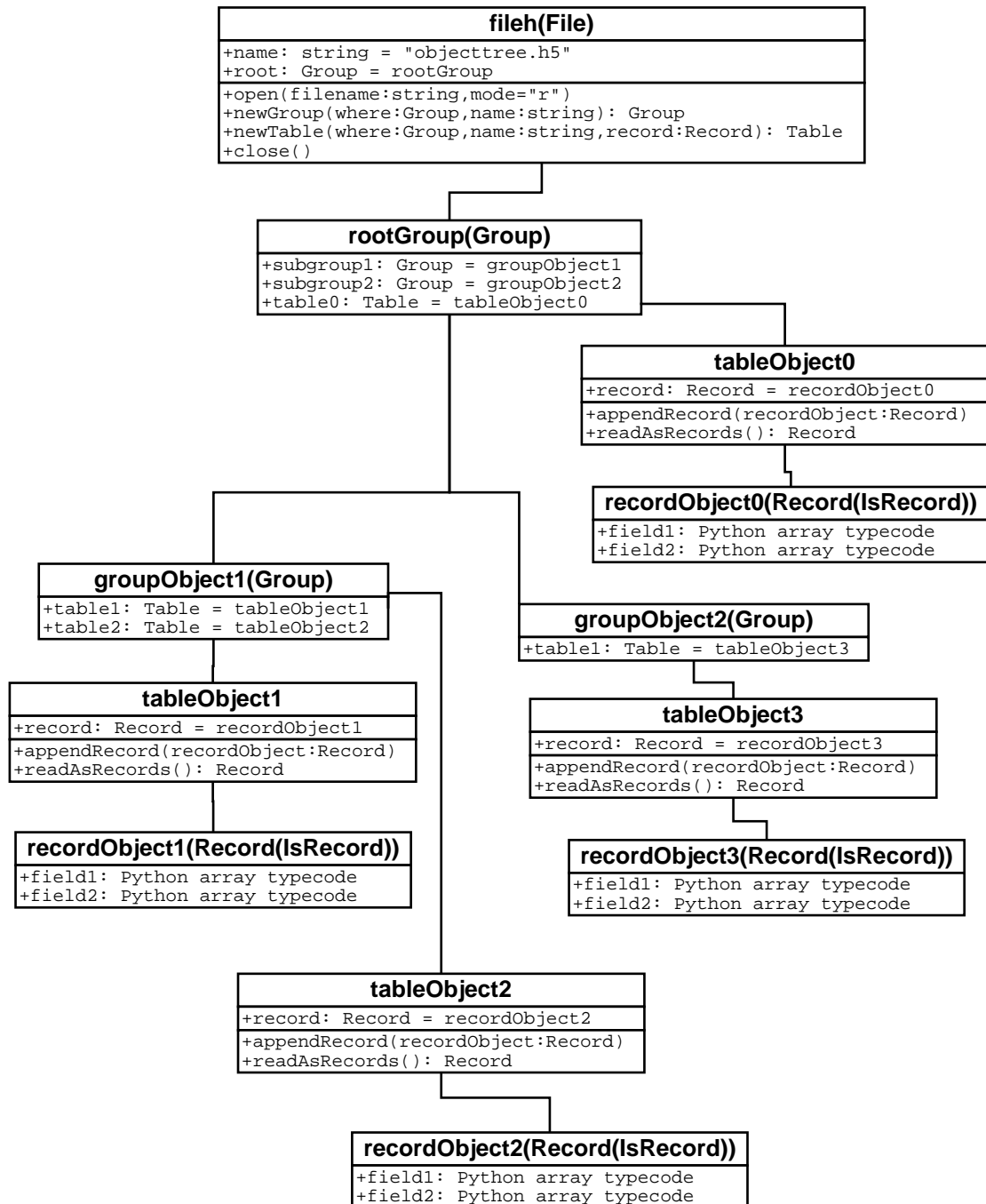


Figure 1.2: An object tree example in PyTables.

Chapter 2

Installation

This are instructions for Unix/Linux system. If you are using Windows, and you get the library to work, please tell me about.

Extensions in `PyTables` has been made using `Pyrex` (see reference 9) and C language. You can rebuild everything from scratch if you got `Pyrex` installed, but this is not necessary, as the `Pyrex` compiled source is included in the distribution. In order to do that, merely replace `setup.py` script in these instructions by `setup-pyrex.py`.

The Python Distutils are used to build and install `PyTables`, so it is fairly simple to get things ready to go.

1. First, make sure that you have `HDF5 1.4.x` and `Numerical Python` installed (I'm using `HDF5 1.4.4` and `Numeric 22.0` currently). If don't, you can find them at <http://hdf.ncsa.uiuc.edu/HDF5> and <http://www.pfdubois.com/numpy>. Compile/install them.

`setup.py` will detect `HDF5` libraries and include files under `/usr` or `/usr/local`; this will catch installations from `RPMs`, `DEBs` and most hand installations under Unix. If `setup.py` can't find your `libhdf5` or if you have several versions installed and want to select one of them, then you can give it a hint either in the environment (using the `HDF5_DIR` environment variable) or on the command line by specifying the directory containing the include and lib directory. For example:

```
--hdf5=/stuff/hdf5-1.4.4
```

If your `HDF5` library was built as shared library, and if this shared library is not in the runtime load path, then you can specify the additional linker flags needed to find the shared library on the command line as well. For example:

```
--lflags="-Xlinker -rpath -Xlinker /stuff/hdf5-1.4.4/lib"
```

or perhaps just

```
--lflags="-R /stuff/hdf5-1.4.4/lib"
```

Check your compiler and linker documentation for correct syntax.

It is also possible to specify linking against different libraries with the `--libs` switch:

```
--libs="-lhdf5-1.4.6"
--libs="-lhdf5-1.4.6 -lnsl"
```

2. From the main `PyTables` distribution directory run this command, (plus any extra flags needed as discussed above):

```
python setup.py build_ext --inplace
```

depending on the compiler flags used when compiling your Python executable, there may appear lots of warnings. Don't worry, almost all of them are caused by variables declared but never used. That's normal in Pyrex extensions.

3. To run the test suite change into the test directory and run this command, (assuming your shell is `sh` or compatible):

```
PYTHONPATH=..  
export PYTHONPATH  
python test_all.py
```

If you would like to see some verbose output from the tests simply add the flag `-v` and/or the word `verbose` to the command line. You can also run just the tests in a particular test module. For example:

```
python test_types.py -v
```

If you run into problems because Python can't load hdf5 shared libraries, try to set the `LD_LIBRARY_PATH` environment variable to point to the directory where the libraries are.

4. To install the entire PyTables Python package, change back to the root distribution directory and run this command as the root user (remember to add any extra flags needed):

```
python setup.py install
```

That's it!. Now, proceed with the next section to see how to use PyTables.

Chapter 3

Usage

This chapter begins with a series of simple, yet comprehensive sections written in a tutorial style that will let you understand the main features that `PyTables` provide. If during the trip you want more information on some specific instance variable, global function or method, go to the library reference in chapter 4. However, if you are reading this in PDF or HTML formats, there should be an hyperlink to its reference near each new introduced entity. Finally, you can get deeper knowledge of `PyTables` internals by reading the last section (3.4) in this chapter.

3.1 Getting started

In this section, we will see how to define our own records from Python and save collections of them (i.e. a **table**) on a file. Then, we will select some data in the table using Python cuts, creating Numerical arrays to keep this selection as separate objects in the tree.

In *examples/tutorial1-1.py* you will find the working version of all the code in this section. However, this tutorial series has been written to allow you reproduce it in a Python interactive console. You are encouraged to take advantage of that by doing parallel testing and inspecting the created objects during the voyage!.

3.1.1 Importing `tables` objects

Before to do anything you need to import the public objects in the `tables` package. You normally do that by issuing:

```
>>> import tables
>>>
```

That is the recommended way to import `tables` if you don't want to pollute too much your namespace. However, `PyTables` has a very reduced set of first-level primitives, so you may consider to use this alternative:

```
>>> from tables import *
>>>
```

which will export in your caller application namespace the next objects: `openFile`, `isHDF5`, `isPyTablesFile` and `IsRecord`. These are a rather small number of objects, and for commodity we will use this last way to access them.

If you are going to deal with Numeric arrays (and normally, you will) you also need to import some objects from it. You can do that in the normal way. So, to access to `PyTables` functionality normally you should start you programs with:

```
>>> from tables import *
>>> from Numeric import *
>>>
```

3.1.2 Declaring a Record

Now, imagine that we have a particle detector and we want to declare a record object in order to save data that comes from it.

Our detector has a TDC (Time to Digital Converter) counter with a dynamic range of 8 bits and an ADC (Analogic to Digital Converter) with a range of 16 bits. For these values, we will define 2 fields in our record object called `TDCcount` and `ADCcount`. We also want to save the grid position in which the particle has been detected and we will add two new fields called `grid_i` and `grid_j`. Our instrumentation also can obtain the pressure and energy of this particle that we want to add in the same way. The resolution of pressure-gauge allows us to use simple-precision float which will be enough to save `pressure` information, while `energy` would need a double-precision float. Finally, to track this particle we want to assign it a name to inform about the kind of the particle and a number identifier unique for each particle. So we will add a couple of fields: `name` will be the a string of up-to 16 characters and because we want to deal with a really huge number of particles, `idnumber` will be an integer of 64-bits.

With all of that, we can declare a new `Particle` class that will keep all this info:

```
>>> class Particle(IsRecord):
...     name          = '16s'    # 16-character String
...     idnumber      = 'Q'      # unsigned long long (i.e. 64-bit integer)
...     TDCcount      = 'B'      # unsigned byte
...     ADCcount      = 'H'      # unsigned short integer
...     grid_i        = 'i'      # integer
...     grid_j        = 'i'      # integer
...     pressure      = 'f'      # float (single-precision)
...     energy        = 'd'      # double (double-precision)
...
>>>
```

This definition class is quite auto-explanatory. Basically, you have to declare a class variable for each field you need, and as its value you put the typecode for this data field. See appendix A for a list of typecodes supported in record classes (`IsRecord` descendants).

From now on, we can use `Particle` instances as a container for our detector data and, as you will see shortly, we will benefit of some magic properties associated with these instances derived from the fact that they are descendants from the class `IsRecord`¹.

In order to do something useful with this record we need to attach it to a `Table` object. But first, we must create a file where all the actual data pushed into `Table` will be saved.

3.1.3 Creating a PyTables file from scratch

To create a PyTables file use the first-level `openFile` (see 4.1.2) function:

```
>>> h5file = openFile("tutorial1.h5", mode = "w", title = "Test file")
```

This `openFile` is one of the objects imported by the `"from tables import *"`, do you remember?. Here, we are telling that we want to create a new file called `"tutorial1.h5"` in `"w"`rite mode and with an informative title string (`"Test file"`). This function tries to open the file, and if successful, returns a `File` (see 4.3) instance which hosts the root of the object tree on its `root` attribute.

3.1.4 Creating a new group

Now, to better organize our data, we will create a group hanging from the root called *detector*. We will use this group to save our particle data there.

¹ `IsRecord` is actually a *metaclass* in object slang, but we don't need to explain nothing more about it in this context. Check the sources if you are interested on how that works.

```
>>> group = h5file.createGroup("/", 'detector', 'Detector information')
>>>
```

Here, we have taken the `File` instance `h5file` and invoked its `createGroup` method (see 4.3.2), telling that we want to create a new group called *detector* hanging from `"/"`, which is other way to refer to the `h5file.root` object we mentioned before. This will create a new `Group` (see 4.4) instance that will be assigned to the `group` variable.

3.1.5 Creating a new table

Let's now create the `Table` (see 4.6) object hanging from the new created group. We do that by calling the `createTable` (see 4.3.2) method from the `h5file` object:

```
>>> table = h5file.createTable(group, 'readout', Particle(), "Readout example")
>>>
```

You can see how we asked to create the `Table` instance hanging from `group`, with name *'readout'*. As the record object we have passed an instance of `Particle`, the class that we have declared before, and finally we attach it a *"Readout example"* title. With all this information, a new `Table` instance is created and assigned to `table` variable.

Now, time to fill this table with some values. But first, we want to get a pointer to the record object in this table instance:

```
>>> particle = table.record
>>>
```

The `record` attribute of `table` points to the `Particle` instance used to create the table, and we assign it to the `particle` variable that will be used as a shortcut. This step is not really necessary, but helps to code legibility (and allows me to introduce the `record` attribute).

We can proceed right now to the filling process:

```
>>> for i in xrange(10):
...     # First, assign the values to the Particle record
...     particle.name = 'Particle: %6d' % (i)
...     particle.TDCcount = i % 256
...     particle.ADCcount = (i * 256) % (1 << 16)
...     particle.grid_i = i
...     particle.grid_j = 10 - i
...     particle.pressure = float(i*i)
...     particle.energy = float(particle.pressure ** 4)
...     particle.idnumber = i * (2 ** 34) # This exceeds long integer range
...     # Insert a new particle record
...     table.appendAsRecord(particle)
...
>>>
```

This code is quite easy to understand. The lines inside the loop just assigned values to the `particle` record object and then a call to the `appendAsRecord` (see 4.6.2) method of `table` instance is made to put this information in the table I/O buffer.

After we have filled all our data, we should flush the I/O buffer for the table if we want to consolidate all this data on disk. We do that by calling the `table.flush` method.

```
>>> table.flush()
>>>
```

3.1.6 Reading (and selecting) data in table

Ok. We have now our data on disk but to this data be useful we need to access it and select some values we are interested in and located at some specific columns. That's is easy to do:

```
>>> table = h5file.root.detector.readout
>>> pressure = [ x.pressure for x in table.readAsRecords()
...              if x.TDCcount > 3 and x.pressure < 50 ]
>>>
```

The first line is only to declare a convenient shortcut to the *readout* table which is a bit deeper on the object tree. As you can see, we have used the **natural naming** schema to access it. We could also have used the `h5file.getNode` method instead, and we certainly do that later on.

The last two lines are a Python comprehensive list. It loops on records returned by `table.readAsRecords()` (see 4.6.2) iterator that returns values until table data is exhausted. This records are filtered using the expression `x.TDCcount > 3 and x.pressure < 50`, and the `pressure` field for satisfying records is selected to form the final list that is assigned to `pressure` variable.

We could have used a normal `for` loop to do that, but I find comprehension syntax more compact and elegant (and faster to execute!).

Let's select the names for the same set of particles:

```
>>> names = [ x.name for x in table.readAsRecords()
...           if x.TDCcount > 3 and x.pressure < 50 ]
>>>
```

Ok. that's enough for selections. Next section will show you how save these selections on file.

3.1.7 Creating new array objects

In order to separate the selected data from the detector data, we will create a new group, called `columns` hanging from the root group:

```
>>> gcolumns = h5file.createGroup(h5file.root, "columns", "Pressure and Name")
>>>
```

Note that this time we have specified the first parameter in a natural naming fashion (`h5file.root`) instead of using an absolute path string (`"/"`).

Now, create the Array objects on file:

```
>>> h5file.createArray(gcolumns, 'pressure', array(pressure),
...                   "Pressure column selection")
<tables.Array.Array object at 0x8217cac>
>>> h5file.createArray('/columns', 'name', array(names),
...                   "Name column selection")
<tables.Array.Array object at 0x814c3dc>
>>>
```

We already know the first two parameters of the `createArray` (see 4.3.2) methods (these are the same as the firsts in `createTable`): they are the parent group *where* Array will be created and the Array instance *name*. You can figure out that the fourth parameter is the *title*. And in the third position we have the `Numeric` object we want to save on disk. They are built from the selection lists we created before, and their `typecodes` are automatically selected by the `array()` constructor to store the list of values. In this case they are double-precision arrays, as we will see in short.

Note that `createArray` method returns an `Array` instance that is not assigned to any variable. Don't worry, this was intentional. The `Array` object has been attached to the object tree and saved in disk. Keep reading, in short I will show you how to retrieve it.

3.1.8 Closing the file and looking at its content

To finish this first tutorial, we use the `close` method of the `h5file` `File` instance to close the file before exiting Python:

```
>>> h5file.close()
>>> ^D
```

With all that, you have created your first `PyTables` file with a table and two arrays. That was easy, admit it. Now, you can have a look at it with some generic `HDF5` tool, like `h5dump` or `h5ls`. Here is the result of passing to `h5ls` the `tutorial1.h5` file:

```
$ h5ls -rd tutorial1.h5
/tutorial1.h5/columns      Group
/tutorial1.h5/columns/name Dataset {1}
  Data:
    (0) ["P","a","r","t","i","c","l","e",":"," "," "," "," "," "," "," "," "," ","4",
    (0)  "P","a","r","t","i","c","l","e",":"," "," "," "," "," "," "," "," "," ","5",
    (0)  "P","a","r","t","i","c","l","e",":"," "," "," "," "," "," "," "," "," ","6",
    (0)  "P","a","r","t","i","c","l","e",":"," "," "," "," "," "," "," "," "," ","7"]
/tutorial1.h5/columns/pressure Dataset {1}
  Data:
    (0) [16,25,36,49]
/tutorial1.h5/detector      Group
/tutorial1.h5/detector/readout Dataset {10/Inf}
  Data:
    (0) {0, 0, 0, 0, 10, 0, "Particle:      0", 0},
    (1) {256, 1, 1, 1, 9, 17179869184, "Particle:      1", 1},
    (2) {512, 2, 256, 2, 8, 34359738368, "Particle:      2", 4},
    (3) {768, 3, 6561, 3, 7, 51539607552, "Particle:      3", 9},
    (4) {1024, 4, 65536, 4, 6, 68719476736, "Particle:      4", 16},
    (5) {1280, 5, 390625, 5, 5, 85899345920, "Particle:      5", 25},
    (6) {1536, 6, 1679616, 6, 4, 103079215104, "Particle:      6", 36},
    (7) {1792, 7, 5764801, 7, 3, 120259084288, "Particle:      7", 49},
    (8) {2048, 8, 16777216, 8, 2, 137438953472, "Particle:      8", 64},
    (9) {2304, 9, 43046721, 9, 1, 154618822656, "Particle:      9", 81}
```

or, using the `"dumpFile.py"` `PyTables` utility (located in `examples/` directory):

```
Filename: tutorial1.h5
All objects:
Filename: tutorial1.h5 \\ Title: "Test file" \\ Format version: 1.0
/ (Group) "Test file"
/columns (Group) "Pressure and Name"
/columns/name Array(4, 16) "Name column selection"
/columns/pressure Array(4,) "Pressure column selection"
/detector (Group) "Detector information"
/detector/readout Table(8, 10) "Readout example"
```

You can pass the `-v` option to `dumpFile.py` if you want more verbosity. Try it!

3.2 Browsing the *object tree* and more

In this section, we will learn how to browse the tree while retrieving meta-information about the actual data, and will finish by appending some rows to the existing table to show how table objects can be enlarged.

In `examples/tutorial1-2.py` you will find the working version of all the code in this section. As before, you are encouraged to use a python shell and inspect the object tree during the voyage.

3.2.1 Traversing the object tree

First of all, let's open the file we have recently created in last tutorial section, as we will take it as a basis for this section:

```
>>> h5file = openFile("tutorial1.h5", "a")
```

This time, we have opened the file in "a"ppend mode. We are using this mode because we want to add more information to the file.

PyTables, following the Python tradition, offers powerful introspection capabilities, i.e. you can easily ask information about any component of the object tree as well as traverse the tree searching for something.

To start with, you can get a first glance image of the object tree, by simply printing the existing File instance:

```
>>> print h5file
Filename: tutorial1.h5 \\ Title: "Test file" \\ Format version: 1.0
/ (Group) "Test file"
/columns (Group) "Pressure and Name"
/columns/name Array(4, 16) "Name column selection"
/columns/pressure Array(4,) "Pressure column selection"
/detector (Group) "Detector information"
/detector/readout Table(8, 10) "Readout example"
>>>
```

That's right, it seems that all our objects are there. We can use the `walkGroups` method (see 4.3.2) of File class to list all the groups on tree:

```
>>> for group in h5file.walkGroups("/"):
...     print group
...
/ (Group) "Test file"
/columns (Group) "Pressure and Name"
/detector (Group) "Detector information"
>>>
```

Note that `walkGroups` actually returns an *iterator*, not a list of objects. And combining it with the `listNodes` method, we can do very powerful things. Let's see an example listing all the arrays in the tree:

```
>>> for group in h5file.walkGroups("/"):
...     for array in h5file.listNodes(group, classname = 'Array'):
...         print array
...
/columns/name Array(4, 16) "Name column selection"
/columns/pressure Array(4,) "Pressure column selection"
>>>
```

`listNodes` (see 4.3.2) lists all the nodes hanging from a group, and if `classname` keyword is specified, the method will filter all instances which are not descendants of it. We have specified it so as to return only the Array instances.

Caveat emptor: `listNodes` (conversely to `walkGroups`) returns an actual list, not an iterator!

As a final example, we will list all the Leaf (i.e. Table and Array instances, see 4.5 for detailed information on leaf class) objects in `/detector` group. Check that only one instance of Table class will be selected in this group (as it should be):

```
>>> for table in h5file.listNodes("/detector", 'Leaf'):
...     print table
...
/detector/readout Table(8, 10) "Readout example"
>>>
```

Of course you can do more sophisticated node selections using these two powerful functions, but first, we need to learn a bit about some important instance variables of PyTables objects.

3.2.2 Getting object metadata

Each object in PyTables has metadata about the actual data on the file. Normally this meta-information is accessible through the node instance variables. Let's see some examples:

```
>>> table = h5file.root.detector.readout
>>> print "Object:", table
Object: /detector/readout Table(8, 10) "Readout example"
>>> print "Table name:", table.name
Table name: readout
>>> print "Table title:", table.title
Table title: Readout example
>>> print "Number of rows in table: %d" % (table.nrows)
Number of rows in table: 10
>>> print "Table variable names (sorted alphanumerically) with their type:"
Table variable names (sorted alphanumerically) with their type:
>>> for i in range(len(table.varnames)):
...     print " ", table.varnames[i], ' := ', table.vartypes[i]
...
ADCcount := H
TDCcount := B
energy := d
grid_i := i
grid_j := i
idnumber := Q
name := 16s
pressure := f
>>>
```

Here, the `name`, `title`, `nrows`, `varnames` and `vartypes` attributes (see 4.3.1 for a complete attribute list) of Table object give us quite a lot of information about actual table data.

Observe how we have used the `getNode` method of File class to access a node in the tree, as well as the natural naming method. Both are useful, and depending on the context you will prefer to use one or another. `getNode` has the advantage that it can get a node from the pathname string (like in this example), and you can force that the node in that location has to be a *classname* instance. However, natural naming is more elegant and quicker to specify (specially if you are using the name completion capability present in interactive console).

Now, print some metadata in `/columns/pressure` Array object:

```
>>> pressureObject = h5file.getNode("/columns", "pressure")
>>> print "Info on the object:", pressureObject
Info on the object: /columns/pressure Array(4,) "Pressure column selection"
>>> print " shape: ==>", pressureObject.shape
shape: ==> (4,)
>>> print " title: ==>", pressureObject.title
title: ==> Pressure column selection
>>> print " typecode ==>", pressureObject.typecode
typecode ==> d
>>>
```

If you look at the `typecode` attribute of the `pressureObject`, you can certify that this is a "double" Numeric array, and that by looking at their `shape` attribute the array on disk is unidimensional and has 4 elements. See 4.7.1 for the complete Array attribute list.

3.2.3 Reading actual data from Array objects

Once you have found the desired Array and decided that you want to retrieve the actual Numeric array from it, you should use the `read` method of the Array object:

```
>>> pressureArray = pressureObject.read()
>>> nameArray = h5file.root.columns.name.read()
>>> print "pressureArray is object of type:", type(pressureArray)
pressureArray is object of type: <type 'array'>
>>> print "nameArray is object of type:", type(nameArray)
nameArray is object of type: <type 'array'>
>>> print "Data on arrays nameArray and pressureArray:"
Data on arrays nameArray and pressureArray:
>>> for i in range(pressureObject.shape[0]):
...     print "".join(nameArray[i]), "-->", pressureArray[i]
...
Particle:      4 --> 16.0
Particle:      5 --> 25.0
Particle:      6 --> 36.0
Particle:      7 --> 49.0
>>>
```

You can verify that `read` method (see 4.7.2) returns an authentic Numeric array looking at the output of the `type()` call. Check also that `nameArray` is actually a 2-dimensional Numeric array. This is because Numeric does not support arrays of strings, and these are represented as arrays of characters plus one dimension (that of the string dimension). This is why we have used the standard `join` method to glue the characters on this extra dimension and get the original arrays.

3.2.4 Appending data to an existing table

To finish this section, let's have a look at how we can add records to an existing on-disk table. Let's use our well-known *readout* Table instance and let's append some new values to it:

```
>>> table = h5file.root.detector.readout
>>> particle = table.record
>>> for i in xrange(10, 15):
...     particle.name = 'Particle: %6d' % (i)
...     particle.TDCcount = i % 256
...     particle.ADCcount = (i * 256) % (1 << 16)
...     particle.grid_i = i
...     particle.grid_j = 10 - i
...     particle.pressure = float(i*i)
...     particle.energy = float(particle.pressure ** 4)
...     particle.idnumber = i * (2 ** 34) # This exceeds long integer range
...     table.appendAsRecord(particle)
...
>>> table.flush()
>>>
```

That works exactly in the same way than filling a new table. PyTables knows that this table is on disk, and when you add new records, they are appended to the end of the table².

If you look carefully at the code you will see that we have used the `table.record` attribute to access to a `Particle` instance and that way we could use it to fill new values. However, it should be stressed that it

² Note that you can only append values to tables, not array objects. However, I plan to support unlimited dimension arrays in short term. Keep tuned.

is not necessary to have the original class definition (`Particle`) in our code to re-create it (in fact, we don't even declared it in our current python session!): it will be created only from metadata existing on file, and it behaves exactly as an original `Particle` instance!.

This is part of the magic that allow the use of *metaclasses* in PyTables, and that will easy the creation of portable applications that can read any PyTables file **regardless** of having access to the original Python record class definition.

Let's have a look at some columns of the resulting table:

```
>>> for x in table.readAsRecords():
...     print "%-16s | %11.1f | %11.4g | %6d | %6d | %8d |" % \
...         (x.name, x.pressure, x.energy, x.grid_i, x.grid_j,
...         x.TDCcount)
...
Particle:      0 |          0.0 |          0 |      0 |      0 |      10 |
Particle:      1 |          1.0 |          1 |      1 |      1 |       9 |
Particle:      2 |          4.0 |        256 |      2 |      8 |       2 |
Particle:      3 |          9.0 |       6561 |      3 |      7 |       3 |
Particle:      4 |         16.0 |    6.554e+04 |      4 |      6 |       4 |
Particle:      5 |         25.0 |    3.906e+05 |      5 |      5 |       5 |
Particle:      6 |         36.0 |    1.68e+06 |      6 |      4 |       6 |
Particle:      7 |         49.0 |    5.765e+06 |      7 |      3 |       7 |
Particle:      8 |         64.0 |    1.678e+07 |      8 |      2 |       8 |
Particle:      9 |         81.0 |    4.305e+07 |      9 |      1 |       9 |
Particle:     10 |        100.0 |    1e+08 |     10 |      0 |      10 |
Particle:     11 |        121.0 |    2.144e+08 |     11 |     -1 |      11 |
Particle:     12 |        144.0 |    4.3e+08 |     12 |     -2 |      12 |
Particle:     13 |        169.0 |    8.157e+08 |     13 |     -3 |      13 |
Particle:     14 |        196.0 |    1.476e+09 |     14 |     -4 |      14 |
>>> print
>>> print "Total numbers of entries after appending new rows:", table.nrows
Total numbers of entries after appending new rows: 15
>>>
```

In figure 3.1 you can see a view of the PyTables file we have created.

We are near the end of this first tutorial. Ei!, do not forget to close the file after you finish all the work:

```
>>> h5file.close()
>>> ^D
$
```

3.3 PyTables automatic sanity checks

Now, time for a more real life example (i.e. with errors in code). Here, we will create a couple of directories (groups, in HDF5 jargon) hanging directly from `root` called `Particles` and `Events`. Then, we will put 3 tables in each group; in `Particles` we will put instances of `Particle` records and in `Events`, instances of `Event`.

After that, we will feed the tables with 257 (you will see soon why I choose such an *esoteric* number) entries each. Finally, we will read the recently created table `/Events/TEvent3` and select some values from it using a comprehension list.

Look at the next script. It seems to do all of that, but a couple of small bugs will be shown up. Note that this `Particle` class is not directly related with the one defined in last example; this is simpler.

```
from tables import *
class Particle(IsRecord):
```

	ADCcount	TDCcount	energy	grid_i	grid_j	idnumber	name	pressure
1	0	0	0.0	0	10	0	Particle: ...	0.0
2	256	1	1.0	1	9	1717986...	Particle: ...	1.0
3	512	2	256.0	2	8	3435973...	Particle: ...	4.0
4	768	3	6561.0	3	7	5153960...	Particle: ...	9.0
5	1024	4	65536.0	4	6	6871947...	Particle: ...	16.0
6	1280	5	390625.0	5	5	8589934...	Particle: ...	25.0
7	1536	6	1679616.0	6	4	1030792...	Particle: ...	36.0
8	1792	7	5764801.0	7	3	1202590...	Particle: ...	49.0
9	2048	8	1.677721...	8	2	1374389...	Particle: ...	64.0
10	2304	9	4.304672...	9	1	1546188...	Particle: ...	81.0
11	2560	10	1.0E8	10	0	1717986...	Particle: ...	100.0
12	2816	11	2.143588...	11	-1	1889785...	Particle: ...	121.0
13	3072	12	4.299816...	12	-2	2061584...	Particle: ...	144.0
14	3328	13	8.157307...	13	-3	2233382...	Particle: ...	169.0
15	3584	14	1.475789...	14	-4	2405181...	Particle: ...	196.0

Figure 3.1: The data file after appending some rows.

```

name          = '16s'  # 16-character String
lati          = 'i'    # integer
longi         = 'i'    # integer
pressure      = 'f'    # float (single-precision)
temperature   = 'd'    # double (double-precision)
class Event(IsRecord):
    name        = '16s'  # 16-character String
    TDCcount    = 'B'    # unsigned char
    ADCcount    = 'H'    # unsigned short
    xcoord      = 'f'    # float (single-precision)
    ycoord      = 'f'    # float (single-precision)
# Open a file in "w"rite mode
fileh = openFile("tutorial2.h5", mode = "w")
# Get the HDF5 root group
root = fileh.root
# Create the groups:
for groupname in ("Particles", "Events"):
    group = fileh.createGroup(root, groupname)
# Now, create and fill the tables in Particles group
gparticles = root.Particles
# Create 3 new tables
for tablename in ("TParticle1", "TParticle2", "TParticle3"):
    # Create a table
    table = fileh.createTable("/Particles", tablename, Particle(),
                              "Particles: "+tablename)
    # Get the record object associated with the table:
    particle = table.record
    # Fill the table with 10 particles
    for i in xrange(257):
        # First, assign the values to the Particle record

```

```

        particle.name = 'Particle: %6d' % (i)
        particle.lati = i
        particle.longi = 10 - i
        particle.pressure = float(i*i)
        particle.temperature = float(i**2)
        # This injects the Record values
        table.appendAsRecord(particle)
    # Flush the table buffers
    table.flush()
# Now, go for Events:
for tablename in ("TEvent1", "TEvent2", "TEvent3"):
    # Create a table in Events group
    table = fileh.createTable(root.Events, tablename, Event(),
                             "Events: "+tablename)
    # Get the record object associated with the table:
    event = table.record
    # Fill the table with 257 events
    for i in xrange(257):
        # First, assign the values to the Event record
        event.name = 'Event: %6d' % (i)
        event.TDCcount = i
        event.ADCcount = i * 2
        event.xcoor = float(i**2)
        event.ycoord = float(i**4)
        # This injects the Record values
        table.appendAsRecord(event)
    # Flush the buffers
    table.flush()
# Read the records from table "/Events/TEvent3" and select some
table = root.Events.TEvent3
e = [ p.TDCcount for p in table.readAsRecords()
      if p.ADCcount < 20 and 4 <= p.TDCcount < 15 ]
print "Last record ==>", p
print "Selected values ==>", e
print "Total selected records ==> ", len(e)
# Finally, close the file
fileh.close()

```

3.3.1 Field name checking

If you have read the code carefully it looks pretty good, but it won't work. When you run this example, you will get the next error:

```

Traceback (most recent call last):
  File "tutorial2.py", line 68, in ?
    event.xcoor = float(i**2)
AttributeError: 'Event' object has no attribute 'xcoor'

```

This error is telling us that we tried to assign a value to a non-existent field in an Event object. By looking carefully at the Event attributes, we see that we misspelled the xcoord field (we wrote xcoor instead). This is very unusual in Python because if you try to assign a value to a non-existent instance variable, a new one is created with that name. Such a feature is not satisfactory when we are dealing with an object that has fixed list of variable names (the user record, that is responsible for defining the table columns). So, thanks to the

magic that provides the `IsRecord` metaclass, all instance variables (data fields) are declared internally as class `__slots__`. This is why the last error appeared.

3.3.2 Data range checking

After correcting the last attribute error in the source, and running the script again... oooops! we find another problem:

```
Traceback (most recent call last):
  File "tutorial2.py", line 69, in ?
    table.appendAsRecord(event)
  File "/usr/lib/python2.2/site-packages/tables/Table.py", line 210, in
appendAsRecord
    self._v_packedtuples.append(recordObject._f_pack2())
  File "/usr/lib/python2.2/site-packages/tables/IsRecord.py", line 121, in
_f_pack2
    self._f_raiseValueError()
  File "/usr/lib/python2.2/site-packages/tables/IsRecord.py", line 130, in
_f_raiseValueError
    raise ValueError, \
ValueError: Error packing record object:
[(('ADCcount', 'H', 256), ('TDCcount', 'B', 256), ('name', '16s', 'Event: 256'),
('xcoord', 'f', 65536.0), ('ycoord', 'f', 4294967296.0))]
Error was: ubyte format requires 0<=number<=255
```

This time the exception is telling us that one of the records is having trouble to be converted to the data types stated in the `Event` class definition. By looking carefully at the record object causing the problem, we see that we are trying to assign a value of 256 to the `TDCcount` field which has a `'B'` (C unsigned char) typecode and the allowed range for it is `0<=TDCcount<=255`. This is a very powerful capability to automatically check for ranges and the message error should be explicit enough to figure out what is happening. In this case you can solve the problem either by promoting the `TDCcount` to `'H'` which is an unsigned 16-bit integer, or, by avoiding the mistake we have probably made in assigning a value greater than 255 to a `'B'` typecode.

If we change the line:

```
event.TDCcount = i
```

by the next one:

```
event.TDCcount = i % (1<<8)
```

you will see that our problem has disappeared, and that the HDF5 file has been created.

3.3.3 Data type checking

Finally, in order to test the type checking, we will change the next line:

```
event.ADCcount = i * 2          # Correct type
```

to read:

```
event.ADCcount = "s"           # Wrong type
```

After this modification, the next exception will be raised when the script is executed:

```
Traceback (most recent call last):
  File "tutorial2.py", line 68, in ?
    table.appendAsRecord(event)
```

	ADCcount	TDCcount	name	xcoord	ycoord
241	480	240	Event: 240	57600.0	3.31776E9
242	482	241	Event: 241	58081.0	3.373402...
243	484	242	Event: 242	58564.0	3.429742...
244	486	243	Event: 243	59049.0	3.486784...
245	488	244	Event: 244	59536.0	3.544535...
246	490	245	Event: 245	60025.0	3.603000...
247	492	246	Event: 246	60516.0	3.662186...
248	494	247	Event: 247	61009.0	3.722098...
249	496	248	Event: 248	61504.0	3.782742...
250	498	249	Event: 249	62001.0	3.844123...
251	500	250	Event: 250	62500.0	3.906249...
252	502	251	Event: 251	63001.0	3.969125...
253	504	252	Event: 252	63504.0	4.032758...
254	506	253	Event: 253	64009.0	4.097152...
255	508	254	Event: 254	64516.0	4.162314...
256	510	255	Event: 255	65025.0	4.228250...
257	512	0	Event: 256	65536.0	4.294967...

Figure 3.2: Table hierarchy for second example.

```

File "/home/faltd/PyTables/pytables-0.2/tables/Table.py", line 279,
in appendAsRecord
    self._v_packedtuples.append(RecordObject._f_pack2())
File "/home/faltd/PyTables/pytables-0.2/tables/IsRecord.py", line
181, in _f_pack2
    self._f_raiseValueError()
File "/home/faltd/PyTables/pytables-0.2/tables/IsRecord.py", line
135, in _f_raiseValueError
    raise ValueError, \
ValueError: Error packing record object:
[('ADCcount', 'H', '0'), ('TDCcount', 'B', 0), ('name', '16s',
'Event:      0'), ('xcoord', 'f', 0.0), ('ycoord', 'f', 0.0)]
Error was: required argument is not an integer

```

that states the error.

You can admire the structure we have created with this (corrected) script in figure 3.2. As before, you will find this example in source file `tutorial2.py` that is located in the directory `examples`.

Feel free to visit the rest of examples in directory `examples`, and try to understand them. I've tried to make several use cases to give you an idea of the PyTables capabilities and its way of dealing with HDF5 objects.

3.4 Optimization tips

PyTables has several places where the user can improve the performance of his application. If you are planning to deal with really large data, you should read carefully this section so as to learn how to get an

important boost for your code. But if your dataset is small or medium size (say, up to 1 MB), you should not worry about that as the default parameters in `PyTables` are already tuned to handle that perfectly.

3.4.1 Compression issues

One of the beauties of `PyTables` is that it comes with compression activated by **default** for tables. This might be a bit controversial feature, because compression has a legend of being a very CPU time resources consumer (but if you are completely against compression, you can disable it; keep reading).

However, there is an usual scenario where users need to save duplicated data in some record fields, while the others have varying values. In a relational database approach such a redundant data can normally be moved to other tables and a relationship between the rows on the separate tables can be created. But that takes analysis and implementation time, and made the underlying libraries more complex and slower.

`PyTables` approach is to not support relationships between tables, but to compress duplicated data in tables. That allows the user to not worry about finding their optimum data tables strategy, but rather use less, not directly related, tables with a larger number of columns while still not cluttering the database too much with duplicated data (compression is responsible to avoid that). As a side effect, data selections can be made more easily because you have more fields available in a single table, and they can be referred in the same loop (or comprehension list).

The compression library used is the **zlib** (see reference 6), and the compression level used by default for `Table` objects is 3. This level is less than 6 which is the default level recommend in `zlib` documentation as a compromise between speed and compression. I've made this decision for two reasons:

- Choosing level 3 is a more conservative (in terms of CPU usage) value. This fact together with the generally available fast CPU today, can make a better balance between CPU usage and I/O performance. It would be even possible in certain situations that reading a compressed table would take less wall-clock time than not using compression at all.
- Normally (except in some degenerate cases), table columns values are stored very closely in memory (i.e. they have a high degree of locality), so the compression algorithm has to make little effort to discover data duplication (as the majority of this duplication would appear in values of the same column). So a small compression level should offer roughly the same results as a big one.

Nonetheless, in some situations you may want to check how compression level affects your application. You can control it by setting the `compress` keyword in the `createTable` method (see 4.3.2). A value of 0 will completely disable compression, 1 is the less CPU time demanding level, while 9 is the maximum level and most CPU intensive.

3.4.2 Informing `PyTables` about expected number of rows in tables

The underlying `HDF5` library that is used by `PyTables` takes the data in bunches of a certain length, so-called *chunks*, to write them on disk as a whole, i.e. the `HDF5` library treats chunks as atomic objects and disk I/O is always made in terms of complete chunks. This allows data filters to be defined by the application to perform tasks such as compression, encryption, checksumming, etc. on entire chunks.

An in-memory B-tree is used to map chunk structures on disk. The more chunks that are allocated for a dataset the larger the B-tree. Large B-trees take memory and causes file storage overhead as well as more disk I/O and higher contention for the meta data cache. Consequently, it's important to balance between memory and I/O overhead (small B-trees) and time to access to data (big B-trees).

`PyTables` can determine an optimum chunk size to make B-trees adequate to your dataset size if you help it by providing an estimation of the number of rows for a table. This must be made in table creation time by passing this value in the `expectedrows` keyword of `createTable` method (see 4.3.2).

When your dataset size is bigger than 1 MB (take this figure only as a reference, not strictly), by providing this guess of the number of rows, you will be optimizing the access to your table data. When the dataset size is larger than, say 100MB, you are **strongly** suggested to provide such a guess; failing to do that may cause your application doing very slow I/O operations and demanding huge amounts of memory. You have been warned!.

3.4.3 Optimized ways to fill and read data from tables

The `appendAsRecord` and `readAsRecords` methods in `Table` class are very convenient to use when you are dealing with small to medium size tables. They are safe and intuitive, **but** they are slow. When you have to deal with large tables, you can use the alternate methods `appendAsValues`, `appendAsTuple` and `readAsTuples`. Look at sections 4.6.2, 4.6.2 and 4.6.2 for a detailed reference of these optimized methods.

These three new methods are different to the two formers in that they accept or return the values to/from rows in table as Python tuples (or independent values in the case of `appendAsValues`). They are much faster (at least a factor two or even more) than `xxxxAsRecord` counterparts, but they are also unsafer, because it is your responsibility to pass the correct order of parameters to be appended to the table (or guess the correct order of fields in tuple when reading). This field order is however well defined as the result of alphanumerically sorting the names of table fields (or columns).

For example, if you have a table with three fields named *"TDCcount"*, *"ADCcount"* and *"energy"*, you have to feed `appendAsValues` with a series of parameters like in:

```
table.appendAsValues(ADCcountValue, TDCcountValue, energyValue)
```

For `readAsTuple` method you have to follow the same rule, i.e. you must unpack the values in the returned tuple in alphanumerical order, like in:

```
(ADCcountValue, TDCcountValue, energyValue) = table.readAsTuple()
```

For a working example that also allows you to do some timings easily, look at the *examples/table-bench.py* script.

Chapter 4

Library Reference

PyTables implements several classes to represent the different nodes in the object tree. They are named `File`, `Group`, `Leaf`, `Table` and `Array`. Another one is responsible to build record objects from a subclass user declaration, and performs field, type and range checks; its name is `IsRecord`. An important function, called `openFile` is responsible to create, open or append to files. In addition, a few utility functions are defined to guess if an user supplied file is a PyTables or HDF5 file. These are called `isPyTablesFile` and `isHDF5`. Finally, several first-level variables are also available to the user that informs about PyTables version, file format version or underlying libraries (as for example HDF5) version number.

Let's start discussing the first-level variables and functions available to the user, then the methods in the classes defined in `PyTables`.

4.1 tables variables and functions

4.1.1 Global variables

__version__ The PyTables version number.

HDF5Version The underlying HDF5 library version number.

ExtVersion The Pyrex extension types version. This might be useful when reporting bugs.

4.1.2 Global functions

openFile(filename, mode='r', title='') Open a PyTables file and returns a `File` object.

filename The name of the file (supports environment variable expansion). It must have any of `".h5"`, `".hdf"` or `".hdf5"` extensions.

mode The mode to open the file. It can be one of the following:

'r' read-only; no data can be modified.

'w' write; a new file is created (an existing file with the same name is deleted).

'a' append; an existing file is opened for reading and writing, and if the file does not exist it is created.

'r+' is similar to `'a'`, but the file must already exist.

title If filename is new, this will set a title for the root group in this file. If filename is not new, the title will be read from disk, and this will not have any effect.

isHDF5(filename) Determines whether filename is in the HDF5 format. When successful, returns a positive value, for `TRUE`, or 0 (zero), for `FALSE`. Otherwise returns a negative value. To this function to work, it needs a closed file.

isPyTablesFile(filename) Determines whether a file is in the `PyTables` format. When successful, returns the format version string, for `TRUE`, or 0 (zero), for `FALSE`. Otherwise returns a negative value. To this function to work, it needs a closed file.

4.2 The `IsRecord` class

This class is in fact a so-called *metaclass* object. There is nothing special on this fact, except that their subclasses attributes are transformed during its instantiation phase, and new methods for instances are defined based on the values of the class attributes.

That way, `PyTables` *force* the resulting instance to only accept assignments on the declared attributes¹. If you try to do an assignment to a non-declared attribute, `PyTables` will raise an error.

To define such a special class, you have to declare it as descendent from `IsRecord`, with many attributes as fields you want in your record. To declare their types, you simply assign to these attributes their *typecode*. See the appendix A for a relation of data types supported in a `IsRecord` class declaration.

That's all, from now on, you can instantiate objects from your new class and use them as a very flexible record objects with safe features like automatic name field, data type and range checks (see the section 3.3 for an example on how it works).

4.3 The `File` class

This class is returned when a `PyTables` is opened with the `openFile` function. It has methods to create, open, flush and close `PyTables` files. Also, `File` class offer methods to traverse the object tree, as well as to create new nodes. One of its attributes (`root`) is quite important because represents the entry point to the object tree attached to the file.

Next, we will discuss the attributes and methods for `File` class².

4.3.1 `File` instance variables

filename Filename opened.

mode Mode in which the filename was opened.

title The title of the root group in file.

root The root group in file. This is the entry point to the object tree.

4.3.2 `File` methods

createGroup(where, name, title='') Create a new `Group` instance with name *name* in *where* location.

where The parent group where the new group will hang. *where* parameter can be a path string (for example `"/Particles/TParticle1"`), or another `Group` instance.

name The name of the new group.

title A description for this group.

createTable(where, name, RecordObject, title='', compress=3, expectedrows=10000) Create a new `Table` instance with name *name* in *where* location.

where The parent group where the new table will hang. *where* parameter can be a path string (for example `"/Particles/TParticle1"`), or `Group` instance.

¹ In fact, descendants of `IsRecord` class has a few more, internal attributes, but they start with prefixes like `"__"`, `"_v_"` or `"_f_"`, so you should not use attribute names starting with these prefixes

² On the following, the term *Leaf* will refer to a `Table` or `Array` node object.

name The name of the new table.

RecordObject An instance of a user-defined class (derived from the `IsRecord` class) where table fields are defined.

title A description for this object.

compress Specifies a compress level for data. The allowed range is 0-9. A value of 0 disables compression. The default is compression level 3, that balances between compression effort and CPU consumption.

expectedrows An user estimate of the number of records that will be on table. If not provided, the default value is appropriate for tables until 1 MB in size (more or less, depending on the record size). If you plan to save bigger tables you should provide a guess; this will optimize the HDF5 B-Tree creation and management process time and memory used. See section 3.4.2 for a detailed justification of that issue.

createArray(where, name, NumericObject, title='') Create a new Array instance with name *name* in *where* location.

where The parent group where the new array will hang. *where* parameter can be a path string (for example `"/Particles/TParticle1"`), or Group instance.

name The name of the new array.

NumericObject The Numeric array to be saved.

title A description for this object.

getNode(where, name='', classname='') Returns the object node *name* under *where* location

where Can be a path string or Group instance. If *where* doesn't exist or has not a child called *name*, a `ValueError` error is raised.

name The object name desired. If *name* is a null string (''), or not supplied, this method assumes to find the object in *where*.

classname If supplied, returns only an instance of this class name. Allowed names in *classname* are: `'Group'`, `'Leaf'`, `'Table'` and `'Array'`. Note that these values are strings.

listNodes(where, classname='') Returns a list with all the object nodes (Group or Leaf) hanging from *where*. The list is alphanumerically sorted by node name.

where The parent group. Can be a path string or Group instance.

classname If a *classname* parameter is supplied, the iterator will return only instances of this class (or subclasses of it). The only supported classes in *classname* are `'Group'`, `'Leaf'`, `'Table'` and `'Array'`. Note that these values are strings.

walkGroups(where='') Iterator that recursively obtains groups (not leaves) hanging from *where*. If *where* is not supplied, the root object is taken as origin. The groups are returned from in a top to bottom order, and alphanumerically sorted when they are at the same level.

where The origin group. Can be a path string or Group instance.

flush() Flush all the leaves existing in the object tree.

close() Flush all the objects in object tree and close the file.

4.4 The Group class

Instances of this class are a grouping structure containing instances of zero or more groups or leaves, together with supporting metadata.

Working with groups and leaves is similar in many ways to working with directories and files, respectively, in a Unix filesystem. As with Unix directories and files, objects in the object tree are often described by giving their full (or absolute) path names. This full path can be specified either as string (like in `'/group1/group2'`) or as a complete object path written in the Pythonic fashion known as *natural name* schema (like in `file.root.group1.group2`) and discussed in the section 1.2.

A collateral effect of the *natural naming* schema is that you must be aware when assigning a new attribute to a Group object to not collide with existing children node names. For this reason and to not pollute the children namespace, it is explicitly forbidden to assign "normal" attributes to Group instances, and the only ones allowed must start with `"_c_"` (for class variables), `"_f_"` (for methods) or `"_v_"` (for instance variables) prefixes. Any attempt to assign a new attribute that does not starts with these prefixes, will raise a `NameError` exception.

4.4.1 Group class variables

`_c_objects` Dictionary with all objects (groups or leaves) on tree.

`_c_objgroups` Dictionary with all object groups on tree.

`_c_objleaves` Dictionary with all object leaves on tree.

4.4.2 Group instance variables

`_v_title` A description for this group.

`_v_name` The name of this group.

`_v_pathname` A string representation of the group location in tree.

`_v_parent` The parent Group instance.

`_v_objchilds` Dictionary with all nodes (groups or leaves) hanging from this instance.

`_v_objgroups` Dictionary with all node groups hanging from this instance.

`_v_objleaves` Dictionary with all node leaves hanging from this instance.

4.4.3 Group methods

Caveat: These methods are documented for completeness, and they can be used without any problem. However, you should use the high-level counterpart methods in the `File` class, because these are most used in documentation and examples, and are a bit more powerful than those exposed here.

`_f_join(name)` Helper method to correctly concatenate a name child object with the pathname of this group.

`_f_listNodes(classname='')` Returns a *list* with all the object nodes hanging from this instance. The list is alphanumerically sorted by node name. If a *classname* parameter is supplied, it will only return instances of this class (or subclasses of it). The supported classes in *classname* are `'Group'`, `'Leaf'`, `'Table'` and `'Array'`.

`_f_walkGroups()` *Iterator* that recursively obtains Groups (not Leaves) hanging from self. The groups are returned from top to bottom, and are alphanumerically sorted when they are at the same level.

4.5 The Leaf class

This is a helper class useful to place common functionality of all Leaf objects. It is also useful for classifying purposes. A Leaf object is an end-node, that is, a node that can hang directly from a group object, but that is not a group itself. Right now this set is composed by Table and Array objects. In fact, Table and Array classes inherit functionality from this class using the *mix-in* technique.

Normally the user will not need to call any method from here, but it is useful to know that it exists because it can be used as a filter in methods like `File.GetNode()` or `File.listNodes()`, against others.

4.6 The Table class

Instances of this class represents table objects in the object tree. It provides methods to create new tables or open existing ones, as well as methods to read/write data and metadata from/to table objects in the file.

Data can be read or written both as records or as tuples and *different* methods are provided to that end. Records are recommended because they are more intuitive and less error prone although they are slow. Using tuples (or value sequences) is faster, but the user must be very careful because when passing the sequence of values, they have to be in the correct order (alphanumerically ordered by field names). If not, unexpected results can appear (most probably `ValueError` exceptions will be raised). See section 3.4.3 for usage details.

4.6.1 Table instance variables

name The node name.

title The title for this node.

record The record object for this table.

nrows The number of rows (records) in this table.

varnames The field names for the table.

vartypes The typecodes for the table fields.

4.6.2 Table methods

appendAsRecord(RecordObject) Append the `RecordObject` to the output buffer of the table instance.

RecordObject An instance of the user-defined record class. It has to be a `IsRecord` descendant instance. If it is not, a `ValueError` exception is raised.

appendAsTuple(tupleValues) Append the *tupleValues* tuple to the output buffer of the table instance. This method is faster (but also unsafer, because requires user to introduce the values in correct order!) than `appendAsRecord` method.

tupleValues is a tuple that has values for all the user record fields. The user has to provide them in the order determined by alphanumerically sorting the record name fields.

appendAsValues(*values) Append the *values* parameters to the table output buffer. This method is faster (and unsafer, because requires user to introduce the values in correct order) than `appendAsRecord` method. It is similar to the `appendAsTuple` method, but accepts separate parameters as values instead of a monolithic tuple.

values Is a series of parameters that provides values for all the user record fields. The user has to provide them in the order determined by alphanumerically sorting the record fields.

readAsRecords() Returns an iterator yielding record instances built from rows in table. This method is a *generator*, i.e. it keeps track on the last record returned so that next time it is invoked it returns the next available record. It is slower than `readAsTuples` but in exchange, it returns full-fledged instance records.

readAsTuples() Returns an iterator yielding tuples built from rows in table. This method is a *generator*, i.e. it keeps track on the last record returned so that next time it is invoked it returns the next available record. This method is twice as faster than `readAsRecords`, but it yields the rows as (alphanumerically ordered) tuples, instead of full-fledged instance records.

flush() Flush the table buffers.

close() Flush the table buffers and close the HDF5 dataset.

4.7 The Array class

Represents a `Numeric` array on file. It provides methods to create new arrays or open existing ones, as well as methods to write/read data and metadata to/from array objects in the file.

Caveat: All `Numeric` typecodes are supported except "F" and "D" which corresponds to complex data types³. See reference 12 to know more about the `Numerical Python` package, and in particular about supported data types.

4.7.1 Array instance variables

name The node name.

title The node title.

shape tuple with the array shape (in the `Numeric` style).

typecode The typecode of the represented array.

4.7.2 Array methods

The methods for this class are very few. Please note that this object has not internal I/O buffers, so there is no need to call `flush()` method. However, it is included for consistency with `Leaf` nodes.

read() Read the array from disk and return it as a `Numeric` object. Note that while this method is not called, the actual array data is resident on disk.

flush() Flush the internal buffers. Remember: this is a do-nothing method.

close() Close the array on file.

³ However, these might be included in short future

Appendix A

Supported data types in tables

`IsRecord` descendants supports a limited set of data types to define the table fields. This is roughly the same that the set supported by the `array` module in Python, with some additions that will be briefly discussed shortly. The supported set is listed on table A.

The additions to the `array` module typecodes are the `'q'`, `'Q'` and `'s'`. The `'q'` and `'Q'` conversion codes are available in native mode only if the platform C compiler supports C long long, or, on Windows, `__int64`. They are always available in standard modes. The `'s'` typecode can be preceded by an integer to indicate the maximum length of the string, so `'16s'` represents a 16-byte string.

Also note that when the `'I'` and `'L'` codetypes are used in records, Python uses internally `Long` integers to represent them, that can (or cannot, depending on what you are trying to do) be a source of inefficiency in your code.

Type Code	Description	C Type	Size (in bytes)	Python Counterpart
<code>'c'</code>	8-bit character	<code>char</code>	1	String of length 1
<code>'b'</code>	8-bit integer	<code>signed char</code>	1	Integer
<code>'B'</code>	8-bit unsigned integer	<code>unsigned char</code>	1	Integer
<code>'h'</code>	16-bit integer	<code>short</code>	2	Integer
<code>'H'</code>	16-bit unsigned integer	<code>unsigned short</code>	2	Integer
<code>'i'</code>	integer	<code>int</code>	4 or 8	Integer
<code>'I'</code>	unsigned integer	<code>unsigned int</code>	4 or 8	Long
<code>'l'</code>	long integer	<code>long</code>	4 or 8	Integer
<code>'L'</code>	unsigned long integer	<code>unsigned long</code>	4 or 8	Long
<code>'q'</code>	long long integer	<code>long long</code>	8	Long
<code>'Q'</code>	unsigned long long integer	<code>unsigned long long</code>	8	Long
<code>'f'</code>	single-precision float	<code>float</code>	4	Float
<code>'d'</code>	double-precision float	<code>double</code>	8	Float
<code>'s'</code>	arbitrary length string	<code>char[]</code>	*	String

Table A.1: Data types supported by `IsRecord` descendants.

Bibliography

1. *What is HDF5?*. Concise description about HDF5 capabilities and its differences from earlier versions (HDF4). <http://hdf.ncsa.uiuc.edu/whatishdf5.html>
2. *Introduction to HDF5*. Introduction to the HDF5 data model and programming model. <http://hdf.ncsa.uiuc.edu/HDF5/doc/H5.intro.html>
3. *HDF5: High Level APIs*. A set of functions built on top of the basic HDF5 library. http://hdf.ncsa.uiuc.edu/HDF5/hdf5_hl/doc/
4. *The HDF5 table programming model*. Examples on using HDF5 tables with the C API. http://hdf.ncsa.uiuc.edu/HDF5/hdf5_hl/doc/RM_hdf5tb_ex.html
5. *HL-HDF*. A High Level Interface to the HDF5 File Format. <ftp://ftp.ncsa.uiuc.edu/HDF/HDF5/contrib/hl-hdf5/README.html>
6. *zlib*. A Massively Spiffy Yet Delicately Unobtrusive Compression Library. <http://www.gzip.org/zlib/>
7. *On the 'Pythonic' treatment of XML documents as objects(II)*. Article describing XML Objectify, a Python module that allows working with XML documents as Python objects. Some of the ideas presented here are used in PyTables. <http://www-106.ibm.com/developerworks/xml/library/xml-matters2/index.html>
8. *gnosis.xml.objectify*. This module is part of the Gnosis utilities, and allows to create a mapping between any XML element to "native" Python objects. http://gnosis.cx/download/Gnosis_Utils-current.tar.gz
9. *Pyrex*. A Language for Writing Python Extension Modules. <http://www.cosc.canterbury.ac.nz/~greg/python/Pyrex>
10. *NetCDF (network Common Data Form)*. This is an interface for array-oriented data access and a library that provides an implementation of the interface. <http://www.unidata.ucar.edu/packages/netcdf/>
11. *NetCDF module on Scientific Python*. ScientificPython is a collection of Python modules that are useful for scientific computing. Its NetCDF module is a powerful interface for NetCDF data format. <http://starship.python.net/~hinsen/ScientificPython/ScientificPythonManual/>
12. *Numerical Python*. Package to speed-up arithmetic operations on arrays of numbers. <http://www.pfdubois.com/numpy/>
13. *Numarray*. Reimplementation of Numeric which adds the ability to efficiently manipulate large numeric arrays in ways similar to Matlab and IDL. Among others, Numarray provides the record array extension. <http://stsdas.stsci.edu/numarray/>