# Francesc Alted PyTables User's Guide

#### Alted, Francesc:

PyTables User's Guide

All rights reserved.
© 2002 Francesc Alted

Day of print: November, 13th

Permission is hereby granted, free of charge, to any person obtaining a copy of this software and associated documentation files (the "Software"), to deal in the Software without restriction, including without limitation the rights to use, copy, modify, merge, publish, distribute, sublicense, and/or sell copies of the Software, and to permit persons to whom the Software is furnished to do so, subject to the following conditions:

The above copyright notice and this permission notice shall be included in all copies or substantial portions of the Software.

THE SOFTWARE IS PROVIDED "AS IS", WITHOUT WARRANTY OF ANY KIND, EXPRESS OR IMPLIED, INCLUDING BUT NOT LIMITED TO THE WARRANTIES OF MERCHANTABILITY, FITNESS FOR A PARTICULAR PURPOSE AND NONINFRINGEMENT. IN NO EVENT SHALL THE AUTHORS OR COPYRIGHT HOLDERS BE LIABLE FOR ANY CLAIM, DAMAGES OR OTHER LIABILITY, WHETHER IN AN ACTION OF CONTRACT, TORT OR OTHERWISE, ARISING FROM, OUT OF OR IN CONNECTION WITH THE SOFTWARE OR THE USE OR OTHER DEALINGS IN THE SOFTWARE.

## Copyright Notice and Statement for NCSA HDF5 (Hierarchical Data Format 5) Software Library and Utilities

NCSA HDF5 (Hierarchical Data Format 5) Software Library and Utilities Copyright 1998, 1999, 2000, 2001, 2002 by the Board of Trustees of the University of Illinois

#### All rights reserved.

Contributors: National Center for Supercomputing Applications (NCSA) at the University of Illinois at Urbana-Champaign (UIUC), Lawrence Livermore National Laboratory (LLNL), Sandia National Laboratories (SNL), Los Alamos National Laboratory (LANL), Jean-loup Gailly and Mark Adler (gzip library). Redistribution and use in source and binary forms, with or without modification, are permitted for any purpose (including commercial purposes) provided that the following conditions are met:

- 1. Redistributions of source code must retain the above copyright notice, this list of conditions, and the following disclaimer.
- 2. Redistributions in binary form must reproduce the above copyright notice, this list of conditions, and the following disclaimer in the documentation and/or materials provided with the distribution.
- 3. In addition, redistributions of modified forms of the source or binary code must carry prominent notices stating that the original code was changed and the date of the change.
- 4. All publications or advertising materials mentioning features or use of this software are asked, but not required, to acknowledge that it was developed by the National Center for Supercomputing Applications at the University of Illinois at Urbana-Champaign and to credit the contributors.
- 5. Neither the name of the University nor the names of the Contributors may be used to endorse or promote products derived from this software without specific prior written permission from the University or the Contributors, as appropriate for the name(s) to be used.
- 6. THIS SOFTWARE IS PROVIDED BY THE UNIVERSITY AND THE CONTRIBUTORS "AS IS" WITH NO WARRANTY OF ANY KIND, EITHER EXPRESSED OR IMPLIED. In no event shall the University or the Contributors be liable for any damages suffered by the users arising out of the use of this software, even if advised of the possibility of such damage.

Portions of HDF5 were developed with support from the University of California, Lawrence Livermore National Laboratory (UC LLNL). The following statement applies to those portions of the product and must be retained in any redistribution of source code, binaries, documentation, and/or accompanying materials: This work was partially produced at the University of California, Lawrence Livermore National Laboratory (UC LLNL) under contract no. W-7405-ENG-48 (Contract 48) between the U.S. Department of Energy (DOE) and The Regents of the University of California (University) for the operation of UC LLNL.

# **Contents**

1	Intr	oduction	1
	1.1	Features	1
	1.2	The Object Tree	2
2	Inst	ıllation	5
3	Usaş	re	7
	3.1	Getting started	7
		3.1.1 Importing tables objects	7
		3.1.2 Declaring a Record	8
		3.1.3 Creating a PyTables file from scratch	8
		3.1.4 Creating a new group	8
		3.1.5 Creating a new table	9
		3.1.6 Reading and selecting table data	10
		3.1.7 Creating new array objects	11
		3.1.8 Traversing the object tree	11
		3.1.9 Getting object metadata	12
		3.1.10 Reading actual data from Array objects	13
		3.1.11 Appending data to an existing table	13
	3.2	Checking data in tables	15
		3.2.1 Field name checking	17
		3.2.2 Data range checking	17
		3.2.3 Data type checking	18
	3.3	Optimization tips	18
		3.3.1 Compression issues	18
		3.3.2 Informing PyTables about expected row number in tables	19
		3.3.3 Optimized ways to fill and read data from tables	20
4	Libr	ary Reference	21
-	4.1	tables Variables and Functions	21
	1.1	4.1.1 Global Variables	21
		4.1.2 Global Functions	21
	4.2	The IsRecord class	22
	4.3	The File class	22
	1.5	4.3.1 File instance variables	22
		4.3.2 File methods	22
	4.4	The Group class	24
		4.4.1 Group class variables	24
		4.4.2 Group instance variables	24
		4.4.3 Group methods	24
	45	The Leaf class	25

	4.6	The Ta	able class	25
		4.6.1	Table instance variables	25
		4.6.2	Table methods	25
	4.7	The Ar	rray class	26
		4.7.1	Array instance variables	26
		4.7.2	Array methods	26
A	РуТ	ables	Supported Data Types	27

## **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 scientifc applications, for example) in an efficient manner that reduces demand on CPU time and I/O.

In order to emulate records (C structs in HDF5) in Python PyTables implements a special metaclass object with the capability to detect errors in field assignments as well as 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):
```

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

then, you will normally instantiate it, fill it 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.

#### 1.1 Features

PyTables has the next capabilities:

- Support of table entities: Allows working with large number of records that don't fit in memory.
- Support of Numerical Python arrays: Numeric arrays are a very useful complement of tables to keep homogeneus table slices (like selections of table columns).

1

- 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 structure and the access to the file objects is made by walking throughout the PyTables object tree, and manipulating them.
- *Incremental I/O:* It supports adding records to already created tables. So you won't need to book large amounts of memory to fill the entire table and then save it to disk but you can do that incrementally, even between different Python sessions.
- Allows field name, data type and range checking: If PyTables does not report an error, you can be 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).
- *Big-Endian/Low-Endian safety:* 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 and read it in other little-endian without problems <sup>1</sup>.

Finally, 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 tool to deal with (very) large amounts of data (i.e., typically bigger than available memory) in tables (heterogeneus data types) and arrays (homogeneus data types) organized in a hierarchical, persistent disk storage. PyTables take advantage of the powerful object orientation and introspection capabilities offered by Python to bring all this power 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. This is achieved by *dynamically* creating an object tree imitating the HDF5 structure on disk. That way, the access to the HDF5 objects is made by walking throughout the PyTables object tree, and manipulating them.

A key aspect of PyTables is that for accessing to the different nodes on the object tree a **natural naming** schema is used, i.e. the attributes of the objects that represent HDF5 elements are the same as the names of the element's children<sup>2</sup>.

For example, to refer to a table object located on directory /subgroup2 of a PyTables file, and called table3, you can use the construction file.root.subgroup2.table3, which is very Pythonic and comfortable in many use cases. See the chapter 3 for a more detailed explanation.

You should note that not all the data present on file is loaded in PyTables tree, but only the *metadata* (i.e. data that actually describes the structure of the actual data). The actual data is not read until you ask for it in a particular node, but by making use of the object tree (the metadata) you can get information on the objects on disk, for example, 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 traverse the tree with the supplied methods, 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.

<sup>&</sup>lt;sup>1</sup> Well, I didn't actually test that in real world, but if you do, please, tell me.

<sup>&</sup>lt;sup>2</sup> I've taken this simple but powerful idea from the excellent Objectify module by David Mertz (see references 6 and 7)

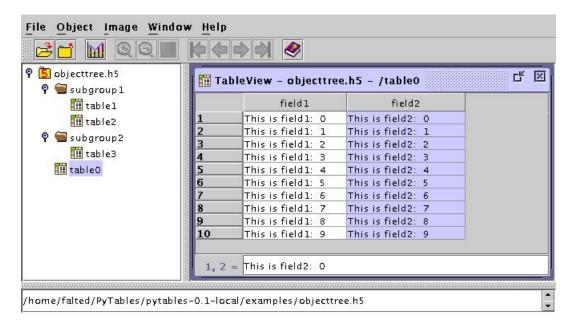


Figure 1.1: An HDF5 example with 2 subgroups and 3 tables.

To better understand the dynamic nature of this object tree, imagine we have made a script (in fact, this script exists; its name is objecttree.py and you can find it in the examples/directory) that creates a simple HDF5 file, with the structure that appears in figure 1.1 (we have used the hdfview application to obtain this image). During creation time, the object tree is updated (using only metadata, remeber) while data is being saved on file and when you close the file, this object is destroyed. If you re-open again this file (in read only mode, for example), the object tree with will be re-constructed from the metadata existent on file, and you can deal 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. If you are going to be a PyTables user, take your time to understand it<sup>3</sup>. That will also make you more proactive by avoiding programming mistakes.

<sup>&</sup>lt;sup>3</sup> 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)

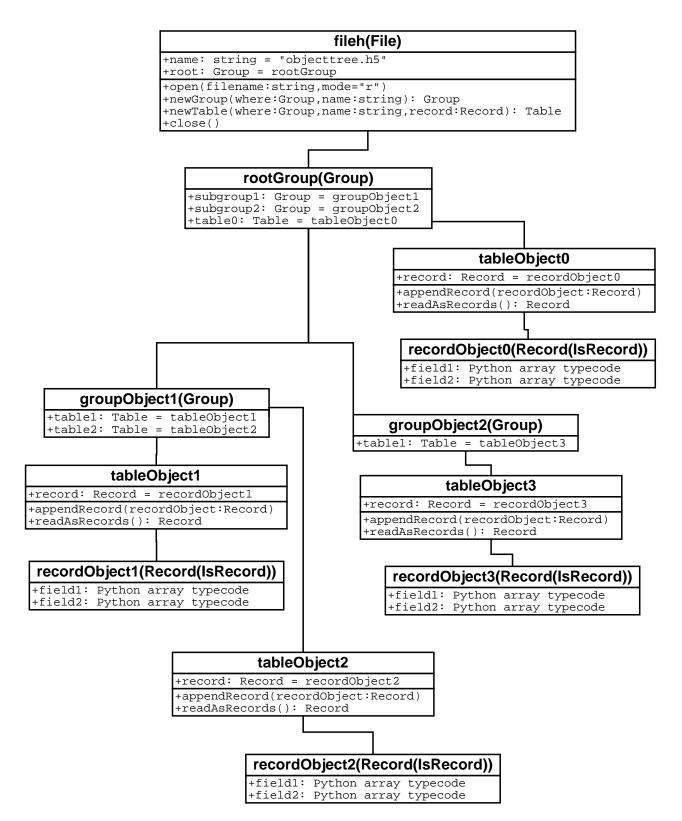


Figure 1.2: An object tree example in PyTables.

## **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 8) and C. 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 evironment 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:

If you would like to see some verbose output from the tests simply add the word verbose to the command line. You can also run only the tests in a particular test module by themselves. For example:

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

4. To install the entire PyTables Python package, change back to the root distribution directory and run this command as the root user:

python setup.py install

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

## **Chapter 3**

## **Usage**

#### 3.1 Getting started

This section is written in a tutorial style. 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 open this freshly created file and we will select some data in the table using Python cuts, creating Numerical arrays to keep this selection as separate objects in the tree. We will see how to browse the tree while retrieving metainformation about the actual data, and will finish by appending some rows to the existing table to show how table objects can be enlarged.

After reading this section you will hopefully learn the main features of PyTables. If you want more information on some specific instance variable, global function or method, go to the library reference in chapter 4. You can get deeper knowledge of PyTables by reading the other sections (XXX which ones?) in this chapter.

You will find in the directory examples the working version of all the code in this section (source file tutorial.py).

#### 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 aplication 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 you will 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, we want to declare a record object in order to save data that comes from our particle detector. Imagine that it 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. We will add two new fields called grid\_i and grid\_j. Our instrumentation also can obtain the pressure and energy of this particle, and we will add them in the same way. A simple-precision float 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 declare a new Particle class that will keep all this info:

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

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

From now on, you can use this class instances as a container for your data, and as you will see shortly, you will get some magic properties associated with instances from Particle, and the class IsRecord<sup>1</sup> from which it is derived is responsible for that magic.

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 funtion:

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

This openFile is one of the objects imported by the "from tables import \*", do you remember?. We are telling that we want to create a new file called "tutorial.h5" in "w"rite mode and with an informative title string ("Test file"). This function tries to open this file, and if successful, returns a File 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.

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

<sup>&</sup>lt;sup>1</sup> IsRecord is actually a *metaclass* in object slang, but we don't need to explain nothing more about it now. Check the sources if you are interested on how that works.

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

#### 3.1.5 Creating a new table

Let's now create the Table object hanging from the new created group. We do that by calling the createTable 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)</pre>
        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 method of table instance is made to put this information in the table I/O buffer.

After we have filled all our data, we must 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()
```

And last, we close the h5file File instance to close the file:

```
>>> h5file.close()
```

With all that, you have created your first PyTables file with a table inside it. 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 tutorial.h5 file:

```
$ h5ls -rd tutorial.h5
/tutorial.h5/detector
                         Group
/tutorial.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):

```
$ python2.2 dumpFile.py tutorial.h5
Filename: tutorial.h5
All objects:
Filename: tutorial.h5 \\ Title: "Test file" \\ Format version: 1.0
/ (Group) "Test file"
/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.

#### 3.1.6 Reading and selecting table data

Ok. We have our data on disk. But we want to access it and select some values we are interested it in some specific columns. That's is easy to do. First, let's open the file we have recently created:

```
>>> h5file = openFile("tutorial.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. But for the moment, our interest is to read an select data from table on disk. The next lines do exactly that:

The first line is only to define a 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 hffile.getNode method instead, and we certainly do that later on.

The last two lines are a Python comprenhensive list. It loops on records returned by table.readAsRecords() iterator that returns values until table data is exhausted. This records are filtered using the *cut* 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 comprehensions syntax more compact and elegant.

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

Ok. that's enough for selections. Now, save these selections on file.

#### 3.1.7 Creating new array objects

In order to separate the selections 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 a path string ("/").

Now, create the Array objects on file:

We already know the first two parameters of the createArray methods (are the same as 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 objects 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 these case, they will become double-precision arrays, as we will see in short.

Note that createArray method returns an Array instance, that we don't keep anywhere. Don't worry, it is attached to the object tree, and can be easily retrieved later on. In fact, you can browse the object tree very easily and retrieve any data you may be interested in. Keep reading.

#### 3.1.8 Traversing the object tree

PyTables, following the Python tradition, offers powerful instropection 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: tutorial.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"
>>>
```

Right, it seems that all our objects are there. We can use the walkGroups method of File class to list all the groups in 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 lists. 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 lists all the nodes hanging from a group, and if *classname* keyword is specified, the method will filter all instances which are not representants of it. We have specified so as to return only the Array instances.

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

As a final example, we will list all the Leaf (i.e. Table or Array) objects in *detector* group. Check that we have only one representant of Table class in this group:

```
>>> 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 this two powerful funtions, but first, we need to learn a bit about important instance variable of PyTables objects.

#### 3.1.9 Getting object metadata

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

```
>>> # Get the "/detector/table"
... table = h5file.getNode("/detector/readout", classname = 'Table')
>>> # Get metadata from table
... 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 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, instead of using 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 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:

```
>>> # Get the object in "/columns pressure"
... pressureObject = h5file.getNode("/columns", "pressure")
>>>
>>> # Get some metadata on this object
... 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 "d"ouble Numeric array, and that by looking at their shape attribute the array on disk is unidimensional and has 4 elements.

#### 3.1.10 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:

```
>>> # Read the 'pressure' actual data
... pressureArray = pressureObject.read()
>>>
>>> # Read the 'name' Array actual data
... nameArray = h5file.root.columns.name.read()
>>>
>>> # Check what kind of object we have created (they should be Numeric arrays)
... 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'>
>>>
```

You can verify that read() returns an authentic Numeric array looking at the output of the type() call.

#### 3.1.11 Appending data to an existing table

To finish this tutorial, 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:

```
>>> # Create a shortcut to table object
... table = h5file.root.detector.readout
>>>
>>> # Get the object record from table
```

```
... particle = table.record
>>>
>>> # Append 5 new particles to table (yes, tables can be enlarged!)
    for i in xrange(10, 15):
        particle.name = 'Particle: %6d' % (i)
. . .
        particle.TDCcount = i % 256
. . .
        particle.ADCcount = (i * 256) % (1 << 16)</pre>
. . .
        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)
. . .
. . .
>>> # Flush this table
... 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 table<sup>2</sup>.

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 is not necessary to have the original class definition (Particle) in our code to re-create it: 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 aplications 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
                                                        10 |
                                                                   0
             1 |
                                        1 |
                                                1 |
                                                         9 |
Particle:
                         1.0
                                                                   1
             2 |
Particle:
                        4.0
                                      256
                                                2
                                                         8
                                                                   2
                        9.0
                                     6561 |
                                                3 |
Particle:
             3
                                                         7 I
                                                                   3
             4
                                6.554e+04
                                                4
Particle:
                       16.0
                                                         6 |
                                                                   4
             5
                        25.0
                                3.906e+05
                                                5
                                                         5
Particle:
                                                                   5
Particle:
              6
                        36.0
                                 1.68e+06
                                                6
                                                         4
                                                                   6
                                                7 |
Particle:
              7
                        49.0
                                5.765e+06
                                                         3 |
                                                                   7
Particle:
             8 |
                        64.0
                                1.678e+07
                                               8 |
                                                         2. |
                                                                   8
                                               9
             9
                                4.305e+07
Particle:
                       81.0
                                                         1 |
                                                                   9
Particle:
           10
                       100.0
                                               10 |
                                                         0 |
                                                                  10
                                    1e+08
Particle:
            11
                       121.0
                                2.144e+08
                                               11 |
                                                        -1 |
                                                                  11
                       144.0 |
Particle:
             12
                                  4.3e+08
                                               12
                                                        -2
                                                                  12
Particle:
             13
                       169.0
                                8.157e+08
                                               13
                                                        -3
                                                                  13
                       196.0
                                1.476e+09
                                               14
Particle:
             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 on this tutorial.

<sup>&</sup>lt;sup>2</sup> 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.

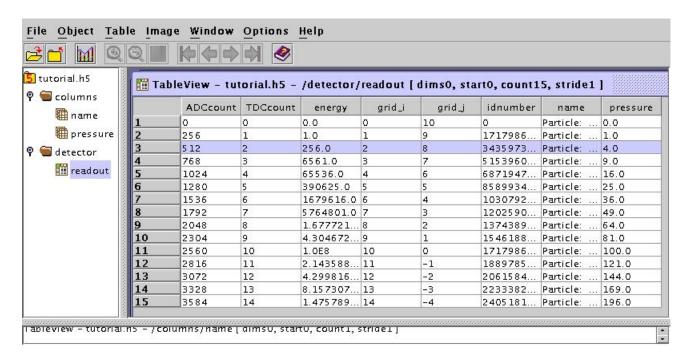


Figure 3.1: The PyTables file created in tutorial.

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

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

#### 3.2 Checking data in tables

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 the root directory 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.

See at the next script. It seems to do all of that, but a couple of small bugs will be shown up:

```
from tables import *
class Particle(IsRecord):
                = '16s'
                          # 16-character String
    name
    lati
                = 'i'
                          # integer
                = 'i'
                          # integer
    longi
                = 'f'
                          # float (single-precision)
    pressure
    temperature = 'd'
                          # double (double-precision)
class Event(IsRecord):
                = '16s'
    name
                          # 16-character String
    TDCcount
                = 'B'
                          # unsigned char
    ADCcount
                = 'H'
                          # unsigned short
                = 'f'
                          # float
                                   (single-precision)
    xcoord
                = 'f'
    ycoord
                          # 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 (this also will flush all the remaining buffers!)
fileh.close()
```

#### 3.2.1 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 inusual 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 resposible 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.

#### 3.2.2 Data range checking

After correcting the last attrribute 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.appendRecord(event)
File "/usr/lib/python2.2/site-packages/tables/Table.py", line 210, in appendRecord
        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</pre>
```

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)</pre>
```

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

#### 3.2.3 Data type checking

Finally, in order to test the type cheking, 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)
  File "/home/falted/PyTables/pytables-0.2/tables/Table.py", line 279,
in appendAsRecord
    self._v_packedtuples.append(RecordObject._f_pack2())
  File "/home/falted/PyTables/pytables-0.2/tables/IsRecord.py", line
181, in f pack2
    self._f_raiseValueError()
  File "/home/falted/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',
                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.

#### 3.3 Optimization tips

PyTables has several places where the user can improve the performace of his application. If you are planning to deal with really large data, you should read carefully this section if you want to get an important boost to your code. But if your dataset is small or medium size (up to 1 MB), you should not worry about that as the default parameters in PyTables are already tuned to handle that perfectly.

#### 3.3.1 Compression issues

One of the beauties of PyTables is that it comes with compression activated by **default** for tables. This may be a bit controversial feature, because compression has a legend of being a very CPU time resources consumer. However, there is an usual scenario where users need to save duplicated data in columns, while the others have changing values. In a relational database approach such a data can normally be moved to other tables and a relationship between the rows 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

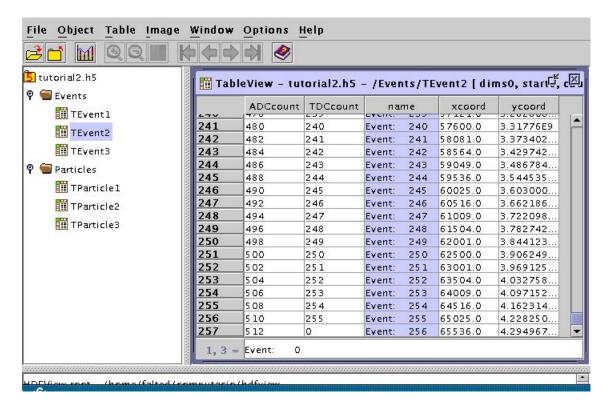


Figure 3.2: Table hierarchy for second example.

more easily because you have more fields available in a single table, and can be referred in the same loop that reads rows of the table.

The compression library used is the **zlib** (http://www.gzip.org/zlib/), 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 is 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 (beware, non-zero!) should offer roughly the same results as a big one.

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

#### 3.3.2 Informing PyTables about expected row number in tables

The underlying HDF5 library that is used by PyTables takes the data in bunches of a certain length (this bunches are 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 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. So, 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 adecuate to your dataset size if you help it by setting an estimated 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 (in File class).

When your dataset size is bigger than 1 MB (take this figure only as a reference, not strictly), by providing createTable with a guess of the number of rows that finally be in table, 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 sloooow I/O operations and huge memory demand. You have been warned!.

#### 3.3.3 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 readAsTuple.

These 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). This methods are much faster (at least a factor two or even more) than xxxxAsRecord equivalents, but they are also unsafer, because it is up to you to pass the correct order of parameters to be appended (or guess the correct order of fields in tuple when reading). This table 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 serie 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 that way:

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

For a working example that also allows you to do some timmings 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 called 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; it is called IsRecord. An important function, called openFile is responsible to create, open or append to PyTables files. In addition, a few utility funtions are defined to guess if an user supplied file is a PyTables file or not. These are called isPyTablesFile and isHDF5. Finally, several 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 global 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 may be useful for reporting bugs.

#### 4.1.2 Global Functions

openFile(filename, mode='r', title="') Open a PyTables file an 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 it, except that their subclasses attributes are transformed during its construction phase, and new methods for the are defined based on the values of the attributes. In that way, we can *force* the resulting instance to only accept assignments on the declared attributes (in fact, it has a few more, but they are hidden with prefixes like "\_\_\_", "\_v\_" or "\_f\_", so please, don't use attributes names starting with these prefixes). If you try to do an assignment to a non-declared attribute, PyTables will raise an error.

To use such a particular class, you have to declare a descendent class from *IsRecord*, with many attributes as fields you want in your record. To declare their types, you simply assign to these attributes their typecode. That's all, from now on, you can instantiate objects from you new class and use them as a very flexible record object with safe features like automatic name field, data type and range checks (see the section 3.2 for an example on how it works).

See the appendix A for a relation of data types supported in a IsRecord class declaration.

#### 4.3 The File class

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

Next, we will discuss the attributes and methods for File class <sup>1</sup>.

#### 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 descrition 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.

<sup>&</sup>lt;sup>1</sup> On the following, the term Leaf will refer to a Table instance. Right now, the only supported Leaf objects are Table and Array, but this list may be increased in the future.

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 descrition for this table.

**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 about 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 try providing a guess; this will optimize the HDF5 B-Tree creation and management process time and memory used.

createArray(where, name, NumericObject, title="') Create a new instance Array 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 table.

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 exists 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'.

**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'.

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 top to bottom, and they are 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 objects on all the HDF5 objects tree.

close() Flush all the objects in HDF5 file 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 no 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 objects (groups or leaves) hanging from this instance.
- \_v\_objgroups Dictionary with all object groups hanging from this instance.
- \_v\_objleaves Dictionaly with all object leaves hanging from this instance.

#### 4.4.3 Group methods

This 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='') Return 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. 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 write/read data and metadata to/from table objects in the file.

Data can be written or read both as records or as tuples. 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).

#### 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 and if 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 serie 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()** Return a record instance from rows in table each time. 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()** Return a tuple from rows in table each time. 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 orderd) 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

Represent a Numeric Array in HDF5 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.

All Numeric typecodes are supported except "F" and "D" which corresponds to complex datatypes. These might be included in short future.

#### 4.7.1 Array instance variables

name The node name.

title. The node title.

**shape** tuple with the array shape (in the Numeric fashion).

**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.

## **Appendix A**

# PyTables Supported Data Types

The supported data types are the same that are supported by the array module in Python, with some additions, which will be briefly discussed shortly. The typecodes for the supported data types are 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	С Туре	Size (in bytes)	Python Counterpart
'c'	8-bit character	char	1	String of lenght 1
'b'	8-bit integer	signed char	1	Integer
'B'	8-bit unsigned integer	unsigned char	1	Integer
'h'	16-bit integer	short	2	Integer
'H'	16-bit unsigned integer	unsigned short	2	Integer
'i'	integer	int	4 or 8	Integer
'I'	unsigned integer	unsigned int	4 or 8	Long
'1'	long integer	long	4 or 8	Integer
'L'	unsigned long integer	unsigned long	4 or 8	Long
'q'	long long integer	long long	8	Long
'Q'	unsigned long long integer	unsigned long long	8	Long
'f'	single-precision float	float	4	Float
'd'	double-precision float	double	8	Float
's'	arbitrary lenght string	char[]	*	String

Table A.1: Data types supported by PyTables

# **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. 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
- 7. *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
- 8. *Pyrex.* A Language for Writing Python Extension Modules. http://www.cosc.canterbury.ac.nz/~greg/python/Pyrex
- 9. *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/net.cdf/
- 10. 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/
- 11. *Numerical Python.* Package to speed-up arithmetic operations on arrays of numbers. http://www.pfdubois.com/numpy/
- 12. 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/