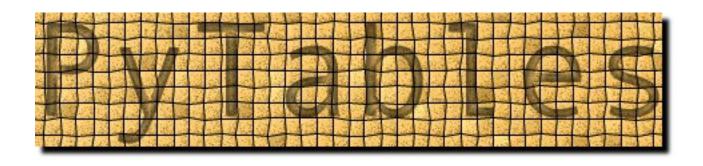
# Francesc Altet • Scott Prater • Ivan Vilata • Tom Hedley

PyTables User's Guide



#### Altet, Francesc:

PyTables User's Guide

Hierarchical datasets in Python Release 0.9

All rights reserved. © 2002, 2003, 2004 Francesc Altet

Typeset by Francesc Altet, Scott Prater, Ivan Vilata and Tom Hedley Day of print: 2004, November, 6th

#### Copyright Notice and Statement for PyTables Software Library and Utilities

Redistribution and use in source and binary forms, with or without modification, are permitted 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 other materials provided with the distribution.

THIS SOFTWARE IS PROVIDED BY THE AUTHOR "AS IS" AND ANY EXPRESS OR IMPLIED WARRANTIES, INCLUDING, BUT NOT LIMITED TO, THE IMPLIED WARRANTIES OF MERCHANTABILITY AND FITNESS FOR A PARTICULAR PURPOSE ARE DISCLAIMED. IN NO EVENT SHALL THE AUTHOR BE LIABLE FOR ANY DIRECT, INDIRECT, INCIDENTAL, SPECIAL, EXEMPLARY, OR CONSEQUENTIAL DAMAGES (INCLUDING, BUT NOT LIMITED TO, PROCUREMENT OF SUBSTITUTE GOODS OR SERVICES; LOSS OF USE, DATA, OR PROFITS; OR BUSINESS INTERRUPTION) HOWEVER CAUSED AND ON ANY THEORY OF LIABILITY, WHETHER IN CONTRACT, STRICT LIABILITY, OR TORT (INCLUDING NEGLIGENCE OR OTHERWISE) ARISING IN ANY WAY OUT OF THE USE OF THIS SOFTWARE, EVEN IF ADVISED OF THE POSSIBILITY OF SUCH DAMAGE.

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

NCSA HDF5 (Hierarchical Data Format 5) Software Library and Utilities Copyright 1998, 1999, 2000, 2001, 2002, 2003, 2004 by the Board of Trustees of the University of Illinois. All rights reserved.

See more information about the terms of this license at: http://hdf.ncsa.uiuc.edu/HDF5/doc/Copyright.html

## **Contents**

1	Intro	ntroduction 1						
	1.1		2					
	1.2	The Object Tree	3					
2	Incto	ation	7					
4	2.1	<del></del>	7					
	2.1		7 7					
		1 · 1 · 1 · 1 · 1 · 1 · 1 · 1 · 1 · 1 ·	, 9					
	2.2	1 F8						
	2.2	·	0					
		1 1	0					
		2.2.2 PyTables package installation	0					
3	Tuto	als 1	1					
	3.1		1					
		· · ·	1					
			2					
			2					
		<i>U</i> 1	2					
			3					
			4					
			5					
		· · ·	6					
	3.2		7					
	3.2		7					
		$\varepsilon$ ,	8					
			1					
			3					
			3 4					
			5					
	2.2		.5 .5					
	3.3	•						
			8					
		8	9					
		3.3.3 Data type checking	9					
4	Libr	ry Reference 3	1					
	4.1	cables variables and functions	1					
		1.1.1 Global variables	1					
			1					
	4.2		3					
			3					
			3					
			7					
	43	1	, R					

		4.3.1	Group instance variables	39
		4.3.2	Group methods	39
		4.3.3	Group special methods	41
	4.4	The Le	af class	41
		4.4.1	Leaf instance variables	42
		4.4.2	Leaf methods	42
	4.5	The Ta	ble class	43
		4.5.1	Table instance variables	43
		4.5.2	Table methods	44
		4.5.3	Table special methods	46
		4.5.4	The Row class	48
		4.5.5	The Cols class	48
	4.6		lumn class	48
	7.0	4.6.1	Column instance variables	48
		4.6.2	Column methods	48
		4.6.3	Column special methods	49
	4.7			50
	4.7	4.7.1	ray class	50
			Array instance variables	
		4.7.2	Array methods	51
	4.0	4.7.3	Array special methods	
	4.8		rray class	
		4.8.1	EArray instance variables	52
		4.8.2	EArray methods	
	4.9		Array class	
			VLArray instance variables	
			VLArray methods	53
			VLArray special methods	55
			Implemented class	56
	4.11		tributeSet class	56
			AttributeSet instance variables	56
		4.11.2	AttributeSet methods	
	4.12	Declara	ative classes	57
		4.12.1	The IsDescription class	57
		4.12.2	The Col class and its descendants	57
		4.12.3	The Atom class and its descendants	58
	4.13	Helper	classes	60
		4.13.1	The Filters class	60
			The IndexProps class	62
			The Index class	62
			The IndexArray class	62
			•	
5	FileN	Node		63
	5.1	What is	SFileNode?	63
	5.2	Current	t limitations	63
	5.3	Finding	g a FileNode node	64
	5.4	Using F	· FileNode	64
		5.4.1	Creating a new file node	64
		5.4.2	Using a file node	65
		5.4.3	Opening an existing file node	65
		5.4.4	Adding metadata to a file node	66
	5.5		ementary notes	67
	5.6		ode module reference	67
	2.0	5.6.1	Global constants	67
		5.6.2	Global functions	67
		3.0.2	Cioum randulum	07

		5.6.3 The FileNode abstract class						
		5.6.4 The ROFileNode class						
		5.6.5 The RWFileNode class						
_								
6	_	timization tips  Informing PyTables about expected number of rows in tables						
	6.1	Informing PyTables about expected number of rows in tables						
	6.2	Accelerating your searches						
		6.2.1 In-kernel searches						
		6.2.2 Indexed searches						
	6.3	Compression issues						
	6.4	Shuffling (or how to make the compression process more effective)						
	6.5	Taking advantage of Psyco						
	6.6	Selecting an User Entry Point (UEP) in your tree						
	6.7	Compacting your PyTables files						
A	Sup	pported data types in PyTables						
	oup,	, october and the property of						
В	Utili	ties						
	B.1	ptdump						
		B.1.1 Usage						
		B.1.2 A small tutorial on ptdump						
	B.2	ptrepack						
		B.2.1 Usage						
		B.2.2 A small tutorial on ptrepack						
	B.3	nctoh5						
		B.3.1 Usage						
C	PvT	ables File Format						
_	C.1	Mandatory attributes for a File						
	C.2	Mandatory attributes for a Group						
	C.3	Mandatory attributes, storage layout and supported datatypes for Leaves						
	C.5	C.3.1 Table format						
		C.3.2 Array format						
		C.3.4 VLArray format						

## **Chapter 1**

## Introduction

La sabiduría no vale la pena si no es posible servirse de ella para inventar una nueva manera de preparar los garbanzos. (Wisdom isn't worth anything if you can't use it to come up with a new way to cook garbanzos).

> —A wise Catalan in "Cien años de soledad" Gabriel García Márquez

The goal of PyTables is to enable the end user to manipulate easily data **tables** and **array** objects in a hierarchical structure. The foundation of the underlying hierarchical data organization is the excellent HDF5 library (see NCSA).

It should be noted that this package is not intended to serve as a complete wrapper for the entire HDF5 API, but only to provide a flexible, *very Pythonic* tool to deal with (arbitrarily) large amounts of data (typically bigger than available memory) in tables and arrays organized in a hierarchical and persistent disk storage structure.

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* may seem to be 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 data aquisition systems, Internet services or scientific applications, for example) in an efficient manner that reduces demand on CPU time and I/O.

In order to emulate in Python records mapped to HDF5 C structs PyTables implements a special *meta-class* object so as to easily define all its fields and other properties. PyTables also provides a powerful interface to mine data in tables. Records in tables are also known in the HDF5 naming scheme as *compound* data types.

For example, you can define arbitrary tables in Python simply by declaring a class with name field and types information, such as in the following example:

```
class Particle(IsDescription):
   name
              = StringCol(16)
                                # 16-character String
    idnumber
             = Int64Col()
                                # Signed 64-bit integer
    ADCcount
             = UInt16Col()
                                # Unsigned short integer
    TDCcount
             = UInt8Col()
                                # unsigned byte
    grid_i
              = Int32Col()
                                # integer
                                # integer (equivalent to Int32Col)
    grid_j
              = IntCol()
    pressure = Float32Col(shape=(2,3)) # 2-D float array (single-precision)
              = FloatCol(shape=(2,3,4)) # 3-D float array (double-precision)
    energy
```

You then pass this class to the table constructor, fill its rows with your values, and save (arbitrarily large) collections of them to a file for persistent storage. After that, the data can be retrieved and post-processed quite easily with PyTables or even with another HDF5 application (in C, Fortran, Java or whatever language that provides a library to interface with HDF5).

Other important entities in PyTables are the **array** objects that are analogous to tables with the difference that all of their components are homogeneous. They come in different flavors, like *generic* (they provide a quick and fast way to deal with for numerical arrays), *enlargeable* (arrays can be extended in any single dimension) and *variable length* (each row in the array can have a different number of elements).

The next section describes the most interesting capabilities of PyTables.

#### 1.1 Main Features

PyTables takes advantage of the object orientation and introspection capabilities offered by Python, the HDF5 powerful data management features and numarray flexibility and high-performance manipulation of large sets of objects organized in grid-like fashion to provide these features:

- Support for table entities: Allows the user to work with a large number of records (up to 2\*\*63), i.e. more than will fit into memory.
- Appendable tables: Supports adding records to already created tables. This can be done even between different Python sessions without copying the dataset or redefining its structure.
- *Multidimensional table cells:* You can declare a column to consist of general array cells as well as scalars, which is the only dimensionality allowed the majority of relational databases.
- *User defined metadata:* Besides suporting system metadata (number of rows of a table, shape, flavor, etc.) the user may specify its own metadata (as for example, room temperature, or protocol for IP traffic that was collected) that complement the meaning of his actual data.
- Support for numerical arrays: Numeric (see Ascher et al.) and numarray (see Greenfield et al.) arrays can be used as a useful complement of tables to store homogeneous data.
- Enlargeable arrays: You can add new elements to existing arrays on disk in any dimension you want (but only one). Besides, you can access to only a slice of your datasets by using the powerful extended slicing mechanism, without need to load all your complete dataset in-memory.
- *Variable length arrays:* The number of elements in these arrays can be variable from row to row. This provides a lot of flexibility when dealing with complex data.
- Supports a hierarchical data model: Allows the user to clearly structure all the 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 through and manipulating this object tree.
- Support of files bigger than 2 GB: PyTables automatically inherits this capability from the underlying HDF5 library (assuming your platform supports the C long long integer, or, on Windows, \_\_int64).
- Ability to read/modify generic HDF5 files: PyTables can access a wide range of objects in generic HDF5 files, like compound type datasets (that can be mapped to Table objects), homogeneous datasets (that can be mapped to Array objects) or variable length record datasets (that can be mapped to VLArray objects). Besides, if a dataset is not supported, it will be mapped into a special UnImplemented class (see 4.10), that will let the user see that the data is there, although it would be unreachable (still, you will be able to access the attributes and some metadata in the dataset). With that, PyTables probably can access and modify most of the HDF5 files out there.
- Data compression: Supports data compression (using the Zlib, LZO and UCL compression libraries) out of the box. This is important when you have repetitive data patterns and don't want to spend time searching for an optimized way to store them (saving you time spent analyzing your data organization).
- *High performance I/O:* On modern systems storing large amounts of data, tables and array objects can be read and written at a speed only limited by the performance of the underlying I/O subsystem. Moreover, if your data is compressible, even that limit is surmountable!
- Architecture-independent: PyTables has been carefully coded (as has HDF5 itself) with little-endian/big-endian byte orderings issues in mind. In principle you can write a file on a big-endian machine (like a Sparc or MIPS) and read it on other little-endian machine (like an Intel or Alpha) without problems. In addition, it has been tested successfully with 64 bit platforms (Intel-64, AMD-64, PowerPC-G5, MIPS, UltraSparc).

#### 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. The HDF5 objects are read by walking through this object tree. You can get a good picture of what kind of data is kept in the object by examining the *metadata* nodes.

The different nodes in the object tree are instances of PyTables classes. There are several types of classes, but the most important ones are the Group and the Leaf classes. Group instances (referred to as *groups* from now on) are a grouping structure containing instances of zero or more groups or leaves, together with supplementary metadata. Leaf instances (referred to as *leaves*) are containers for actual data and cannot contain further groups or leaves. The Table, Array, EArray, VLArray and UnImplemented classes are descendents of Leaf, and inherit all its properties.

Working with groups and leaves is similar in many ways to working with directories and files on a Unix filesystem. As is the case 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 (such as '/subgroup2/table3') or as a complete object path written in a format known as the *natural name* schema (such as file.root.subgroup2.table3).

Support for *natural naming* is a key aspect of PyTables. It means that the names of instance variables of the node objects are the same as the names of the element's children<sup>1</sup>. This is very *Pythonic* and intuitive in many cases. Check the tutorial section 3.1.6 for usage examples.

You should also be aware that not all the data present in a file is loaded into the object tree. Only the *metadata* (i.e. special data that describes the structure of the actual data) is loaded. The actual data is not read until you request it (by calling a method on a particular node). Using the object tree (the metadata) you can retrieve information about the objects on disk such as table names, titles, name columns, data types in columns, numbers of rows, or, in the case of arrays, the shapes, typecodes, etc. of the array. You can also search through the tree for specific kinds of data then read it and process it. In a certain sense, you can think of PyTables as a tool that applies the same introspection capabilities of Python objects to large amounts of data in persistent storage.

To better understand the dynamic nature of this object tree entity, let's start with a sample PyTables script (you can find it in examples/objecttree.py) to create a HDF5 file:

```
from tables import *
class Particle(IsDescription):
    identity = StringCol(length=22, dflt=" ", pos = 0)
                                                        # character String
    idnumber = Int16Col(1, pos = 1) # short integer
             = Float32Col(1, pos = 2) # single-precision
    speed
# Open a file in "w"rite mode
fileh = openFile("objecttree.h5", mode = "w")
# Get the HDF5 root group
root = fileh.root
# Create the groups:
group1 = fileh.createGroup(root, "group1")
group2 = fileh.createGroup(root, "group2")
# Now, create an array in the root group
array1 = fileh.createArray(root, "array1",
                           ["this is", "a string array"], "String array")
# Create 2 new tables in group1 and group2
table1 = fileh.createTable(group1, "table1", Particle)
table2 = fileh.createTable("/group2", "table2", Particle)
```

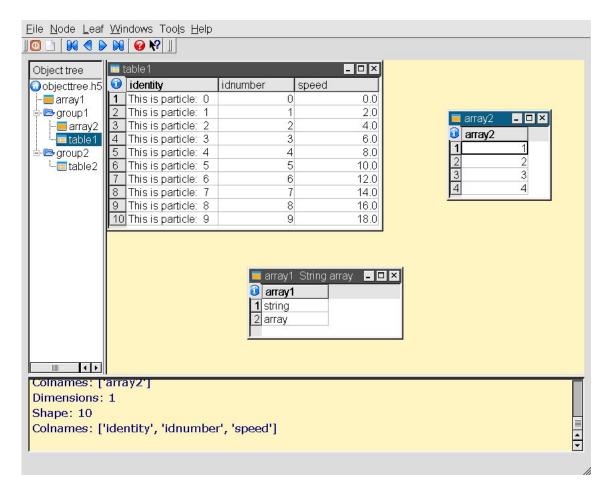
 $<sup>^{1}</sup>$  I got this simple but powerful idea from the excellent Objectify module by David Mertz (see Mertz)

```
# Create one more Array in group1
array2 = fileh.createArray("/group1", "array2", [1,2,3,4])
# Now, fill the tables:
for table in (table1, table2):
    # Get the record object associated with the table:
   row = table.row
    # Fill the table with 10 records
    for i in xrange(10):
        # First, assign the values to the Particle record
       row['identity'] = 'This is particle: %2d' % (i)
        row['idnumber'] = i
        row['speed'] = i * 2.
        # This injects the Record values
       row.append()
    # Flush the table buffers
    table.flush()
# Finally, close the file (this also will flush all the remaining buffers!)
fileh.close()
```

This small program creates a simple HDF5 file called objecttree.h5 with the structure that appears in figure 1.1. When the file is created, the metadata in the object tree is updated in memory while the actual data is saved to disk. When you close the file the object tree is no longer available. However, when you reopen this file the object tree will be reconstructed in memory from the metadata on disk, allowing you to work with it in exactly the same way as when you originally created it.

In figure 1.2 you can see an example of the object tree created when the above objecttree.h5 file is read (in fact, such an object is always created when reading any supported generic HDF5 file). It's worthwhile to take your time to understand it<sup>2</sup>. It will help you to avoid programming mistakes.

<sup>&</sup>lt;sup>2</sup> Bear in mind, however, that this diagram is **not** a standard UML class diagram; it is rather meant to show the connections between the PyTables objects and some of its most important attributes and methods.



**Figure 1.1:** An HDF5 example with 2 subgroups, 2 tables and 1 array.

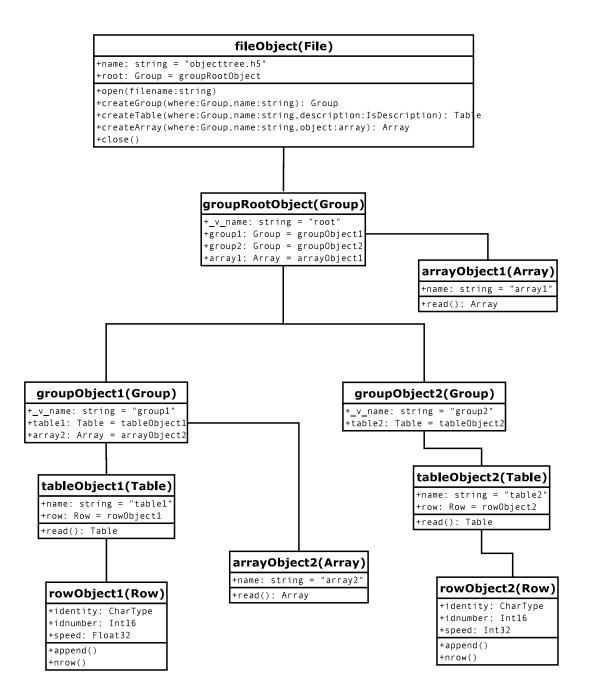


Figure 1.2: A PyTables object tree example.

### Chapter 2

## Installation

The Python Distutils are used to build and install PyTables, so it is fairly simple to get the application up and running. If you want to install the package from sources go to the next section. But if you are running Windows and want to install precompiled binaries jump to section 2.2). In addition, packages are starting to appear in different Linux distributions, for instance RockLinux, Debian, Fedora or Gentoo. There also packages for other Unices like FreeBSD or MacOSX

#### 2.1 Installation from source

These instructions are for both Unix/Linux and Windows systems. If you are using Windows, it is assumed that you have a recent version of MS  $Visual\ C++\ (>=6.0)$  compiler installed. A GCC compiler is assumed for Unix, but other compilers should work as well.

Extensions in PyTables have been developed in Pyrex (see Ewing) and C language. You can rebuild everything from scratch if you have Pyrex installed, but this is not necessary, as the Pyrex compiled source is included in the distribution.

To compile PyTables you will need a recent version of the HDF5 (C flavor) library and the numarray (see Greenfield *et al.*) package. Although you won't need Numerical Python (see Ascher *et al.*) in order to compile PyTables, it is supported; you only need a reasonably recent version of it (>= 21.x) if you plan on using its methods in your applications. PyTables has been successfully tested with Numeric 21.3, 22.0 and 23.0. If you already have Numeric installed, the test driver module will detect it and will run the tests for Numeric automatically.

#### 2.1.1 Prerequisites

First, make sure that you have at least HDF5 1.6.3-patch and numarray 1.1 or higher installed (I'm using HDF5 1.6.3-patch<sup>1</sup> and numarray 1.1 currently). If you don't, fetch and install them before proceeding.

Compile and install these packages (but see section 2.2.1 for instructions on how to install precompiled binaries if you are not willing to compile the prerequisites on Windows systems).

For compression (and possibly improved performance), you will need to install the Zlib (see Gailly and Adler), which is also required by HDF5 as well. You may also optionally install the excellent LZO and UCL compression libraries (see Oberhumer and section 6.3).

Unix setup.py will detect HDF5, LZO or UCL libraries and include files under /usr or /usr/local; this will cover most manual installations as well as installations from packages. If setup.py can't find libhdf5 or libz (or liblzo or libucl that you may wish to use) or if you have several versions of a library installed and want to use a particular one, then you can set the path to the resource in the environment, setting the values of the HDF5\_DIR, LZO\_DIR or UCL\_DIR environment variables to the

<sup>&</sup>lt;sup>1</sup> Unfortunately, HDF5 1.6.3 was released with a bug that causes a segmentation fault when an index is deleted. The 1.6.3-patch and higher versions solve this.

path to the particular resource. You may also specify the locations of the resource root directories on the setup.py command line. For example:

```
--hdf5=/stuff/hdf5-1.6.3
--lzo=/stuff/lzo-1.08
--ucl=/stuff/ucl-1.03
```

If your HDF5 library was built as a shared library 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/hdf5-1.6.3/lib"

or perhaps just
```

```
--rpath="/stuff/hdf5-1.6.3/lib"
```

Check your compiler and linker documentation as well as the Python Distutils documentation for the correct syntax.

It is also possible to link with specific libraries by setting the LIBS environment variable:

```
LIBS="hdf5-1.6.5"
LIBS="hdf5-1.6.5 nsl"
```

**Windows** Once you have installed the prerequisites, setup.py needs to know where the necessary library *stub* (.lib) and *header* (.h) files are installed. Set the following environment variables:

**HDF5\_DIR** Points to the root HDF5 directory (where the include/ and dll/ directories can be found). *Mandatory*.

**LZO\_DIR** Points to the root LZO directory (where the include/ and lib/ directories can be found). *Optional*.

**UCL\_DIR** Points to the root UCL directory (where the include/ and lib/ directories can be found). *Optional*.

For example:

```
set HDF5_DIR=c:\stuff\5-162-win2k\c\release
set UCL_DIR=c:\stuff\ucl-1-02
set LZO_DIR=c:\stuff\lzo-1-08
```

Or, you can pass this information to setup.py by setting the appropriate arguments on the command line. For example:

```
--hdf5=c:\stuff\5-162-win2k\c\release
--lzo=c:\stuff\lzo-1-08
--ucl=c:\stuff\ucl-1-02
```

#### 2.1.2 PyTables package installation

Once you have installed the HDF5 library and numarray packages, you can proceed with the PyTables package itself:

1. Run this command from the main PyTables distribution directory, including any extra command line arguments as discussed above:

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

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

2. To run the test suite, change into the test directory and execute this command:

Unix In the shell sh and its variants:

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

Windows Open a DOS terminal and type:

```
set PYTHONPATH=..
python test_all.py
```

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

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

If a test fails, please enable verbose output (the -v flag **and** verbose option), run the failing test module again, and, very important, get your PyTables version information by running the command:

```
python test_all.py --show-versions-only
```

and send back the output to developers so that we may continue improving PyTables.

If you run into problems because Python can't load the HDF5 library or other shared libraries:

**Unix** Try setting the LD\_LIBRARY\_PATH environment variable to point to the directory where the missing libraries can be found.

Windows Put the DLL libraries (hdf5dll.dll and, optionally, lzo.dll and ucl.dll) in a directory listed in your PATH environment variable. The setup.py installation program will print out a warning to that effect if the libraries can't be found.

3. To install the entire PyTables Python package, change back to the root distribution directory and run the following command (make sure you have sufficient permissions to write to the directories where the PyTables files will be installed):

```
python setup.py install
```

Of course, you will need super-user privileges if you want to install PyTables on a system-protected area. You can select, though, a different place to install the package using the --prefix flag:

```
python setup.py install --prefix="/home/myuser/mystuff"
```

Have in mind, however, that if you use the --prefix flag to install in a non-standard place, you should properly setup your PYTHONPATH environment variable, so that the Python interpreter would be able to find your new PyTables installation.

You have more installation options available in the distutils package. Issue a:

```
python setup.py install --help
```

for more information on that subject.

That's it! Now you can skip to the next chapter to learn how to use PyTables.

#### 2.2 Binary installation (Windows)

This section is intended for installing precompiled binaries on Windows platforms. You may also find it useful for instructions on how to install *binary prerequisites* even if you want to compile PyTables itself on Windows.

#### 2.2.1 Windows prerequisites

First, make sure that you have HDF5 1.6.3-patch<sup>2</sup> or higher and numarray 1.1 or higher installed (I have built the PyTables binaries using HDF5 1.6.3-patch and numarray 1.1).

For the HDF5 it should be enough to manually copy the hdf5dll.dll, zlib1.dll and szipdll.dll files to a directory in your PATH environment variable (for example C:\WINDOWS\SYSTEM).

To enable compression with optional LZO and UCL libraries (see the section 6.3 for hints about how they may be used to improve performance), fetch and install the LZO and UCL binaries from:

http://gnuwin32.sourceforge.net/. Normally, you will only need to fetch and install the <package>-<version>-bin.zip file and copy the lzo.dll or ucl.dll files in a directory in the PATH environment variable, so that they can be found by the PyTables extensions.

**Note:** If you are reading this because you have been redirected from the section 2.1 (*Installation from source*), some of the headers you will need are in the cpackage>-<version>-lib.zip file.

#### 2.2.2 PyTables package installation

Download the tables-<version>.win32-py<version>.exe (tables-<version>-LU.win32-py<version>.exe if you want support for LZO and UCL libraries) file and execute it.

You can (you should) test your installation by unpacking the source tar-ball, changing to the test/subdirectory and executing the test\_all.py script. If all the tests pass (possibly with a few warnings, related to the potential unavailability of LZO and UCL libs) you already have a working, well-tested copy of PyTables installed! If any test fails, please try to locate which test module is failing and execute:

```
python test_<module>.py -v verbose
```

and also:

```
python test_all.py --show-versions-only
```

and mail the output to the developers so that the problem can be fixed in future releases.

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

<sup>&</sup>lt;sup>2</sup> Unfortunately, HDF5 1.6.3 was released with a bug that causes a segmentation fault when an index is deleted. The 1.6.3-patch and higher versions solve this. You can find a binary version of libraries in ftp://hdf.ncsa.uiuc.edu/HDF5/hdf5-1.6.3/src/patches/bin/WinXP-patch.tar.gz

Serás la clau que obre tots els panys, seràs la llum, la llum il.limitada, seràs confí on l'aurora comença, seràs forment, escala il.luminada!

> —M'aclame a tu Lyrics: Vicent Andrés i Estellés Music: Ovidi Montllor

# Chapter 3

## **Tutorials**

This chapter consists of a series of simple yet comprehensive tutorials that will enable you to understand PyTables' main features. If you would like more information about some particular instance variable, global function, or method, look at the doc strings or go to the library reference in chapter 4. If you are reading this in PDF or HTML formats, follow the corresponding hyperlink near each newly introduced entity.

Please note that throughout this document the terms *column* and *field* will be used interchangeably, as will the terms *row* and *record*.

#### 3.1 Getting started

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

In *examples/tutorial1-1.py* you will find the working version of all the code in this section. Nonetheless, this tutorial series has been written to allow you reproduce it in a Python interactive console. I encourage you to do parallel testing and inspect the created objects (variables, docs, children objects, etc.) during the course of the tutorial!

#### 3.1.1 Importing tables objects

Before starting you need to import the public objects in the tables package. You normally do that by executing:

```
>>> import tables
```

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

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

which will export in your caller application namespace the following objects: openFile, isHDF5, isPyTablesFile and IsDescription. This is a rather reduced set of objects, and for convenience, we will use this technique to access them.

If you are going to work with numarray or Numeric arrays (and normally, you will) you will also need to import objects from them. So most PyTables programs begin with:

#### 3.1.2 Declaring a Column Descriptor

Now, imagine that we have a particle detector and we want to create a table object in order to save data retrieved from it. You need first to define the table, the number of columns it has, what kind of object is contained in each column, and so on.

Our particle detector has a TDC (Time to Digital Converter) counter with a dynamic range of 8 bits and an ADC (Analogical 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, so we will add two new fields called grid\_i and grid\_j. Our instrumentation also can obtain the pressure and energy of the particle. The resolution of the pressure-gauge allows us to use a simple-precision float to store pressure readings, while the energy value will need a double-precision float. Finally, to track the particle we want to assign it a name to identify the kind of the particle it is and a unique numeric identifier. So we will add two more fields: name will be a string of up to 16 characters, and idnumber will be an integer of 64 bits (to allow us to store records for extremely large numbers of particles).

Having determined our columns and their types, we can now declare a new Particle class that will contain all this information:

```
>>> class Particle(IsDescription):
                  = StringCol(16)
                                     # 16-character String
        name
. . .
        idnumber
                  = Int64Col()
                                     # Signed 64-bit integer
. . .
        ADCcount = UInt16Col()
                                     # Unsigned short integer
. . .
        TDCcount = UInt8Col()
                                     # unsigned byte
. . .
                  = Int32Col()
                                     # integer
        grid_i
. . .
                  = IntCol()
                                     # integer (equivalent to Int32Col)
        grid_j
        pressure = Float32Col()
                                     # float (single-precision)
        energy
                  = FloatCol()
                                     # double (double-precision)
. . .
. . .
>>>
```

This definition class is self-explanatory. Basically, you declare a class variable for each field you need. As its value you assign an instance of the appropriate Col subclass, according to the kind of column defined (the data type, the length, the shape, etc). See the section 4.12.2 for a complete description of these subclasses. See also appendix A for a list of data types supported by the Col constructor.

From now on, we can use Particle instances as a descriptor for our detector data table. We will see later on how to pass this object to construct the table. But first, we must create a file where all the actual data pushed into our table will be saved.

#### 3.1.3 Creating a PyTables file from scratch

Use the first-level openFile (see 4.1.2) function to create a PyTables file:

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

openFile (see 4.1.2) is one of the objects imported by the "from tables import \*" statement. Here, we are saying that we want to create a new file in the current working directory called "tutorial1.h5" in "w"rite mode and with an descriptive title string ("Test file"). This function attempts to open the file, and if successful, returns the File (see 4.2) object instance h5file. The root of the object tree is specified in the instance's root attribute.

#### 3.1.4 Creating a new group

Now, to better organize our data, we will create a group called *detector* that branches from the root node. We will save our particle data table in this group.

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

Here, we have taken the File instance h5file and invoked its createGroup method (see 4.2.2) to create a new group called *detector* branching from "/" (another way to refer to the h5file.root object we mentioned above). This will create a new Group (see 4.3) object instance that will be assigned to the variable group.

#### 3.1.5 Creating a new table

Let's now create a Table (see 4.5) object as a branch off the newly-created group. We do that by calling the createTable (see 4.2.2) method of the h5file object:

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

We create the Table instance under group. We assign this table the node name "readout". The Particle class declared before is the *description* parameter (to define the columns of the table) and finally we set "Readout example" as the Table title. With all this information, a new Table instance is created and assigned to the variable table.

If you are curious about how the object tree looks right now, simply print the File instance variable *h5file*, and examine the output:

```
>>> print h5file
Filename: 'tutorial1.h5' Title: 'Test file' Last modif.: 'Sun Jul 27 14:00:13 2003'
/ (Group) 'Test file'
/detector (Group) 'Detector information'
/detector/readout (Table(0,)) 'Readout example'
```

As you can see, a dump of the object tree is displayed. It's easy to see the Group and Table objects we have just created. If you want more information, just type the variable containing the File instance:

```
>>> h5file
File(filename='tutorial1.h5', title='Test file', mode='w', trMap={}, rootUEP='/')
/ (Group) 'Test file'
/detector (Group) 'Detector information'
/detector/readout (Table(0,)) 'Readout example'
description := {
    "ADCcount": Col('UInt16', shape=1, itemsize=2, dflt=0),
    "TDCcount": Col('UInt8', shape=1, itemsize=1, dflt=0),
    "energy": Col('Float64', shape=1, itemsize=8, dflt=0.0),
    "grid_i": Col('Int32', shape=1, itemsize=4, dflt=0),
    "grid_j": Col('Int32', shape=1, itemsize=4, dflt=0),
    "idnumber": Col('Int64', shape=1, itemsize=8, dflt=0),
    "name": Col('CharType', shape=1, itemsize=16, dflt=None),
    "pressure": Col('Float32', shape=1, itemsize=4, dflt=0.0) }
byteorder := little
```

More detailed information is displayed about each object in the tree. Note how Particle, our table descriptor class, is printed as part of the *readout* table description information. In general, you can obtain much more information about the objects and their children by just printing them. That introspection capability is very useful, and I recommend that you use it extensively.

The time has come to fill this table with some values. First we will get a pointer to the Row (see 4.5.4) instance of this table instance:

```
>>> particle = table.row
```

The row attribute of table points to the Row instance that will be used to write data rows into the table. We write data simply by assigning the Row instance the values for each row as if it were a dictionary (although it is actually an *extension class*), using the column names as keys.

Below is an example of how to write rows:

```
>>> for i in xrange(10):
        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)
        particle.append()
. . .
. . .
>>>
```

This code should be easy to understand. The lines inside the loop just assign values to the different columns in the Row instance particle (see 4.5.4). A call to its append() method writes this information to the table I/O buffer.

After we have processed all our data, we should flush the table's I/O buffer if we want to write all this data to disk. We achieve that by calling the table.flush() method.

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

#### 3.1.6 Reading (and selecting) data in a table

Ok. We have our data on disk, and now we need to access it and select from specific columns the values we are interested in. See the example below:

The first line creates a "shortcut" to the *readout* table deeper on the object tree. As you can see, we use the **natural naming** schema to access it. We also could have used the h5file.getNode() method, as we will do later on.

You will recognize the last two lines as a Python list comprehension. It loops over the rows in *table* as they are provided by the table.iterrows() iterator (see 4.5.2). The iterator returns values until all the data in table is exhausted. These rows are filtered using the expression:

```
x['TDCcount'] > 3 and x['pressure'] < 50
```

We select the value of the pressure column from filtered records to create the final list and assign it to pressure variable.

We could have used a normal for loop to accomplish the same purpose, but I find comprehension syntax to be more compact and elegant.

Let's select the name column for the same set of cuts:

```
>>> names=[ x['name'] for x in table if x['TDCcount']>3 and 20<=x['pressure']<50 ]
>>> names
['Particle: 5', 'Particle: 6', 'Particle: 7']
```

Note how we have omitted the iterrows() call in the list comprehension. The Table class has an implementation of the special method \_\_iter\_\_() that iterates over all the rows in the table. In fact, iterrows() internally calls this special \_\_iter\_\_() method. Accessing all the rows in a table using this method is very convenient, especially when working with the data interactively.

That's enough about selections. The next section will show you how to save these select results to a file.

#### 3.1.7 Creating new array objects

In order to separate the selected data from the mass of detector data, we will create a new group columns branching off the root group. Afterwards, under this group, we will create two arrays that will contain the selected data. First, we create the group:

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

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

Now, create the first of the two Array objects we've just mentioned:

We already know the first two parameters of the createArray (see 4.2.2) methods (these are the same as the first two in createTable): they are the parent group *where* Array will be created and the Array instance *name*. The third parameter is the *object* we want to save to disk. In this case, it is a Numeric array that is built from the selection list we created before. The fourth parameter is the *title*.

Now, we will save the second array. It contains the list of strings we selected before: we save this object as-is, with no further conversion.

```
>>> h5file.createArray(gcolumns, 'name', names, "Name column selection")
/columns/name Array(4,) 'Name column selection'
  type = 'CharType'
  itemsize = 16
  flavor = 'List'
  byteorder = 'little'
```

As you can see, <code>createArray()</code> accepts *names* (which is a regular Python list) as an *object* parameter. Actually, it accepts a variety of different regular objects (see 4.2.2) as parameters. The flavor attribute (see the output above) saves the original kind of object that was saved. Based on this *flavor*, <code>PyTables</code> will be able to retrieve exactly the same object from disk later on.

Note that in these examples, the createArray method returns an Array instance that is not assigned to any variable. Don't worry, this is intentional to show the kind of object we have created by displaying its representation. The Array objects have been attached to the object tree and saved to disk, as you can see if you print the complete object tree:

```
>>> print h5file
Filename: 'tutorial1.h5' Title: 'Test file' Last modif.: 'Sun Jul 27 14:00:13 2003'
/ (Group) 'Test file'
/columns (Group) 'Pressure and Name'
/columns/name (Array(3,)) 'Name column selection'
/columns/pressure (Array(3,)) 'Pressure column selection'
/detector (Group) 'Detector information'
/detector/readout (Table(10,)) 'Readout example'
```

#### 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 object to close the file before exiting Python:

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

You have now created your first PyTables file with a table and two arrays. You can examine it with any generic HDF5 tool, such as h5dump or h51s. Here is what the tutorial1.h5 looks like when read with the h51s program:

```
$ h5ls -rd tutorial1.h5
/columns
                         Group
/columns/name
                         Dataset {3}
   Data:
       (0) "Particle:
                            5", "Particle:
                                               6", "Particle:
                                                                    7 "
/columns/pressure
                        Dataset {3}
   Data:
        (0) 25, 36, 49
/detector
                         Group
/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}
```

Here's the outputs as displayed by the "ptdump" PyTables utility (located in utils / directory):

```
$ ptdump tutorial1.h5
Filename: 'tutorial1.h5' Title: 'Test file' Last modif.: 'Sun Jul 27 14:40:51 2003'
/ (Group) 'Test file'
/columns (Group) 'Pressure and Name'
/columns/name (Array(3,)) 'Name column selection'
/columns/pressure (Array(3,)) 'Pressure column selection'
/detector (Group) 'Detector information'
```

```
/detector/readout (Table(10,)) 'Readout example'
```

You can pass the -v or -d options to ptdump if you want more verbosity. Try them out!

#### 3.2 Browsing the *object tree* and appending to tables

In this section, we will learn how to browse the tree and retrieve meta-information about the actual data, then append some rows to an 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 course of the tutorial.

#### 3.2.1 Traversing the object tree

Let's start by opening the file we created in last tutorial section.

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

This time, we have opened the file in "a"ppend mode. We use this mode 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 search the tree.

To start with, you can get a preliminary overview of the object tree by simply printing the existing File instance:

```
>>> print h5file
Filename: 'tutorial1.h5' Title: 'Test file' Last modif.: 'Sun Jul 27 14:40:51 2003'
/ (Group) 'Test file'
/columns (Group) 'Pressure and Name'
/columns/name (Array(3,)) 'Name column selection'
/columns/pressure (Array(3,)) 'Pressure column selection'
/detector (Group) 'Detector information'
/detector/readout (Table(10,)) 'Readout example'
```

It looks like all of our objects are there. Now let's make use of the File iterator to see to list all the nodes in the object tree:

```
>>> for node in h5file:
... print node
...
/ (Group) 'Test file'
/columns (Group) 'Pressure and Name'
/detector (Group) 'Detector information'
/columns/name (Array(3,)) 'Name column selection'
/columns/pressure (Array(3,)) 'Pressure column selection'
/detector/readout (Table(10,)) 'Readout example'
```

We can use the walkGroups method (see 4.2.2) of the File class to list only 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. Using this iterator with the listNodes() method is a powerful combination. Let's see an example listing of all the arrays in the tree:

```
>>> for group in h5file.walkGroups("/"):
...     for array in h5file.listNodes(group, classname = 'Array'):
...         print array
...
/columns/name Array(3,) 'Name column selection'
/columns/pressure Array(3,) 'Pressure column selection'
```

listNodes() (see 4.2.2) returns a list containing all the nodes hanging off a specific Group. If the *classname* keyword is specified, the method will filter out all instances which are not descendants of the class. We have asked for only Array instances.

We can combine both calls by using the walkNodes(where, classname) special method of the File object (see 4.2.2). For example:

```
>>> for array in h5file.walkNodes("/", "Array"):
... print array
...
/columns/name (Array(3,)) 'Name column selection'
/columns/pressure (Array(3,)) 'Pressure column selection'
```

This is a nice shortcut when working interactively.

Finally, we will list all the Leaf, i.e. Table and Array instances (see 4.4 for detailed information on Leaf class), in the /detector group. Note that only one instance of the Table class (i.e. readout) will be selected in this group (as should be the case):

```
>>> for leaf in h5file.root.detector._f_walkNodes('Leaf'):
... print leaf
...
/detector/readout (Table(10,)) 'Readout example'
```

We have used a call to the  $Group._f_walkNodes(classname, recursive)$  method (4.3.2), using the *natural naming* path specification.

Of course you can do more sophisticated node selections using these powerful methods. But first, let's take a look at some important PyTables object instance variables.

#### 3.2.2 Setting and getting user attributes

PyTables provides an easy and concise way to complement the meaning of your node objects on the tree by using the AttributeSet class (see section 4.11). You can access this object through the standard attribute attrs in Leaf nodes and \_v\_attrs in Group nodes.

For example, let's imagine that we want to save the date indicating when the data in /detector/readout table has been acquired, as well as the temperature during the gathering process:

```
>>> table = h5file.root.detector.readout
>>> table.attrs.gath_date = "Wed, 06/12/2003 18:33"
>>> table.attrs.temperature = 18.4
>>> table.attrs.temp_scale = "Celsius"
```

Now, let's set a somewhat more complex attribute in the /detector group:

```
>>> detector = h5file.root.detector
>>> detector._v_attrs.stuff = [5, (2.3, 4.5), "Integer and tuple"]
```

Note how the AttributeSet instance is accessed with the \_v\_attrs attribute because detector is a Group node. In general, you can save any standard Python data structure as an attribute node. See section 4.11 for a more detailed explanation of how they are serialized for export to disk.

Retrieving the attributes is equally simple:

```
>>> table.attrs.gath_date
'Wed, 06/12/2003 18:33'
>>> table.attrs.temperature
18.39999999999999
>>> table.attrs.temp_scale
'Celsius'
>>> detector._v_attrs.stuff
[5, (2.29999999999998, 4.5), 'Integer and tuple']
```

You can probably guess how to delete attributes:

```
>>> del table.attrs.gath_date
```

If you want to examine the current complete attribute set of /detector/table, you can print its representation (try hitting the TAB key twice if you are on a Unix Python console with the rlcompleter module active):

```
>>> table.attrs
/detector/readout (AttributeSet), 14 attributes:
   [CLASS := 'TABLE',
   FIELD_0_NAME := 'ADCcount',
   FIELD_1_NAME := 'TDCcount',
   FIELD_2_NAME := 'energy',
   FIELD_3_NAME := 'grid_i',
   FIELD_4_NAME := 'grid_j',
    FIELD_5_NAME := 'idnumber',
   FIELD_6_NAME := 'name',
   FIELD_7_NAME := 'pressure',
   NROWS := 10,
   TITLE := 'Readout example',
    VERSION := '2.0',
    tempScale := 'Celsius',
    temperature := 18.399999999999999]
```

You can get a list of only the user or system attributes with the \_f\_list() method.

```
>>> print table.attrs._f_list("user")
['temp_scale', 'temperature']
>>> print table.attrs._f_list("sys")
['CLASS', 'FIELD_0_NAME', 'FIELD_1_NAME', 'FIELD_2_NAME', 'FIELD_3_NAME',
    'FIELD_4_NAME', 'FIELD_5_NAME', 'FIELD_6_NAME', 'FIELD_7_NAME', 'NROWS',
    'TITLE', 'VERSION']
```

You can also rename attributes:

```
chapter 3. Tutorials

>>> table.attrs._f_rename("temp_scale","tempScale")
>>> print table.attrs._f_list()
['tempScale', 'temperature']

However, you can't set, delete or rename read-only attributes:
>>> table.attrs._f_rename("VERSION", "version")
Traceback (most recent call last):
    File ">stdin>", line 1, in ?
    File "/home/falted/PyTables/pytables-0.7/tables/AttributeSet.py",
    line 249, in _f_rename
        raise RuntimeError, \
RuntimeError: Read-only attribute ('VERSION') cannot be renamed

If you would terminate your session now, you would be able to use the h5ls command to read the /detector/readout attributes from the file written to disk:

$ h5ls -vr tutorial1.h5/detector/readout
```

```
Opened "tutorial1.h5" with sec2 driver.
/detector/readout Dataset {10/Inf}
Attribute: CLASS scalar
       Type:
               6-byte null-terminated ASCII string
       Data: "TABLE"
   Attribute: VERSION scalar
       Type:
               4-byte null-terminated ASCII string
       Data: "2.0"
   Attribute: TITLE
                       scalar
               16-byte null-terminated ASCII string
       Data: "Readout example"
   Attribute: FIELD_0_NAME scalar
       Type:
                  9-byte null-terminated ASCII string
       Data: "ADCcount"
   Attribute: FIELD 1 NAME scalar
                  9-byte null-terminated ASCII string
       Type:
       Data: "TDCcount"
   Attribute: FIELD_2_NAME scalar
                  7-byte null-terminated ASCII string
       Type:
       Data: "energy"
   Attribute: FIELD_3_NAME scalar
       Type:
               7-byte null-terminated ASCII string
       Data: "grid_i"
   Attribute: FIELD_4_NAME scalar
       Type:
                 7-byte null-terminated ASCII string
       Data: "grid_j"
   Attribute: FIELD 5 NAME scalar
                  9-byte null-terminated ASCII string
       Type:
       Data: "idnumber"
   Attribute: FIELD_6_NAME scalar
                  5-byte null-terminated ASCII string
       Type:
       Data: "name"
   Attribute: FIELD_7_NAME scalar
                  9-byte null-terminated ASCII string
       Data: "pressure"
   Attribute: tempScale scalar
```

```
8-byte null-terminated ASCII string
   Type:
   Data: "Celsius"
Attribute: temperature {1}
   Type:
          native double
   Data: 18.4
Attribute: NROWS
                    {1}
              native int
   Type:
   Data: 10
Location: 0:1:0:1952
Links:
Modified: 2003-07-24 13:59:19 CEST
          {2048} 96256 bytes
Chunks:
Storage:
          470 logical bytes, 96256 allocated bytes, 0.49% utilization
          struct {
Type:
              "ADCcount"
                                 +0
                                      native unsigned short
              "TDCcount"
                                +2
                                      native unsigned char
                                +3
                                      native double
              "energy"
              "grid_i"
                                +11 native int
              grid_j"
                                +15
                                     native int
              "idnumber"
                                +19
                                     native long long
              "name"
                                +27
                                      16-byte null-terminated ASCII string
              "pressure"
                                +43
                                     native float
           } 47 bytes
```

Attributes are a useful mechanism to add persistent (meta) information to your data.

#### 3.2.3 Getting object metadata

Each object in PyTables has *metadata* information about the data in the file. Normally this *metainformation* is accessible through the node instance variables. Let's take a look at some examples:

```
>>> print "Object:", table
Object: /detector/readout Table(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:", table.nrows
Number of rows in table: 10
>>> print "Table variable names with their type and shape:"
Table variable names with their type and shape:
>>> for name in table.colnames:
      print name, ':= %s, %s' % (table.coltypes[name], table.colshapes[name])
. . .
ADCcount := UInt16, 1
TDCcount := UInt8, 1
energy := Float64, 1
grid_i := Int32, 1
grid_j := Int32, 1
idnumber := Int64, 1
name := CharType, 1
pressure := Float32, 1
```

Here, the name, title, nrows, colnames, coltypes and colshapes attributes (see 4.2.1 for a complete attribute list) of the Table object gives us quite a bit of information about the table data.

You can interactively retrieve general information about the public objects in PyTables by printing their internal doc strings:

```
>>> print table.__doc_
Represent a table in the object tree.
    It provides methods to create new tables or open existing ones, as
    well as to write/read data to/from table objects over the
    file. A method is also provided to iterate over the rows without
    loading the entire table or column in memory.
    Data can be written or read both as Row instances or as numarray
    (NumArray or RecArray) objects.
    Methods:
        __getitem__(key)
        __iter__()
         _setitem__(key, value)
        append(rows)
        flushRowsToIndex()
        iterrows(start, stop, step)
        itersequence(sequence)
        modifyRows(start, rows)
        modifyColumns(start, columns, names)
        read([start] [, stop] [, step] [, field [, flavor]])
        reIndex()
        reIndexDirty()
        removeRows(start, stop)
        removeIndex(column)
        where(condition [, start] [, stop] [, step])
        whereIndexed(condition [, start] [, stop] [, step])
        whereInRange(condition [, start] [, stop] [, step])
        getWhereList(condition [, flavor])
    Instance variables:
        description -- the metaobject describing this table
        row -- a reference to the Row object associated with this table
        nrows -- the number of rows in this table
        rowsize -- the size, in bytes, of each row
        cols -- accessor to the columns using a natural name schema
        colnames -- the field names for the table (list)
        coltypes -- the type class for the table fields (dictionary)
        colshapes -- the shapes for the table fields (dictionary)
        colindexed -- whether the table fields are indexed (dictionary)
        indexed -- whether or not some field in Table is indexed
        indexprops -- properties of an indexed Table. Exists only
```

The help function is also a handy way to see PyTables reference documentation online. Try it yourself with other object docs:

if the Table is indexed

```
>>> help(table.__class__)
>>> help(table.removeRows)
```

To examine metadata in the /columns/pressure Array object:

```
>>> pressureObject = h5file.getNode("/columns", "pressure")
>>> print "Info on the object:", repr(pressureObject)
Info on the object: /columns/pressure (Array(3,)) 'Pressure column selection'
    type = Float64
    itemsize = 8
    flavor = 'NumArray'
    byteorder = 'little'
>>> print " shape: ==>", pressureObject.shape
    shape: ==> (3,)
>>> print " title: ==>", pressureObject.title
    title: ==> Pressure column selection
>>> print " type: ==>", pressureObject.type
    type: ==> Float64
```

Observe that we have used the getNode() method of the File class to access a node in the tree, instead of the natural naming method. Both are useful, and depending on the context you will prefer one or the other. getNode() has the advantages that it can get a node from the pathname string (as in this example) and can also act as a filter to show only nodes in a particular location that are instances of class *classname*. In general, however, I consider natural naming to be more elegant and easier to use, especially if you are using the name completion capability present in interactive console. Try this powerful combination of natural naming and completion capabilities present in most Python consoles, and see how pleasant it is to browse the object tree (at least, as pleasant as such an activity can be).

If you look at the type attribute of the pressureObject object, you can verify that it is a "Float64" array. By looking at its shape attribute, you can deduce that the array on disk is unidimensional and has 3 elements. See 4.7.1 or the internal string docs for the complete Array attribute list.

#### 3.2.4 Reading data from Array objects

Once you have found the desired Array, use the read() method of the Array object to retrieve its data:

```
>>> pressureArray = pressureObject.read()
>>> pressureArray
array([ 25., 36.,
                   49.])
>>> print "pressureArray is an object of type:", type(pressureArray)
pressureArray is an object of type: <class 'numarray.numarraycore.NumArray'>
>>> nameArray = h5file.root.columns.name.read()
>>> nameArray
                                                          7′]
['Particle:
                 5', 'Particle:
                                     6', 'Particle:
>>> print "nameArray is an object of type:", type(nameArray)
nameArray is an object of type: <type 'list'>
>>>
>>> print "Data on arrays nameArray and pressureArray:"
Data on arrays nameArray and pressureArray:
>>> for i in range(pressureObject.shape[0]):
      print nameArray[i], "-->", pressureArray[i]
Particle:
               5 --> 25.0
               6 --> 36.0
Particle:
               7 --> 49.0
Particle:
```

```
>>> pressureObject.name
'pressure'
```

You can see that the read() method (see section 4.7.2) returns an authentic numarray object for the pressureObject instance by looking at the output of the type() call. A read() of the nameObject object instance returns a native Python list (of strings). The type of the object saved is stored as an HDF5 attribute (named FLAVOR) for objects on disk. This attribute is then read as Array metainformation (accessible through in the Array.attrs.FLAVOR variable), enabling the read array to be converted into the original object. This provides a means to save a large variety of objects as arrays with the guarantee that you will be able to later recover them in their original form. See section 4.2.2 for a complete list of supported objects for the Array object class.

#### 3.2.5 Appending data to an existing table

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

```
>>> table = h5file.root.detector.readout
>>> particle = table.row
>>> 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)
. . .
        particle.append()
. . .
>>> table.flush()
```

It's the same method we used to fill 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 1.

If you look carefully at the code you will see that we have used the table.row attribute to create a table row and fill it with the new values. Each time that its append() method is called, the actual row is committed to the output buffer and the row pointer is incremented to point to the next table record. When the buffer is full, the data is saved on disk, and the buffer is reused again for the next cycle.

**Caveat emptor**: Do not forget to always call the .flush() method after a write operation, or else your tables will not be updated!

Let's have a look at some rows in the modified table and verify that our new data has been appended:

```
>>> for r in table.iterrows():
        print "%-16s | %11.1f | %11.4g | %6d | %6d | %8d | " % \
           (r['name'], r['pressure'], r['energy'], r['grid_i'], r['grid_j'],
. . .
            r['TDCcount'])
. . .
               0
                                             0 |
                                                                           0 |
Particle:
                            0.0
                                                      0 |
                                                              10 l
Particle:
               1
                            1.0 |
                                            1 |
                                                      1 |
                                                               9 |
                                                                           1 |
Particle:
               2 |
                                          256
                                                      2 |
                                                               8 |
                                                                           2 |
                            4.0
                                                               7 |
               3
Particle:
                            9.0
                                         6561
                                                      3
                                                                           3
```

<sup>&</sup>lt;sup>1</sup> Note that you can append not only scalar values to tables, but also fully multidimensional array objects.

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

#### 3.2.6 And finally... how to delete rows from a table

We'll finish this tutorial by deleting some rows from the table we have. Suppose that we want to delete the the 5th to 9th rows (inclusive):

```
>>> table.removeRows(5,10)
5
```

removeRows(start, stop) (see 4.5.2) deletes the rows in the range (start, stop). It returns the number of rows effectively removed.

We have reached the end of this first tutorial. Don't forget to close the file when you finish:

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

In figure 3.1 you can see a graphical view of the PyTables file with the datasets we have just created. In figure 3.2 are displayed the general properties of the table /detector/readout.

#### 3.3 Multidimensional table cells and automatic sanity checks

Now it's time for a more real-life example (i.e. with errors in the code). We will create two groups that branch directly from the root node, Particles and Events. Then, we will put three tables in each group. In Particles we will put tables based on the Particle descriptor and in Events, the tables based the Event descriptor.

Afterwards, we will provision the tables with a number of records. Finally, we will read the newly-created table /Events/TEvent3 and select some values from it, using a comprehension list.

Look at the next script (you can find it in examples/tutorial2.py). It appears to do all of the above, but it contains some small bugs. Note that this Particle class is not directly related to the one defined in last tutorial; this class is simpler (note, however, the *multidimensional* columns called pressure and temperature).

We also introduce a new manner to describe a Table as a dictionary, as you can see in the Event description. See section 4.2.2 about the different kinds of descriptor objects that can be passed to the createTable() method.

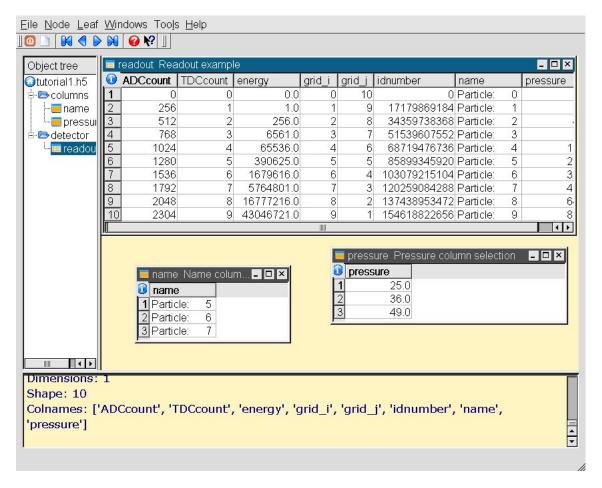
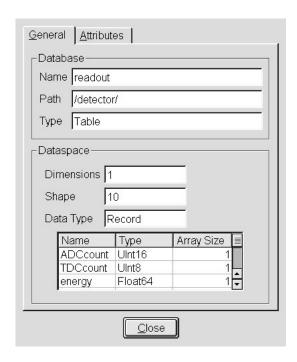


Figure 3.1: The final version of the data file for tutorial 1, with a view of the data objects.



**Figure 3.2:** General properties of the /detector/readout table.

```
lati
              = IntCol()
                                       # integer
    longi
              = IntCol()
                                       # integer
    pressure = Float32Col(shape=(2,3)) # array of floats (single-precision)
    temperature = FloatCol(shape=(2,3))  # array of doubles (double-precision)
# Another way to describe the columns of a table
Event = {
    "name"
             : Col('CharType', 16), # 16-character String
    "TDCcount": Col("UInt8", 1),
                                      # unsigned byte
                                     # Unsigned short integer
    "ADCcount": Col("UInt16", 1),
    "xcoord" : Col("Float32", 1),
                                      # integer
                                    # integer
    "ycoord" : Col("Float32", 1),
    }
# 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 the 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.row
    # Fill the table with data for 257 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
        ######### Detectable errors start here. Play with them!
        particle['pressure'] = array(i*arange(2*3), shape=(2,4)) # Incorrect
        #particle['pressure'] = array(i*arange(2*3), shape=(2,3)) # Correct
        ######## End of errors
        particle['temperature'] = (i**2)
                                             # Broadcasting
        # This injects the Record values
        particle.append()
    # Flush the table buffers
    table.flush()
# Now Events:
for tablename in ("TEvent1", "TEvent2", "TEvent3"):
    # Create a table in the Events group
    table = fileh.createTable(root.Events, tablename, Event,
                          "Events: "+tablename)
    # Get the record object associated with the table:
    event = table row
    # Fill the table with data on 257 events
```

```
for i in xrange(257):
        # First, assign the values to the Event record
        event['name'] = 'Event: %6d' % (i)
        event['TDCcount'] = i % (1<<8)</pre>
                                        # Correct range
        ######### Detectable errors start here. Play with them!
        #event['xcoord'] = float(i**2) # Correct spelling
        event['xcoor'] = float(i**2)
                                       # Wrong spelling
        event['ADCcount'] = i * 2
                                        # Correct type
        #event['ADCcount'] = "sss"
                                            # Wrong type
        ######## End of errors
        event['ycoord'] = float(i)**4
        # This injects the Record values
        event.append()
    # 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
      if p['ADCcount'] < 20 and 4 <= p['TDCcount'] < 15 ]</pre>
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()
```

#### 3.3.1 Shape checking

If you look at the code carefully, you'll see that it won't work. You will get the following error:

```
$ python tutorial2.py
Traceback (most recent call last):
   File "tutorial2.py", line 53, in ?
     particle['pressure'] = array(i*arange(2*3), shape=(2,4)) # Incorrect
   File "/usr/local/lib/python2.2/site-packages/numarray/numarraycore.py",
   line 281, in array
   a.setshape(shape)
   File "/usr/local/lib/python2.2/site-packages/numarray/generic.py",
   line 530, in setshape
     raise ValueError("New shape is not consistent with the old shape")
ValueError: New shape is not consistent with the old shape
```

This error indicates that you are trying to assign an array with an incompatible shape to a table cell. Looking at the source, we see that we were trying to assign an array of shape (2,4) to a pressure element, which was defined with the shape (2,3).

In general, these kinds of operations are forbidden, with one valid exception: when you assign a *scalar* value to a multidimensional column cell, all the cell elements are populated with the value of the scalar. For example:

```
particle['temperature'] = (i**2) # Broadcasting
```

The value i\*\*2 is assigned to all the elements of the temperature table cell. This capability is provided by the numarray package and is known as *broadcasting*.

#### 3.3.2 Field name checking

After fixing the previous error and rerunning the program, we encounter another error:

```
$ python tutorial2.py
Traceback (most recent call last):
   File "tutorial2.py", line 74, in ?
     event['xcoor'] = float(i**2)  # Wrong spelling
   File "/home/falted/PyTables/pytables-0.8/src/hdf5Extension.pyx",
   line 1812, in hdf5Extension.Row.__setitem__
     raise KeyError, "Error setting \"%s\" field.\n %s" % \
KeyError: Error setting "xcoor" field.
Error was: "exceptions.KeyError: xcoor"
```

This error indicates that we are attempting to assign a value to a non-existent field in the *event* table object. By looking carefully at the Event class attributes, we see that we misspelled the xcoord field (we wrote xcoor instead). This is unusual behavior for Python, as normally when you assign a value to a non-existent instance variable, Python creates a new variable with that name. Such a feature can be dangerous when dealing with an object that contains a fixed list of field names. PyTables checks that the field exists and raises a KeyError if the check fails.

#### 3.3.3 Data type checking

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

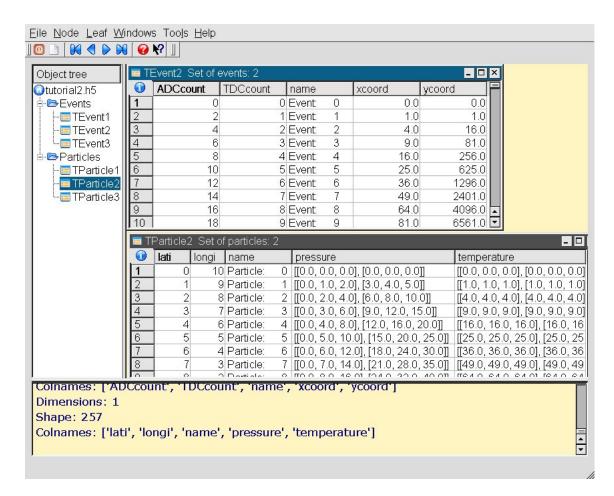
```
event.ADCcount = i * 2  # Correct type
to read:
    event.ADCcount = "sss"  # Wrong type
```

This modification will cause the following TypeError exception to be raised when the script is executed:

```
$ python tutorial2.py
Traceback (most recent call last):
   File "tutorial2.py", line 76, in ?
      event['ADCcount'] = "sss"  # Wrong type
   File "/home/falted/PyTables/pytables-0.8/src/hdf5Extension.pyx",
   line 1812, in hdf5Extension.Row.__setitem__
      raise KeyError, "Error setting \"%s\" field.\n %s" % \
KeyError: Error setting "ADCcount" field.
Error was: "exceptions.TypeError: NA_setFromPythonScalar: bad value type."
```

You can see the structure created with this (corrected) script in figure 3.3. In particular, note the multidimensional column cells in table /Particles/TParticle2.

Feel free to examine the rest of examples in directory examples, and try to understand them. I've written several practical sample scripts to give you an idea of the PyTables capabilities, its way of dealing with HDF5 objects, and how it can be used in the real world.



**Figure 3.3:** Table hierarchy for tutorial 2.

# **Chapter 4**

# **Library Reference**

PyTables implements several classes to represent the different nodes in the object tree. They are named File, Group, Leaf, Table, Array, EArray, VLArray and UnImplemented. Another one allows the user to complement the information on these different objects; its name is AttributeSet. Finally, another important class called IsDescription allows to build a Table record description by declaring a subclass of it. Many other classes are defined in PyTables, but they can be regarded as helpers whose goal is mainly to declare the *data type properties* of the different first class objects and will be described at the end of this chapter as well.

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 the user supplied file is a *PyTables* or *HDF5* file. These are called isPyTablesFile and isHDF5, respectively. Finally, there exists a function called whichLibVersion that informs about the versions of the underlying C libraries (for example, the HDF5 or the Zlib).

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

## 4.1 tables variables and functions

## 4.1.1 Global variables

\_\_version\_\_ The PyTables version number.

**ExtVersion** The version of the Pyrex extension module. This might be useful when reporting bugs.

**HDF5Version** The underlying HDF5 library version number.

## 4.1.2 Global functions

copyFile(srcFilename=None, dstFilename=None, title=None, filters=None, copyuserattrs=1, overwrite=0)

Copy a closed PyTables (or generic HDF5) file specified by *srcFilename* to *dstFilename*. Returns a tuple in the form (ngroups, nleaves, nbytes) specifiying the number of groups, leaves and bytes copied.

title The title for the new file. If not specified, the source file title will be copied.

**filters** A Filters instance (see 4.13.1). If specified, it will override the original filter properties in **all** source nodes.

**copyuserattrs** You can prevent the user attributes from being copied by setting this parameter to 0. The default is to copy them.

**overwrite** If dstFilename file already exists and overwrite is 1, it will be silently overwritten. The default is not overwriting.

## isHDF5(filename)

Determines whether filename is in the HDF5 format or not. 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.

## openFile(filename, mode='r', title=", trMap={}, rootUEP="/", filters=None)

Open a PyTables (or generic HDF5) file and returns a File object.

**filename** The name of the file (supports environment variable expansion). It is suggested that it should have any of ".h5", ".hdf" or ".hdf5" extensions, although this is not mandatory.

**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 would be 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.
- **trMap** A dictionary to map names in the object tree Python namespace into different HDF5 names in file namespace. The keys are the Python names, while the values are the HDF5 names. This is useful when you need to use HDF5 node names with invalid or reserved words in Python.
- rootUEP The root User Entry Point. This is a group in the HDF5 hierarchy which will be taken as the starting point to create the object tree. The group has to be named after its HDF5 name and can be a path. If it does not exist, a RuntimeError exception is issued. Use this if you do not want to build the entire object tree, but rather only a subtree of it.
- filters An instance of the Filters class (see section 4.13.1) that provides information about the desired I/O filters applicable to the leaves that hangs directly from *root* (unless other filters properties are specified for these leaves). Besides, if you do not specify filter properties for its child groups, they will inherit these ones. So, if you open a new file with this parameter set, all the leaves that would be created in the file will recursively inherit this filtering properties (again, if you don't prevent that from happening by specifying other filters on the child groups or leaves).

## whichLibVersion(libname)

Returns info about versions of the underlying C libraries. **libname** can be whether "hdf5", "zlib", "lzo" or "ucl". It always returns a tuple of 3 elements. When successful, the first element of this tuple has a positive value, and is 0 (zero) when library is not available (for example LZO or UCL). In case the library is available, the second element of tuple contains the library version and the third element the date (if available) of that version.

## 4.2 The File class

This class is returned when a PyTables file is opened with the openFile function. It has methods to flush and close files. Also, the File class offers methods to create, rename and delete nodes, as well as to traverse the object tree. One of its attributes (rootUEP) represents the *user entry point* to the object tree attached to the file.

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

#### 4.2.1 File instance variables

filename Filename opened.

format\_version The PyTables version number of this file.

**isopen** It takes the value 1 if the underlying file is open. 0 otherwise.

**mode** Mode in which the filename was opened.

root The root of the object tree hierarchy. It is a Group instance.

rootUEP The UEP (User Entry Point) group in file (see 4.1.2).

**title** The title of the root group in file.

**trMap** This is a dictionary that maps node names between python and HDF5 domain names. Its initial values are set from the *trMap* parameter passed to the openFile function. You can change its contents *after* a file is opened and the new map will take effect over any new object added to the tree.

**filters** Container for filter properties associated to this file. See section 4.13.1 for more information on this object.

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

groups Dictionary with all object groups on tree.

leaves Dictionary with all object leaves on tree.

## 4.2.2 File methods

copyChildren(whereSrc, whereDst, recursive=0, filters=None, copyuserattrs=1, start=0, stop=None, step=1, overwrite = 0)

Copy (recursively) the children of a group into another location. Returns a tuple in the form (ngroups, nleaves, nbytes) specifiying the number of groups, leaves and bytes copied.

where Src The parent group where the children to be copied are hanging on. This parameter can be a path string (for example "/level1/group5"), or another Group instance.

whereDst The parent group where the source children will be copied to. This group must exist or a LookupError will be issued. This parameter can be a path string (for example "/level1/group6"), or another Group instance.

recursive Specifies whether the copy should recurse into subgroups or not. The default is not recurse.

**filters** Whether or not override the original filter properties present in source nodes. This parameter must be an instance of the Filters class (see section 4.13.1). The default is to copy the filter attributes from source children.

**copyuserattrs** You can prevent the user attributes from being copied by setting this parameter to 0. The default is to copy them.

 $<sup>^{1}</sup>$  On the following, the term Leaf will refer to either a Table, Array, EArray, VLArray or UnImplemented node object.

start, stop, step Specifies the range of rows in child leaves to be copied; the default is to copy all the rows.

**overwrite** Whether the possible existing children hanging from whereDst and having the same names than whereSrc children should overwrite the destination nodes or not.

## copyFile(dstFilename=None, title=None, filters=None, copyuserattrs=1, overwrite=0)

Copy the contents of this file to *dstFilename*. If the filename already exists it won't be overwritten unless *overwrite* is set to true (see later). Returns a tuple in the form (ngroups, nleaves, nbytes) specifying the number of groups, leaves and bytes copied.

title The title for the new file. If not specified, the source file title will be copied.

**filters** Whether or not override the original filter properties present in source nodes. This parameter must be an instance of the Filters class (see section 4.13.1). The default is to copy the filter attributes from source children.

**copyuserattrs** You can prevent the user attributes from being copied by setting this parameter to 0. The default is to copy them.

**copyuserattrs** You can prevent the user attributes from being copied by setting this parameter to 0. The default is to copy them.

**overwrite** Whether overwrite or not the possibly existing *dstFilename* file. The default is not overwrite it.

## createGroup(where, name, title="', filters=None)

Create a new Group instance with name name in where location.

where The parent group where the new group will hang from. *where* parameter can be a path string (for example "/level1/group5"), or another Group instance.

name The name of the new group.

title A description for this group.

filters An instance of the Filters class (see section 4.13.1) that provides information about the desired I/O filters applicable to the leaves that hangs directly from this new group (unless other filters properties are specified for these leaves). Besides, if you do not specify filter properties for its child groups, they will inherit these ones.

## createTable(where, name, description, title=", filters=None, expectedrows=10000)

Create a new Table instance with name name in where location.

where The parent group where the new table will hang from. where parameter can be a path string (for example "/level1/leaf5"), or Group instance.

name The name of the new table.

description An instance of a user-defined class (derived from the IsDescription class) where table fields are defined. However, in certain situations, it is more handy to allow this description to be supplied as a dictionary (for example, when you do not know beforehand which structure will have your table). In such a cases, you can pass the description as a dictionary as well. See section 3.3 for an example of use. Finally, a Recarray object from the numarray package is also accepted, and all the information about columns and other metadata is used as a basis to create the Table object. Moreover, if the Recarray has actual data this is also injected on the newly created Table object.

title A description for this object.

**filters** An instance of the Filters class (see section 4.13.1) that provides information about the desired I/O filters to be applied during the life of this object.

**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 10 MB in size (more or less). 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 6.1 for a discussion on that issue.

## createArray(where, name, object, title=")

Create a new Array instance with name name in where location.

**object** The regular array to be saved. Currently accepted values are: lists, tuples, scalars (int and float), strings and (multidimensional) Numeric and NumArray arrays (including CharArrays string arrays). However, these objects must be regular (i.e. they cannot be like, for example, [[1,2],2]). Also, objects that have some of their dimensions equal to zero are not supported (use an EArray object if you want to create an array with one of its dimensions equal to 0).

See createTable description 4.2.2 for more information on the where, name and title, parameters.

## createEArray(where, name, atom, title=", filters=None, expectedrows=1000)

Create a new EArray instance with name *name* in *where* location.

**atom** An Atom instance representing the *shape*, *type* and *flavor* of the atomic objects to be saved. One (and only one) of the shape dimensions **must** be 0. The dimension being 0 means that the resulting EArray object can be extended along it. Multiple enlargeable dimensions are not supported right now. See section 4.12.3 for the supported set of Atom class descendants.

**expectedrows** In the case of enlargeable arrays this represents an user estimate about the number of row elements that will be added to the growable dimension in the EArray object. If not provided, the default value is 1000 rows. If you plan to create both much smaller or much bigger EArrays try providing a guess; this will optimize the HDF5 B-Tree creation and management process time and the amount of memory used.

See createTable description 4.2.2 for more information on the *where*, *name*, *title*, and *filters* parameters.

## createVLArray(where, name, atom=None, title=", filters=None, expectedsizeinMB=1.0)

Create a new VLArray instance with name *name* in *where* location. See the section 4.9 for a description of the VLArray class.

**atom** An Atom instance representing the shape, type and flavor of the atomic object to be saved. See section 4.12.3 for the supported set of Atom class descendants.

**expectedsizeinMB** An user estimate about the size (in MB) in the final VLArray object. If not provided, the default value is 1 MB. If you plan to create both much smaller or much bigger VLA's try providing a guess; this will optimize the HDF5 B-Tree creation and management process time and the amount of memory used.

See createTable description 4.2.2 for more information on the *where*, *name*, *title*, and *filters* parameters.

## 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 already 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. Possible values are: 'Group', 'Leaf', 'Table', 'Array', 'EArray', 'VLArray' and 'UnImplemented'. Note that these values are strings.

## getAttrNode(where, attrname, name="')

Returns the attribute attrname under where.name 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.

attrname The name of the attribute to get.

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

#### setAttrNode(where, attrname, attrvalue, name=")

Sets the attribute attrname with value attrvalue under where.name 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.

attrname The name of the attribute to set on disk.

attrvalue The value of the attribute to set. Any scalar (string, ints or floats) attribute is supported natively. However, (c)Pickle is automatically used so as to serialize other kind of objects (like lists, tuples, dicts, small Numeric/numarray objects, ...) that you might want to save.

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

#### delAttrNode(where, attrname, name = "")

Delete the attribute attrname in where.name 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.

attrname The name of the attribute to delete on disk.

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

## listNodes(where, classname=")

Returns a list with all the object nodes (Group or Leaf) hanging from *where*. The list is alpha-numerically 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', 'Array', 'EArray', 'VLArray' and 'UnImplemented'. Note that these values are strings.

## removeNode(where, name = "", recursive=0)

Removes 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 LookupError error is raised.

**name** The name of the node to be removed. If not provided, the *where* node is changed.

**recursive** If not supplied, the object will be removed only if it has no children. If supplied with a true value, the object and all its descendants will be completely removed.

#### renameNode(where, newname, name)

Rename 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 LookupError error is raised.

**newname** Is the new name to be assigned to the node.

**name** The name of the node to be changed. If not provided, the *where* node is changed.

## walkGroups(where='/')

*Iterator* that returns the list of Groups (not Leaves) hanging from *where*. If *where* is not supplied, the root object is taken as origin. The returned Group list is in a top-bottom order, and alpha-numerically sorted when they are at the same level.

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

```
walkNodes(where="/", classname="")
```

Recursively iterate over the nodes in the File instance. It takes two parameters:

where If supplied, the iteration starts from this group.

**classname** (String) If supplied, only instances of this class are returned.

Example of use:

```
# Recursively print all the nodes hanging from '/detector'
print "Nodes hanging from group '/detector':"
for node in h5file.walkNodes("/detector"):
    print node
```

## flush()

Flush all the leaves in the object tree.

## close()

Flush all the leaves in object tree and close the file.

## 4.2.3 File special methods

Following are described the methods that automatically trigger actions when a File instance is accessed in a special way.

```
__iter__()
```

Iterate over the children on the File instance. However, this does not accept parameters. This iterator *is recursive*.

Example of use:

```
# Recursively list all the nodes in the object tree
h5file = tables.openFile("vlarray1.h5")
print "All nodes in the object tree:"
for node in h5file:
    print node
```

#### \_\_str\_\_()

Prints a short description of the File object.

Example of use:

```
>>> f=tables.openFile("data/test.h5")
>>> print f
data/test.h5 (File) 'Table Benchmark'
Last modif.: 'Mon Sep 20 12:40:47 2004'
Object Tree:
/ (Group) 'Table Benchmark'
/tuple0 (Table(100L,)) 'This is the table title'
/group0 (Group) ''
/group0/tuple1 (Table(100L,)) 'This is the table title'
/group0/group1 (Group) ''
/group0/group1/tuple2 (Table(100L,)) 'This is the table title'
/group0/group1/group2 (Group) ''
```

\_\_repr\_\_()

Prints a detailed description of the File object.

## 4.3 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 a string (like in '/group1/group2') or as a complete object path written in *natural name* schema (like in file.root.group1) as 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 variable 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 some reserved prefixes, like "\_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.

Other effect is that you cannot use reserved Python names or other non-allowed python names (like for example "\$a" or "44") as node names. You can, however, make use of the trMap (translation map dictionary) parameter in the openFile function (see section 4.1.2) in order to use non-valid Python names as node names in the file.

## 4.3.1 Group instance variables

- \_v\_title A description for this group.
- \_v\_name The name of this group.
- \_v\_hdf5name The name of this group in HDF5 file namespace.
- \_v\_pathname A string representation of the group location in tree.
- \_v\_parent The parent Group instance.
- \_v\_rootgroup Pointer to the root group object.
- \_v\_file Pointer to the associated File object.
- \_v\_depth The depth level in tree for this group.
- \_v\_nchildren The number of children (groups or leaves) hanging from this instance.
- \_v\_children Dictionary with all nodes (groups or leaves) hanging from this instance.
- \_v\_groups Dictionary with all node groups hanging from this instance.
- \_v\_leaves Dictionary with all node leaves hanging from this instance.
- \_v\_attrs The associated AttributeSet instance (see 4.11).
- \_v\_filters Container for filter properties. See section 4.13.1 for more information on this object.

## 4.3.2 Group methods

This class define the \_\_setattr\_\_, \_\_getattr\_\_ and \_\_delattr\_\_ and they work as normally intended. So, you can access, assign or delete children to a group by just using the next constructs:

```
# Add a Table child instance under group with name "tablename"
group.tablename = Table(recordDict, "Record instance")
table = group.tablename  # Get the table child instance
del group.tablename  # Delete the table child instance
```

**Caveat:** The following 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\_rename(newname)

Change the name of this group to newname.

## \_f\_remove(recursive=0)

Remove this object. If recursive is true, force the removal even if this group has children.

## \_f\_getAttr(attrname)

Gets the HDF5 attribute attrname of this group.

#### \_f\_setAttr(attrname, attrvalue)

Sets the attribute *attrname* of this group to the value *attrvalue*. Any scalar (string, ints or floats) attribute is supported natively. However, (c)Pickle is automatically used so as to serialize other kind of objects (like lists, tuples, dicts, small Numeric/numarray objects, ...) that you might want to save.

#### \_f\_delAttr(attrname)

Delete the attribute *attrname* of this group.

## \_f\_listNodes(classname="')

Returns a *list* with all the object nodes hanging from this instance. The list is alpha-numerically 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', 'EArray', 'VLArray' and 'UnImplemented'.

## \_f\_walkGroups()

Iterate over the list of Groups (not Leaves) hanging from *self*. The returned Group list is in a top-bottom order, and alpha-numerically sorted when they are at the same level.

## \_f\_walkNodes(classname="", recursive=0)

Iterate over the nodes in the Group instance. It takes two parameters:

**classname** (String) If supplied, only instances of this class are returned.

**recursive** (*Integer*) If false, only children hanging immediately after the group are returned. If true, a recursion over all the groups hanging from it is performed.

Example of use:

```
# Recursively print all the arrays hanging from '/'
print "Arrays the object tree '/':"
for array in h5file.root._f_walkNodes("Array", recursive=1):
    print array
```

## \_f\_close()

Close this group, making it and its children unaccessible in the object tree.

# \_f\_copyChildren(where, recursive=0, filters=None, copyuserattrs=1, start=0, stop=None, step=1, overwrite=0)

Copy (recursively) the children of this group into another location specified by *where* (it can be a path string or a Group object). Returns a tuple in the form (ngroups, nleaves, nbytes) specifying the number of groups, leaves and bytes copied.

recursive Specifies whether the copy should recurse into subgroups or not. The default is not recurse.

**filters** Whether or not override the original filter properties present in source nodes. This parameter must be an instance of the Filters class (see section 4.13.1). The default is to copy the filter attributes from source children.

**copyuserattrs** You can prevent the user attributes from being copied by setting this parameter to 0. The default is to copy them.

start, stop, step Specifies the range of rows in child leaves to be copied; the default is to copy all the rows.

**overwrite** Whether the possible existing children hanging from this group and having the same names than where children should overwrite the destination nodes or not.

## 4.3.3 Group special methods

Following are described the methods that automatically trigger actions when a Group instance is accessed in a special way.

```
__iter__()
```

Iterate over the children on the group instance. However, this does not accept parameters. This iterator is **not** recursive.

Example of use:

```
# Non-recursively list all the nodes hanging from '/detector'
print "Nodes in '/detector' group:"
for node in h5file.root.detector:
    print node
```

```
__str__()
```

Prints a short description of the Group object.

Example of use:

```
>>> f=tables.openFile("data/test.h5")
>>> print f.root.group0
/group0 (Group) 'First Group'
>>>
```

```
__repr__()
```

Prints a detailed description of the Group object.

Example of use:

```
>>> f=tables.openFile("data/test.h5")
>>> f.root.group0
/group0 (Group) 'First Group'
  children := ['tuple1' (Table), 'group1' (Group)]
>>>
```

## 4.4 The Leaf class

The goal of this class is to provide a place to put common functionality of all its descendants as well as provide a way to help classifying objects on the tree. 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 and, thus, it cannot have descendents. Right now, the set of end-nodes is composed by Table, Array, EArray, VLArray and UnImplemented class instances. In fact, all the previous classes inherit from the Leaf class.

## 4.4.1 Leaf instance variables

The public variables and methods that class descendants inherits from Leaf are listed below.

name The Leaf node name in Python namespace.

**hdf5name** The Leaf node name in HDF5 namespace.

**objectID** The HDF5 object ID of the Leaf node.

title The Leaf title (actually a property rather than a plain attribute).

shape The shape of the associated data in the Leaf.

byteorder The byteorder of the associated data of the Leaf.

attrs The associated AttributeSet instance (see 4.11).

filters Container for filter properties. See section 4.13.1 for more information on this object.

Besides, the next instance variables are also defined and have similar meaning as its counterparts in the Group class:

- \_v\_hdf5name The name of this leaf in HDF5 file namespace.
- \_v\_pathname A string representation of the leaf location in tree.
- \_v\_parent The parent Group instance.
- \_v\_rootgroup Pointer to the root Group object.
- \_v\_file Pointer to the associated File object.
- \_v\_depth The depth level in tree for this leaf.

## 4.4.2 Leaf methods

copy(where, name, title=None, filters=None, copyuserattrs=1, start=0, stop=None, step=1, overwrite=0)

Copy this leaf into another location. It returns a tuple (object, nbytes) where object is the newly created object and nbytes is the number of bytes copied. The meaning of the parameters is explained below:

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

name The name of the destination node.

title The new title for destination. If None, the original title is copied.

**filters** An instance of the Filters (see section 4.13.1) class. A None value means that the source properties are copied *as is*.

**copyuserattrs** Whether copy the user attributes of the source leaf to the destination or not. The default is to copy them.

start, stop, step Specifies the range of rows to be copied; the default is to copy all the rows.

**overwrite** If the destination node *name* already exists this specifies whether it should be overwritten or not. The default is not overwrite it.

## remove()

Remove this leaf.

#### rename(newname)

Change the name of this leaf to newname.

#### getAttr(attrname)

Gets the HDF5 attribute attrname of this leaf.

## setAttr(attrname, attrvalue)

Sets the attribute *attrname* of this leaf to the value *attrvalue*.

#### delAttr(attrname)

Delete the HDF5 attribute attrname of this leaf.

#### flush()

Flush the leaf buffers (if any).

## close()

Flush the leaf buffers (if any) and close the dataset.

## 4.5 The Table class

Instances of this class represents table objects in the object tree. It provides methods to read/write data and from/to table objects in the file.

Data can be read from or written to tables by accessing to an special object that hangs from Table. This object is an instance of the Row class (see 4.5.4). See the tutorial sections chapter 3 on how to use the Row interface. The columns of the tables can also be easily accessed (and more specifically, they can be read but not written) by making use of the Column class, through the use of an *extension* of the natural naming schema applied inside the tables. See the section 4.6 for some examples of use of this capability.

Note that this object inherits all the public attributes and methods that Leaf already has.

## 4.5.1 Table instance variables

description The metaobject describing this table.

**row** The Row instance for this table (see 4.5.4).

**nrows** The number of rows in this table.

**rowsize** The size, in bytes, of each row.

cols A Cols (see section 4.5.5) instance that serves as accessor to Column (see section 4.6) objects.

colnames The field names for the table (list).

**coltypes** The data types for the table fields (dictionary).

**colshapes** The shapes for the table fields (dictionary).

colindexed Whether the table fields are indexed (dictionary).

indexed Whether the table fields are indexed (dictionary).

**indexprops** Properties of an indexed Table (see 4.13.2). This attribute (dictionary) exists only if the Table is indexed.

## 4.5.2 Table methods

#### append(rows=None)

Append a series of rows to this Table instance. *rows* is an object that can keep the rows to be append in several formats, like a RecArray, a list of tuples, list of Numeric/NumArray/CharArray objects, string, Python buffer or None (no append will result). Of course, this *rows* object has to be compliant with the underlying format of the Table instance or a ValueError will be issued.

Example of use:

```
from tables import *
class Particle(IsDescription):
   name = StringCol(16, pos=1) # 16-character String
                                   # integer
   lati
             = IntCol(pos=2)
   longi
             = IntCol(pos=3)
                                    # integer
   pressure = Float32Col(pos=4)
                                    # float (single-precision)
   temperature = FloatCol(pos=5)
                                     # double (double-precision)
fileh = openFile("test4.h5", mode = "w")
table = fileh.createTable(fileh.root, 'table', Particle, "A table")
# Append several rows in only one call
                         10", 10, 0, 10*10, 10**2),
table.append([("Particle:
                            11", 11, -1, 11*11, 11**2),
             ("Particle:
             ("Particle:
                            12", 12, -2, 12*12, 12**2)])
fileh.close()
```

## iterrows(start=None, stop=None, step=1)

Returns an iterator yielding Row (see section 4.5.4) instances built from rows in table. If a range is supplied (i.e. some of the *start*, *stop* or *step* parameters are passed), only the appropriate rows are returned. Else, all the rows are returned. See also the \_\_iter\_\_() special method in section 4.5.3 for a shorter way to call this iterator.

The meaning of the *start*, *stop* and *step* parameters is the same as in the range() python function, except that negative values of step are not allowed. Moreover, if only start is specified, then stop will be set to start+1. If you do not specify neither *start* nor *stop*, then **all the rows** in the object are selected.

Example of use:

#### itersequence(sequence=None)

Iterate over a *sequence* of row coordinates. *sequence* can be any object that supports the \_\_getitem\_\_ special method, like lists, tuples, Numeric/numarray objects, etc.

## read(start=None, stop=None, step=1, field=None, flavor="numarray")

Returns the actual data in Table. If *field* is not supplied, it returns the data as a RecArray object table.

The meaning of the *start*, *stop* and *step* parameters is the same as in the range() python function, except that negative values of step are not allowed. Moreover, if only start is specified, then stop will be set to start+1. If you do not specify neither *start* nor *stop*, then all the rows in the object are selected.

The rest of the parameters are described next:

**field** If specified, only the column *field* is returned as a NumArray object. If this is not supplied, all the fields are selected and a RecArray is returned.

**flavor** When a field in table is selected, passing a *flavor* parameter make an additional conversion to happen in the default "numarray" returned object. *flavor* must have any of the next values: "numarray" (i.e. no conversion is made), "Numeric", "Tuple" or "List".

## modifyRows(start=None, stop=None, step=1, rows=None)

Modify a series of rows in the [start:stop:step] extended slice range. If you pass None to stop, all the rows existing in rows will be used.

rows can be either a RecArray object or a structure that is able to be converted to a RecArray and compliant with the table format.

Returns the number of modified rows.

It raises an ValueError in case the rows parameter could not be converted to an object compliant with table description.

It raises an IndexError in case the modification will exceed the length of the table.

## modifyColumns(start=None, stop=None, step=1, columns=None, names=None)

Modify a series of rows in the [start:stop:step] extended slice row range. If you pass None to stop, all the rows existing in columns will be used.

columns can be either a RecArray or a list of arrays (the columns) that is able to be converted to a RecArray compliant with the specified column *names* subset of the table format.

names specifies the column names of the table to be modified.

Returns the number of modified rows.

It raises an ValueError in case the *columns* parameter could not be converted to an object compliant with table description.

It raises an IndexError in case the modification will exceed the length of the table.

## removeRows(start=None, stop=None)

Removes a range of rows in the table. If only *start* is supplied, this row is to be deleted. If a range is supplied, i.e. both the *start* and *stop* parameters are passed, all the rows in the range are removed. A *step* parameter is not supported, and it is not foreseen to implement it anytime soon.

**start** Sets the starting row to be removed. It accepts negative values meaning that the count starts from the end. A value of 0 means the first row.

**stop** Sets the last row to be removed to *stop* - 1, i.e. the end point is omitted (in the Python range tradition). It accepts, likewise *start*, negative values. A special value of None (the default) means removing just the row supplied in start.

## removeIndex(index=None)

Remove the index associated with the specified column. Only Index instances (see 4.13.3) are accepted as parameter. This index can be recreated again by calling the createIndex (see 4.6.2) method of the appropriate Column object.

## flushRowsToIndex()

Add remaining rows in buffers to non-dirty indexes. This can be useful when you have chosen non-automatic indexing for the table (see section 4.13.2) and want to update the indexes on it.

## reIndex()

Recompute all the existing indexes in table. This can be useful when you suspect that, for any reason, the index information for columns is no longer valid and want to rebuild the indexes on it.

## reIndexDirty()

Recompute the existing indexes in table, but *only* if they are dirty. This can be useful when you have set the reindex parameter to 0 in IndexProps constructor (see 4.13.2) for the table and want to update the indexes after a invalidating index operation (Table.removeRows, for example).

## where(condition, start=None, stop=None, step=None)

Returns an iterator yielding Row (see section 4.5.4) instances built from rows in table that satisfy a *condition* over a column. If the column to which the condition is applied is indexed, this index will be used in order to accelerate the search. Else, the *in-kernel* iterator (with better performance than the regular iterator) will be choosed instead.

Moreover, if a range is supplied (i.e. some of the *start*, *stop* or *step* parameters are passed), only the rows in that range *and* fullfilling the *condition* are returned. Else, all the rows that fullfill the *condition* are returned.

The meaning of the *start*, *stop* and *step* parameters is the same as in the range() python function, except that negative values of step are not allowed. Moreover, if only start is specified, then stop will be set to start+1. If you do not specify neither *start* nor *stop*, then **all the rows** that fullfill the *condition* are selected.

You can mix this method with regular selections in order to have complex queries. It is strongly recommended that you pass the most restrictive condition as the parameter to this method if you want to achieve maximum performance.

Example of use:

```
passvalues=[]
for row in table.iterrows(0>table.cols.col1<0.3, step=5):
    if row['var1'] <= 20:
        passvalues.append(row['var2'])
print "Values that passes the cuts:", passvalues</pre>
```

See also the whereIndexed and whereInRange methods below for more specific ways to call this iterator.

## whereIndexed(condition, start=None, stop=None, step=None)

Iterator that selects values fulfilling the *condition* parameter. This *only* works for conditions over a *indexed* column. If you try to use it over non-indexed column, an AssertionError will be raised.

The meaning of the *condition*, *start*, *stop* and *step* parameters is the same as in the where method (see 4.5.2) described above.

## whereInRange(condition, start=None, stop=None, step=None)

Iterator that selects values fulfilling the *condition* parameter. This method will use the *in-kernel* search method, i.e. it won't take advantage of a possible indexed column.

The meaning of the *condition*, *start*, *stop* and *step* parameters is the same as in the where method (see 4.5.2) described above.

## getWhereList(condition, flavor="List")

Get the row coordinates that fulfill the *condition* param. This method will take advantage of an indexed column to speed-up the search.

flavor is the desired type of the returned list. It can take the 'List' (the default), 'Tuple' or 'NumArray' values.

## 4.5.3 Table special methods

Following are described the methods that automatically trigger actions when a Table instance is accessed in a special way (e.g., table["var2"] will be equivalent to a call to table.\_\_getitem\_\_("var2")).

```
__iter__()
```

It returns the same iterator than Table.iterrows(0,0,1). However, this does not accept parameters. Example of use:

Which is equivalent to:

```
__getitem__(key)
```

It takes different actions depending on the type of the key parameter:

key is an Integer The corresponding table row is returned as a RecArray. Record object.

**key is a Slice** The row slice determined by key is returned as a RecArray object.

**key is a String** The key is interpreted as a *column* name of the table, and, if it exists, it is read and returned as a NumArray or CharArray object (whatever is appropriate).

Example of use:

```
record = table[4]
recarray = table[4:1000:2]
narray = table["var2"]
```

Which is equivalent to:

```
record = table.read(start=4)[0]
recarray = table.read(start=4, stop=1000, step=2)
narray = table.read(field="var2")
```

```
__setitem__(key, value)
```

It takes different actions depending on the type of the  ${\tt key}$  parameter:

**key is an Integer** The corresponding table row is set to *value*. *value* must be a List or Tuple capable of being converted to the table field format.

**key is a Slice** The row slice determined by key is set to *value*. *value* must be a RecArray object or a list of rows capable of being converted to the table field format.

Example of use:

Which is equivalent to:

## 4.5.4 The Row class

This class is used to fetch and set values on the table fields. It works very much like a dictionary, where the keys are the field names of the associated table and the values are the values of those fields in a specific row.

This object turns out to actually be an extension type, so you won't be able to access its documentation interactively. Neither you won't be able to access its internal attributes (they are not directly accessible from Python), although *accessors* (i.e. methods that return an internal attribute) have been defined for the most important variables.

#### **Row methods**

**append()** Once you have filled the proper fields for the current row, calling this method actually commits these data to the disk (actually data are written to the output buffer).

**nrow**() Accessor that returns the current row number in the table. It is useful to know which row is being dealt with in the middle of a loop.

## 4.5.5 The Cols class

This class is used as an *accessor* to the table columns following the natural name convention, so that you can access the different columns because there exist one attribute with the name of the columns for each associated Column instances. Besides, and like the Row class, it works similar to a dictionary, where the keys are the column names of the associated table and the values are Column instances. See section 4.6 for examples of use.

## 4.6 The Column class

Each instance of this class is associated with one column of every table. These instances are mainly used to fetch and set actual data from the table columns, but there are a few other associated methods to deal with indexes.

## 4.6.1 Column instance variables

table The parent Table instance.

name The name of the associated column.

**type** The data type of the column.

index The associated Index object (see 4.13.3) to this column (None if doesn't exist).

dirty Whether the index is dirty or not (property).

#### 4.6.2 Column methods

```
createIndex()
```

Create an Index (see 4.13.3) object for this column.

#### reIndex()

Recompute the index associated with this column. This can be useful when you suspect that, for any reason, the index information is no longer valid and want to rebuild it.

#### reIndexDirty()

Recompute the existing index only if it is dirty. This can be useful when you have set the reindex parameter to 0 in IndexProps constructor (see 4.13.2) for the table and want to update the column's index after a invalidating index operation (Table.removeRows, for example).

#### removeIndex()

Delete the associated column's index. After doing that, you will loose the indexation information on disk. However, you can always re-create it using the createIndex() method (see 4.6.2).

#### closeIndex()

Close the index of this column. After that, the column will look as if it has no index, although it will re-appear when the file would be re-opened later on.

## 4.6.3 Column special methods

```
__getitem__(key)
```

Returns a column element or slice. It takes different actions depending on the type of the key parameter:

**key is an Integer** The corresponding element in the column is returned as a scalar object or as a NumArray/CharArray object, depending on its shape.

**key is a Slice** The row range determined by this slice is returned as a NumArray or CharArray object (whichever is appropriate).

## Example of use:

```
print "Column handlers:"
for name in table.colnames:
    print table.cols[name]
print
print "Some selections:"
print "Select table.cols.name[1]-->", table.cols.name[1]
print "Select table.cols.name[1:2]-->", table.cols.name[1:2]
print "Select table.cols.lati[1:3]-->", table.cols.lati[1:3]
print "Select table.cols.pressure[:]-->", table.cols.pressure[:]
print "Select table.cols['temperature'][:]-->", table.cols['temperature'][:]
```

and the output of this for a certain arbitrary table is:

```
Column handlers:
/table.cols.name (Column(1,), CharType)
/table.cols.lati (Column(2,), Int32)
/table.cols.longi (Column(1,), Int32)
/table.cols.pressure (Column(1,), Float32)
/table.cols.temperature (Column(1,), Float64)
Some selections:
Select table.cols.name[1]--> Particle: 11
```

```
Select table.cols.name[1:2]--> ['Particle: 11']
Select table.cols.lati[1:3]--> [[11 12]
       [12 13]]
Select table.cols.pressure[:]--> [ 90. 110. 132.]
Select table.cols['temperature'][:]--> [ 100. 121. 144.]
```

See the examples/table2.py for a more complete example.

```
_setitem__(key, value)
```

It takes different actions depending on the type of the key parameter:

**key is an Integer** The corresponding element in the column is set to *value*. *value* must be a scalar or NumArray/CharArray, depending on column's shape.

**key is a Slice** The row slice determined by *key* is set to *value*. *value* must be a list of elements or a NumArray/CharArray.

Example of use:

```
# Modify row 1
table.cols.col1[1] = -1
# Modify rows 1 and 3
table.cols.col1[1::2] = [2,3]
```

Which is equivalent to:

```
# Modify row 1
table.modifyColumns(start=1, columns=[[-1]], names=["col1"])
# Modify rows 1 and 3
columns = numarray.records.fromarrays([[2,3]], formats="i4")
table.modifyColumns(start=1, step=2, columns=columns, names=["col1"])
```

## 4.7 The Array class

Represents an array on file. It provides methods to write/read data to/from array objects in the file. This class does not allow you to enlarge the datasets on disk; see the EArray descendant in section 4.8 if you want enlargeable dataset support and/or compression features.

The array data types supported are the same as the set provided by Numeric and numerray. For details of these data types see appendix A, or the numerray reference manual (Greenfield *et al.*).

Note that this object inherits all the public attributes and methods that Leaf already provides.

## 4.7.1 Array instance variables

**flavor** The object representation for this array. It can be any of "NumArray", "CharArray" "Numeric", "List", "Tuple", "String", "Int" or "Float" values.

**nrows** The length of the first dimension of Array.

**nrow** On iterators, this is the index of the current row.

**type** The type class of the represented array.

itemsize The size of the base items. Specially useful for CharArray objects.

## 4.7.2 Array methods

Note that, as this object has no internal I/O buffers, it is not necessary to use the flush() method inherited from Leaf in order to save its internal state to disk. When a writing method call returns, all the data is already on disk.

## iterrows(start=None, stop=None, step=1)

Returns an iterator yielding numarray instances built from rows in array. The return rows are taken from the first dimension in case of an Array instance and the enlargeable dimension in case of an EArray instance. If a range is supplied (i.e. some of the *start*, *stop* or *step* parameters are passed), only the appropriate rows are returned. Else, all the rows are returned. See also the and \_\_iter\_\_() special methods in section 4.7.3 for a shorter way to call this iterator.

The meaning of the *start*, *stop* and *step* parameters is the same as in the range() python function, except that negative values of step are not allowed. Moreover, if only start is specified, then stop will be set to start+1. If you do not specify neither *start* nor *stop*, then all the rows in the object are selected.

Example of use:

```
result = [ row for row in arrayInstance.iterrows(step=4) ]
```

## read(start=None, stop=None, step=1)

Read the array from disk and return it as a numarray (default) object, or an object with the same original flavor that it was saved. It accepts start, stop and step parameters to select rows (the first dimension in the case of an Array instance and the *enlargeable* dimension in case of an EArray) for reading.

The meaning of the *start*, *stop* and *step* parameters is the same as in the range() python function, except that negative values of step are not allowed. Moreover, if only start is specified, then stop will be set to start+1. If you do not specify neither *start* nor *stop*, then all the rows in the object are selected.

## 4.7.3 Array special methods

Following are described the methods that automatically trigger actions when an Array instance is accessed in a special way (e.g., array[ $2:3,\ldots,::2$ ] will be equivalent to a call to

```
array.__getitem__(slice(2,3, None), Ellipsis, slice(None, None, 2))).
```

```
__iter__()
```

It returns the same iterator than Array.iterrows(0,0,1). However, this does not accept parameters. Example of use:

```
result = [ row[2] for row in array ]
```

Which is equivalent to:

```
result = [ row[2] for row in array.iterrows(0, 0, 1) ]
```

```
__getitem__(key)
```

It returns a numarray (default) object (or an object with the same original *flavor* that it was saved) containing the slice of rows stated in the key parameter. The set of allowed tokens in key is the same as extended slicing in python (the Ellipsis token included).

Example of use:

```
array1 = array[4]  # array1.shape == array.shape[1:]
array2 = array[4:1000:2]  # len(array2.shape) == len(array.shape)
array3 = array[::2, 1:4, :]
array4 = array[1, ..., ::2, 1:4, 4:]  # General slice selection
```

## \_\_setitem\_\_(key, value)

Sets an Array element, row or extended slice. It takes different actions depending on the type of the key parameter:

**key is an integer:** The corresponding row is assigned to value. If needed, this value is broadcasted to fit the specified row.

key is a slice: The row slice determined by it is assigned to value. If needed, this value is broadcasted to fit in the desired range. If the slice to be updated exceeds the actual shape of the array, only the values in the existing range are updated, i.e. the index error will be silently ignored. If value is a multidimensional object, then its shape must be compatible with the slice specified in key, otherwhise, a ValueError will be issued.

Example of use:

```
a1[0] = 333  # Assign an integer to a Integer Array row
a2[0] = "b"  # Assign a string to a string Array row
a3[1:4] = 5  # Broadcast 5 to slice 1:4
a4[1:4:2] = "xXx" # Broadcast "xXx" to slice 1:4:2
# General slice update (a5.shape = (4,3,2,8,5,10)
a5[1, ..., ::2, 1:4, 4:] = arange(1728, shape=(4,3,2,4,3,6))
```

## 4.8 The Earray class

This is a child of the Array class (see 4.7) and as such, EArray represents an array on the file. The difference is that EArray allows to enlarge datasets along any single dimension<sup>2</sup> you select. Another important difference is that it also supports compression.

So, in addition to the attributes and methods that EArray inherits from Array, it supports a few more that provide a way to enlarge the arrays on disk. Following are described the new variables and methods as well as some that already exist in Array but that differ somewhat on the meaning and/or functionality in the EArray context.

## 4.8.1 Earray instance variables

atom The class instance chosen for the atom object (see section 4.12.3).

extdim The enlargeable dimension.

**nrows** The length of the enlargeable dimension.

## 4.8.2 Earray methods

## append(object)

Appends an object to the underlying dataset. Obviously, this object has to have the same type as the EArray instance; otherwise a TypeError is issued. In the same way, the dimensions of the object have

<sup>&</sup>lt;sup>2</sup> In the future, multiple enlargeable dimensions might be implemented as well.

to conform to those of EArray, that is, all the dimensions have to be the same except, of course, that of the enlargeable dimension which can be of any length (even 0!).

Example of use (code available in examples/earray1.py):

```
import tables
from numarray import strings
fileh = tables.openFile("earray1.h5", mode = "w")
a = tables.StringAtom(shape=(0,), length=8)
# Use 'a' as the object type for the enlargeable array
array c = fileh.createEArray(fileh.root, 'array c', a, "Chars")
array_c.append(strings.array(['a'*2, 'b'*4], itemsize=8))
array_c.append(strings.array(['a'*6, 'b'*8, 'c'*10], itemsize=8))
# Read the string EArray we have created on disk
for s in array_c:
    print "array_c[%s] => '%s'" % (array_c.nrow, s)
# Close the file
fileh.close()
  and the output is:
      array_c[0] => 'aa'
      array_c[1] => 'bbbb'
      array_c[2] => 'aaaaaa'
      array_c[3] => 'bbbbbbbb'
      array_c[4] => 'ccccccc'
```

## 4.9 The VLArray class

Instances of this class represents array objects in the object tree with the property that their rows can have a **variable** number of (homogeneous) elements (called *atomic* objects, or just *atoms*). Variable length arrays (or *VLA*'s for short), similarly to Table instances, can have only one dimension, and likewise Table, the compound elements (the *atoms*) of the rows of VLArrays can be fully multidimensional objects.

VLArray provides methods to read/write data from/to variable length array objects residents on disk. Also, note that this object inherits all the public attributes and methods that Leaf already has.

## 4.9.1 VLArray instance variables

**atom** The class instance chosen for the atom object (see section 4.12.3).

**nrow** On iterators, this is the index of the current row.

**nrows** The total number of rows.

## 4.9.2 VLArray methods

```
append(object1, object2, ...)
```

Append the objects passed as parameters to a single row in the VLArray instance. The type of the objects has to be compliant with the VLArray.atom instance type.

Example of use (code available in examples/vlarray1.py):

```
import tables
from Numeric import *
                        # or, from numarray import *
# Create a VLArray:
fileh = tables.openFile("vlarray1.h5", mode = "w")
vlarray = fileh.createVLArray(fileh.root, 'vlarray1',
tables.Int32Atom(flavor="Numeric"),
                 "ragged array of ints", Filters(complevel=1))
# Append some (variable length) rows
# All these different parameter specification are accepted:
vlarray.append(array([5, 6]))
vlarray.append(array([5, 6, 7]))
vlarray.append([5, 6, 9, 8])
vlarray.append(5, 6, 9, 10, 12)
# Now, read it through an iterator
for x in vlarray:
    print vlarray.name+"["+str(vlarray.nrow)+"]-->", x
# Close the file
fileh.close()
```

And the output for this looks like:

```
vlarray1[0]--> [5 6]
vlarray1[1]--> [5 6 7]
vlarray1[2]--> [5 6 9 8]
vlarray1[3]--> [ 5 6 9 10 12]
```

#### iterrows(start=None, stop=None, step=1)

Returns an iterator yielding one row per iteration. If a range is supplied (i.e. some of the *start*, *stop* or *step* parameters are passed), only the appropriate rows are returned. Else, all the rows are returned. See also the \_\_iter\_\_() special methods in section 4.9.3 for a shorter way to call this iterator.

The meaning of the *start*, *stop* and *step* parameters is the same as in the range() python function, except that negative values of step are not allowed. Moreover, if only start is specified, then stop will be set to start+1. If you do not specify neither *start* nor *stop*, then all the rows in the object are selected.

Example of use:

```
for row in vlarray.iterrows(step=4):
    print vlarray.name+"["+str(vlarray.nrow)+"]-->", row
```

## read(start=None, stop=None, step=1)

Returns the actual data in VLArray. As the lengths of the different rows are variable, the returned value is a python list, with as many entries as specified rows in the range parameters.

The meaning of the *start*, *stop* and *step* parameters is the same as in the range() python function, except that negative values of step are not allowed. Moreover, if only start is specified, then stop will be set to start+1. If you do not specify neither *start* nor *stop*, then all the rows in the object are selected.

## 4.9.3 VLArray special methods

Following are described the methods that automatically trigger actions when a VLArray instance is accessed in a special way (e.g., vlarray[2:5] will be equivalent to a call to vlarray. \_\_getitem\_\_(slice(2,5,None)).

```
__iter__()
```

It returns the same iterator than VLArray.iterrows(0,0,1). However, this does not accept parameters. Example of use:

```
result = [ row for row in vlarray ]
```

Which is equivalent to:

```
result = [ row for row in vlarray.iterrows() ]
```

```
__getitem__(key)
```

It returns the slice of rows determined by key, which can be an integer index or an extended slice. The returned value is a list of objects of type array.atom.type.

Example of use:

```
list1 = vlarray[4]
list2 = vlarray[4:1000:2]
```

```
__setitem__(keys, value)
```

Updates a vlarray row described by keys by setting it to value. Depending on the value of keys, the action taken is different:

**keys is an integer:** It refers to the number of row to be modified. The value object must be type and shape compatible with the object that exists in the vlarray row.

**keys is a tuple:** The first element refers to the row to be modified, and the second element to the range (so, it can be an integer or an slice) of the row that will be updated. As above, the value object must be type and shape compatible with the object specified in the vlarray row *and* range.

**Note:** When updating VLStrings (codification UTF-8) or Objects atoms, there is a problem: one can only update values with *exactly* the same bytes than in the original row. With UTF-8 encoding this is problematic because, for instance, 'c' takes 1 byte, but 'ç' takes two. The same applies when using Objects atoms, because when cPickle applies to a class instance (for example), it does not guarantee to return the same number of bytes than over other instance, even of the same class than the former. These facts effectively limit the number of objects than can be updated in VLArrays.

Example of use:

```
vlarray[0] = vlarray[0]*2+3
vlarray[99,3:] = arange(96)*2+3
# Negative values for start and stop (but not step) are supported
vlarray[99,-99:-89:2] = vlarray[5]*2+3
```

## 4.10 The UnImplemented class

Instances of this class represents an unimplemented dataset in a generic HDF5 file. When reading such a file (i.e. one that has not been created with PyTables, but with some other HDF5 library based tool), chances are that the specific combination of *datatypes* and/or *dataspaces* in some dataset might not be supported by PyTables yet. In such a case, this dataset will be mapped into the UnImplemented class and hence, the user will still be able to build the complete object tree of this generic HDF5 file, as well as enabling the access (both read and *write*) of the attributes of this dataset and some metadata. Of course, the user won't be able to read the actual data on it.

This is an elegant way to allow users to work with generic HDF5 files despite the fact that some of its datasets would not be supported by PyTables. However, if you are really interested in having access to an unimplemented dataset, please, get in contact with the developer team.

This class does not have any public instance variables, except those inherited from the Leaf class (see 4.4).

## 4.11 The AttributeSet class

Represents the set of attributes of a node (Leaf or Group). It provides methods to create new attributes, open, rename or delete existing ones.

Like in Group instances, AttributeSet instances make use of the *natural naming* convention, i.e. you can access the attributes on disk like if they were *normal* AttributeSet attributes. This offers the user a very convenient way to access (but also to set and delete) node attributes by simply specifying them like a *normal* attribute class.

**Caveat:** All Python data types are supported. The scalar ones (i.e. String, Int and Float) are mapped directly to the HDF5 counterparts, so you can correctly visualize them with any HDF5 tool. However, the rest of the data types and more general objects are serialized using cPickle, so you will be able to correctly retrieve them only from a Python-aware HDF5 library. Hopefully, the list of supported native attributes will be extended to fully multidimensional arrays sometime in the future.

## 4.11.1 AttributeSet instance variables

- \_v\_node The parent node instance.
- \_v\_attrnames List with all attribute names.
- \_v\_attrnamessys List with system attribute names.
- v attrnamesuser List with user attribute names.

## 4.11.2 AttributeSet methods

Note that this class define the \_\_setattr\_\_, \_\_getattr\_\_ and \_\_delattr\_\_ and they work as normally intended. Any scalar (string, ints or floats) attribute is supported natively as an attribute. However, (c)Pickle is automatically used so as to serialize other kind of objects (like lists, tuples, dicts, small Numeric/numarray objects, ...) that you might want to save.

With these special methods, you can access, assign or delete attributes on disk by just using the next constructs:

```
leaf.attrs.myattr = "str attr"  # Set a string (native support)
leaf.attrs.myattr2 = 3  # Set an integer (native support)
leaf.attrs.myattr3 = [3,(1,2)]  # A generic object (Pickled)
attrib = leaf.attrs.myattr  # Get the attribute myattr
del leaf.attrs.myattr  # Delete the attribute myattr
```

**\_f\_copy(where)** Copy the user attributes to *where* object. *where* has to be a Group or Leaf instance.

\_f\_list(attrset = "user") Return the list of attributes of the parent node. attrset selects the attribute set to be returned. An "user" value returns only the user attributes and this is the default. "sys" returns only the system (some of which are read-only) attributes. "readonly" returns the system read-only attributes. "all" returns both the system and user attributes.

**\_f\_rename(oldattrname, newattrname)** Rename an attribute.

## 4.12 Declarative classes

In this section a series of classes that are meant to *declare* datatypes that are required for primary PyTables (like Table or VLArray) objects are described.

## 4.12.1 The IsDescription 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.

It is designed to be used as an easy, yet meaningful way to describe the properties of Table objects through the use of classes that inherit properties from it. In order to define such a special class, you have to declare it as descendant of *IsDescription*, with many attributes as columns you want in your table. The name of these attributes will become the name of the columns, while its values are the properties of the columns that are obtained through the use of the Col 4.12.2 class constructor.

Then, you can pass an instance of this object to the Table constructor, where all the information it contains will be used to define the table structure. See the section 3.3 for an example on how that works.

Moreover, you can change the properties of the index creation process by using an instance of the Index-Props 4.13.2 class and assign it to a special attribute called \_v\_indexprops.

## 4.12.2 The Col class and its descendants

The Col class is used as a mean to declare the different properties of a table column. In addition, a series of descendant classes are offered in order to make these column descriptions easier to the user. In general, it is recommended to use these descendant classes, as they are more meaningful when found in the middle of the code.

Note that the only public method accessible in these classes is the constructor itself.

Col(dtype="Float64", shape=1, dflt=None, pos=None, indexed=0) Declare the properties of a Table column.

- **dtype** The data type for the column. All types listed in appendix A are valid data types for columns. The type description is accepted both in string format and as a numarray data type.
- **shape** An integer or a tuple, that specifies the number of *dtype* items for each element (or shape, for multidimensional elements) of this column. For CharType columns, the last dimension is used as the length of the character strings. However, for this kind of objects, the use of StringCol subclass is strongly recommended.
- **dflt** The default value for elements of this column. If the user does not supply a value for an element while filling a table, this default value will be written to disk. If the user supplies an scalar value for a multidimensional column, this value is automatically *broadcasted* to all the elements in the column cell. If *dflt* is not supplied, an appropriate zero value (or *null* string) will be chosen by default.
- **pos** By default, columns are arranged in memory following an alpha-numerical order of the column names. In some situations, however, it is convenient to impose a user defined ordering. *pos* parameter allows the user to force the desired ordering.

**indexed** Whether this column should be indexed for better performance in table selections.

**StringCol(length=None, dflt=None, shape=1, pos=None, indexed=0)** Declare a column to be of type CharType. The *length* parameter sets the length of the strings. The meaning of the other parameters are like in the Col class.

**BoolCol(dflt=0, shape=1, pos=None, indexed=0)** Define a column to be of type Bool. The meaning of the parameters are the same of those in the Col class.

IntCol(dflt=0, shape=1, itemsize=4, sign=1, pos=None, indexed=0) Declare a column to be of type IntXX, depending on the value of *itemsize* parameter, that sets the number of bytes of the integers in the column. *sign* determines whether the integers are signed or not. The meaning of the other parameters are the same of those in the Col class.

This class has several descendants:

Int8Col(dflt=0, shape=1, pos=None, indexed=0) Define a column of type Int8.

UInt8Col(dflt=0, shape=1, pos=None, indexed=0) Define a column of type UInt8.

Int16Col(dflt=0, shape=1, pos=None, indexed=0) Define a column of type Int16.

UInt16Col(dflt=0, shape=1, pos=None, indexed=0) Define a column of type UInt16.

**Int32Col(dflt=0, shape=1, pos=None, indexed=0)** Define a column of type Int32.

UInt32Col(dflt=0, shape=1, pos=None, indexed=0) Define a column of type UInt32.

Int64Col(dflt=0, shape=1, pos=None, indexed=0) Define a column of type Int64.

UInt64Col(dflt=0, shape=1, pos=None, indexed=0) Define a column of type UInt64.

FloatCol(dflt=0.0, shape=1, itemsize=8, pos=None, indexed=0) Define a column to be of type FloatXX, depending on the value of itemsize. The itemsize parameter sets the number of bytes of the floats in the column and the default is 8 bytes (double precision). The meaning of the other parameters are the same as those in the Col class.

This class has two descendants:

Float32Col(dflt=0.0, shape=1, pos=None, indexed=0) Define a column of type Float32. Float64Col(dflt=0.0, shape=1, pos=None, indexed=0) Define a column of type Float64.

ComplexCol(dflt=0.+0.j, shape=1, itemsize=16, pos=None) Define a column to be of type ComplexXX, depending on the value of itemsize. The itemsize parameter sets the number of bytes of the complex types in the column and the default is 16 bytes (double precision complex). The meaning of the other parameters are the same as those in the Col class.

This class has two descendants:

Complex32Col(dflt=0.+0.j, shape=1, pos=None) Define a column of type Complex32. Float64Col(dflt=0+0.j, shape=1, pos=None) Define a column of type Complex64.

ComplexCol columns and its descendants do not support indexation.

#### 4.12.3 The Atom class and its descendants.

The Atom class is meant to declare the different properties of the *base element* (also known as *atom*) of EArray and VLArray objects. The Atom instances have the property that their length is always the same. However, you can grow objects along the extendable dimension in the case of EArray or put a variable number of them on a VLArray row. Moreover, the atoms are not restricted to scalar values, and they can be fully multidimensional objects.

A series of descendant classes are offered in order to make the use of these element descriptions easier. In general, it is recommended to use these descendant classes, as they are more meaningful when found in the middle of the code. Note that the only public methods accessible in these classes are the atomsize() method and the constructor itself. The atomsize() method returns the total length, in bytes, of the element base atom.

A description of the different constructors with their parameters follows:

- **Atom(dtype="Float64", shape=1, flavor="NumArray")** Define properties for the base elements of EArray and VLArray objects.
  - **dtype** The data type for the base element. See the appendix A for a relation of data types supported. The type description is accepted both in string format and as numarray data type.
  - **shape** In a EArray context, it is a **tuple** specifing the shape of the object, and one (and only one) of its dimensions **must** be 0, meaning that the EArray object will be enlarged along this axis. In the case of a VLArray, it can be an integer with a value of 1 (one) or a tuple, that specifies whether the atom is an scalar (in the case of a 1) or has multiple dimensions (in the case of a tuple). For CharType elements, the last dimension is used as the length of the character strings. However, for this kind of objects, the use of StringAtom subclass is strongly recommended.
  - flavor The object representation for this atom. It can be any of "CharArray" or "String" for the CharType type and "NumArray", "Numeric", "List" or "Tuple" for the rest of the types. If the specified values differs from CharArray or NumArray values, the read atoms will be converted to that specific flavor. If not specified, the atoms will remain in their native format (i.e. CharArray or NumArray).
- **StringAtom(shape=1, length=None, flavor="CharArray")** Define an atom to be of CharType type. The meaning of the *shape* parameter is the same as in the Atom class. *length* sets the length of the strings atoms. *flavor* can be whether "CharArray" or "String". Unicode strings are not supported by this type; see the VLStringAtom class if you want Unicode support (only available for VLAtom objects).
- **BoolAtom**(shape=1, flavor="NumArray") Define an atom to be of type Bool. The meaning of the parameters are the same of those in the Atom class.
- IntAtom(shape=1, itemsize=4, sign=1, flavor="NumArray") Define an atom to be of type IntXX, depending on the value of *itemsize* parameter, that sets the number of bytes of the integers that conform the atom. *sign* determines whether the integers are signed or not. The meaning of the other parameters are the same of those in the Atom class.

This class has several descendants:

Int8Atom(shape=1, flavor="NumArray") Define an atom of type Int8.

**UInt8Atom(shape=1, flavor="NumArray")** Define an atom of type UInt8.

Int16Atom(shape=1, flavor="NumArray") Define an atom of type Int16.

UInt16Atom(shape=1, flavor="NumArray") Define an atom of type UInt16.

Int32Atom(shape=1, flavor="NumArray") Define an atom of type Int32.

UInt32Atom(shape=1, flavor="NumArray") Define an atom of type UInt32.

Int64Atom(shape=1, flavor="NumArray") Define an atom of type Int64.

**UInt64Atom(shape=1, flavor="NumArray")** Define an atom of type UInt64.

FloatAtom(shape=1, itemsize=8, flavor="NumArray") Define an atom to be of FloatXX type, depending on the value of itemsize. The itemsize parameter sets the number of bytes of the floats in the atom and the default is 8 bytes (double precision). The meaning of the other parameters are the same as those in the Atom class.

This class has two descendants:

Float32Atom(shape=1, flavor="NumArray") Define an atom of type Float32.

Float64Atom(shape=1, flavor="NumArray") Define an atom of type Float64.

ComplexAtom(shape=1, itemsize=16, flavor="NumArray") Define an atom to be of ComplexXX type, depending on the value of itemsize. The itemsize parameter sets the number of bytes of the floats in the atom and the default is 16 bytes (double precision complex). The meaning of the other parameters are the same as those in the Atom class.

This class has two descendants:

Complex32Atom(shape=1, flavor="NumArray") Define an atom of type Complex32.

Complex64Atom(shape=1, flavor="NumArray") Define an atom of type Complex64.

Now, there come two special classes, ObjectAtom and VLString, that actually do not descend from Atom, but which goal is so similar that they should be described here. The difference between them and the Atom and descendents classes is that these special classes does not allow multidimensional atoms, nor multiple values per row. A *flavor* can't be specified neither as it is immutable (see below).

**Caveat emptor:** You are only allowed to use these classes to create VLArray objects, not EArray objects.

ObjectAtom() This class is meant to fit *any* kind of object in a row of an VLArray instance by using cPickle behind the scenes. Due to the fact that you cannot foresee how long will be the output of the cPickle serialization (i.e. the atom already has a *variable* length), you can only fit a representant of it per row. However, you can still pass several parameters to the VLArray.append() method as they will be regarded as a *tuple* of compound objects (the parameters), so that we still have only one object to be saved in a single row. It does not accept parameters and its flavor is automatically set to "Object", so the reads of rows always returns an arbitrary python object. You can regard ObjectAtom types as an easy way to save an arbitrary number of generic python objects in a VLArray object.

**VLStringAtom()** This class describes a *row* of the VLArray class, rather than an *atom*. It differs from the StringAtom class in that you can only add one instance of it to one specific row, i.e. the VLArray.append() method only accepts one object when the base atom is of this type. Besides, it supports Unicode strings (contrarily to StringAtom) because it uses the UTF-8 codification (this is why its atomsize() method returns always 1) when serializing to disk. It does not accept any parameter and because its *flavor* is automatically set to "VLString", the reads of rows always returns a python string. See the appendix C.3.4 if you are curious on how this is implemented at the low-level. You can regard VLStringAtom types as an easy way to save generic variable length strings.

See examples/vlarray1.py and examples/vlarray2.py for further examples on VLArrays, including object serialization and Unicode string management.

## 4.13 Helper classes

In this section are listed classes that does not fit in any other section and that mainly serves for ancillary purposes.

## 4.13.1 The Filters class

This class is meant to serve as a container that keeps information about the filter properties associated with the enlargeable leaves, that is Table, EArray and VLArray.

The public variables of Filters are listed below:

**complevel** The compression level (0 means no compression).

complib The compression filter used (in case of compressed dataset).

**shuffle** Whether the shuffle filter is active or not.

**fletcher32** Whether the fletcher32 filter is active or not.

There are no Filters public methods with the exception of the constructor itself that is described next.

```
Filters(complevel=0, complib="zlib", shuffle=1, fletcher32=0)
```

The parameters that can be passed to the Filters class constructor are:

- **complevel** Specifies a compress level for data. The allowed range is 0-9. A value of 0 disables compression. The default is that compression is disabled, that balances between compression effort and CPU consumption.
- **complib** Specifies the compression library to be used. Right now, "zlib" (default), "lzo" and "ucl" values are supported. See section 6.3 for some advice on which library is better suited to your needs.
- **shuffle** Whether or not to use the *shuffle* filter present in the HDF5 library. This is normally used to improve the compression ratio (at the cost of consuming a little bit more CPU time). A value of 0 disables shuffling and 1 makes it active. The default value depends on whether compression is enabled or not; if compression is enabled, shuffling defaults to be active, else shuffling is disabled.
- **fletcher32** Whether or not to use the *fletcher32* filter in the HDF5 library. This is used to add a checksum on each data chunk. A value of 0 disables the checksum and it is the default.

Of course, you can also create an instance and then assign the ones you want to change. For example:

```
import numarray as na
from tables import *
fileh = openFile("test5.h5", mode = "w")
atom = Float32Atom(shape=(0,2))
filters = Filters(complevel=1, complib = "lzo")
filters.fletcher32 = 1
arr = fileh.createEArray(fileh.root, 'earray', atom, "A growable array",
                         filters = filters)
# Append several rows in only one call
arr.append(na.array([[1., 2.],
                     [2., 3.],
                     [3., 4.]], type=na.Float32))
# Print information on that enlargeable array
print "Result Array:"
print repr(arr)
fileh.close()
```

This enforces the use of the LZO library, a compression level of 1 and a fletcher32 checksum filter as well. See the output of this example:

```
Result Array:
/earray (EArray(3L, 2), fletcher32, shuffle, lzo(1)) 'A growable array'
type = Float32
shape = (3L, 2)
itemsize = 4
nrows = 3
extdim = 0
flavor = 'NumArray'
byteorder = 'little'
```

## 4.13.2 The IndexProps class

You can use this class to set/unset the properties in the indexing process of a Table column. To use it, create an instance, and assign it to the special attribute \_v\_indexprops in a table description 4.12.1 class or dictionary.

The public variables of IndexProps are listed below:

auto Whether an existing index should be updated or not after a table append operation.

reindex Whether the table columns are to be re-indexed after an invalidating index operation.

filters The filter settings for the different Table indexes.

There are no IndexProps public methods with the exception of the constructor itself that is described next.

#### IndexProps(auto=1, reindex=1, filters=None)

The parameters that can be passed to the IndexProps class constructor are:

**auto** Specifies whether an existing index should be updated or not after a table append operation. The default is enable automatic index updates.

**reindex** Specifies whether the table columns are to be re-indexed after an invalidating index operation (like for example, after a Table.removeRows call). The default is to reindex after operations that invalidate indexes.

**filters** Sets the filter properties for Column indexes. It has to be an instance of the Filters (see section 4.13.1) class. A None value means that the default settings for the Filters object are selected.

## 4.13.3 The Index class

This class is used to keep the indexing information for table columns. It is actually a descendant of the Group class, with some added functionality.

It has no methods intented for programmer's use, but it has some attributes that maybe interesting for him.

## Index instance variables

**column** The column object this index belongs to.

**type** The type class for the index.

itemsize The size of the atomic items. Specially useful for columns of CharType type.

**nelements** The total number of elements in index.

dirty Whether the index is dirty or not.

**sorted** The IndexArray object (see 4.13.4) with the sorted values information.

**indices** The IndexArray object (see 4.13.4) with the sorted indices information.

**filters** The Filters (see section 4.13.1) instance for this index.

## 4.13.4 The IndexArray class

This class is used to keep part of the indexing information for table columns. It is actually a descendant of the EArray class, with some added functionality.

It has no methods intented for programmer's use, and although it has some attributes with potentially useful information, all of it is accessible through Index class (see 4.13.3), so it will not be replicated here.

# Chapter 5

## **FileNode**

## 5.1 What is FileNode?

FileNode is a module which enables you to create a PyTables database of nodes which can be used like regular opened files in Python. In other words, you can store a file in a PyTables database, and read and write it as you would do with any other file in Python. Used in conjunction with PyTables hierarchical database organisation, you can have your database turned into an open, extensible, efficient, high capacity, portable and metadata-rich filesystem for data exchange with other systems (including backup purposes).

Between the main features of FileNode, one can list:

- Open: Since it relies on PyTables, which in turn, sits over HDF5 (see NCSA), a standard hierarchical data format from NCSA.
- Extensible: You can define new types of nodes, and their instances will be safely preserved (as are normal groups, leafs and attributes) by PyTables applications having no knowledge of their types. Moreover, the set of possible attributes for a node is not fixed, so you can define your own node attributes.
- *Efficient:* Thanks to PyTables' proven extreme efficiency on handling huge amounts of data. FileNode can make use of PyTables' on-the-fly compression and decompression of data.
- *High capacity:* Since PyTables and HDF5 are designed for massive data storage (they use 64-bit addressing even where the platform does not support it natively).
- *Portable:* Since the HDF5 format has an architecture-neutral design, and the HDF5 libraries and PyTables are known to run under a variety of platforms. Besides that, a PyTables database fits into a single file, which poses no trouble for transportation.
- *Metadata-rich:* Since PyTables can store arbitrary key-value pairs (even Python objects!) for every database node. Metadata may include authorship, keywords, MIME types and encodings, ownership information, access control lists (ACL), decoding functions and anything you can imagine!

## 5.2 Current limitations

FileNode is still a young piece of software, so it lacks some functionality. This is a list of known current limitations:

- 1. Node file names are constrained to PyTables node names (i.e. most valid Python identifiers). For the moment, if you want arbitrary names you will have to use a translation map (see 4.1.2) or the node title. The same restriction applies to attribute names.
- 2. Node files can only be opened for read-only or read and append mode. This will be enhanced in the future.

- 3. There is no universal newline support yet. This is likely to be implemented in a near future.
- 4. Sparse files (files with lots of zeros) are not treated specially; if you want them to take less space, you should be better off using compression.

These limitations still make FileNode entirely adequate to work with most binary and text files. Of course, suggestions and patches are welcome.

## 5.3 Finding a FileNode node

FileNode nodes can be recognised because they have a \_type attribute with a 'file' value. It is recommended that you use the getAttrNode() method (see 4.2.2) of tables.File class to get the \_type attribute independently of the nature (group or leaf) of the node, so you do not need to care about.

## 5.4 Using FileNode

The FileNode module is part of the nodes sub-package of PyTables. The recommended way to import the module is:

```
>>> from tables.nodes import FileNode
```

However, FileNode exports very few symbols, so you can import \* for interactive usage. In fact, you will most probably only use the NodeType constant and the newNode() and openNode() calls.

The NodeType constant contains the value that the \_type attribute of a node file is expected to contain ('file', as we have seen). Although this is not expected to change, you should use FileNode.NodeType instead of the literal 'file' when possible.

newNode() and openNode() are the equivalent to the Python file() call (alias open()) for ordinary files. Their arguments differ from that of file(), but this is the only point where you will note the difference between working with a node file and working with an ordinary file.

For this little tutorial, we will assume that we have a PyTables database opened for writing. Also, if you are somewhat lazy at typing sentences, the code that we are going to explain is included in the examples/filenodes1.py file.

You can create a brand new file with these sentences:

```
>>> import tables
>>> h5file = tables.openFile('fnode.h5', 'w')
```

## 5.4.1 Creating a new file node

Creation of a new file node is achieved with the newNode() call. You must tell it in which PyTables file you want to create it, where in the PyTables hierarchy you want to create the node and which will be its name. The PyTables file is the first argument to newNode(); it will be also called the 'host PyTables file'. The other two arguments must be given as keyword arguments where and name, respectively. As a result of the call, a brand new appendable and readable file node object is returned.

So let us create a new node file in the previously opened h5file PyTables file, named 'fnode\_test' and placed right under the root of the database hierarchy. This is that command:

```
>>> fnode = FileNode.newNode(h5file, where='/', name='fnode_test')
```

That is basically all you need to create a file node. Simple, isn't it? From that point on, you can use fnode as any opened Python file (i.e. you can write data, read data, lines of text and so on).

newNode() accepts some more keyword arguments. You can give a title to your file with the title argument. You can use PyTables' compression features with the filters argument. If you know beforehand the size that your file will have, you can give its final file size in bytes to the expectedsize argument so that the PyTables library would be able to optimise the data access.

newNode() creates a PyTables node where it is told to. To prove it, we will try to get the \_type attribute from the newly created node.

```
>>> print h5file.getAttrNode('/fnode_test', '_type')
file
```

## 5.4.2 Using a file node

As stated above, you can use the new node file as any other opened file. Let us try to write some text in and read it.

```
>>> print >> fnode, "This is a test text line."
>>> print >> fnode, "And this is another one."
>>> print >> fnode
>>> fnode.write("Of course, file methods can also be used.")
>>>
>>> fnode.seek(0) # Go back to the beginning of file.
>>>
>>> for line in fnode:
... print repr(line)
'This is a test text line.\n'
'And this is another one.\n'
'\n'
'Of course, file methods can also be used.'
```

This was run on a Unix system, so newlines are expressed as  $'\n'$ . In fact, you can override the line separator for a file by setting its lineSeparator property to any string you want.

While using a file node, you should take care of closing it **before** you close the PyTables host file. Because of the way PyTables works, your data it will not be at a risk, but every operation you execute after closing the host file will fail with a ValueError. To close a file node, simply delete it or call its close() method.

```
>>> fnode.close()
>>> print fnode.closed
True
```

## 5.4.3 Opening an existing file node

If you have a file node that you created using newNode(), you can open it later by calling openNode(). Its arguments are similar to that of file() or open(): the first argument is the PyTables node that you want to open (i.e. a node with a \_type attribute having a 'file' value), and the second argument is a mode string indicating how to open the file. Contrary to file(), openNode() can not be used to create a new file node.

File nodes can be opened in read-only mode ('r') or in read-and-append mode ('a+'). Reading from a file node is allowed in both modes, but appending is only allowed in the second one. Just like Python files do, writing data to an appendable file places it after the file pointer if it is on or beyond the end of the file, or otherwise after the existing data. Let us see an example:

```
>>> node = h5file.root.fnode_test
>>> fnode = FileNode.openNode(node, 'a+')
>>> print repr(fnode.readline())
'This is a test text line.\n'
>>> print fnode.tell()
```

```
26
>>> print >> fnode, "This is a new line."
>>> print repr(fnode.readline())
,,
```

Of course, the data append process places the pointer at the end of the file, so the last readline() call hit EOF. Let us seek to the beginning of the file to see the whole contents of our file.

```
>>> fnode.seek(0)
>>> for line in fnode:
... print repr(line)
'This is a test text line.\n'
'And this is another one.\n'
'\n'
'Of course, file methods can also be used.This is a new line.\n'
```

As you can check, the last string we wrote was correctly appended at the end of the file, instead of overwriting the second line, where the file pointer was positioned by the time of the appending.

## 5.4.4 Adding metadata to a file node

You can associate arbitrary metadata to any open node file, regardless of its mode, as long as the host PyTables file is writable. Of course, you could use the setAttrNode() method of tables.File to do it directly on the proper node, but FileNode offers a much more comfortable way to do it. FileNode objects have an attrs property which gives you direct access to their corresponding AttributeSet object.

For instance, let us see how to associate MIME type metadata to our file node:

```
>>> fnode.attrs.content_type = 'text/plain; charset=us-ascii'
```

As simple as A-B-C. You can put nearly anything in an attribute, which opens the way to authorship, keywords, permissions and more. Moreover, there is not a fixed list of attributes. However, you should avoid names in all caps or starting with '\_', since PyTables and FileNode may use them internally. Some valid examples:

```
>>> fnode.attrs.author = "Ivan Vilata i Balaguer"
>>> fnode.attrs.creation_date = '2004-10-20T13:25:25+0200'
>>> fnode.attrs.keywords_en = ["FileNode", "test", "metadata"]
>>> fnode.attrs.keywords_ca = ["FileNode", "prova", "metadades"]
>>> fnode.attrs.owner = 'ivan'
>>> fnode.attrs.acl = {'ivan': 'rw', '@users': 'r'}
```

You can check that these attributes get stored by running the ptdump command on the host PyTables file:

```
$ ptdump -a fnode.h5:/fnode_test
/fnode_test (EArray(113, 1)) ''
   /fnode_test.attrs (AttributeSet), 14 attributes:
   [CLASS := 'EARRAY',
    EXTDIM := 0,
   FLAVOR := 'NumArray',
   TITLE := '',
   VERSION := '1.0',
   _type := 'file',
```

```
_type_version := 1,
acl := {'ivan': 'rw', '@users': 'r'},
author := 'Ivan Vilata i Balaguer',
content_type := 'text/plain; charset=us-ascii',
creation_date := '2004-10-20T13:25:25+0200',
keywords_ca := ['FileNode', 'prova', 'metadades'],
keywords_en := ['FileNode', 'test', 'metadata'],
owner := 'ivan']
```

Please note that FileNode makes no assumptions about the meaning of your metadata, so its handling is entirely left to your needs and imagination.

### 5.5 Complementary notes

You can use FileNodes and PyTables groups to mimic a filesystem with files and directories. Since you can store nearly anything you want as file metadata, this enables you to use a PyTables file as a portable compressed backup, even between radically different platforms. Take this with a grain of salt, since node files are restricted in their naming (only valid Python identifiers are valid); however, remember that you can use node titles and metadata to overcome this limitation. Also, you may need to devise some strategy to represent special files such as devices, sockets and such (not necessarily using FileNode).

We are eager to hear your opinion about FileNode and its potential uses. Suggestions to improve FileNode and create other node types are also welcome. Do not hesitate to contact us!

#### 5.6 FileNode module reference

#### 5.6.1 Global constants

**NodeType** Value for \_type node attribute.

**NodeTypeVersions** Supported values for \_type\_version node attribute.

#### 5.6.2 Global functions

```
newNode(h5file, where, name, title="", filters=None, expectedsize=1000)
```

Creates a new file node object in the specified PyTables file object. Additional named arguments where and name must be passed to specify where the file node is to be created. Other named arguments such as title and filters may also be passed. The special named argument expectedsize, indicating an estimate of the file size in bytes, may also be passed. It returns the filenode object.

```
openNode(node, mode = 'r')
```

Opens an existing file node. Returns a file node object from the existing specified PyTables node. If mode is not specified or it is 'r', the file can only be read, and the pointer is positioned at the beginning of the file. If mode is 'a+', the file can be read and appended, and the pointer is positioned at the end of the file.

#### 5.6.3 The FileNode abstract class

This is the ancestor of ROFileNode and RWFileNode (see below). Instances of these classes are returned when newNode() or openNode() are called. It represents a new file node associated with a PyTables node, providing a standard Python file interface to it.

This abstract class provides only an implementation of the reading methods needed to implement a file-like object over a PyTables node. The attribute set of the node becomes available via the attrs property.

You can add attributes there, but try to avoid attribute names in all caps or starting with '\_', since they may clash with internal attributes.

The node used as storage is also made available via the read-only attribute node. Please do not tamper with this object unless unavoidably, since you may break the operation of the file node object.

The lineSeparator property contains the string used as a line separator, and defaults to os.linesep. It can be set to any reasonably-sized string you want.

The constructor sets the closed, softspace and \_lineSeparator attributes to their initial values, as well as the node attribute to None. Sub-classes should set the node, mode and offset attributes.

Version 1 implements the file storage as a UInt8 uni-dimensional EArray.

#### FileNode methods

getLineSeparator() Returns the line separator string.

setLineSeparator() Sets the line separator string.

getAttrs() Returns the attribute set of the file node.

**close()** Flushes the file and closes it. The node attribute becomes None and the attrs property becomes no longer available.

next() Returns the next line of text. Raises StopIteration when lines are exhausted. See file.next.\_\_doc\_\_ for more information.

read(size=None) Reads at most size bytes. See file.read.\_\_doc\_\_ for more information

readline(size=-1) Reads the next text line. See file.readline.\_\_doc\_\_ for more information

readlines(sizehint=-1) Reads the text lines. See file.readlines.\_\_doc\_\_ for more information.

seek(offset, whence=0) Moves to a new file position. See file.seek.\_\_doc\_\_ for more information.

tell() Gets the current file position. See file.tell.\_\_doc\_\_ for more information.

xreadlines() For backward compatibility. See file.xreadlines.\_\_doc\_\_ for more information.

#### 5.6.4 The ROFileNode class

Instances of this class are returned when openNode() is called in read-only mode ('r'). This is a descendant of FileNode class, so it inherits all its methods. Moreover, it does not define any other useful method, just some protections against users intents to write on file.

#### 5.6.5 The RWFileNode class

Instances of this class are returned when either newNode() is called or when openNode() is called in append mode ('a+'). This is a descendant of FileNode class, so it inherits all its methods. It provides additional methods that allow to write on file nodes.

flush() Flushes the file node. See file.flush.\_\_doc\_\_ for more information.

**truncate**(size=None) Truncates the file node to at most size bytes. Currently, this method only makes sense to grow the file node, since data can not be rewritten nor deleted. See file.truncate.\_\_doc\_\_ for more information.

write(string) Writes the string to the file. Writing an empty string does nothing, but requires the file to be open. See file.write.\_\_doc\_\_ for more information.

writelines(sequence) Writes the sequence of strings to the file. See file.writelines.\_\_doc\_\_ for more information.

... durch planmässiges Tattonieren.
[... through systematic, palpable experimentation.]

—Johann Karl Friedrich Gauss [asked how he came upon his theorems]

# **Chapter 6**

# **Optimization tips**

On this chapter, you will get deeper knowledge of PyTables internals. 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 in order to learn how to get an important boost for your code. But if your dataset is small or medium size (say, up to 10 MB), you should not worry about that as the default parameters in PyTables are already tuned to handle that perfectly.

### 6.1 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 cause file storage overhead as well as more disk I/O and higher contention for the metadata cache. Consequently, it's important to balance between memory and I/O overhead (small B-trees) and time to access 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 4.2.2).

When your table size is bigger than 10 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 data. When the table 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!.

### 6.2 Accelerating your searches

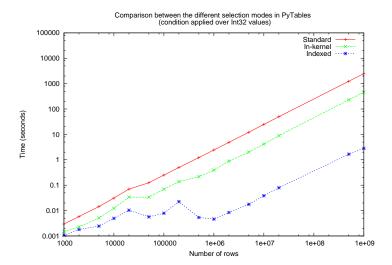
If you are going to use a lot of searches like the next one:

```
row = table.row
result = [ row['var2'] for row in table if row['var1'] <= 20 ]</pre>
```

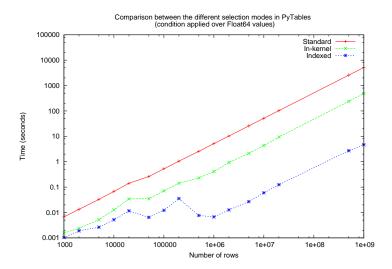
(for future reference, we will call this the *standard* selection mode) and want to improve the time taken by it, keep reading.

#### 6.2.1 In-kernel searches

PyTables provides a way to accelerate data selections when they are simple, i.e. only a column is implied in the selection process, through the use of the where iterator (see 4.5.2). We will call this mode of selecting



**Figure 6.1:** Times for different selection modes over Int32 values. Benchmark made on a machine with Itanium (IA64) @ 900 MHz processors with SCSI disk @ 10K RPM.



**Figure 6.2:** Times for different selection modes over Float64 values. Benchmark made on a machine with Itanium (IA64) @ 900 MHz processors with SCSI disk @ 10K RPM.

data as *in-kernel*. Let's see an example of *in-kernel* selection based on the *standard* selection mentioned above:

```
row = table
result = [ row['var2'] for row in table.where(table.cols.var1 <= 20)]</pre>
```

This simple change of mode selection can account for an improvement in search times up to a factor of 10 (see the figure 6.1).

So, where is the trick? It's easy. In the *standard* selection mode the data for column var1 has to be carried up to Python space so as to evaluate the condition and decide if the var2 value should be added to the result list. On the contrary, in the *in-kernel* mode, the *condition* is passed to the PyTables kernel, written in C (hence the name), and evaluated there at C speed (with some help of the numarray package), so that the only values that were brought to the Python space where the references for rows that fulfilled the condition.

You should note, however, that currently the where method only accepts conditions along a single column<sup>1</sup>. Fortunately, you can mix the *in-kernel* and *standard* selection modes for evaluating arbitrarily complex conditions along several columns at once. Look at this example:

here, we have used a *in-kernel* selection to filter the rows whose var3 field is equal to string "foo". Then, we apply a *standard* selection to complete the query.

Of course, when you mix the *in-kernel* and *standard* selection modes you should pass the most restrictive condition to the *in-kernel* part, i.e. to the where iterator. In situations where it is not clear which is the most restrictive condition, you might want to experiment a bit in order to find the best combination.

#### 6.2.2 Indexed searches

When you need more speed than *in-kernel* selections can offer you, PyTables offer a third selection method, so-called *indexed* mode. On this mode, you have to decide which column(s) are you going to do your selections and index them. Indexing is just a kind of sort operation, so that next searches along a column will look at the sorted information using a *binary search* which is much faster than a *sequential search*.

You can index your selected columns in several ways:

**Declaratively** In this mode, you can declare a column as being indexed by passing the *indexed* parameter to the column descriptor. That is:

```
class Example(IsDescription):
    var1 = StringCol(length=4, dflt="", pos=1, indexed=1)
    var2 = BoolCol(0, indexed=1, pos = 2)
    var3 = IntCol(0, indexed=1, pos = 3)
    var4 = FloatCol(0, indexed=0, pos = 4)
```

In this case, we are telling that var1, var2 and var3 columns will be indexed automatically when you add rows to the table with this description.

**Calling Column.createIndex()** In this mode, you can create an index even on an already created table. For example:

```
indexrows = table.cols.var1.createIndex()
indexrows = table.cols.var2.createIndex()
indexrows = table.cols.var3.createIndex()
```

will create indexes for all var1, var2 and var3 columns, and after doing that, they will behave as regular indexes.

After you have indexed a column, you can proceed to use it through the use of Table.where method:

```
row = table
result = [ row['var2'] for row in table.where(table.cols.var1 == "foo")]
```

or, if you want to add more conditions, you can mix the indexed selection with a standard one:

<sup>&</sup>lt;sup>1</sup> Although this may change in the future

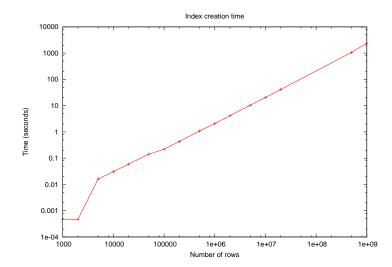


Figure 6.3: Times for indexing a couple of columns of datatypes Int32 and Float64. Benchmark made on a machine with Itanium (IA64) @ 900 MHz processors with SCSI disk @ 10K RPM.

rememeber to pass the most restictive condition to the where iterator.

You can see in figures 6.1 and 6.2 that indexing can accelerate quite a lots your data selections in tables. For moderately large tables (> one million rows), you can see that you can achieve speed-ups in the order of 100x respect to *in-kernel* selections and in the order of 1000x respect to *standard* selections.

One important aspect of indexation in PyTables is that it has been implemented with the goal of being capable to manage effectively very large tables. In figure 6.3, you can see that the times to index columns in tables always grows *linearly*. In particular, the time to index a couple of columns with 1 billion of rows each is 40 min. (roughly 20 min. each), which is a quite reasonable figure. This is because PyTables has choosed an algorithm that do a *partial* sorting of the columns in order to ensure that the indexing time grows *linearly*. On the contrary, most of relational databases try to do a *complete* sorting of columns, and this makes the time to index to grow *quadratically* with the number of rows.

The fact that relational databases uses a complete sorting algorithm for indexes means that their index would be more effective (but not by a large extent) for searching purposes that the PyTables approach. However, for relatively large tables (> 10 millions of rows) the time required for completing such a sort can be so large, that indexing is not normally worth the effort. In other words, PyTables indexing scales much better than relational databases. So, don't worry if you have extremely large columns to index: PyTables is designed to handle with that perfectly.

#### 6.3 Compression issues

One of the beauties of PyTables is that it supports compression on tables and arrays<sup>2</sup>, although it is disabled by default. Compression of big amounts of data might be a bit controversial feature, because compression has a legend of being a very big CPU time resources consumer. However, if you are willing to check if compression can help not only reducing your dataset file size but **also** improving your I/O efficiency, keep reading.

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 redundant data can normally be moved to other

 $<sup>^2</sup>$  More precisely, it is supported in EArray and VLArray objects, not in Array objects itself.

Compr. Lib	File size (MB)	Time writing (s)	Time reading (s)	Speed writing (Krow/s)	Speed reading (Krow/s)
NO COMPR	244.0	24.4	16.0	18.0	27.8
Zlib (lvl 1)	8.5	17.0	3.11	26.5	144.4
Zlib (lvl 6)	7.1	20.1	3.10	22.4	144.9
Zlib (lvl 9)	7.2	42.5	3.10	10.6	145.1
LZO (lvl 1)	9.7	14.6	1.95	30.6	230.5
UCL (lvl 1)	6.9	38.3	2.58	11.7	185.4

**Table 6.1:** Comparison between different compression libraries. The tests have been conducted on a Pentium 4 at 2 GHz and a hard disk at 4200 RPM.

tables and a relationship between the rows on the separate tables can be created. But that takes analysis and implementation time, and makes the underlying libraries more complex and slower.

PyTables transparent compression allows the users to not worry about finding which is 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. This process may normally end in a simpler, yet powerful manner to process your data (although you should still be careful about in which kind of scenarios compression use is convenient or not).

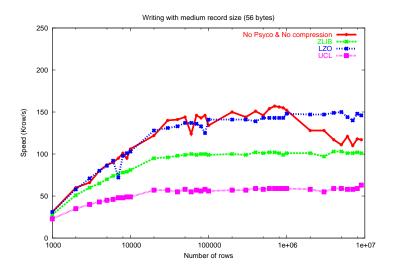
The compression library used by default is the **Zlib** (see Gailly and Adler), and as HDF5 *requires* it, you can safely use it and expect that your HDF5 files will be readable on any other platform that has HDF5 libraries installed. Zlib provides good compression ratio, although somewhat slow, and reasonably fast decompression. Because of that, it is a good candidate to be used for compressing you data.

However, in many situations (i.e. write *once*, read *multiple*), it is critical to have *very good* decompression speed (at expense of whether less compression or more CPU wasted on compression, as we will see soon). This is why support for two additional compressors has been added to PyTables: LZO and UCL (see Oberhumer). Following his author (and checked by the author of this manual), LZO offers pretty fast compression (although small compression ratio) and extremely fast decompression while UCL achieves an excellent compression ratio (at the price of spending much more CPU time) while allowing very fast decompression (and *very close* to the LZO one). In fact, LZO and UCL are so fast when decompressing that, in general (that depends on your data, of course), writing and reading a compressed table is actually faster (and sometimes **much faster**) than if it is uncompressed. This fact is very important, specially if you have to deal with very large amounts of data.

Be aware that the LZO and UCL support in PyTables is not standard on HDF5, so if you are going to use your PyTables files in other contexts different from PyTables you will not be able to read them. Still, see the appendix B.2 where the ptrepack utility is described to find a way to free your files from LZO or UCL dependencies, so that you can use these compressors locally with the warranty that you can replace them with ZLIB (or even remove compression completely) if you want to export the files to other HDF5 tools afterwards.

In order to give you a raw idea of what ratios would be achieved, and what resources would be consumed, look at the table 6.1. This table has been obtained from synthetic data and with a somewhat outdated PyTables version (0.5), so take this just as a guide because your mileage will probably vary. Have also a look at the graphs 6.4 and 6.5 (these graphs have been obtained with tables with different row sizes and PyTables version than the previous example, so do not try to directly compare the figures). They show how the speed of writing/reading rows evolves as the size (the row number) of tables grows. Even though in these graphs the size of one single row is 56 bytes, you can most probably extrapolate this figures to other row sizes. If you are curious about how well compression can perform together with Psyco, look at the graphs 6.6 and 6.7. As you can see, the results are pretty interesting.

By looking at graphs, you can expect that, generally speaking, LZO would be the fastest both compressing and uncompressing, but the one that achieves the worse compression ratio (although that may be just ok for many situations). UCL is the slowest when compressing, but is faster than Zlib when decompressing, and, besides, it achieves very good compression ratios (generally better than Zlib). Zlib represents a balance



**Figure 6.4:** Writing tables with several compressors.

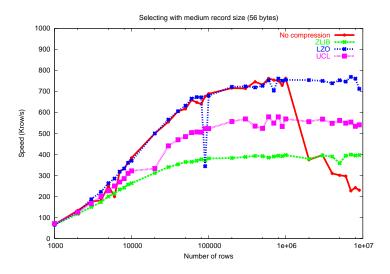


Figure 6.5: Reading tables with several compressors.



Figure 6.6: Writing tables with several compressors and Psyco.

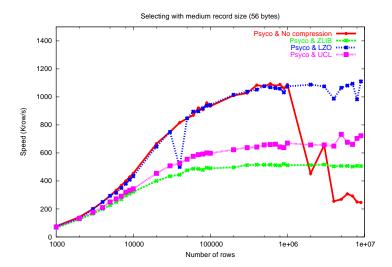


Figure 6.7: Reading tables with several compressors and Psyco.

between them: it's somewhat slow compressing, the slowest during decompression, but it normally achieves fairly good compression ratios.

So, if your ultimate goal is reading as fast as possible, choose LZO. If you want to reduce as much as possible your data, while retaining good read speed, choose UCL. If you don't mind too much about the above parameters and/or portability is important for you, Zlib is your best bet.

The compression level that I recommend to use for all compression libraries is 1. This is the lowest level of compression, but if you take the approach suggested above, normally the redundant data is to be found in the same row, so the redundant data locality is very high and such a small level of compression should be enough to achieve a good compression ratio on your data tables, saving CPU cycles for doing other things. Nonetheless, in some situations you may want to check how compression level affects your application.

You can select the compression library and level by setting the complib and compress keywords in the Filters class (see 4.13.1). A compression level of 0 will completely disable compression (the default), 1 is the less CPU time demanding level, while 9 is the maximum level and most CPU intensive. Finally, have in mind that LZO is not accepting a compression level right now, so, when using LZO, 0 means that compression is not active, and any other value means that LZO is active.

# 6.4 Shuffling (or how to make the compression process more effective)

The HDF5 library provides an interesting filter that can leverage the results of your favorite compressor. Its name is *shuffle*, and because it can greatly benefit compression and it doesn't take many CPU resources, it is active by *default* in PyTables whenever compression is activated (independently of the chosen compressor). It is of course deactivated when compression is off (which is the default, as you already should know).

From the HDF5 reference manual: "The *shuffle* filter de-interlaces a block of data by reordering the bytes. All the bytes from one consistent byte position of each data element are placed together in one block; all bytes from a second consistent byte position of each data element are placed together a second block; etc. For example, given three data elements of a 4-byte datatype stored as 012301230123, shuffling will re-order data as 000111222333. This can be a valuable step in an effective compression algorithm because the bytes in each byte position are often closely related to each other and putting them together can increase the compression ratio."

In table 6.2 you can see a benchmark that shows how the *shuffle* filter can help to the different libraries to compress data in three table datasets. Generally speaking, *shuffle* makes the writing process (shuffling+compressing) faster (between 7% and 22%), which is an interesting result in itself. However, the reading process (unshuffling+decompressing) is slower, but by a lesser extent (between 3% and 18%).

Compr. Lib	File size (MB)	Time writing (s)	Time reading (s)	Speed writing (MB/s)	Speed reading (MB/s)
NO COMPR	165.4	24.5	17.13	6.6	9.6
Zlib (lvl 1)	26.4	22.2	5.77	7.3	28.4
Zlib+shuffle	4.0	19.0	5.94	8.6	27.6
LZO (lvl 1)	44.9	17.8	4.13	9.2	39.7
LZO+shuffle	4.3	16.4	5.03	9.9	32.6
UCL (lvl 1)	27.4	48.8	5.02	3.3	32.7
UCL+shuffle	3.5	38.1	5.31	4.3	30.9

**Table 6.2:** Comparison between different compression libraries, with and without shuffling. The tests have been conducted on a Pentium 4 at 2 GHz and a hard disk at 4200 RPM.

But the most remarkable fact is the level of compression that compressor filters can achieve after *shuffle* has passed over the data: the total file size can be up to 40 times smaller than the uncompressed file, and up to 5 times smaller than the already compressed files (!). Of course, the data for doing this test is synthetic, and *shuffle* seems to do a great work with it, so in general, the results will vary in your case. However, due to the small drawbacks (reads are slowed down by a small extent) and its potential gains (faster writing, but specially much better compression level), I do believe that it is a good thing to have such a filter enabled by default in the battle for discovering redundancy in your data.

### 6.5 Taking advantage of Psyco

Psyco (see Rigo) is a kind of specialized compiler for Python that typically accelerates Python applications with no change in source code. You can think of Psyco as a kind of just-in-time (JIT) compiler, a little bit like Java's, that emits machine code on the fly instead of interpreting your Python program step by step. The result is that your unmodified Python programs run faster.

Psyco is very easy to install and use, so in most scenarios it is worth to give it a try. However, it only runs on Intel 386 architectures, so if you are using other architectures, you are out of luck (at least until Psyco will support yours).

As an example, imagine that you have a small script that reads and selects data over a series of datasets, like this:

```
def readFile(filename):
    "Select data from all the tables in filename"

fileh = openFile(filename, mode = "r")
    result = []
    for table in fileh("/", 'Table'):
        result = [ p['var3'] for p in table if p['var2'] <= 20 ]

    fileh.close()
    return e

if __name__ == "__main__":
    print readFile("myfile.h5")</pre>
```

In order to accelerate this piece of code, you can rewrite your main program to look like:

```
if __name__ == "__main__":
    import pysco
    psyco.bind(readFile)
    print readFile("myfile.h5")
```

That's all!. From now on, each time that you execute your Python script, Psyco will deploy its sophisticated algorithms so as to accelerate your calculations.

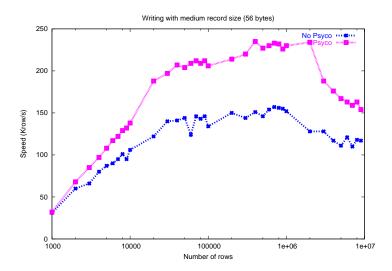


Figure 6.8: Writing tables with/without Psyco.

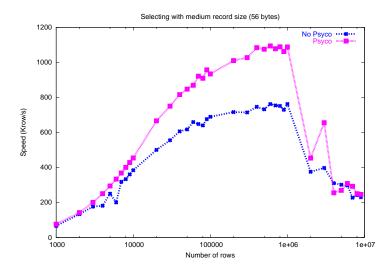


Figure 6.9: Reading tables with/without Psyco.

You can see in the graphs 6.8 and 6.9 how much I/O speed improvement you can get by using Psyco. By looking at this figures you can get an idea if these improvements are of your interest or not. In general, if you are not going to use compression you will take advantage of Psyco if your tables are medium sized (from a thousand to a million rows), and this advantage will disappear progressively when the number of rows grows well over one million. However if you use compression, you will probably see improvements even beyond this limit (see section 6.3). As always, there is no substitute for experimentation with your own dataset.

### 6.6 Selecting an User Entry Point (UEP) in your tree

If you have a **huge** tree in your data file with many nodes on it, creating the object tree would take long time. Many times, however, you are interested only in access to a part of the complete tree, so you won't strictly need PyTables to build the entire object tree in-memory, but only the *interesting* part.

This is where the rootUEP parameter of openFile function (see 4.1.2) can be helpful. Imagine that you have a file called "test.h5" with the associated tree that you can see in figure 6.10, and you are interested

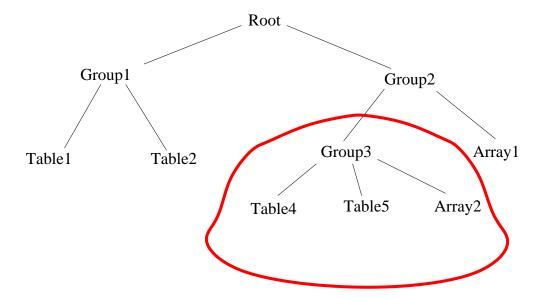


Figure 6.10: Complete tree in file test. h5, and subtree of interest for the user.

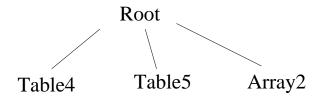


Figure 6.11: Resulting object tree derived from the use of the rootUEP parameter.

only in the section marked in red. You can avoid the build of all the object tree by saying to openFile that your root will be the /Group2/Group3 group. That is:

```
fileh = openFile("test.h5", rootUEP="/Group2/Group3")
```

As a result, the actual object tree built will be like the one that can be seen in figure 6.11.

Of course this has been a simple example and the use of the rootUEP parameter was not very necessary. But when you have *thousands* of nodes on a tree, you will certainly appreciate the rootUEP parameter.

### 6.7 Compacting your PyTables files

Let's suppose that you have a file on which you have made a lot of row deletions on one or more tables, or deleted many leaves or even entire subtrees. These operations might leave *holes* (i.e. space that is not used anymore) in your files, that may potentially affect not only the size of the files but, more importantly, the performance of I/O. This is because when you delete a lot of rows on a table, the space is not automatically recovered on-the-flight. In addition, if you add many more rows to a table than specified in the expectedrows keyword in creation time this may affect performace as well, as explained in section 6.1.

In order to cope with these issues, you should be aware that a handy PyTables utility called ptrepack can be very useful, not only to compact your already existing *leaky* files, but also to adjust some internal parameters (both in memory and in file) in order to create adequate buffer sizes and chunk sizes for optimum I/O speed. Please, check the appendix B.2 for a brief tutorial on its use.

Another thing that you might want to use ptrepack for is changing the compression filters or compression levels on your existing data for different goals, like checking how this can affect both final size and I/O performance, or getting rid of the optional compressors like LZO or UCL in your existing files in case you want to use them with generic HDF5 tools that do not have support for these filters.

# **Appendix A**

# Supported data types in PyTables

The Table, Array, VLArray and EArray classes can all handle the complete set of data types supported by the numarray package (see Greenfield *et al.*) and Numeric (see Ascher *et al.*) in Python. The data types for table fields can be set via the constructor for the Col class and its descendants (see 4.12.2 while array elements can be set through the use of the Atom class and its descendants (see 4.12.3).

A quick reference to the complete set of data types supported by PyTables is given in table A.

**Table A.1:** Data types supported for array elements and tables columns in PyTables.

Type Code	Description	C Type	Size (in bytes)	Python Counterpart
Bool	boolean	unsigned char	1	Boolean
Int8	8-bit integer	signed char	1	Integer
UInt8	8-bit unsigned integer	unsigned char	1	Integer
Int16	16-bit integer	short	2	Integer
UInt16	16-bit unsigned integer	unsigned short	2	Integer
Int32	integer	int	4	Integer
UInt32	unsigned integer	unsigned int	4	Long
Int64	64-bit integer	long long	8	Long
UInt64	unsigned 64-bit integer	unsigned long long	8	Long
Float32	single-precision float	float	4	Float
Float64	double-precision float	double	8	Float
Complex32	single-precision complex	struct {float r, i;}	8	Complex
Complex64	double-precision complex	struct {double r, i;}	16	Complex
CharType	arbitrary length string	char[]	*	String

## **Appendix B**

## **Utilities**

PyTables comes with a couple of utilities that make the life easier to the user. One is called ptdump and lets you see the contents of a PyTables file (or generic HDF5 file, if supported). The other one is named ptrepack that allows to (recursively) copy sub-hierarchies of objects present in a file into another one, changing, if desired, some of the filters applied to the leaves during the copy process.

Normally, these utilities will be installed somewhere in your PATH during the process of installation of the PyTables package, so that you can invoke them from any place in your filesystem after the installation has successfully finished.

### B.1 ptdump

As has been said before, ptdump utility allows you look into the contents of your PyTables files. It lets you see not only the data but also the metadata (that is, the *structure* and additional information in the form of *attributes*).

#### B.1.1 Usage

For instructions on how to use it, just pass the -h flag to the command:

```
$ ptdump -h
```

to see the message usage:

```
usage: ptdump [-R start,stop,step] [-a] [-h] [-d] [-v] file[:nodepath]
  -R RANGE -- Select a RANGE of rows in the form "start,stop,step"
  -a -- Show attributes in nodes (only useful when -v or -d are active)
  -c -- Show info of columns in tables (only useful when -v or -d are active)
  -i -- Show info of indexed columns (only useful when -v or -d are active)
  -d -- Dump data information on leaves
  -h -- Print help on usage
  -v -- Dump more metainformation on nodes
```

#### B.1.2 A small tutorial on ptdump

Let's suppose that we want to know only the *structure* of a file. In order to do that, just don't pass any flag, just the file as parameter:

```
$ ptdump vlarray1.h5
Filename: 'vlarray1.h5' Title: '' , Last modif.: 'Fri Feb 6 19:33:28 2004' ,
rootUEP='/', filters=Filters(), Format version: 1.2
```

```
/ (Group) ''
/vlarray( (VLArray(4,), shuffle, zlib(1)) 'ragged array of ints'
```

we can see that the file contains a just a leaf object called vlarray1, that is an instance of VLArray, has 4 rows, and two filters has been used in order to create it: shuffle and zlib (with a compression level of 1).

```
Let's say we want more metainformation. Just add the -v (verbose) flag:
```

```
$ ptdump -v vlarray1.h5
/ (Group) ''
  children := ['vlarray1' (VLArray)]
/vlarray1 (VLArray(4,), shuffle, zlib(1)) 'ragged array of ints'
  atom = Atom(type=Int32, shape=1, flavor='Numeric')
  nrows = 4
  flavor = 'Numeric'
  byteorder = 'little'
```

so we can see more info about the atoms that are the components of the vlarray1 dataset, i.e. they are scalars of type Int32 and with Numeric flavor.

If we want information about the attributes on the nodes, we must add the -a flag:

```
$ ptdump -va vlarray1.h5
/ (Group) ''
 children := ['vlarray1' (VLArray)]
  /._v_attrs (AttributeSet), 5 attributes:
  [CLASS := 'GROUP',
   FILTERS := None,
   PYTABLES_FORMAT_VERSION := '1.2',
    TITLE := '',
    VERSION := '1.0']
/vlarray1 (VLArray(4,), shuffle, zlib(1)) 'ragged array of ints'
 atom = Atom(type=Int32, shape=1, flavor='Numeric')
 nrows = 4
 flavor = 'Numeric'
 byteorder = 'little'
  /vlarray1.attrs (AttributeSet), 4 attributes:
   [CLASS := 'VLARRAY',
    FLAVOR := 'Numeric',
    TITLE := 'ragged array of ints',
    VERSION := '1.0']
  Let's have a look at the real data:
$ ptdump -d vlarray1.h5
/ (Group) ''
/vlarray1 (VLArray(4,), shuffle, zlib(1)) 'ragged array of ints'
```

we see here a data dump of the 4 rows in vlarray1 object, in the form of a list. Because the object is a VLA, we see a different number of integers on each row.

[array([5, 6]), array([5, 6, 7]), array([5, 6, 9, 8]), array([5, 6, 9, 10, 12])]

Say that we are interested only on a specific row range of the /vlarray1 object:

```
ptdump -R2,4 -d vlarray1.h5:/vlarray1
/vlarray1 (VLArray(4,), shuffle, zlib(1)) 'ragged array of ints'
   Data dump:
[array([5, 6, 9, 8]), array([ 5, 6, 9, 10, 12])]
```

Here, we have specified the range of rows between 2 and 4 (the upper limit excluded, as usual in Python). See how we have selected only the /vlarray1 object for doing the dump (vlarray1.h5:/vlarray1).

Finally, you can mix several information at once:

```
$ ptdump -R2,4 -vad vlarray1.h5:/vlarray1
/vlarray1 (VLArray(4,), shuffle, zlib(1)) 'ragged array of ints'
  atom = Atom(type=Int32, shape=1, flavor='Numeric')
  nrows = 4
  flavor = 'Numeric'
  byteorder = 'little'
  /vlarray1.attrs (AttributeSet), 4 attributes:
  [CLASS := 'VLARRAY',
    FLAVOR := 'Numeric',
    TITLE := 'ragged array of ints',
    VERSION := '1.0']
  Data dump:
[array([5, 6, 9, 8]), array([ 5, 6, 9, 10, 12])]
```

#### B.2 ptrepack

This utility is a very powerful one and let's you to copy any leaf, group or complete subtree into another file. During the copy process you are allowed to change the filter properties if you want so. Also, in the case of duplicated pathnames, you can decide if you want to overwrite already existing nodes on the destination file. Generally speaking, ptrepack can be useful in may situations, like replicating a subtree in another file, change the filters in objects and see how affect this to the compression degree or I/O performance, consolidating specific data in repositoris or even *importing* generic HDF5 files and create true PyTables counterparts.

#### B.2.1 Usage

For instructions on how to use it, just pass the -h flag to the command:

```
$ ptrepack -h
```

to see the message usage:

```
the source is copied).

--dont-copy-userattrs -- Do not copy the user attrs (default is to do it)

--overwrite-nodes -- Overwrite destination nodes if they exist. Default is to not overwrite them.

--complevel=(0-9) -- Set a compression level (0 for no compression, which is the default).

--complib=lib -- Set the compression library to be used during the copy. lib can be set to "zlib", "lzo" or "ucl". Defaults to "zlib".

--shuffle=(0|1) -- Activate or not the shuffling filter (default is active if complevel>0).

--fletcher32=(0|1) -- Whether to activate or not the fletcher32 filter (not active by default).

--keep-source-filters -- Use the original filters in source files. The default is not doing that if any of --complevel, --complib, --shuffle or --fletcher32 option is specified.
```

#### B.2.2 A small tutorial on ptrepack

Imagine that we have ended the tutorial 1 (see the output of examples/tutorial1-1.py), and we want to copy our reduced data (i.e. those datasets that hangs from the /column group) to another file. First, let's remember the content of the examples/tutorial1.h5:

```
$ ptdump tutorial1.h5
Filename: 'tutorial1.h5' Title: 'Test file' , Last modif.: 'Fri Feb 6
  19:33:28 2004', rootUEP='/', filters=Filters(), Format version: 1.2
/ (Group) 'Test file'
/columns (Group) 'Pressure and Name'
/columns/name (Array(3,)) 'Name column selection'
/columns/pressure (Array(3,)) 'Pressure column selection'
/detector (Group) 'Detector information'
/detector/readout (Table(10L,)) 'Readout example'
Now, copy the /columns to other non-existing file. That's easy:
$ ptrepack tutorial1.h5:/columns reduced.h5
That's all. Let's see the contents of the newly created reduced. h5 file:
$ ptdump reduced.h5
Filename: 'reduced.h5' Title: '' , Last modif.: 'Fri Feb 20 15:26:47 2004' ,
rootUEP='/', filters=Filters(), Format version: 1.2
/ (Group) ''
/name (Array(3,)) 'Name column selection'
/pressure (Array(3,)) 'Pressure column selection'
```

so, you have copied the childs of /columns group into the root of the reduced. h5 file.

Now, you suddenly realized that what you intended to do was to copy all the hierarchy, the group /columns itself included. You can do that by just specificing the destination group:

```
$ ptrepack tutorial1.h5:/columns reduced.h5:/columns
ptdump reduced.h5
Filename: 'reduced.h5' Title: '' , Last modif.: 'Fri Feb 20 15:39:15 2004' ,
rootUEP='/', filters=Filters(), Format version: 1.2
```

```
/ (Group) ''
/name (Array(3,)) 'Name column selection'
/pressure (Array(3,)) 'Pressure column selection'
/columns (Group) ''
/columns/name (Array(3,)) 'Name column selection'
/columns/pressure (Array(3,)) 'Pressure column selection'
Ok. Much better. But you want to get rid of the existing nodes on the new file. You can achieve this by adding
the -o flag:
$ ptrepack -o tutorial1.h5:/columns reduced.h5:/columns
$ ptdump reduced.h5
Filename: 'reduced.h5' Title: '' , Last modif.: 'Fri Feb 20 15:41:57 2004' ,
rootUEP='/', filters=Filters(), Format version: 1.2
/ (Group) ''
/columns (Group) ''
/columns/name (Array(3,)) 'Name column selection'
/columns/pressure (Array(3,)) 'Pressure column selection'
where you can see how the old contents of the reduced. h5 file has been overwritten.
   You can copy just one single node in the repacking operation and change its name in destination:
$ ptrepack tutorial1.h5:/detector/readout reduced.h5:/rawdata
$ ptdump reduced.h5
Filename: 'reduced.h5' Title: '' , Last modif.: 'Fri Feb 20 15:52:22 2004',
 rootUEP='/', filters=Filters(), Format version: 1.2
/ (Group) ''
/rawdata (Table(10L,)) 'Readout example'
/columns (Group) ''
/columns/name (Array(3,)) 'Name column selection'
/columns/pressure (Array(3,)) 'Pressure column selection'
where the /detector/readout has been copied to /rawdata in destination.
   We can change the filter properties as well:
$ ptrepack --complevel=1 tutorial1.h5:/detector/readout reduced.h5:/rawdata
Problems doing the copy from 'tutorial1.h5:/detector/readout' to
'reduced.h5:/rawdata'
The error was --> exceptions. Value Error: The destination
 (/rawdata (Table(10L,)) 'Readout example') already exists.
 Assert the overwrite parameter if you really want to overwrite it.
The destination file looks like:
Filename: 'reduced.h5' Title: ''; Last modif.: 'Fri Feb 20 15:52:22 2004';
 rootUEP='/'; filters=Filters(), Format version: 1.2
/ (Group) ''
/rawdata (Table(10L,)) 'Readout example'
/columns (Group) ''
/columns/name (Array(3,)) 'Name column selection'
/columns/pressure (Array(3,)) 'Pressure column selection'
Traceback (most recent call last):
  File "../utils/ptrepack", line 358, in ?
    start=start, stop=stop, step=step)
  File "../utils/ptrepack", line 111, in copyLeaf
```

```
raise RuntimeError, "Please, check that the node names are not duplicated in destination, and if so, add the --overwrite-nodes flag if desired."

RuntimeError: Please, check that the node names are not duplicated in destination, and if so, add the --overwrite-nodes flag if desired.
```

ooops!. We ran into problems: we forgot that /rawdata pathname already existed in destination file. Let's add the --overwrite-nodes, as the verbose error suggested:

```
$ ptrepack --overwrite-nodes --complevel=1 tutorial1.h5:/detector/readout
reduced.h5:/rawdata
$ ptdump reduced.h5
Filename: 'reduced.h5' Title: ''; Last modif.: 'Fri Feb 20 16:02:20 2004';
rootUEP='/'; filters=Filters(), Format version: 1.2
/ (Group) ''
/rawdata (Table(10L,), shuffle, zlib(1)) 'Readout example'
/columns (Group) ''
/columns/name (Array(3,)) 'Name column selection'
/columns/pressure (Array(3,)) 'Pressure column selection'
```

you can check how the filter properties has been changed for the /rawdata table. Check as the other nodes still exists.

Finally, let's copy a *slice* of the readout table in origin to destination, under a new group called /slices and with the name, for example, aslice:

```
$ ptrepack -R1,8,3 tutorial1.h5:/detector/readout reduced.h5:/slices/aslice
$ ptdump reduced.h5
Filename: 'reduced.h5' Title: ''; Last modif.: 'Fri Feb 20 16:17:13 2004';
  rootUEP='/'; filters=Filters(); Format version: 1.2
/ (Group) ''
/rawdata (Table(10L,), shuffle, zlib(1)) 'Readout example'
/columns (Group) ''
/columns/name (Array(3,)) 'Name column selection'
/columns/pressure (Array(3,)) 'Pressure column selection'
/slices (Group) ''
/slices/aslice (Table(3L,)) 'Readout example'
```

note how only 3 rows of the original readout table has been copied to the new aslice destination. Note as well how the previously inexistent slices group has been created in the same operation.

#### B.3 nctoh5

This tool is able to convert a file in NetCDF format to a PyTables file (and hence, to a HDF5 file). However, for this to work, you will need the NetCDF interface for Python that comes with the excellent Scientific Python (see Hinsen) package. This script was initially contributed by Jeff Whitaker. It has been updated to support selectable filters from the command line and some other small improvements.

If you want other file formats to be converted to PyTables, have a look at the SciPy (see Jones *et al.*) project (subpackage io), and look for different methods to import them into Numeric/numarray objects. Following the SciPy documentation, you can read, among other formats, ASCII files (read\_array), binary files in C or Fortran (fopen) and MATLAB (version 4 or 5) files (loadmat). Once you have the content of your files as Numeric/numarray objects, you can save them as regular (E)Arrays in PyTables files. Remember, if you end with a nice conversor, do not forget to contribute it back to the community. Thanks!

#### B.3.1 Usage

For instructions on how to use it, just pass the -h flag to the command:

```
$ nctoh5 -h
```

to see the message usage:

```
usage: nctoh5 [-h] [-v] [-o] [--complevel=(0-9)] [--complib=lib] [--shuffle=(0|1)]
[--fletcher32=(0|1)] netcdffilename hdf5filename
-h -- Print usage message.
-v -- Show more information.
-o -- Overwite destination file.
--complevel=(0-9) -- Set a compression level (0 for no compression, which is the default).
--complib=lib -- Set the compression library to be used during the copy.
    lib can be set to "zlib", "lzo" or "ucl". Defaults to "zlib".
--shuffle=(0|1) -- Activate or not the shuffling filter (default is active if complevel>0).
--fletcher32=(0|1) -- Whether to activate or not the fletcher32 filter (not active by default).
```

If you have followed the small tutorial on the ptrepack utility (see B.2), you should easily realize what the different flags would mean.

## Appendix C

# PyTables File Format

PyTables has a powerful capability to deal with native HDF5 files created with another tools. However, there are situations were you may want to create truly native PyTables files with those tools while retaining fully compatibility with PyTables format. That is perfectly possible, and in this appendix is presented the format that you should endow to your own-generated files in order to get a fully PyTables compatible file.

We are going to describe the **1.3 version of PyTables file format** (introduced in PyTables version 0.9). At this stage, this file format is considered stable enough to do not introduce significant changes during a reasonable amount of time. As time goes by, some changes will be introduced (and documented here) in order to cope with new necessities. However, the changes will be carefully analyzed so as to ensure backward compatibility whenever is possible.

A PyTables file is composed with arbitrarily large amounts of HDF5 groups (Groups in PyTables naming scheme) and datasets (Leaves in PyTables naming scheme). For groups, the only requirements are that they must have some *system attributes* available. By convention, system attributes in PyTables are written in upper case, and user attributes in lower case but this is not enforced by the software. In the case of datasets, besides the mandatory system attributes, some conditions are further needed in their storage layout, as well as in the datatypes used in there, as we will see shortly.

As a final remark, you can use any filter as you want to create a PyTables file, provided that the filter is a standard one in HDF5, like *zlib*, *shuffle* or *szip* (although the last one cannot be used from within PyTables to create a new file, datasets compressed with szip can be read, because it is the HDF5 library which do the decompression transparently).

### C.1 Mandatory attributes for a File

The File object is, in fact, an special HDF5 *group* structure that is *root* for the rest of the objects on the object tree. The next attributes are mandatory for the HDF5 *root group* structure in PyTables files:

**CLASS** This attribute should always be set to 'GROUP' for group structures.

**PYTABLES\_FORMAT\_VERSION** It represents the internal format version, and currently should be set to the '1.2' string.

**TITLE** A string where the user can put some description on what is this group used for.

**VERSION** Should contains the string '1.0'.

#### C.2 Mandatory attributes for a Group

The next attributes are mandatory for group structures:

**CLASS** This attribute should always be set to 'GROUP' for group structures.

**TITLE** A string where the user can put some description on what is this group used for.

**VERSION** Should contains the string '1.0'.

There exist a special Group, called the *root*, that, in addition to the attributes listed above, it requires the next one:

**PYTABLES\_FORMAT\_VERSION** It represents the internal format version, and currently should be set to the '1.3' string.

# C.3 Mandatory attributes, storage layout and supported datatypes for Leaves

This depends on the kind of Leaf. The format for each type follows.

#### C.3.1 Table format

#### **Mandatory attributes**

The next attributes are mandatory for table structures:

**CLASS** Must be set to 'TABLE'.

**TITLE** A string where the user can put some description on what is this dataset used for.

**VERSION** Should contain the string '2.2'.

**FIELD\_X\_NAME** It contains the names of the different fields. The x means the number of the field (beware, order do matter). You should add as many attributes of this kind as fields you have in your records.

**NROWS** This should contain the number of *compound* datatype entries in the dataset. It must be an *int* datatype.

#### **Storage Layout**

A Table has a dataspace with a 1-dimensional chunked layout.

#### **Datatypes supported**

The datatype of the elements (rows) of Table must be the H5T\_COMPOUND *compound* datatype, and each of these compound components must be built with only the next HDF5 datatypes *classes*:

**H5T\_BITFIELD** This class is used to represent the Bool type. Such a type must be build using a H5T\_NATIVE\_B8 datatype, followed by a HDF5 H5Tset\_precision call to set its precision to be just 1 bit.

**H5T\_INTEGER** This includes the next datatypes:

- **H5T\_NATIVE\_SCHAR** This represents a *signed char* C type, but it is effectively used to represent an Int8 type.
- **H5T\_NATIVE\_UCHAR** This represents an *unsigned char* C type, but it is effectively used to represent an UInt8 type.
- **H5T\_NATIVE\_SHORT** This represents a *short* C type, and it is effectively used to represent an Int16 type.
- **H5T\_NATIVE\_USHORT** This represents an *unsigned short* C type, and it is effectively used to represent an UInt16 type.

- **H5T\_NATIVE\_INT** This represents an *int* C type, and it is effectively used to represent an Int32 type.
- **H5T\_NATIVE\_UINT** This represents an *unsigned int* C type, and it is effectively used to represent an UInt32 type.
- **H5T\_NATIVE\_LONG** This represents a *long* C type, and it is effectively used to represent an Int32 or an Int64, depending on whether you are running a 32-bit or 64-bit architecture.
- **H5T\_NATIVE\_ULONG** This represents an *unsigned long* C type, and it is effectively used to represent an UInt32 or an UInt64, depending on whether you are running a 32-bit or 64-bit architecture.
- **H5T\_NATIVE\_LLONG** This represents a *long long* C type (\_\_int64, if you are using a Windows system) and it is effectively used to represent an Int64 type.
- **H5T\_NATIVE\_ULLONG** This represents an *unsigned long long* C type (beware: this type does not have a correspondence on Windows systems) and it is effectively used to represent an UInt64 type.
- **H5T\_FLOAT** This includes the next datatypes:
  - **H5T\_NATIVE\_FLOAT** This represents a *float* C type and it is effectively used to represent an Float32 type.
  - **H5T\_NATIVE\_DOUBLE** This represents a *double* C type and it is effectively used to represent an Float64 type.
- **H5T\_STRING** The datatype used to describe strings in PyTables is H5T\_C\_S1 (i.e. a *string* C type) followed with a call to the HDF5 H5Tset\_size() function to set their length.
- **H5T\_ARRAY** This allows the construction of homogeneous, multi-dimensional arrays, so that you can include such objects in compound records. The types supported as elements of H5T\_ARRAY datatypes are the ones described above. Currently, PyTables does not support nested H5T\_ARRAY types.
- **H5T\_COMPOUND** This allows the support of complex numbers. Its format is described below:

The H5T\_COMPOUND type class contains two members. Both members must have the H5T\_FLOAT atomic datatype class. The name of the first member should be "r" and represents the real part. The name of the second member should be "i" and represents the imaginary part. The *precision* property of both of the H5T\_FLOAT members must be either 32 significant bits (e.g. H5T\_NATIVE\_FLOAT) or 64 significant bits (e.g. H5T\_NATIVE\_DOUBLE). They represent Complex32 and Complex64 types respectively.

Currently, PyTables does not support nested H5T\_COMPOUND types, the only exception being supporting complex numbers in Table objects as described above.

#### C.3.2 Array format

#### **Mandatory attributes**

The next attributes are mandatory for array structures:

- **CLASS** Must be set to 'ARRAY'.
- **FLAVOR** This is meant to provide the information about the kind of object kept in the Array, i.e. when the dataset is read, it will be converted to the indicated flavor. It can take one the next string values:
  - "NumArray" The dataset will be returned as a NumArray object (from the numarray package).
  - "CharArray" The dataset will be returned as a CharArray object (from the numarray package).
  - "Numeric" The dataset will be returned as an array object (from the Numeric package).

- "List" The dataset will be returned as a Python List object.
- "Tuple" The dataset will be returned as a Python Tuple object.
- "Int" The dataset will be returned as a Python Int object. This is meant mainly for scalar (i.e. without dimensions) integer values.
- "Float" The dataset will be returned as a Python Float object. This is meant mainly for scalar (i.e. without dimensions) floating point values.
- "String" The dataset will be returned as a Python String object. This is meant mainly for scalar (i.e. without dimensions) string values.
- **TITLE** A string where the user can put some description on what is this dataset used for.

**VERSION** Should contain the string '2.1'.

#### Storage Layout

An Array has a *dataspace* with a *N-dimensional contiguous* layout (if you prefer a *chunked* layout see EArray below).

#### **Datatypes supported**

The elements of Array must have either HDF5 *atomic* datatypes or a *compound* datatype representing a complex number. The atomic datatypes can currently be one of the next HDF5 datatype *classes*: H5T\_BITFIELD, H5T\_INTEGER, H5T\_FLOAT and H5T\_STRING. See the Table format description in section C.3.1 for more info about these types.

In addition to the HDF5 atomic datatypes, the Array format supports complex numbers with the H5T\_COMPOUND datatype class. See the Table format description in section C.3.1 for more info about this special type.

You should note that H5T\_ARRAY class datatypes are not allowed in Array objects.

#### C.3.3 Earray format

#### **Mandatory attributes**

The next attributes are mandatory for earray structures:

**CLASS** Must be set to 'EARRAY'.

- **EXTDIM** (*Integer*) Must be set to the extensible dimension. Only one extensible dimension is supported right now.
- **FLAVOR** This is meant to provide the information about the kind of objects kept in the EArray, i.e. when the dataset is read, it will be converted to the indicated flavor. It can take the same values as the Array object (see C.3.2), except "Int" and "Float".
- **TITLE** A string where the user can put some description on what is this dataset used for.

**VERSION** Should contain the string '1.1'.

#### Storage Layout

An EArray has a dataspace with a N-dimensional chunked layout.

#### **Datatypes supported**

The elements of EArray are allowed to have the same datatypes as for the elements in the Array format. They can be one of the HDF5 *atomic* datatype *classes*: H5T\_BITFIELD, H5T\_INTEGER, H5T\_FLOAT or H5T\_STRING, see the Table format description in section C.3.1 for more info about these types. They can also be a H5T\_COMPOUND datatype representing a complex number, see the Table format description in section C.3.1.

You should note that H5T\_ARRAY class datatypes are not allowed in EArray objects.

#### C.3.4 VLArray format

#### Mandatory attributes

The next attributes are mandatory for *vlarray* structures:

**CLASS** Must be set to 'VLARRAY'.

- **FLAVOR** This is meant to provide the information about the kind of objects kept in the VLArray, i.e. when the dataset is read, it will be converted to the indicated flavor. It can take one of the next values:
  - "NumArray" The elements in dataset will be returned as NumArray objects (from the numarray package).
  - "CharArray" The elements in dataset will be returned as CharArray objects (from the numarray package).
  - "String" The elements in the dataset will be returned as Python String objects of *fixed* length (and not as CharArrays).
  - "Numeric" The elements in the dataset will be returned as array objects (from the Numeric package).
  - "List" The elements in the dataset will be returned as Python List objects.
  - "Tuple" The elements in the dataset will be returned as Python Tuple objects.
  - "Object" The elements in the dataset will be interpreted as pickled (i.e. serialized objects through the use of the Pickle Python module) objects and returned as Python generic objects. Only one of such objects will be supported per entry. As the Pickle module is not normally available in other languages, this flavor won't be useful in general.
  - "VLString" The elements in the dataset will be returned as Python String objects of *any* length, with the twist that Unicode strings are supported as well (provided you use the UTF-8 codification, see below). However, only one of such objects will be supported per entry.
- TITLE A string where the user can put some description on what is this dataset used for.

**VERSION** Should contain the string '1.1'.

#### Storage Layout

An VLArray has a dataspace with a 1-dimensional chunked layout.

#### **Datatypes supported**

The datatype of the elements (rows) of VLArray objects must be the H5T\_VLEN *variable-length* (or VL for short) datatype, and the base datatype specified for the VL datatype can be of any *atomic* HDF5 datatype that is listed in the Table format description section C.3.1. That includes the classes:

- H5T BITFIELD
- H5T\_INTEGER

- H5T\_FLOAT
- H5T\_STRING
- H5T\_ARRAY

They can also be a H5T\_COMPOUND datatype representing a complex number, see the Table format description in section C.3.1 for a detailed description.

You should note that this does not include another VL datatype, or a compound datatype that does not fit the description of a complex number. Note as well that, for <code>Object</code> and <code>VLString</code> special flavors, the base for the VL datatype is always a <code>H5T\_NATIVE\_UCHAR</code>. That means that the complete row entry in the dataset has to be used in order to fully serialize the object or the variable length string.

In addition, if you plan to use a VLString flavor for your text data and you are using ascii-7 (7 bits ASCII) codification for your strings, but you don't know (or just don't want) to convert it to the required UTF-8 codification, you should not worry too much about that because the ASCII characters with values in the range [0x00, 0x7f] are directly mapped to Unicode characters in the range [U+0000, U+007F] and the UTF-8 encoding has the useful property that an UTF-8 encoded ascii-7 string is indistinguishable from a traditional ascii-7 string. So, you will not need any further conversion in order to save your ascii-7 strings and have an VLString flavor.

# **Bibliography**

ASCHER, David, Paul F. DUBOIS, Konrad HINSEN, Jim HUGUNIN, and Travis OLIPHANT, : *Numerical Python*. Package to speed-up arithmetic operations on arrays of numbers.

URL http://www.pfdubois.com/numpy/ 2,7,79

EWING, Greg,: Pyrex. A Language for Writing Python Extension Modules.

URL http://www.cosc.canterbury.ac.nz/~greg/python/Pyrex 7

GAILLY, JeanLoup and Mark ADLER, : zlib. A Massively Spiffy Yet Delicately Unobtrusive Compression Library. A standard library for compression purposes.

URL http://www.gzip.org/zlib/ 7,73

GREENFIELD, Perry, Todd MILLER, Richard L. WHITE, *et al.*, : *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.

URL http://stsdas.stsci.edu/numarray/ 2,7,50,79

HINSEN, Konrad,: *Scientific Python*. Collection of Python modules useful for scientific computing. URL http://starship.python.net/~hinsen/ScientificPython/ 86

JONES, Eric, Travis OLIPHANT, Pearu PETERSON, et al., : SciPy. Scientific tools for Python. SciPy supplements the popular Numeric module, gathering a variety of high level science and engineering modules together as a single package.

URL http://www.scipy.org 86

MERTZ, David, : *Objectify. 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.

URL http://www-106.ibm.com/developerworks/xml/library/xml-matters2/index. html 3

NCSA,: What is HDF5? Concise description about HDF5 capabilities and its differences from earlier versions (HDF4).

URL http://hdf.ncsa.uiuc.edu/whatishdf5.html 1,63

OBERHUMER, Markus F.X.J., : LZO and UCL. A couple of portable lossless data compression libraries. They offer pretty fast compression and extremly fast decompression.

URL http://www.oberhumer.com/opensource/ 7,73

RIGO, Armin, : *Psyco. A Python specializing compiler.* Run existing Python software faster, with no change in your source.

URL http://psyco.sourceforge.net 76