PyTables & Family

Analyzing and Sharing HDF5 Data with Python

Francesc Altet

Cárabos Coop. V.

HDF Workshop November 30, 2005 - December 2, 2005.

Who are we?

- Cárabos is the company committed to the PyTables suite development and deployment.
- We have years of experience in designing software solutions for handling extremely large datasets.
- What we provide:
  - Commercial support for the PyTables suite.
  - PyTables-based applications.
  - Consulting services for managing complex data environments.

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- Flexible data structures $\Rightarrow$ Malleability
- Minimalistic grammar $\Rightarrow$ Easy to learn
- Very complete library (*Batteries included*) $\Rightarrow$ Boosts productivity

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Very Suitable for Scientific/Engineer Fields

- Interactivity has always been very appreciated for increasing productivity.
- Being interpreted does not necessarily mean being inefficient. Python has solutions for linking C & Fortran libraries in an easy way.
- Programming is normally considered a *necessary evil*. Rich expressivity of Python normally reduces the amount of code to solve real problems.
- Many efficient scientific libraries have been developed for Python: Numeric, numarray, SciPy, Scientific-Python, matplotlib...

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Basic Matrix Handling

Numeric

- Very mature but lacking some features.
- Still has a huge user base.

scipy.core

- Called to substitute both Numeric & numarray. When finished, it is supposed to have all the advantages of Numeric & numarray together.

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- Better handling of large arrays, heterogeneous data...

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SciPy

- Optimization, integration, special functions
- Signal and image processing
- Genetic algorithms, ODE solvers...

Scientific Python

- Quaternions, automatic derivatives, (linear) interpolation, polinomials, ...
- Overlaps somewhat SciPy, but it has...
- A nice netCDF module for I/O

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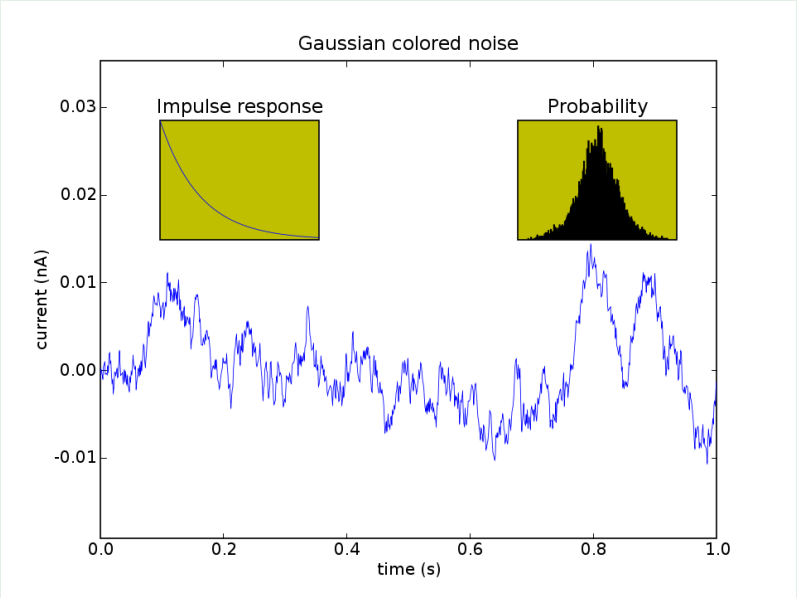
Plotting (2D)

matplotlib

- Great interactivity.
- Produces publication quality figures.

matplotlib example

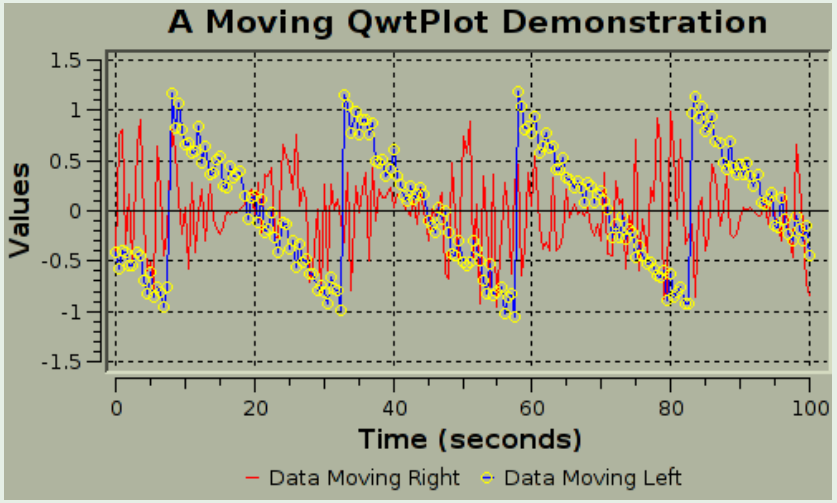


Plotting (2D)

PyQwt

- Fast plotting.
- Nice to be embedded in Qt apps.

PyQwt example

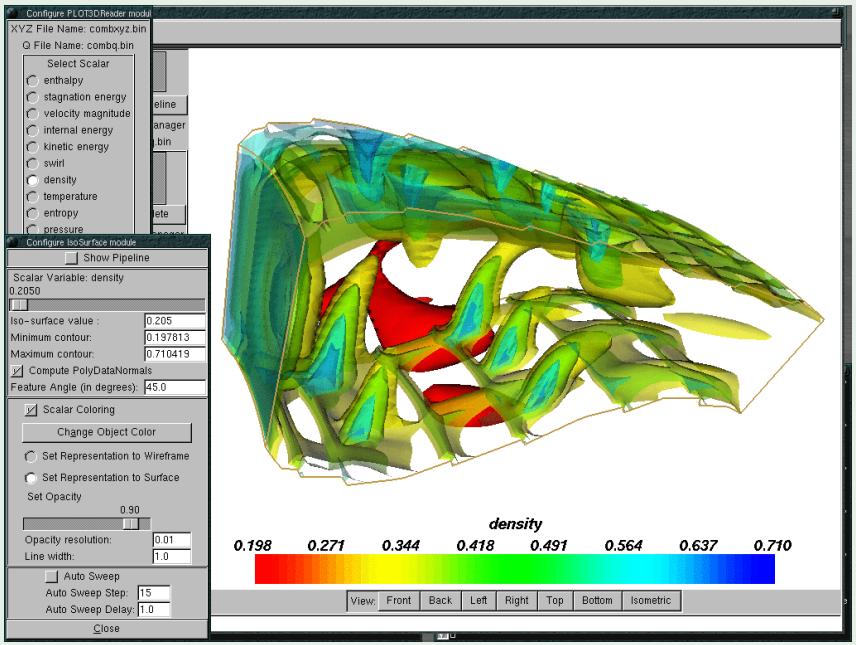


Plotting (3D)

MayaVi

- 3D-oriented scientific data visualizer.
- Uses the Visualization Toolkit (VTK).

MayaVi example



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Programming as a Necessary Evil

Evaluate $E_n(x) = \int_1^\infty \frac{e^{-xt}}{t^n} dt$ for each value of n

```
from scipy import *
from scipy.integrate import quad, Inf
def integrand(t,n,x):
    return exp(-x*t) / t**n
def expint(n,x):
    return quad(integrand, 1, Inf, args=(n, x))[0]
v_expint = vectorize(expint)
print v_expint(3,arange(1.0,4.0,0.5))
```

The output

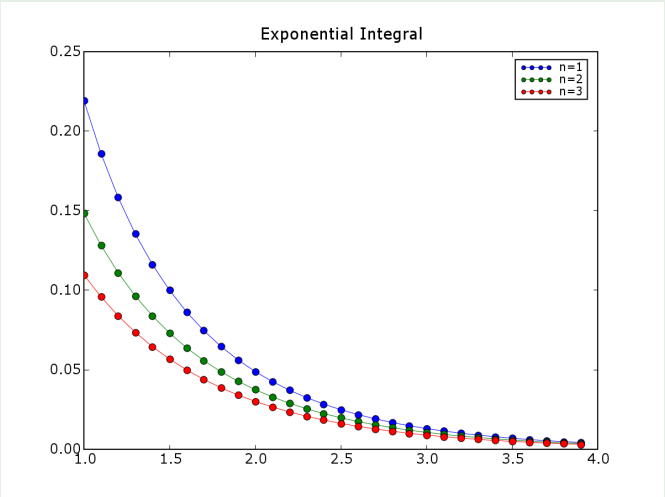
```
[ 0.10969197, 0.05673949, 0.03013338, 0.01629537,
0.00893065, 0.00494538,]
```

Programming as a Necessary Evil

The plotting code (matplotlib)

```
xrng = arange(1.0,4.0,0.1)
plot(xrng, v_expint(1, xrng))
plot(xrng, v_expint(2, xrng))
plot(xrng, v_expint(3, xrng))
legend(("n=1", "n=2", "n=3"))
title('Exponential Integral')
```

The output



Resources

- Introductory material:
  - docs.python.org/tut/tut.html
  - www.python.org/doc/Intros.html
- Lutz & Ascher, "Learning Python": good introduction.
- Martelli, "Python in a Nutshell": useful reference.
- Martelli & Ascher, "Python Cookbook": more specialized, useful recipes for particular problems.
- Hans P. Langtangen, "Python Scripting for Computational Science": teaches computational scientists and engineers how to write small Python scripts efficiently.

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What is PyTables?

Simply stated: a database for Python based on HDF5.

- Designed to deal with extremely large datasets.
- Provides an easy-to-use interface.
- Supports many of the features of HDF5 and others that are not present in it (e.g. indexation).
- It is Open Source software (BSD license).

Why HDF5?

I started looking for different backends for saving large datasets, but HDF5 was the final winner.

- Thought out for managing very large datasets in an efficient way.
- Let you organize datasets hierchically.
- Very flexible and well tested in scientific environments.
- Good maintenance and improvement rate.
- It is Open Source software.

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What Does *Extremely Large* Exactly Mean?

The Hitch Hiker's Guide to the Galaxy *offers this definition of the word "Infinite":*

Infinite: *Bigger than the biggest thing ever and then some. Much bigger than that in fact, really amazingly immense, a totally stunning size, real "wow, that's big". Infinity is just so big that, by comparison, bigness looks really titchy. Gigantic multiplied by colossal multiplied by staggeringly huge is the sort of concept we're trying to get across here.*

Disclaimer

Agreed, *'Extremely Large'* may not exactly mean *'Infinite'*, although it is pretty close to this definition.

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Which *ELD* Features Does PyTables Support?

- A good base library (HDF5).
- Support for 64-bit in all data addressing.
  - Need to overcome a Python slicing limitation: only 32-bit addresses are supported.
- Buffered I/O.
- A LRU cache system for an efficient reuse of objects.
- Fast indexing and searching capabilities for tables.

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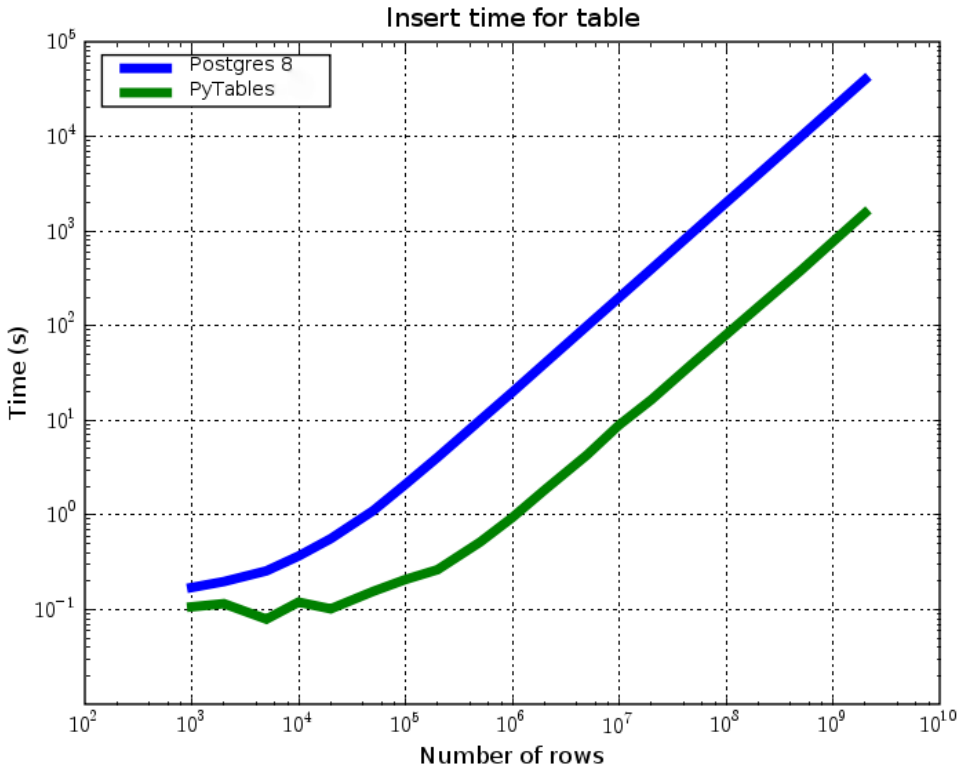
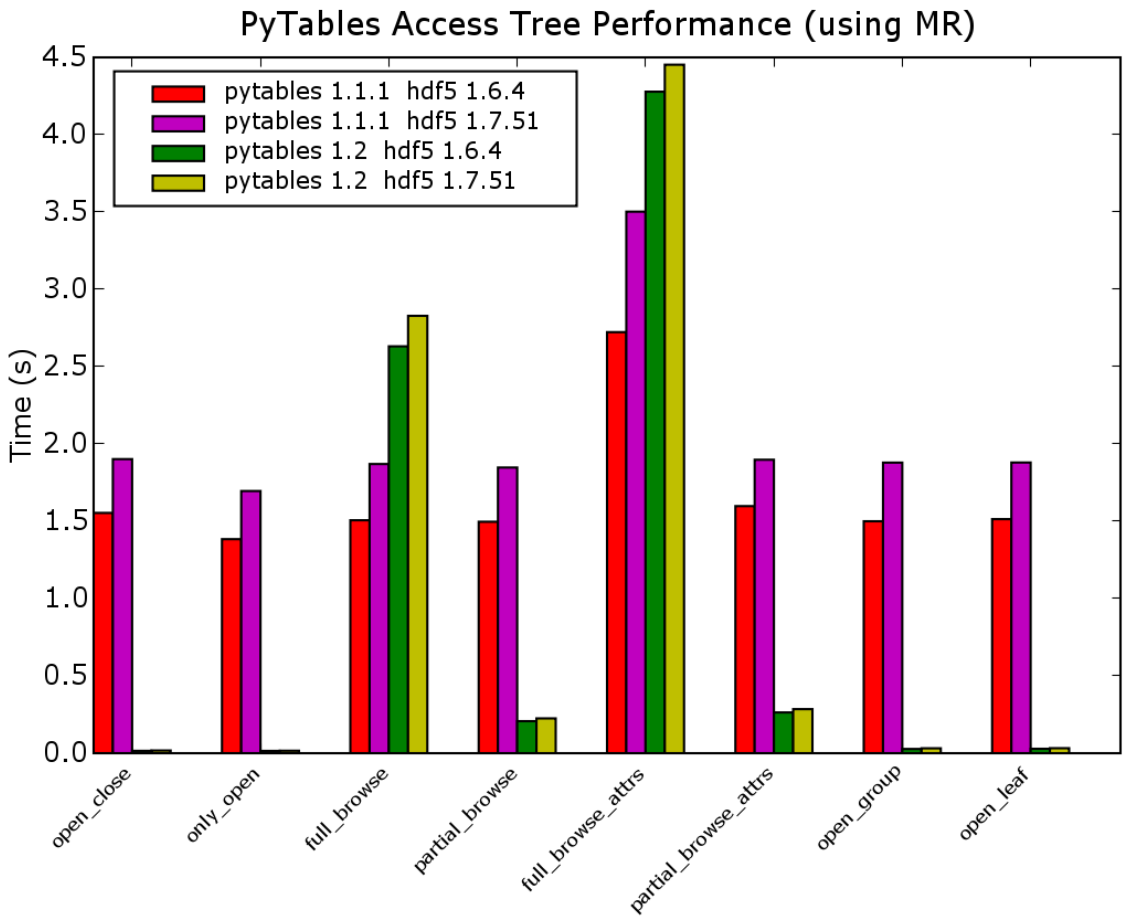
Why Buffered I/O?

Because of speed (what else?):



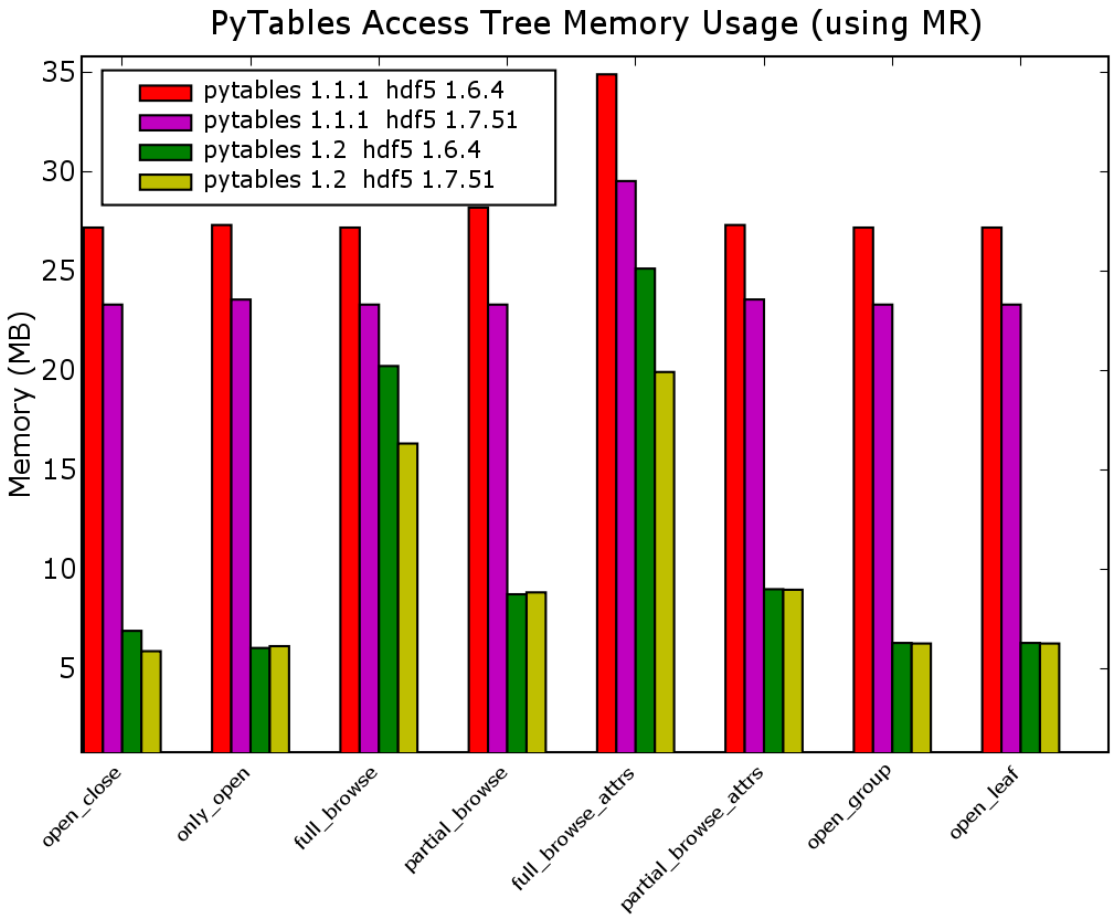
Why a Cache System?

1.- To achieve better open file times:



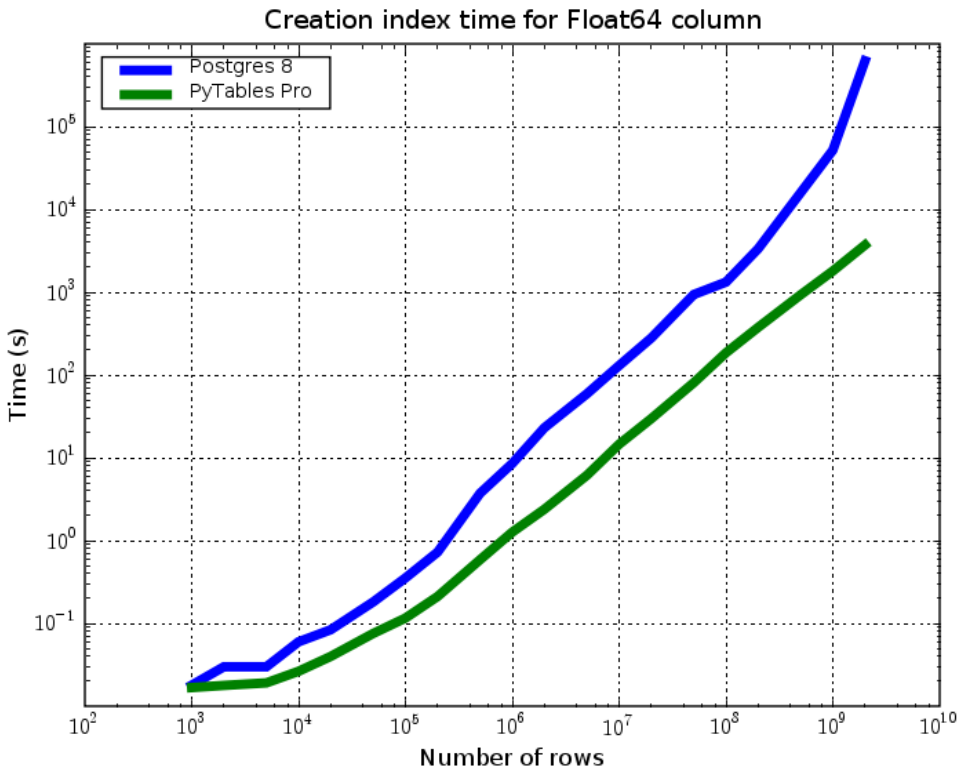
Why a Cache System?

2.- To achieve a conservative usage of the memory:



Why Fast Indexing?

It is not trifling in terms of time when you have to index tables with more than one billion of rows:



Ease of Use

Natural naming

```
# access to file:/group1/table
table = file.root.group1.table
```

Support for generalized slicing

```
# step means a stride in the slice
table[start:stop:step]
```

Support for iterators

```
# get the values in col1 that satisfy the
# (1.3 < col3 <= 2.) condition in table
col3 = table.cols.col3
[r['col1'] for r in table.where(1.3 < col3 <= 2.)]
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Supported Objects in PyTables

- **Table**: Lets you deal with heterogeneous datasets. Chunked. Enlargeable. Support for nested types.
- **Array**: Provides quick and dirty array handling. Not chunked. Non enlargeable.
- **CArray**: Provides compressed array support. Chunked. Not enlargeable.
- **EArray**: Most general array support. Chunked. Enlargeable.
- **VLArray**: Collections of homogeneous data with a variable number of entries. Chunked. Enlargeable.
- **Group**: The *structural* component.

What's New in PyTables 1.2?

- Added a new cache for the object tree.
  - Allows a contained use of memory (even with huge trees).
  - Almost instantaneous opening of files (good news for interactive use!).
- New NetCDF module (contributed by Jeff Whitaker).
  - Provides API emulation for `Scientific.IO.NetCDF`.
  - netCDF-3 $\Leftrightarrow$ HDF5 conversions.
  - tables.NetCDF datasets can be shared over the internet with the OPeNDAP protocol.
  - Plans to write data natively in netCDF-4 format in the future.

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Some Metrics on PyTables 1.2

- Core Library
  - ~ 7.5 thousand LOC (Python)
  - ~ 2.8 thousand LOC (Pyrex)
  - ~ 4.0 thousand LOC (C)
- Test Units
  - ~ 3.1 thousand test units (Python)
  - ~ 23 thousand LOC (Python)
- Documentation
  - ~ 5.0 thousand lines of on-line doc strings
  - ~ 160 pages of Users' Guide in PDF (and HTML)

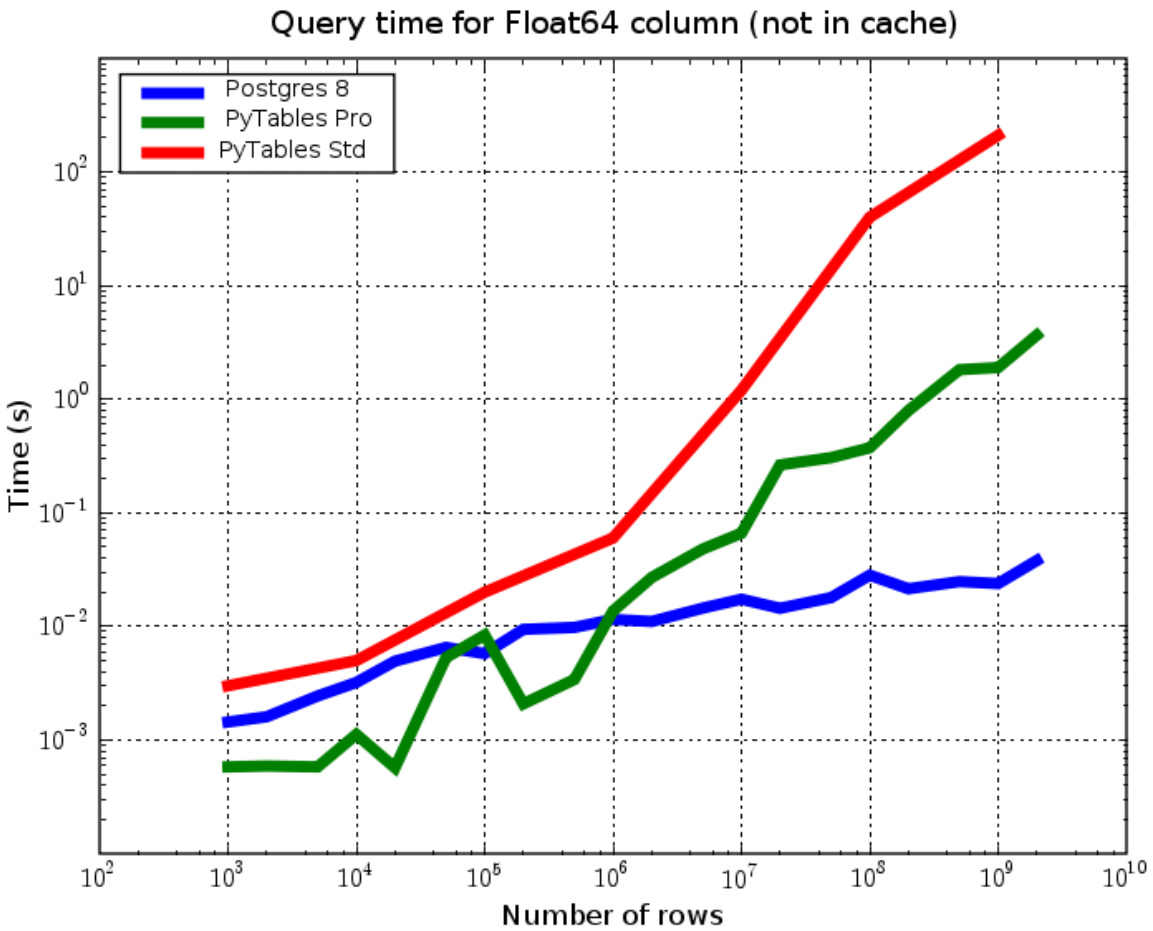
Outline

What is PyTables Pro?

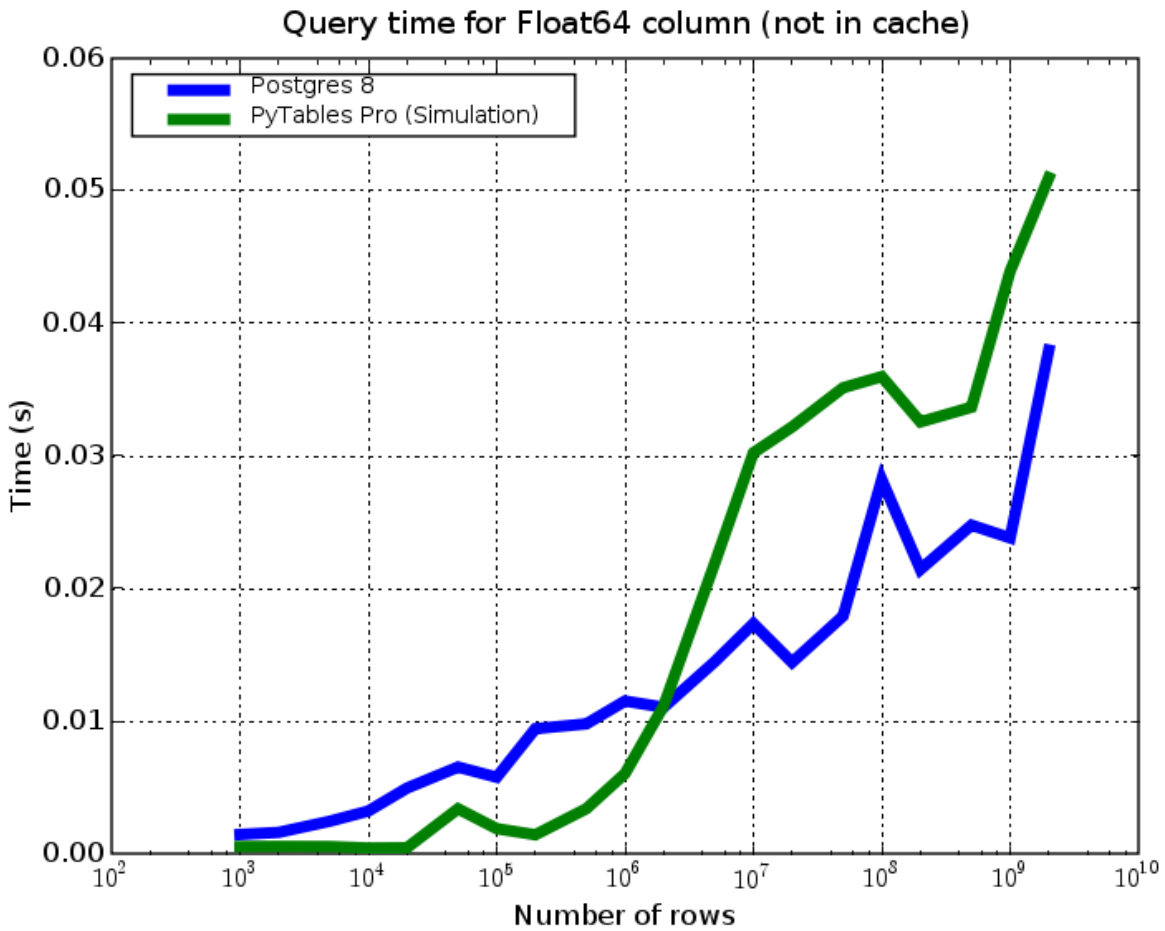
It's just a regular PyTables but with enhanced features:

- **Improved search speed**: Selections in tables with > 1 billion rows will be typically done in less than 1 second.
- **Complex queries**: Supports an unlimited combination of conditions.
- **Query optimizer**: Queries are analyzed, reordered and classified to get an optimum response time.
- **Support for complex indices**: Expressions like *col1 + col2*col3 + col4**3* can be indexed and used for selections afterwards.

Index Selection Speed



Index Selection Speed: The Goal

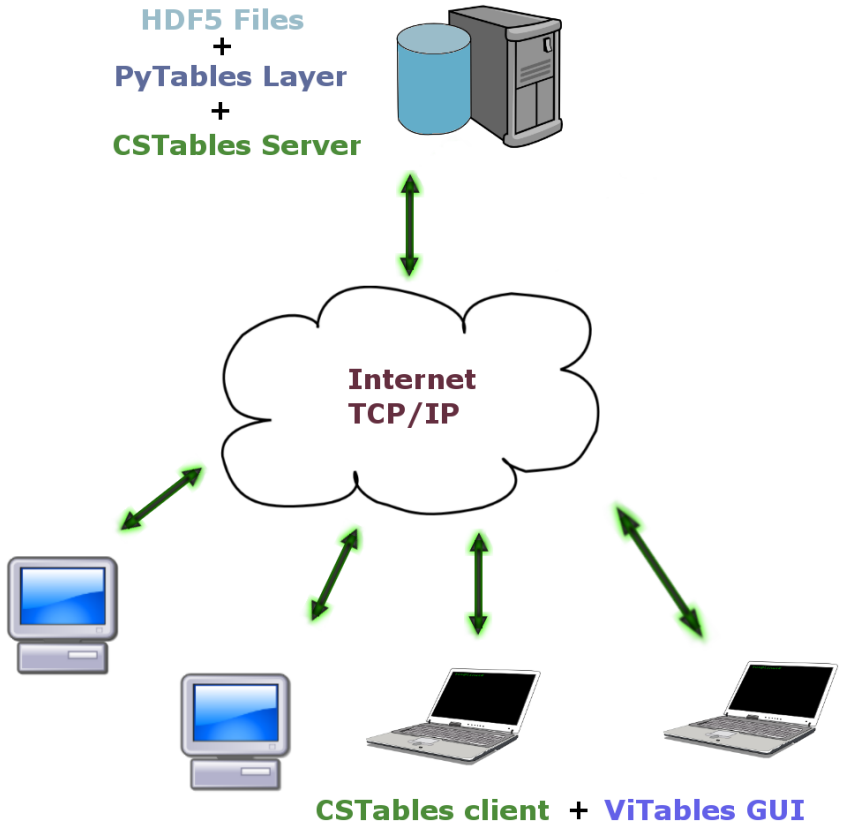


Current Status for PyTables Pro

- Improving the query response time.
- Remains to be done:
  - Complex queries.
  - Query optimizer.
- Date of release: 2nd quarter 2006 (tentative).

Outline

CSTables: PyTables Goes Client-Server



Outline

Design Goals

- Concurrency: Allows multiple access to the same file at the same time.
  - Locking system: Avoids corruption of data.
- High Throughput: Data is transmitted in large blocks. High-speed compressor/decompressor used.
- Client Cache: Metadata is kept in the client-side when an object is first accessed.
- Full PyTables API compatibility: Existing PyTables programs can be re-used to access remote files without changing virtually anything.

Concurrency Issues

- **Question**: CSTables does not provide threading or asynchronous features yet. So, how does it deal with several requests at a time?
- **Answer**: Large data read and write requests are split into small chunks. This considerably improves server response time.
- In addition, CSTables provides a *lock mechanism* that allows applications to explicitly put a lock on a node or on an entire subtree.
  - Different locking access modes: READ, WRITE and ALL

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Client Cache More in Depth

- CSTables caches some of the metadata of the PyTables object tree.
- When a client makes a change to the metadata, this change is *pushed* to the other clients' caches.
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  - You should try to cache primarily read-only attributes.

Caveat emptor:

Caching attributes that are updated very often might generate more traffic than attributes that are not cached at all!

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Two Different APIs

PyTables API (prefix with `csclient -ip=server_IP`)

```
import tables
fileh = tables.openFile("file.h5")
print fileh.root.table.cols.col1[:]
fileh.close()
```

CSTables API (no need to be prefixed)

```
from cstables.client import client
c=client.Session()
app=c.connect("your_FQDN_server")
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CSTables Status & Availability

- The main design features are already implemented and working.
- Beta available (caveat: only works against PyTables 1.0).
- Focus now is on checking & debugging possible errors, improving the throughput and bettering the Users' Guide.
- Future directions: threading, asynchronous communications.

The PyTables Suite Is Getting Shape

PyTables

The basic layer for the other components.

PyTables Pro

PyTables with a twist: Complex searches and ultra-fast selections in tables.

CSTables

The client-server PyTables. It supports as well generic HDF5 files.

ViTables

A data viewer for PyTables (and HDF5) files.

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Summary

- Python is a joy for scientific computing. Start using it now!
- The PyTables suite is designed to work with HDF5 files in an interactive, efficient and, most importantly, easy way.

- Outlook
  - Working hard to release CSTables in the first quarter of 2006. PyTables Pro will come later on (~ 2nd quarter of 2006).
  - It would be nice to produce a parallel version of PyTables (long term goal).

Thank You!

Thanks also to:

- Elena Pourmal, for inviting us to the Workshop.
- Frank Baker, for being kind.
- **The HDF Group** for pushing forward PyTables.