HDF5 is for Lovers 

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Which you will learn today!

A Note on the Format

Intermixed, there will be:

- Slides
- Interactive Hacking
- Exercises

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Feel free to:

- Ask questions at anytime
- Explore at your own pace.

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Allow me to recomend this tutorial with DWF's "Intro to Scientific Computing" tutorial. So...

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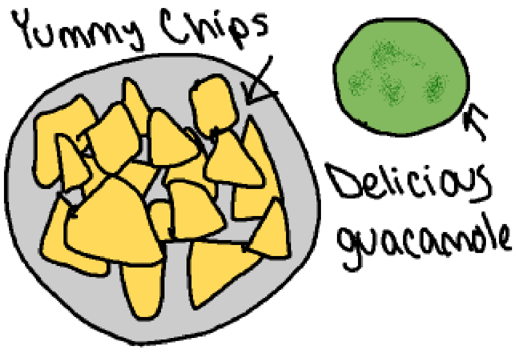
Get the Program Committee!



~go to that one too! (img http://mayorgia.blogspot.ca/2012/03/and-then-i-ate-worlds-best-burrito.html)

Also

Happy 10th Birthday, PyTables!

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Continuum Analytics has a promotion right now for PyConCa for 25% off of the professional version of Anaconda, their Python distribution.

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It comes with HDF5 and PyTables (and h5py).

Class Makeup

By a show of hands, how many people have used:

- HDF5 before?

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By a show of hands, how many people have used:

- HDF5 before?
- PyTables?
- h5py?
- the HDF5 C API?
- SQL?
- Other binary data formats?

Setup

Please clone the repo:

```
git clone git://github.com/scopatz/hdf5-is-for-lovers.git
```

Or download a tarball from:

https://github.com/scopatz/hdf5-is-for-lovers

Warm up exercise

In IPython:

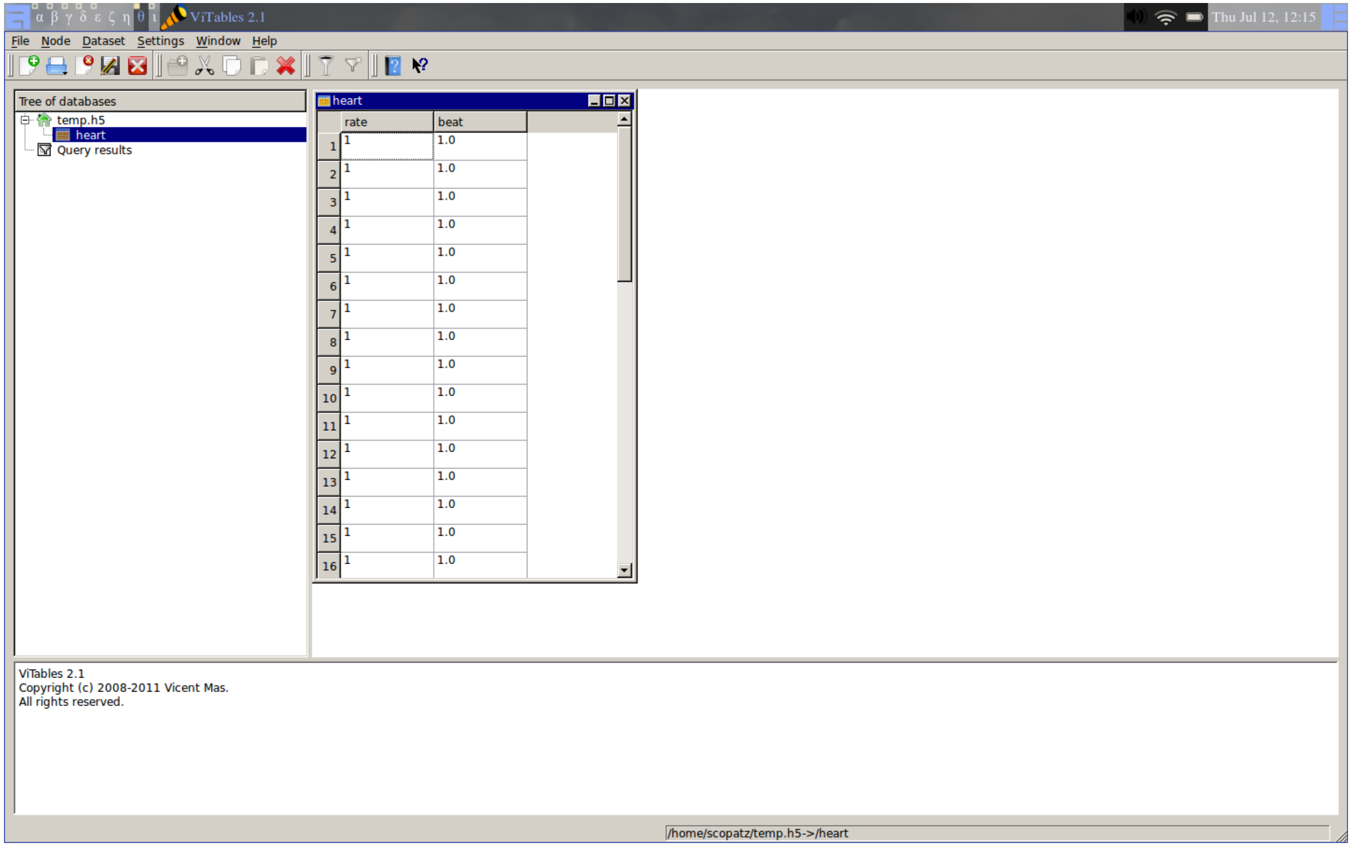
```
import numpy as np
import tables as tb

f = tb.openFile('temp.h5', 'a')
heart = np.ones(42, dtype=[('rate', int), ('beat', float)])
f.createTable('/', 'heart', heart)
f.close()
```

Or run `python exer/warmup.py`

Warm up exercise

You should see in ViTables:



A Brief Introduction

For persisting structured numerical data, binary formats are superior to plaintext.

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For one thing, they are often smaller:

```
# small ints           # med ints
42    (4 bytes)        123456   (4 bytes)
'42'  (2 bytes)        '123456' (6 bytes)

# near-int floats      # e-notation floats
12.34   (8 bytes)      42.424242E+42   (8 bytes)
'12.34' (5 bytes)      '42.424242E+42' (13 bytes)
```

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> ***Note***
>
> This is the mechanism behind `numpy.save()` and `numpy.savez()`.

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In effect, HDF5 is a file system within a file.

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In effect, HDF5 is a file system within a file.

(More on this later.)

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All of these must be composed of atomic types.

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- float: Floating point types. 16, 32 and 64 (default) bits.
- complex: Complex number. 64 and 128 (default) bits.
- string: Raw string types. 8-bit positive multiples.

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PyTables docs may be found at http://pytables.github.com/

Opening Files

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import tables as tb
f = tb.openFile('/path/to/file', 'a')
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- *'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+'*: It is similar to 'a', but the file must already exist.

Using the Hierarchy

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Creating new nodes must be done on the file handle:

```
f.createGroup('/', 'a_group', "My Group")
f.root.a_group
```

Creating Datasets

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Appropriate create methods live on the file handle:

```
# integer array
f.createArray('/a_group', 'arthur_count', [1, 2, 5, 3])
```

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```
# integer array
f.createArray('/a_group', 'arthur_count', [1, 2, 5, 3])
```

```
# tables, need descriptions
dt = np.dtype([('id', int), ('name', 'S10')])
knights = np.array([(42, 'Lancelot'), (12, 'Bedivere')], dtype=dt)
f.createTable('/', 'knights', dt)
f.root.knights.append(knights)
```

Reading Datasets

Arrays and Tables try to preserve the original flavor that they were created with.

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```
>>> print f.root.a_group.arthur_count[:]
[1, 2, 5, 3]

>>> type(f.root.a_group.arthur_count[:])
list

>>> type(f.root.a_group.arthur_count)
tables.array.Array
```

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```
>>> f.root.knights[1]
(12, 'Bedivere')

>>> f.root.knights[:1]
array([(42, 'Lancelot')], dtype=[('id', '<i8'), ('name', 'S10')])

>>> mask = (f.root.knights.cols.id[:] < 28)
>>> f.root.knights[mask]
array([(12, 'Bedivere')], dtype=[('id', '<i8'), ('name', 'S10')])

>>> f.root.knights[([1, 0],)]
array([(12, 'Bedivere'), (42, 'Lancelot')], dtype=[('id', '<i8'), ('name', 'S10')])
```

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>>> f.root.knights[([1, 0],)]
array([(12, 'Bedivere'), (42, 'Lancelot')], dtype=[('id', '<i8'), ('name', 'S10')])
```

Data accessed in this way is *memory mapped*.

Exercise

exer/peaks_of_kilimanjaro.py

Exercise

sol/peaks_of_kilimanjaro.py

Hierarchy Layout

Suppose there is a big table of like-things:

```
# people:  name,            profession,    home
people = [('Arthur',        'King',        'Camelot'),
          ('Lancelot',      'Knight',      'Lake'),
          ('Bedevere',      'Knight',      'Wales'),
          ('Witch',         'Witch',       'Village'),
          ('Guard',         'Man-at-Arms', 'Swamp Castle'),
          ('Ni',            'Knight',      'Shrubbery'),
          ('Strange Woman', 'Lady',        'Lake'),
          ...
          ]
```

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          ('Ni',                 'Knight',       'Shrubbery'),
          ('Strange Woman',      'Lady',         'Lake'),
          ...
          ]
```

It is tempting to throw everyone into a big `people` table.

Hierarchy Layout

However, a search over a class of people can be eliminated by splitting these tables up:

```
knight = [('Lancelot',       'Knight',       'Lake'),
          ('Bedevere',       'Knight',       'Wales'),
          ('Ni',             'Knight',       'Shrubbery'),
          ]

others = [('Arthur',         'King',         'Camelot'),
          ('Witch',          'Witch',        'Village'),
          ('Guard',          'Man-at-Arms', 'Swamp Castle'),
          ('Strange Woman', 'Lady',          'Lake'),
          ...
          ]
```

Hierarchy Layout

The profession column is now redundant:

```
knight = [('Lancelot', 'Lake'),
          ('Bedevere', 'Wales'),
          ('Ni',       'Shrubbery'),
          ]

others = [('Arthur',        'King',        'Camelot'),
          ('Witch',         'Witch',       'Village'),
          ('Guard',         'Man-at-Arms', 'Swamp Castle'),
          ('Strange Woman', 'Lady',        'Lake'),
          ...
          ]
```

Hierarchy Layout

Information can be embedded implicitly in the hierarchy as well:

```
root
  | - England
  |       | - knight
  |       | - others
  |
  | - France
  |       | - knight
  |       | - others
```

Hierarchy Layout

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Ultimately, it is all about *speed*, especially for big tables.

Access Time Analogy

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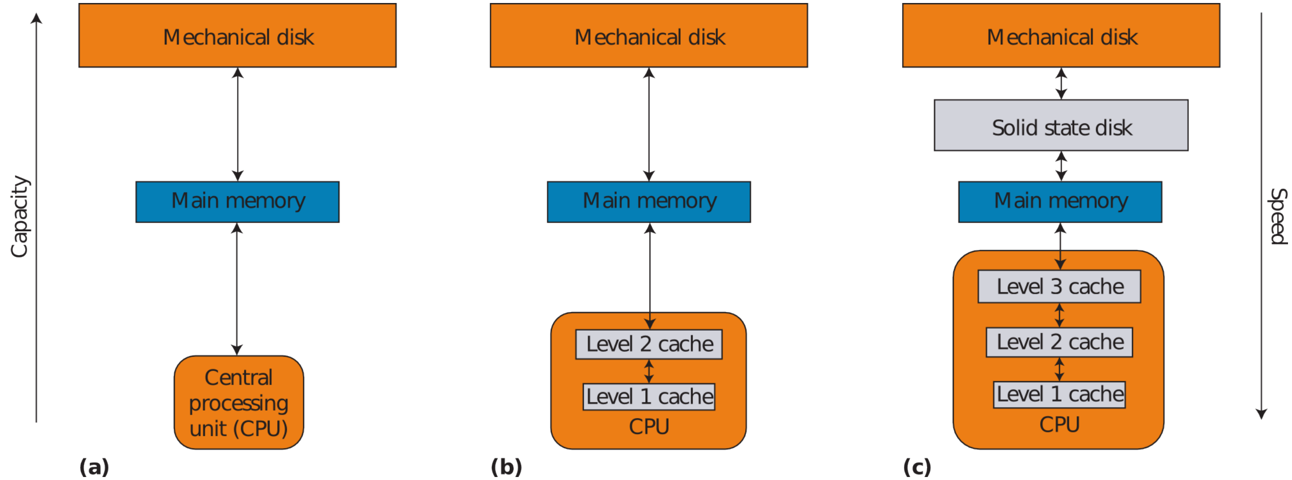
Accessing a (mechanical) HDD is leaving your office, leaving your building, wandering the planet for a year and four months to return to your desk with the information finally made available.

Thanks K. Smith & http://duartes.org/gustavo/blog/post/what-your-computer-does-while-you-wait

Starving CPU Problem

Waiting around for access times prior to computation is known as the *Starving CPU Problem*.



Francesc Alted. 2010. Why Modern CPUs Are Starving and What Can Be Done about It. IEEE Des. Test 12, 2 (March 2010), 68-71. DOI=10.1109/MCSE.2010.51
http://dx.doi.org/10.1109/MCSE.2010.51

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In fact, the struct / dtype / description concept is only a convenient way to assign meaning to bytes:

```
|  ids  |       first       |        last       |
|-------|-------------------|-------------------|
| | | | | | | | | | | | | | | | | | | | | | | | |
```

Tables

Data types may be nested (though they are stored in flattened way).

```
dt = np.dtype([('id', int),
               ('first', 'S5'),
               ('last',  'S5'),
               ('parents', [
                    ('mom_id', int),
                    ('dad_id', int),
                ]),
              ])

people = np.fromstring(np.random.bytes(dt.itemsize * 10000), dt)
f.createTable('/', 'random_peeps', people)
```

Tables

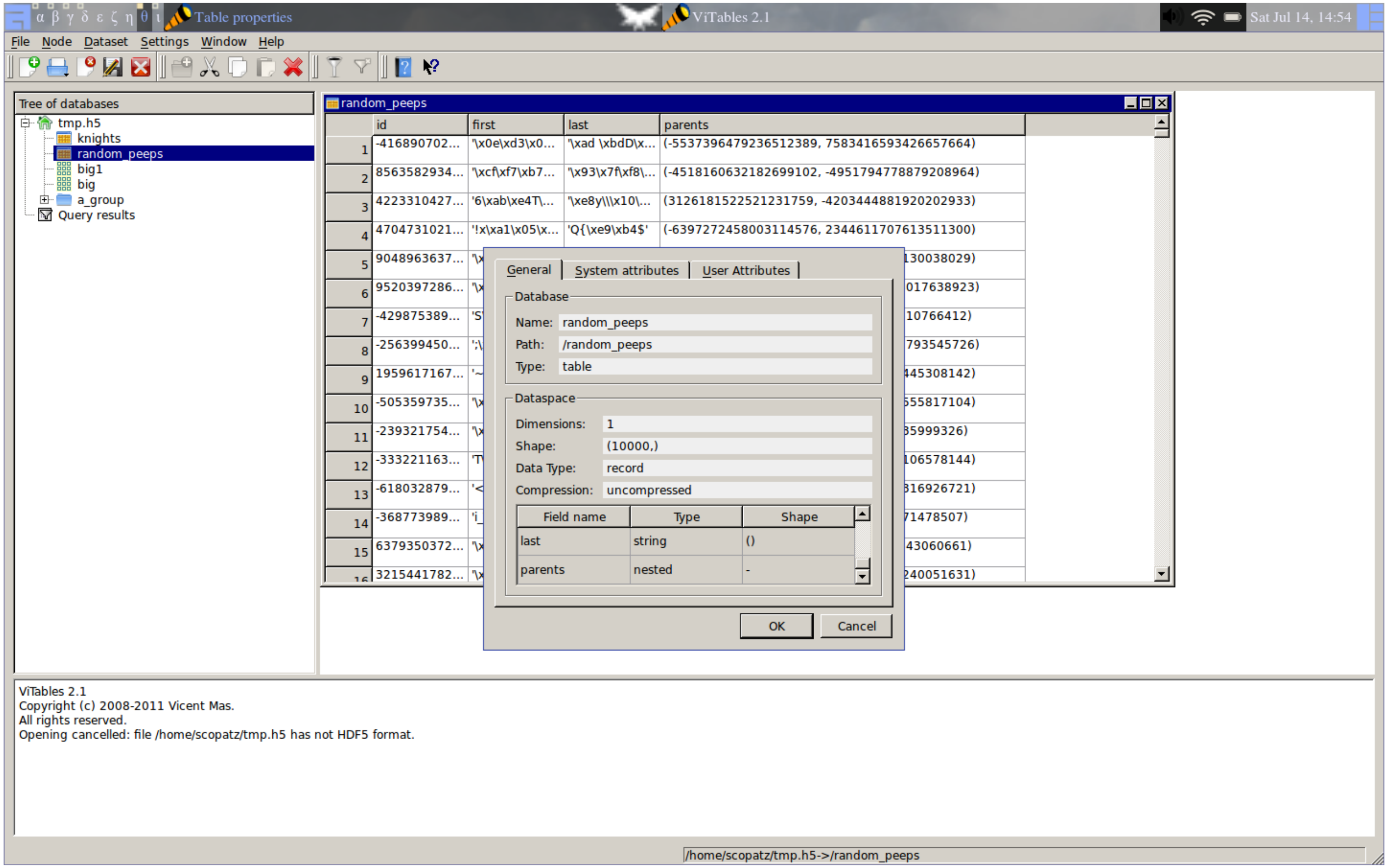
Table properties
ViTables 2.1
Sat Jul 14, 14:54
File Node Dataset Settings Window Help
Tree of databases
tmp.h5
knights
random_peeps
big1
big
a_group
Query results
random_peeps
id
first
last
parents
General
System attributes
User Attributes
Database
Name: random_peeps
Path: /random_peeps
Type: table
Dataspace
Dimensions: 1
Shape: (10000,)
Data Type: record
Compression: uncompressed
Field name
Type
Shape
last
string
()
parents
nested
-
OK
Cancel
ViTables 2.1
Copyright (c) 2008-2011 Vicent Mas.
All rights reserved.
Opening cancelled: file /home/scopatz/tmp.h5 has not HDF5 format.
/home/scopatz/tmp.h5->/random_peeps

Tables

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This is accomplished in compiled languages through normal memory allocation and careful byte counting:

```
typedef struct mat {
  double mass;
  int atoms_per_mol;
  double comp [];
} mat;
```

Tables

```
typedef struct mat {
  double mass;
  int atoms_per_mol;
  double comp [];
} mat;

size_t mat_size = sizeof(mat) + sizeof(double)*comp_size;
hid_t desc = H5Tcreate(H5T_COMPOUND, mat_size);
hid_t comptype = H5Tarray_create2(H5T_NATIVE_DOUBLE, 1, nuc_dims);

// make the data table type
H5Tinsert(desc, "mass", HOFFSET(mat, mass), H5T_NATIVE_DOUBLE);
H5Tinsert(desc, "atoms_per_mol", HOFFSET(mat, atoms_per_mol), H5T_NATIVE_DOUBLE);
H5Tinsert(desc, "comp", HOFFSET(mat, comp), comp_type);

// make the data array for a single row, have to over-allocate
mat * mat_data  = new mat[mat_size];

// ...fill in data array...

// Write the row
H5Dwrite(data_set, desc, mem_space, data_hyperslab, H5P_DEFAULT, mat_data);
```

Exercise

exer/boatload.py

Exercise

sol/boatload.py

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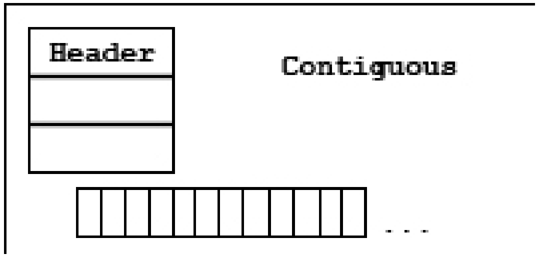
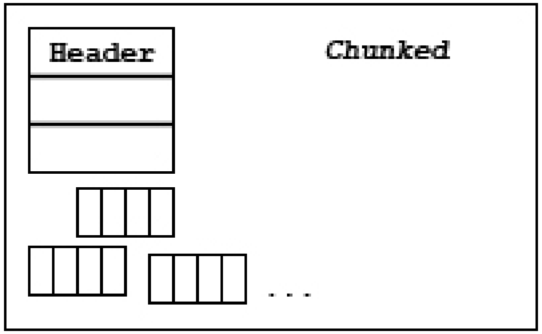
Note: Currently, PyTables only allows one extendable dim.

Chunking



Contiguous Dataset



Chunked Dataset

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- small chunks are good for accessing some of data
- large chunks are good for accessing lots of data

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Any chunked dataset allows you to set the chunksize.

```
f.createTable('/', 'omnomnom', data, chunkshape=(42,42))
```

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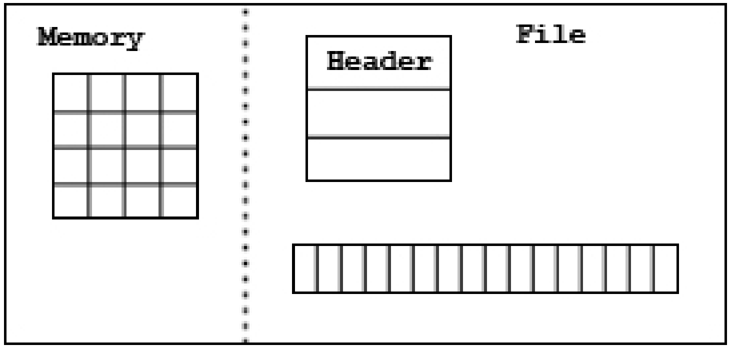
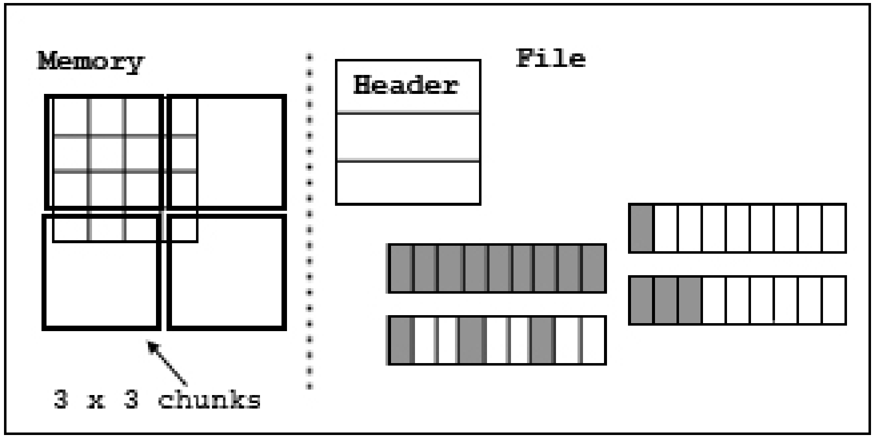
However, it could not have a 12x12 chunksize, since the ranks must be less than or equal to that of the array.

Manipulating the chunksize is a great way to fine-tune an application.

Chunking



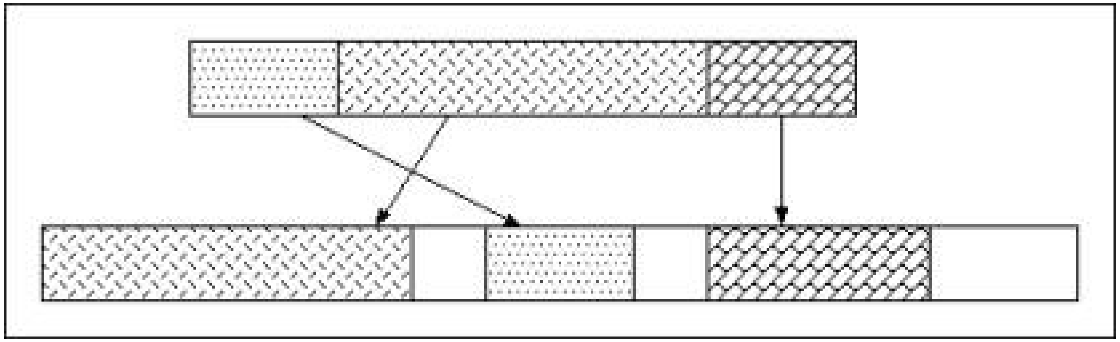
Contiguous 4x4 Dataset



Chunked 4x4 Dataset

Chunking

Note that the addresses of chunks in dataspace (memory) has no bearing on their arrangement in the actual file.



Dataspace (top) vs File (bottom) Chunk Locations

In-Core vs Out-of-Core

Calculations depend on the current memory layout.

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Recall access time analogy (wander Earth for 16 months).

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Definitions:

- Operations which require all data to be in memory are *in-core* and may be memory bound (NumPy).
- Operations where the dataset is external to memory are *out-of-core* (or *in-kernel*) and may be CPU bound.

In-Core Operations

Say, `a` and `b` are arrays sitting in memory:

```
a = np.array(...)
b = np.array(...)
c = 42 * a + 28 * b + 6
```

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For `N` operations, `N-1` temporaries are made.

Wastes memory and is slow. Pulling from disk is slower.

In-Core Operations

A less memory intensive implementation would be an element-wise evaluation:

```
c = np.empty(...)
for i in range(len(c)):
    c[i] = 42 * a[i] + 28 * b[i] + 6
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Even with in memory NumPy arrays, there are problems with gratuitous Python type checking.

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```
for i in range(0, len(a), 256):
    r0, r1 = a[i:i+256], b[i:i+256]
    multiply(r0, 42, r2)
    multiply(r1, 28, r3)
    add(r2, r3, r2); add(r2,  6, r2)
    c[i:i+256] = r2
```

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PyTables implements a `tb.Expr` class which backends to the numexpr VM but has additional optimizations for disk reading and writing.

The full array need never be in memory.

Out-of-Core Operations

Fully out-of-core expression example:

```
shape = (10, 10000)
f = tb.openFile("/tmp/expression.h5", "w")

a = f.createCArray(f.root, 'a', tb.Float32Atom(dflt=1.), shape)
b = f.createCArray(f.root, 'b', tb.Float32Atom(dflt=2.), shape)
c = f.createCArray(f.root, 'c', tb.Float32Atom(dflt=3.), shape)
out = f.createCArray(f.root, 'out', tb.Float32Atom(dflt=3.), shape)

expr = tb.Expr("a*b+c")
expr.setOutput(out)
d = expr.eval()

print "returned-->", repr(d)
f.close()
```

Querying

The most common operation is asking an existing dataset whether its elements satisfy some criteria. This is known as *querying*.

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```
tb.Table.where(cond)
tb.Table.getWhereList(cond)
tb.Table.readWhere(cond)
tb.Table.whereAppend(dest, cond)
```

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The `where()` method itself returns an iterator over all matched (hit) rows:

```
for row in table.where('(col1 < 42) & (col2 == col3)'):
    # do something with row
```

Querying

For a speed comparison, here is a complex query using regular Python:

```
result = [row['col2'] for row in table if (
          ((row['col4'] >= lim1 and row['col4'] < lim2) or
          ((row['col2'] > lim3 and row['col2'] < lim4])) and
          ((row['col1']+3.1*row['col2']+row['col3']*row['col4']) > lim5)
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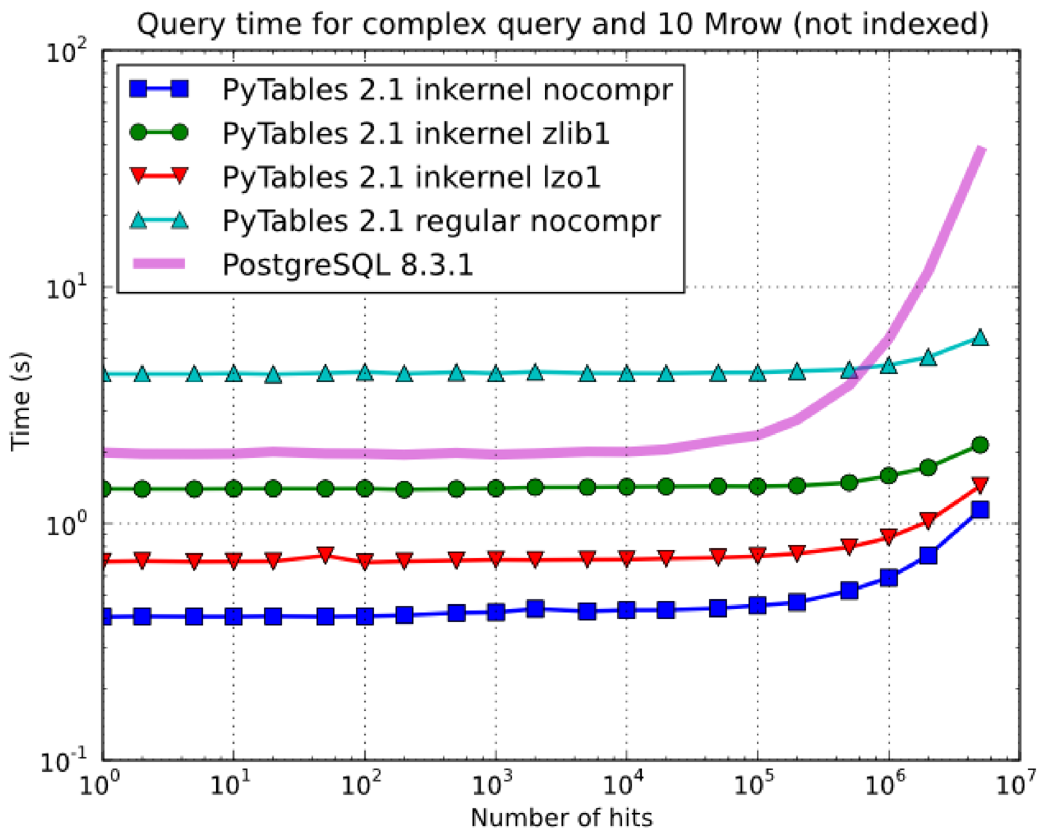
          )]
```

And this is the equivalent out-of-core search:

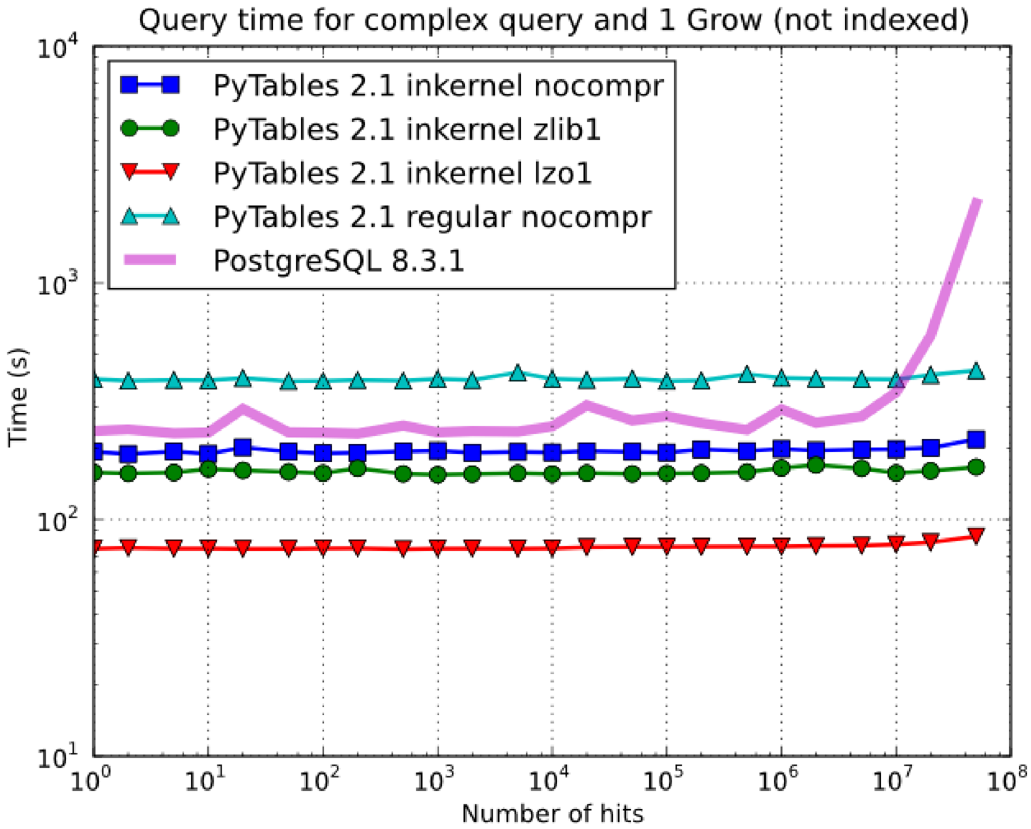
```
result = [row['col2'] for row in table.where(
            '(((col4 >= lim1) & (col4 < lim2)) | '
            '((col2 > lim3) & (col2 < lim4)) &   '
            '((col1+3.1*col2+col3*col4) > lim5)) ')]
```

Querying



Complex query with 10 million rows. Data fits in memory.

Querying



Complex query with 1 billion rows. Too big for memory.

Exercise

exer/crono.py

Exercise

sol/crono.py

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Compression is when the dataset is piped through a zipping algorithm on write and the inverse unzipping algorithm on read.

Each chunk is compressed independently, so chunks end up with a varying number bytes.

Has some storage overhead, but may drastically reduce file sizes for very regular data.

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Compression/Decompression is clearly more CPU intensive than simply blitting an array into memory.

However, because there is *less total information* to transfer, the time spent unpacking the array can be far less than moving the array around wholesale.

This is kind of like power steering, you can either tell wheels how to turn manually or you can tell the car how you want the wheels turned.

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PyTables supports:

• zlib (default), • lzo, • bzip2, and • blosc.

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Filters only act on chunked datasets.

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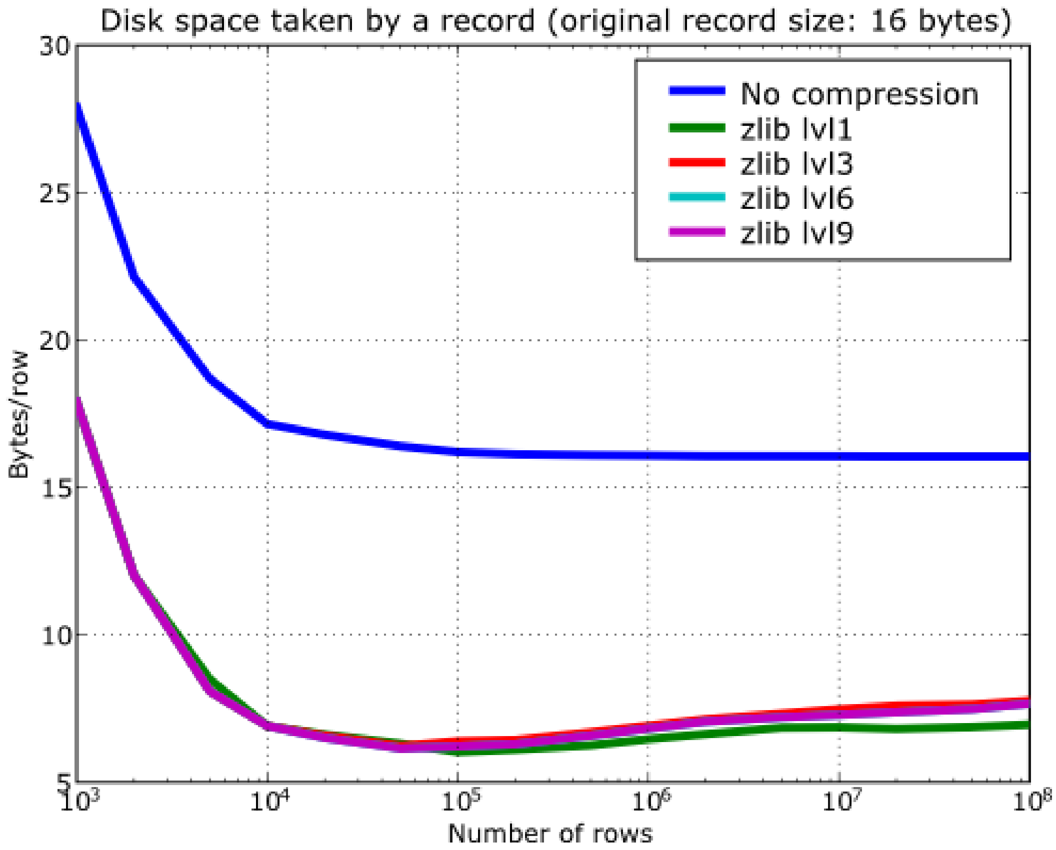
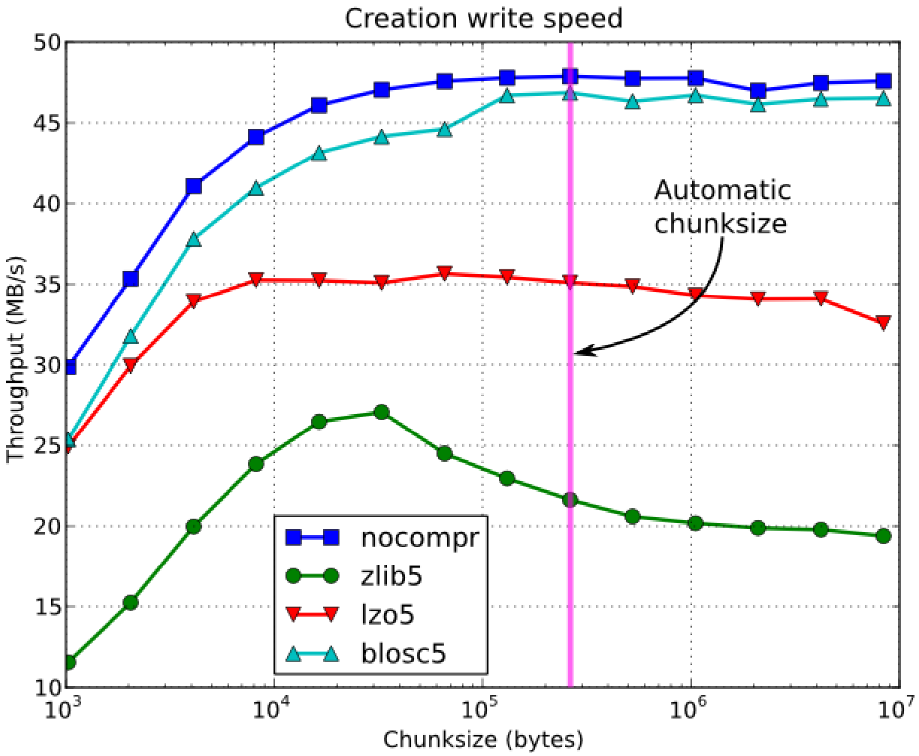
But why? (I don't have time to go into the details of blosc. However here are some justifications...)

Compression



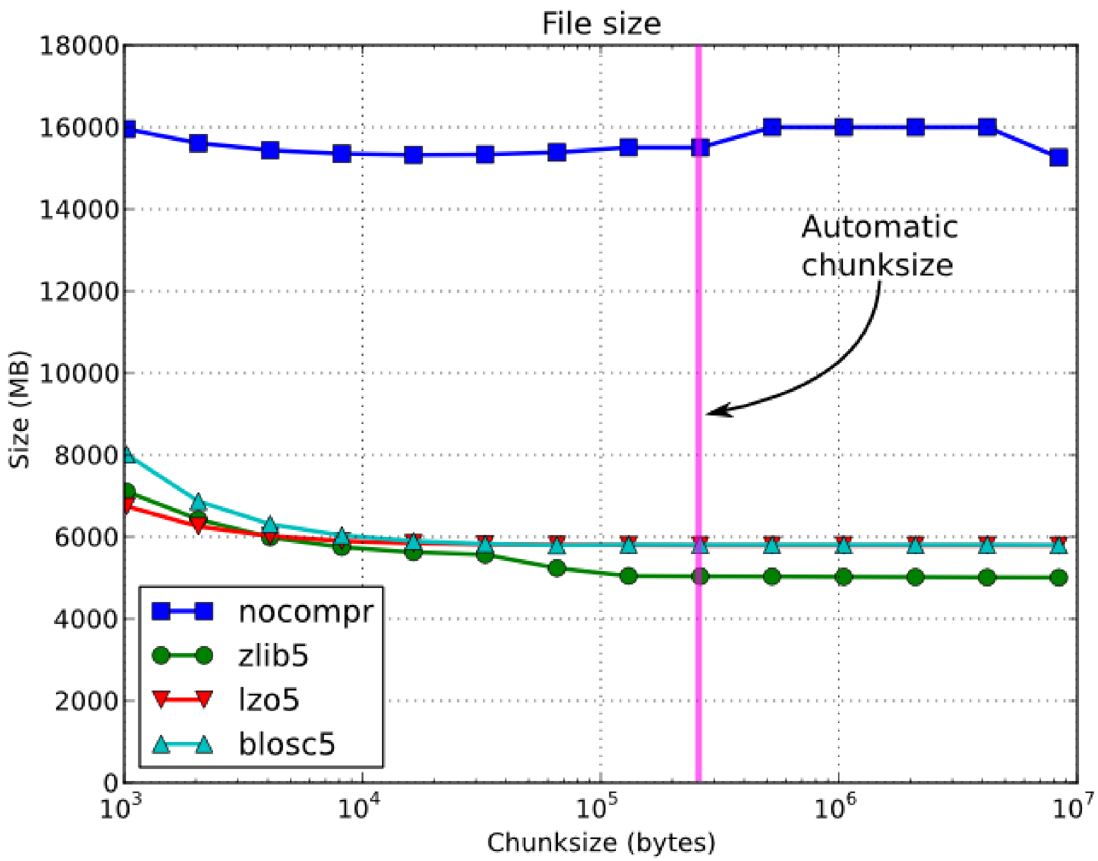
Comparison of different compression levels of zlib.

Compression



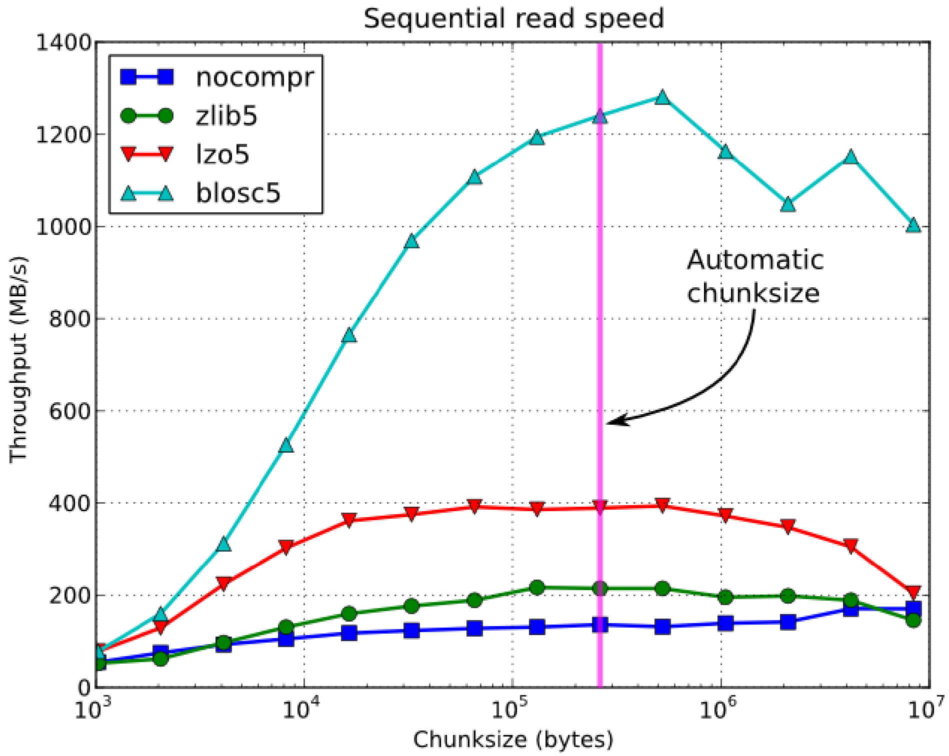
Creation time per element for a 15 GB EArray and different chunksizes.

Compression



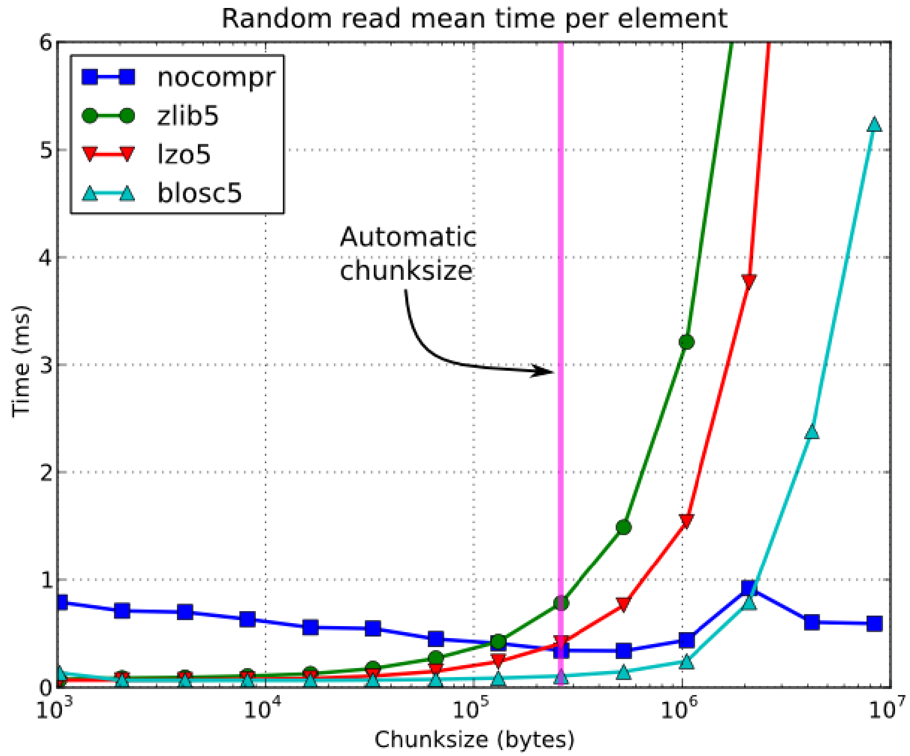
File sizes for a 15 GB EArray and different chunksizes.

Compression



Sequential access time per element for a 15 GB EArray and different chunksizes.

Compression



Random access time per element for a 15 GB EArray and different chunksizes.

Exercise

exer/spam_filter.py

Exercise

sol/spam_filter.py

Other Python Data Structures

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Using lists or tuples instead of arrays follows analogously.

It is data structures like sets and dictionaries which do not quite map.

However, as long as all elements may be cast into the same atomic type, these structures can be stored in HDF5 with relative ease.

Sets

Example of serializing and deserializing sets:

```
>>> s = {1.0, 42, 77.7, 6E+01, True}

>>> f.createArray('/', 's', [float(x) for x in s])
/s (Array(4,)) ''
  atom := Float64Atom(shape=(), dflt=0.0)
  maindim := 0
  flavor := 'python'
  byteorder := 'little'
  chunkshape := None

>>> set(f.root.s)
set([1.0, 42.0, 77.7, 60.0])
```

Exercise

exer/dict_table.py

Exercise

sol/dict_table.py

What Was Missed

- Walking Nodes
- File Nodes
- Indexing
- Migrating to / from SQL
- HDF5 in other database formats
- Other Databases in HDF5
- HDF5 as a File System

Acknowledgements

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- The PyTables Governance Team:
  - Josh Moore, • Antonio Valentino, • Josh Ayers

Acknowledgements

(Cont.)

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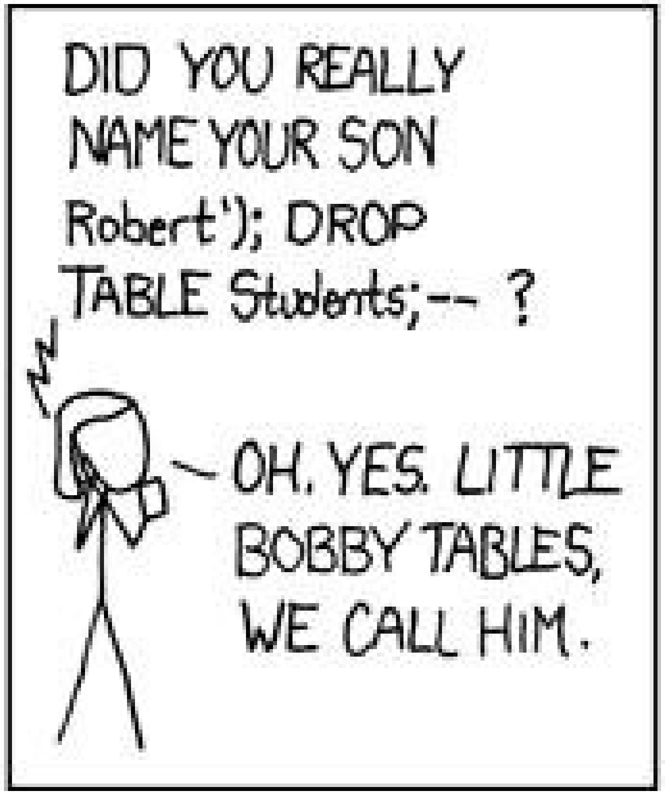
Shameless Plug: *We are always looking for more hands. Join Now!*

Questions


DID YOU REALLY NAME YOUR SON Robert'); DROP TABLE Students;-- ?
OH. YES. LITTLE BOBBY TABLES, WE CALL HIM.