NUMERICAL PYTHON

Python for computational science

16 – 18 October 2017

CINECA

m.cestari@cineca.it

What do you notice?

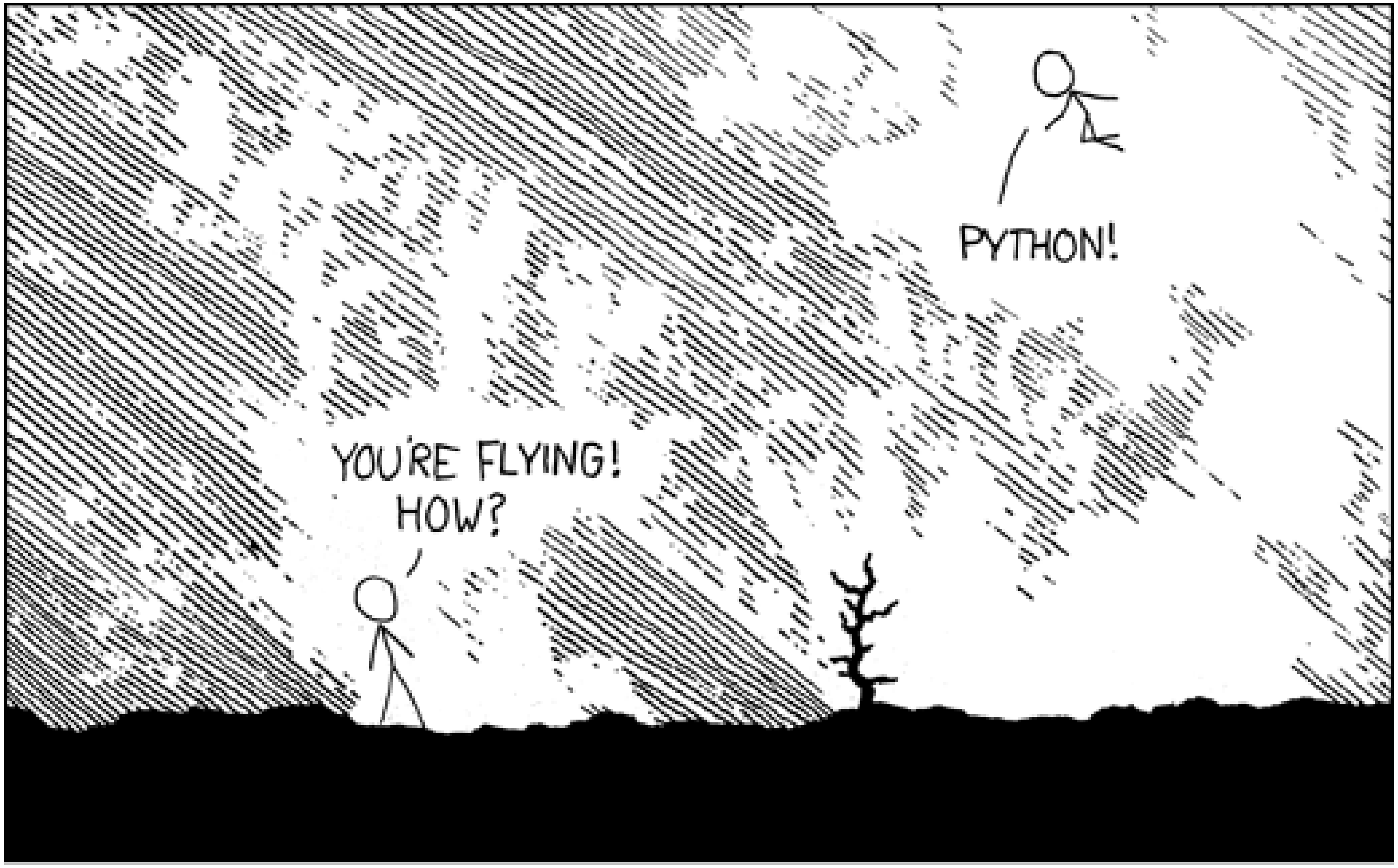
https://en.wikipedia.org/wiki/Rubber_duck_debugging

Goal of the lecture

Learn:

- overall use of the objects provided by numpy
- how to read data from files and manipulate it
- how to integrate python with plotting
- and of course ...

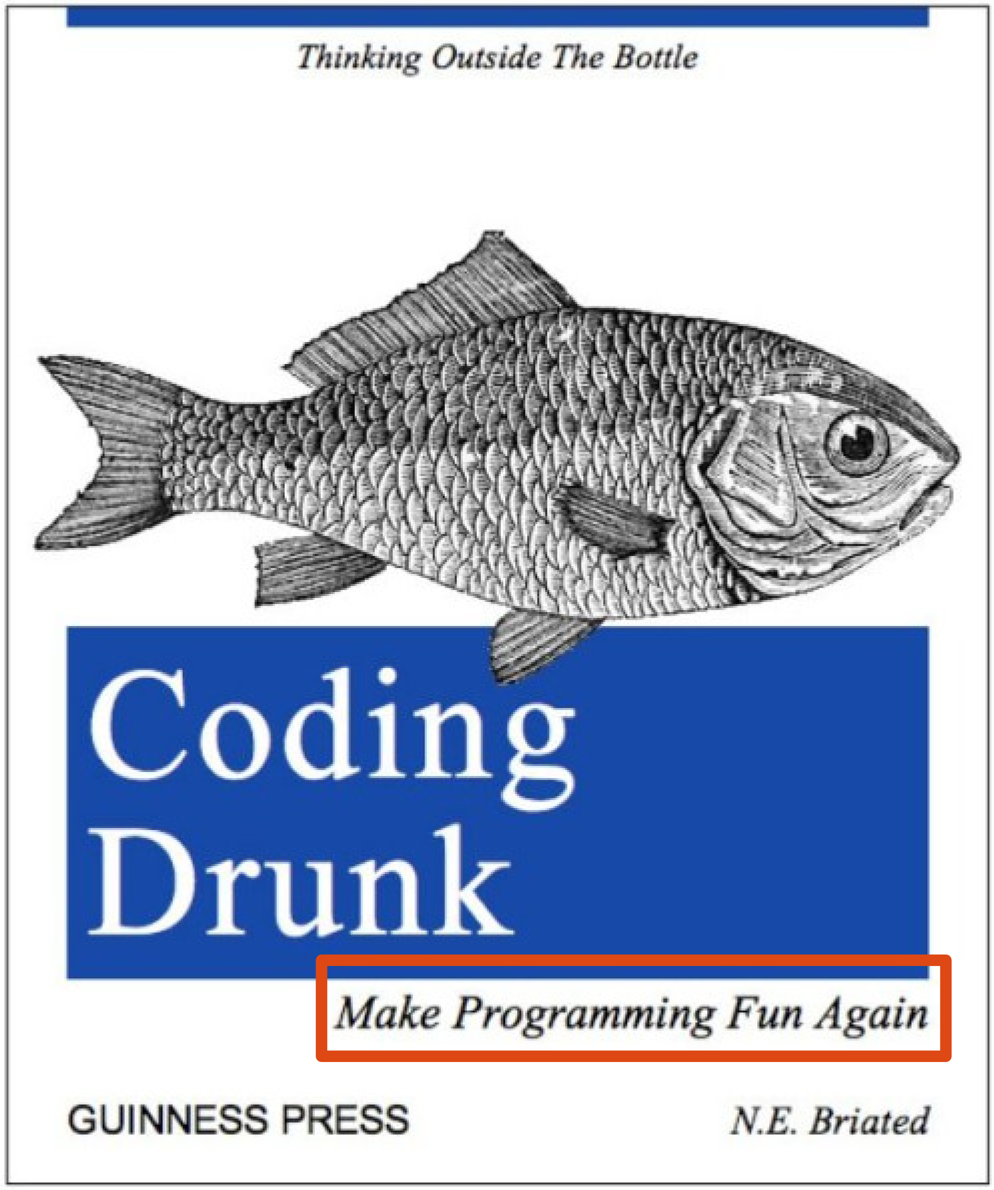
… how to have fun with it …



Try on a python prompt :

```
>>> import antigravity
```

but don't get TOO excited …


Thinking Outside The Bottle

Coding Drunk

Make Programming Fun Again

GUINNESS PRESS

N.E. Briated

Where are the bottlenecks?

- Let’s start by trying to understand why high level languages like Python are **slower** than compiled code
- In Python the main reasons of the "slowness" of the code are:
  - Dynamic Typing
  - Data (memory) Access

Dynamic typing

- Consider the operation a+b
  - If a and b are integers, then a+b requires **sum** of integers
  - If a and b are strings, then a+b requires **string concatenation**
  - If a and b are lists, then a+b requires **list concatenation**
- The operator + is **overloaded**: its action depends on the type of the objects on which it acts
- As a result, Python must check the type of the objects and then call the correct operation: this involves substantial **overheads**

Static typing

```
#include <stdio.h>


int main(void) {
    int i;
    int sum = 0;
    for (i = 1; i <= 10; i++) {
        sum = sum + i;
    }
    printf("sum = %d\n", sum);
    return 0;
}
```

The variables i and sum are explicitly declared to be integers, hence the meaning of addition here is completely unambiguous.

Introduction (1): history

- Numerical Python: evolution

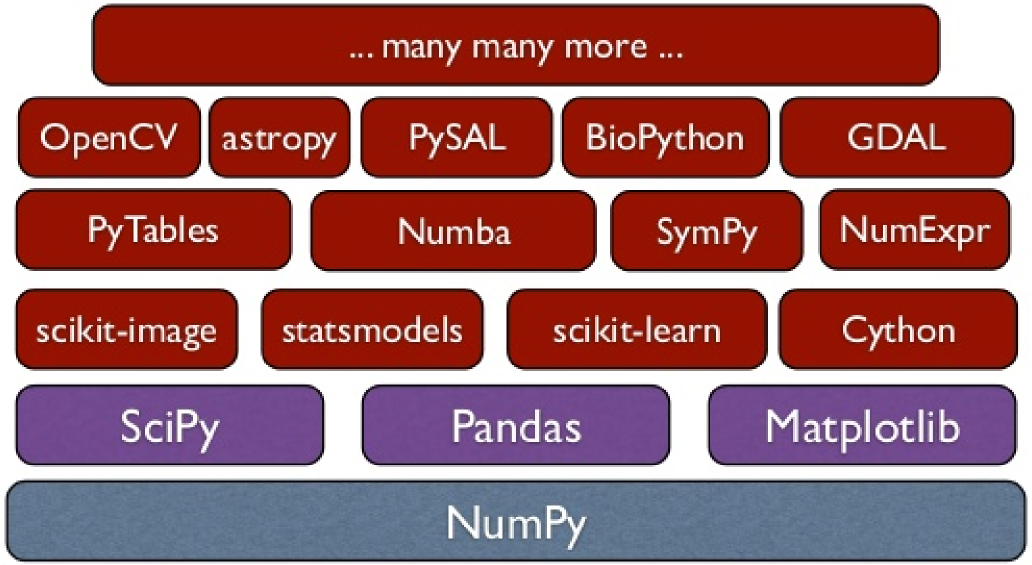
  - ➔ In origin, 2 different libraries Numeric and Numarray

  - They became NumPy (2006). All the features of the two original libraries (plus more..) converging in one library

Introduction (2): why bother?

- NumPy offers efficient array storing and computation
- Python scientific libraries (i.e. scipy, matplotlib, pandas) make use of NumPy objects
- NumPy is the *de facto* **standard**

NumPy Stack (cry for conda...)



CONTINUUM ANALYTICS

Introduction (3): what's inside the box

Sub-Packages	**Purpose**	**Comments**
core	basic objects	**all names exported to numpy**
lib	Addintional utilities	**all names exported to numpy**
linalg	Basic linear algebra	LinearAlgebra derived from Numeric
fft	Discrete Fourier transforms	FFT derived from Numeric
random	Random number generators	RandomArray derived from Numeric
distutils	Enhanced build and distribution	improvements built on standard distutils
testing	unit-testing	utility functions useful for testing
f2py	Automatic wrapping of Fortran code	Utility to extend the language

Introduction (4)

- Default for this presentation (and for the standard documentation)

```
>>> import numpy as np
```

NumPy (main) objects

- NumPy provides two main objects:
  - **ndarray**;
  - **ufunc**;

`ndarray`

- Like lists, tuples and sets, ndarrays are **collection** of items

```
>>> my_array, type(my_array)
(array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9]),
numpy.ndarray)
```

ndarray (2)

Examples:

```
>>> a = np.array([1, 2, 3])

>>> b = np.array([[1.5, 2.2, 34.4], [2.3, 4, 6.5]])

>>> c = np.array(['lof', 'l', 'ga'])

>>> d = np.array([2, 3,'lof']) # doesn't work as
                                 expected
```

`ndarray` (3)

* ndarray is a collection of **homogeneous** items

- Each item occupies the same number of bytes

* Items typically are numerical type...

* ... but an arbitrary **record** of (non) numerical types can be used

ndarray (4)

(numpy/core/include/numpy/ndarrayobject.h)

```
typedef struct PyArrayObject {
    char *data;              /* pointer to raw data buffer */
    PyArray_Descr *descr;    /* Pointer to type structure */
    int nd;                  /* number of dimensions, also
                               called ndim */
    npy_intp *dimensions;    /* size in each dimension (shape) */
    npy_intp *strides;       /* bytes to jump to get to the next
                               element in each dimension */
    PyObject *base;          /* This object should be decref'd
                               upon deletion of array */
                             /* For views it points to the
                                original array */
    int flags;               /* Flags describing array */
} PyArrayObject;
```

ndarray: data

```
char *data;      /* pointer to raw data buffer */
PyArray_Descr *descr; /* pointer to type structure */
```

- data is just a pointer to bytes in memory
- data needs some sort of descriptor (dtype) to be interpreted

```
In [1]: a = np.array([1, 2, 3]) # buffer of 12 bytes
In [2]: a.dtype
Out[2]: dtype('int32')          # interpreted as 3 ints
In [3]: b = a.astype(np.float)  # dtype('float64')
```

NOTE: int**32**: 32 bits (4bytes) for integer representation

ndarray: some dtype types

Data Type	np.dtype	char. code	Description
bool	np.bool	'b'	Boolean (True or False) stored as a byte
string	'S'	'S', 'a'	String datatype
int	np.int	'i4' or 'i8'	Platform integer (normally either int32 or int64)
int8	np.int8	'i1'	Byte (-128 to 127)
int16	np.int16	'i2'	Integer (-32768 to 32767)
int32	np.int32	'i4'	Integer (-2147483648 to 2147483647)
int64	np.int64	'i8'	Integer (-9223372036854775808 to 9223372036854775807)
uint32	np.uint32	'u4'	Unsigned integer (0 to 4294967295)
uint64	np.uint64	'u8'	Unsigned integer (0 to 18446744073709551615)
float	np.float	'f8'	Shorthand for float64
float32	np.float32	'f4'	Single precision float, sign bit, 8 bits exponent, 23 bits mantissa
float64	np.float64	'f8'	Double precision float, sign bit, 11 bits exponent, 52 bits mantissa
complex64	np.complex64	'c8'	Complex number represented by two 32-bit floats
complex128	np.complex128	'c16'	Complex number represented by two 64-bit floats

ndarray: dtype cont'ed

- the elements of ndarrays can be specified with a dtype object:

numerical

```
>>> np.dtype(np.int32)  # 32 are the bits used to
    dtype('np.int32')   # represent the integer
                        # (4 bytes int)
```

strings

```
>>> np.dtype('S3')      # mind the capital case here
                        # 3 means 3 bytes
```

both

```
>>> np.dtype([('f1', np.uint), ('f2', 'S3')])
    dtype([('f1', '<u4'), ('f2', '|S3')]) # list of tuples
```

You! Enough theory...

- Let's get our (dirty) hands on this new toy

- During this course, most of the things we learn will be used to solve an exercise

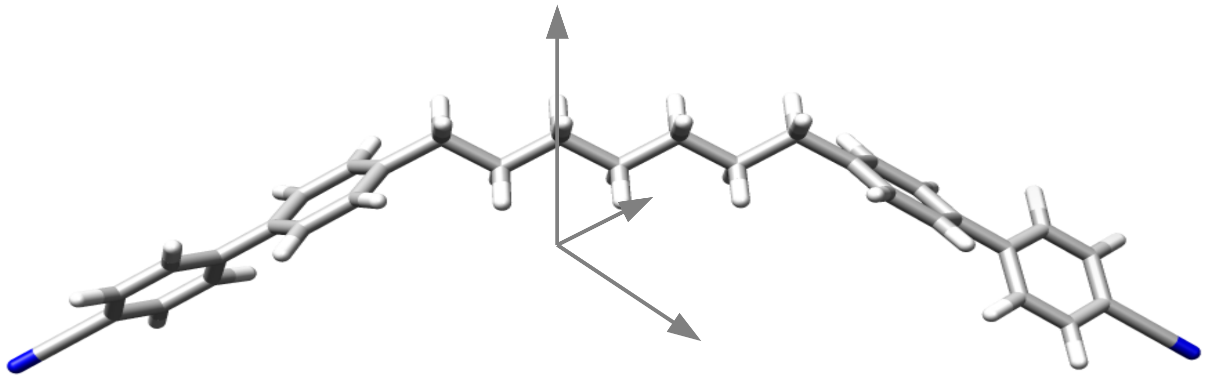
- It's about ...

chemistry

before it was cool

Exercise

- Rotate a molecule along the axes that diagonalize the moment of inertia tensor



```
C   12             -0.102  -0.301  -0.276
C   12             -0.024  -0.189   1.125
C   12              1.254  -0.165   1.713
C   12              2.406  -0.245   0.941
…
```

- Step by step guided solution through this course

Exercise 1: dtype

- Try to construct a dtype object to represent an atom in a 3d space. It should contain:
    - a string ('S3') to represent the symbol (i.e. Na, Cl, H, O)
    - an integer (np.int) for the atomic weight (i.e. 11, 17, 1)
    - 3 floats 64 bits (np.float64) for the cartesian coordinates

- Help needed? Try (after having imported numpy):

```
>>> help(np.dtype)          (python)
>>> np.dtype?               (ipython)
```

Exercise 1: dtype

- Solution

```
>>> dt = np.dtype([('symb','S3'),('PA',np.int),
('x',np.float64),('y',np.float64),('z',np.float64)])
```

```
   dtype([('symb', '|S3'), ('PA', '<i4'), ('x', '<f8'), ('y',
   '<f8'), ('z', '<f8')])
```

ndarray (4)

(numpy/core/include/numpy/ndarrayobject.h)

```
typedef struct PyArrayObject {
    char *data;              /* pointer to raw data buffer */
    PyArray_Descr *descr; /* Pointer to type structure */
    int nd;                  /* number of dimensions, also
                              called ndim */

    npy_intp *dimensions; /* size in each dimension (shape) */
    npy_intp *strides;    /* bytes to jump to get to the next
                              element in each dimension */
    PyObject *base;       /* This object should be decref'd
                              upon deletion of array */
                           /* For views it points to the
                                original array */
    int flags;               /* Flags describing array */
} PyArrayObject;
```

ndarray: dimensions

```
int nd;              /* number of dimensions,
                      also called ndim */

npy_intp *dimensions;      /* size in each dimension */
```

```
In [1]: b = np.array([[1,2], [3,4]])
In [2]: b.ndim
Out[2]: 2
In [3]: b.shape
Out[3]: (2, 2)
b.shape = 1,4   # to reshape an array
```

ndarray: strides

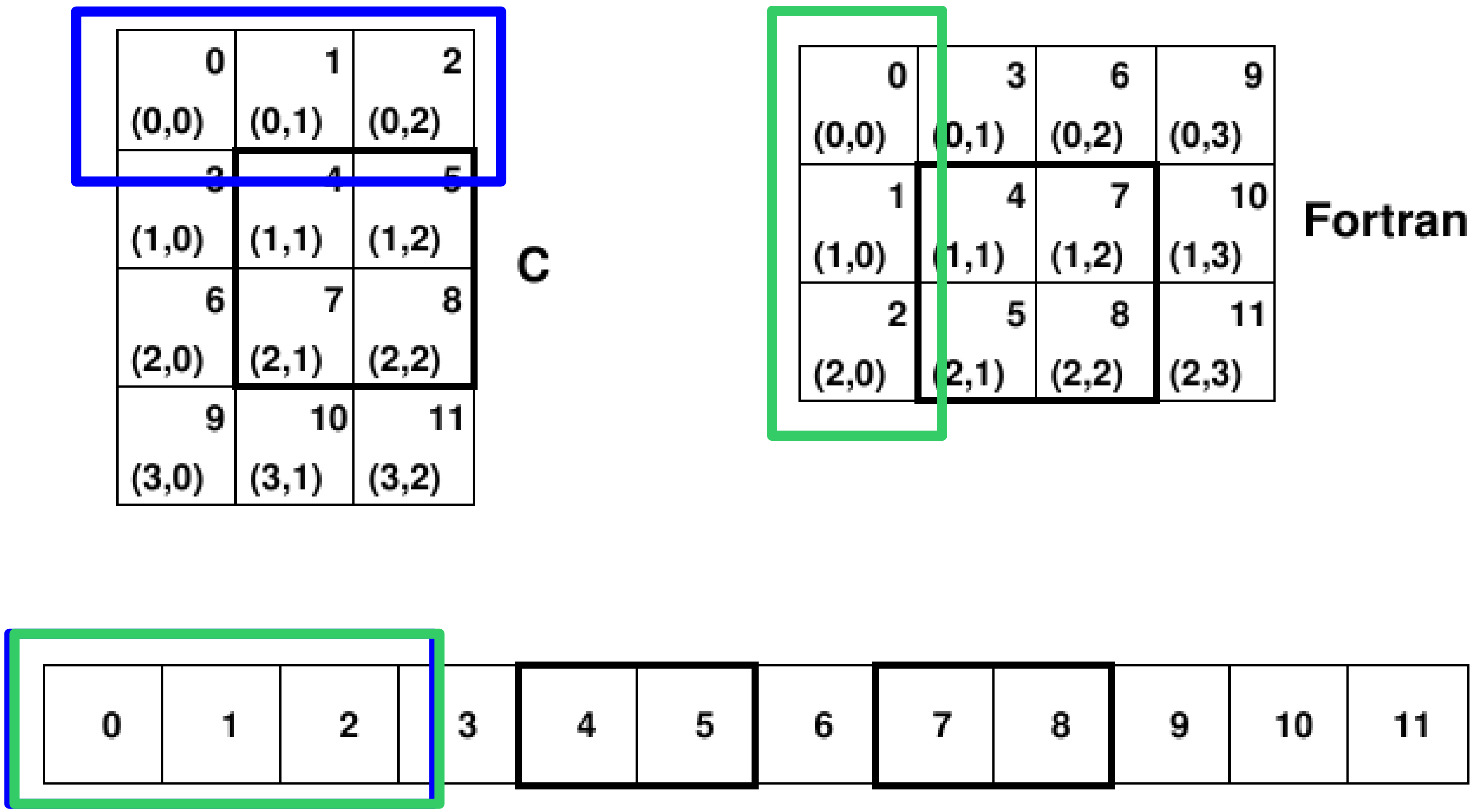
```
npy_intp *strides;     /* bytes to jump to get to the
                         next element of each dimensions */
```

```
In [36]: b
Out[36]:
array([[1, 2],
       [3, 4]])
In [37]: b.dtype.itemsize
Out[37]: 4            # bytes to represent item
In [38]: b.strides
Out[38]: (8, 4)       # (skip_bytes_row, skip_bytes_col)
                      # (2*itemsize, itemsize)
```

ndarray: flags

```
int flags;        /* Flags describing array
                   see below */

In [36]: b.flags
Out[39]:
 C_CONTIGUOUS : True
 F_CONTIGUOUS : False
 OWNDATA : True          # are we responsible for memory
                         # handling?
 WRITEABLE : True        # may we change the data?
 ALIGNED : True          # appropriate hardware alignment
 UPDATEIFCOPY : False    # update .base w/ its data on
                         # deallocation
```

ndarrays memory layout



- In C-style the last index varies first, than the second-to-last varies second, and so on (**default behavior for numpy**).
- Algorithms that work on N-dimensional arrays that are written in Fortran typically expect Fortran-style arrays

ndarray: base pointer

```
PyObject *base;   /* This object should be decref'd
                     upon deletion of array. For views it
                     points to the original array */
```

```
In [60]: a = b.view()    #  a = array([[1, 2],
                                       [3, 4]])

In [61]: a.flags

 C_CONTIGUOUS : True

 F_CONTIGUOUS : False

 OWNDATA : False


In [62]: a[0] = 1, 5      # now also b = array([[1, 5],
                                                [3, 4]])
```

Creating arrays (1)

5 general mechanism to create arrays:

(1) Conversion from other Python structures (e.g. lists, tuples): np.array function

```
>>> list = [0,2,3,7]
>>> a = np.array(list)    # or np.array([0,2,3,7])
    Array([0, 2, 3, 7])
>>> b = np.array([l, m])   # l, m python lists
>>> b = np.asarray(b)      # convert b to an array if b is,
                           # i.e, a list; otherwise do
                           # nothing
```

Creating arrays (2)

(2) Intrinsic NumPy array creation functions (e.g. arange, ones, zeros, etc.)

```
>>> a = np.zeros(10)

>>> a = np.ones((3,2))

>>> a = np.linspace(0,10,11) # start, stop, npoints

array([  0.,   1.,   2.,   3.,   4.,   5.,   6.,
7.,   8.,   9.,  10.])

>>> a = np.arange(10)

array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])

>>> a = np.arange(1,10,2) # start, stop, step

array([1, 3, 5, 7, 9])
```

Creating arrays (3)

Try the shortcut: **np.r_**

```
>>> a = np.r_[0,1,2]      # ~ np.array
>>> a = np.r_[0:10:0.1]  #   np.arange
>>> a = np.r_[0:10:100j] #   np.linspace
```

(3) Creating arrays from strings or buffers

```
>>> np.fromstring('1, 2', dtype=np.int, sep=',')
    array([1, 2])
```

Creating arrays (4)

(4) Reading arrays from disk, either from standard or custom formats (mind the **byte order!!**)

- `loadtxt, genfromtxt` `# custom` **`ASCII`** `formats`
- `fromfile(), <ndarray>.tofile()` **`# custom binary`**
- `HDF5: h5py, pytables` **`# binary standard formats`**
- `netcdf: netcdf-python`

Creating arrays (5)

- Reading from ASCII text files

loadtxt(fname[, dtype=, comments=, delimiter=, skiprows=, coverters=, usecolums=, ...])	Load data from a text file.
savetxt(fname, X[, fmt=, delimiter=])	Save an array to a text file (auto recognizes if .gz) X is the array
genfromtxt(fname[, dtype=, comments=, missing= ...])	Load data from a text file, with missing values handled as specified.

- loadtxt is faster but less flexible
- genfromtxt runs two loops, the first reads all the lines (→ strings), the second parses the line and converts each string to a data type
  - It has the advantage of taking into account missing data

Exercise 2: creating array

1. Create a ndarray of 6x5 elements, all set to 1

```
>>> help(np.ones)
```

1a. Reshape the array to 3x10

2. Download 'mol.xyz' from here and build a new array of atom dtype

```
>>> help(np.loadtxt)
```

Exercise 2: creating array

Solutions

1.

```
>>> a = np.ones((6,5))
>>> a.shape = 3,10
```

2.

```
>>> dt = np.dtype([('symb','|S3'),('PA',np.int),
('x',np.float64),('y',np.float64),('z',np.float64)])
>>> arr = np.loadtxt('mol.xyz',dtype=dt)
```

Creating arrays (6)

- From the ndarray just built we can save a binary file with the ndarray data

```
>>> arr.tofile('mol_bin')
```

- It can be read with np.fromfile

```
>>> arr2 = np.fromfile('mol_bin', dtype=dt)
```

- Be careful when using np.fromfile w/ fortran binary files
  - You may need to deal with field separators...

Creating arrays (7)

(5) Special library functions (e.g. random, …) or *ad hoc* defined function

```
>>> def func(i,j):
      return i*j+1
>>> a = np.fromfunction(func, (3,4)) # meshgrid
array([[ 1.,  1.,  1.,  1.],          i = 1, j = 3
       [ 1.,  2.,  3.,  4.],
       [ 1.,  3.,  5.,  7.]])
In [1]: np.random.rand(4)
Out[1]:
array([ 0.14046702,  0.31755881,  0.44131823,
0.1219652])
```

(some) `ndarray` attributes

- Some useful `ndarray` attributes are: (let `arr` be the array)
  - `arr.`**`shape`** returns a tuple with the size of the array. Changing the tuple re-shapes the array
  - `arr.`**`dtype`** data-type object for this array

    ```
    a = np.ones(10);    a.dtype
    dtype('float64')
    ```
  - `arr.`**`ndim`** number of dimension in array
  - `arr.`**`size`** total number of elements

(some) `ndarray` functions

Some useful `ndarray` functions are:

- `arr.`**`copy`**`()` returns a copy of the array
- `arr.`**`view`**`()` returns a new view of the array using the same data of `arr` `#` **`save memory space`**
- `arr.`**`reshape`**`()` returns an array with a new shape
- `arr.`**`transpose`**`()` returns an array view with the shape transposed
- `arr.`**`ravel`**`()` return a flattered array

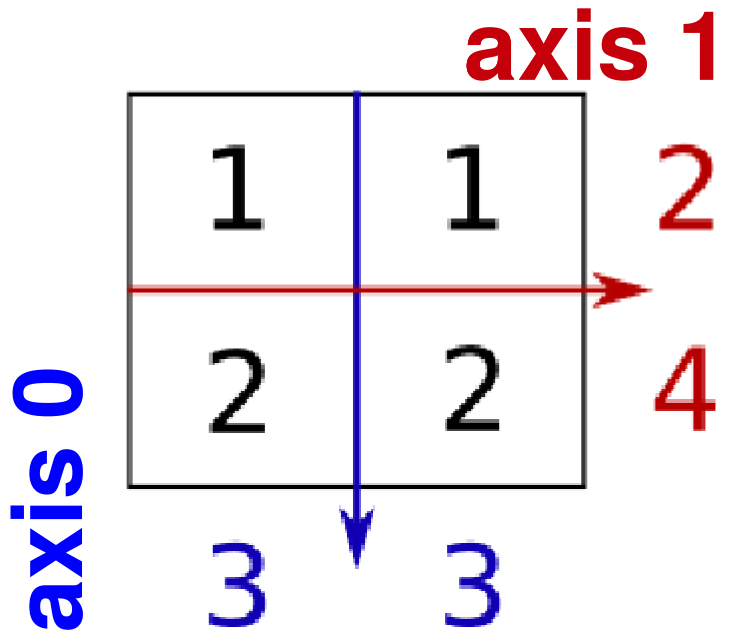
(some) ndarray functions (2)

- arr.**sum**()

```
>>> a = np.array([[1,4,2],[3,1,8]])
>>> a.sum(axis=0)
>>> array([ 4,  5, 10])
```

(some) ndarray functions (2) cont'd

```
>>> a = np.array([[1,1],[2,2]])
>>> a.sum(axis=0)
>>> array([ 3,  3])
```



(some) ndarray functions (2)

- `arr.`**`min|max`**`()` return min (or max) value
- `arr.`**`argmin|argmax`**`()` return the index of min (max) value
- `arr.`**`var|mean|std|prod`**`()` take the usual meaning

(some) ndarray functions (3)

- **sort** array sorting

```
>>> a = np.array([[1,4],[3,1]])
>>> np.sort(a)     # sort along the last axis
 array([[1, 4],
        [1, 3]])
 >>> np.sort(a, axis=0)    # sort along x axis
 array([[1, 1],
        [3, 4]])
>>> np.sort(a, axis=None)  # sort the flattened
                           # array
 array([1, 1, 3, 4])
>>> np.sort(a, order=field)  # 'field' of a
                             # structured array
```

Basic routines overview

- Creating arrays routines (mentioned earlier in this presentation)
- Operation on two or more arrays (`dot, ...`)
- Shape functions (`split`, `resize, concatenate, stack`)
- Basic functions (`average`, `cov`, `vectorize,`...)
- Two-dimensional array functions (`eye`, `diag`, ...)

Indexing

- Indexing means selecting some of the array's values
- ndarrays can be indexed using the following syntax:

X**[obj]**

- Depending on **obj**, a different indexing is triggered:
  - **Basic slicing** when obj is an integer, or a tuple (or list) of integers, and slice objects.
    - always returns a **view** of the array
  - **Record access** when obj is the string of a field of structured array
  - **Advanced selection** when obj contains a ndarray of data type integer or bool.
    - always returns a **copy** of the array

Basic slicing (1)

- A slice object is represented by X[**I**:**J**:**K**]
  - I = **first element** (included, default is 0)
  - J = **last element** (excluded, default is length of the array)
  - K = **step or stride** (default is 1)

- Slicing for `ndarray` works similarly to standard Python sequences but can be done over **multiple dimensions**

Basic slicing (2)

- Examples: given a two dimensional 5x10 `ndarray` "A"

  - `A[3] = A[3,:] = A[3,::]`

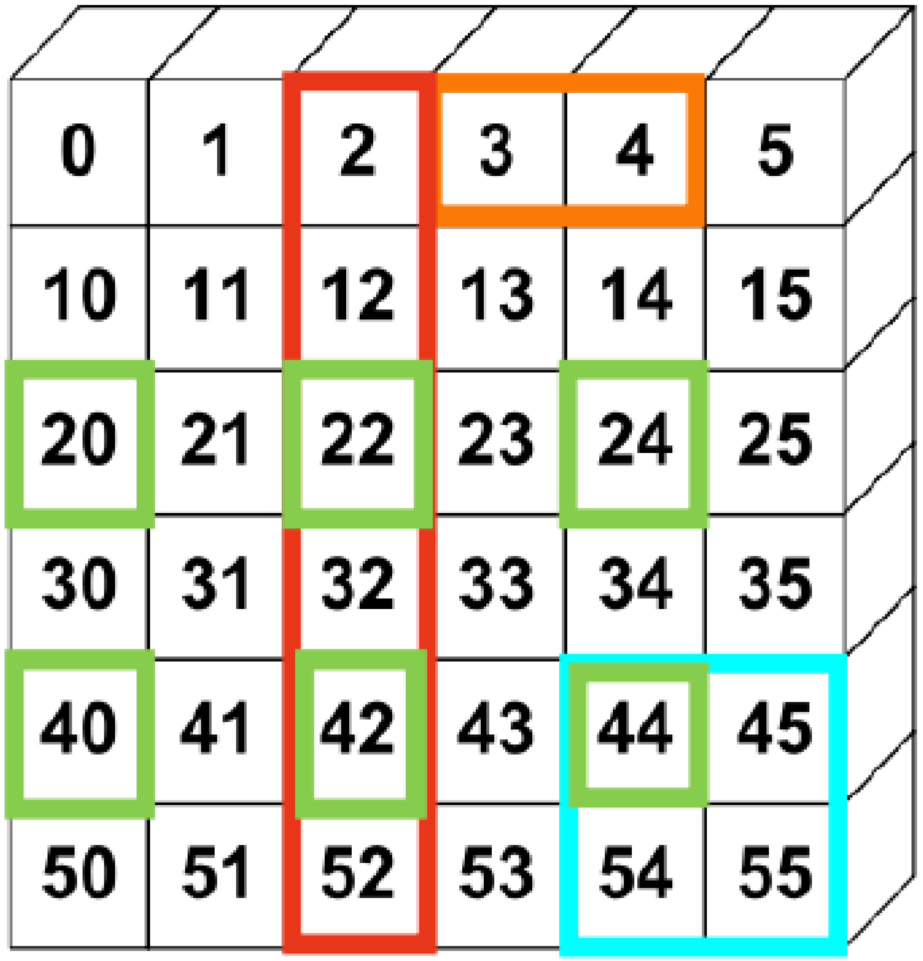
    represents the **4th row** of the array (10 elements)

  - `A[:,1] = A[::,1]`

    represents the **2nd column** of the array (5 elements)

Basic slicing (3)

```
>>> a[0,3:5]

>>> a[4:,4:]

>>> a[:,2]

>>> a[2::2,::2]
```



Basic slicing (4)

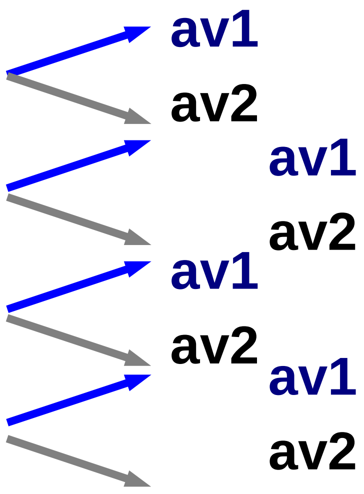
- **Ellipses** (`...`) can be used to replace zero or more ":" terms so that the total number of dimensions in the slicing tuple **matches the shape** of the `ndarray`

```
a = np.arange(60); a.shape=(3,4,5)
print a[...,3]   # print a[:,:,3] → (3,4)
print a[1,...,3] # print a[1,:,3] → (4)
```

Exercise 3: Basic slicing

- Build a 2-dim array, then calculate all the average values along the rows for its odd and even columns.

```
[ 0,  1,  2,  3,  4,  5]
[ 6,  7,  8,  9, 10, 11]
[12, 13, 14, 15, 16, 17]
[18, 19, 20, 21, 22, 23]
```



```
hint:  np.mean() or arr.mean()
```

Exercise 3: Basic slicing

```
>>> a = np.arange(24).reshape(4,6)
>>> a[:,0::2].mean(axis=1)
>>> a[:,1::2].mean(axis=1)

or alternatively
>>> np.mean(a[:,0::2],axis=1)  # [2., 8., 14., 20.]
>>> np.mean(a[:,1::2],axis=1)  # [3., 9., 15., 21.]
```

Record access

- The fields of structured arrays can be accessed by indexing the array with string

-
```
>>> ra
array([(b'H', 1), (b'C', 6)],
      dtype=[('at', 'S3'), ('Z', '<i4')])


ra['at']   # array(['H', 'C'], dtype='|S3')
```

Advanced selection

- Indexing arrays with other arrays

- This means X[obj] → obj is a `ndarray`

- There are two different ways:
  - **Boolean (mask) index arrays**. Involve giving a boolean array of the proper shape to indicate the values to be selected

  - **Integer index arrays**. Use one or more arrays of index values.

Adv. selection: boolean index arrays

- `a = np.array([True, False, True]) # dtype('bool')`

- Boolean arrays must be of the (or broadcastable to the) same shape of the array being indexed

```
>>> y
array([[ 0,  1,  2,  3,  4,  5],
       [ 6,  7,  8,  9, 10, 11],
       [12, 13, 14, 15, 16, 17]])
>>> b = y>10
>>> y[b]   # y[y>10]
array([11, 12, 13, 14, 15, 16, 17]    # 1-d array
```

Exercise 4 ndarray selection

- From the atoms array calculate the contribution to the molecular weight for each of the different kind of atoms (C, N, H, O) making use of the Numpy selection

$$PM_C = \sum PA_C$$

Hint: use the advanced boolean selection

Exercise 4 ndarray selection

- Solution

```
>>> arr[arr['symb']=='C']['PA'].sum() # 372
>>> arr[arr['symb']=='H']['PA'].sum() # 26
>>> arr[arr['symb']=='N']['PA'].sum() # 28
>>> arr[arr['symb']=='O']['PA'].sum() # 32
```

(does it break some of The Zen of Python's rules??)

ndarray selection

To summarize, selection:

- can save you **time** (and code lines)
- enhances the code **performances**
  - avoid traversing array through python loops

  (internal (C) loops are still performed... more on that later)
- can save **memory** (in place selection)

NumPy (main) objects

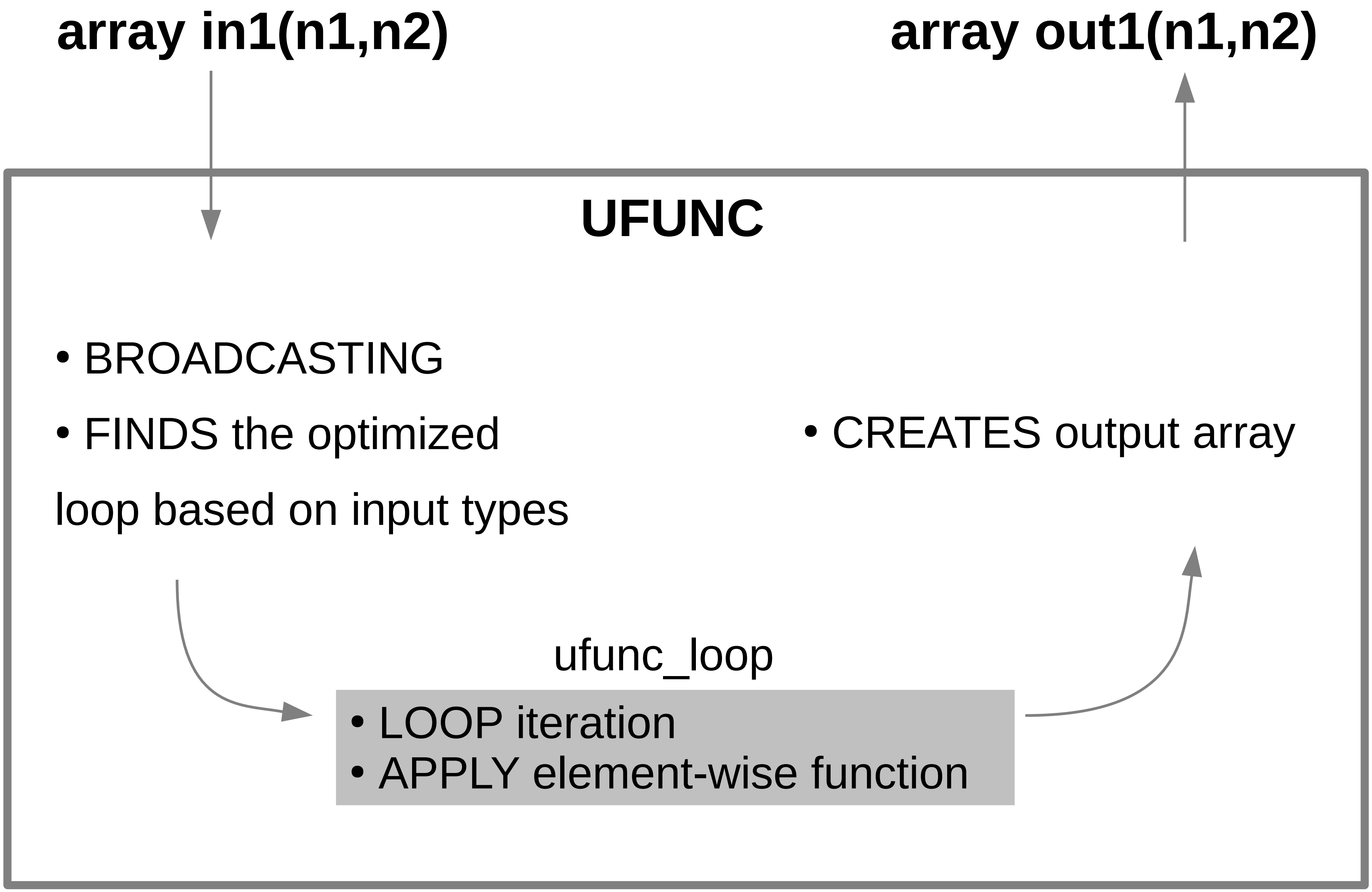
- NumPy provides two fundamental objects:
  - **`ndarray`**;
  - **`ufunc`**; functions that operate on one or more `ndarrays` **element-by-element**

ufunc

Universal functions (1)

- Universal functions, ufuncs are functions that **operate** on the ndarray objects
- all ufuncs are instances of a general class, thus they behave the same. All ufuncs perform **element-by-element** operations on the entire ndarray(s)
- These functions are **wrapper** of some core functions, typically implemented in compiled (C or Fortran) code

Universal functions (2)



Universal functions (2)

- Ufunc loop may look something like

```
void ufunc_loop(void **args, int *dimensions, int *steps,
                void *data)
{
 /* int8 output = elementwise_function(int8 input_1, int8
  * input_2)
  *
  * This function must compute the ufunc for many values at
  * once, in the way shown below.
 */

  char *input_1 = (char*)args[0];
  char *input_2 = (char*)args[1];
  char *output = (char*)args[2];
  int i;
  for (i = 0; i < dimensions[0]; ++i) {
    *output = elementwise_function(*input_1, *input_2);
    input_1 += steps[0];
    input_2 += steps[1];
    output += steps[2];
  }
}
```

Universal functions (2)

- Examples:

>>> a = np.array([a_1,a_2,...,a_n]) # a -> ndarray

np.cos(a) = ([cos(a_1),cos(a_2),...,cos(a_n)])

element-wise function

```
>>> b = 1.5*a + 2   #   * + / -  all ufuncs
```

  - all the elements of "a" are multiplied by 1.5; result stored in a **temporary array**
  - All the elements of the temp array are increased by 2; result stored in another **temporary array**
  - b becomes a reference to the 2nd temp array

Universal functions (3)

- What happens when `ufunc` has to operate on **two arrays** of **different dimensions**?

$$\begin{bmatrix} \texttt{[0,11,21,3,4,15]} \\ \texttt{[6,17,8,9,10,11]} \\ \texttt{[1,13,4,11,16,1]} \\ \texttt{[18,1,2,21,2,23]} \\ \texttt{[24,2,26,7,28,9]} \end{bmatrix} + \begin{bmatrix} \texttt{[1,2,3,4,5,10]} \end{bmatrix}$$

- → To be efficient, element-wise operations are required
- → To operate element-by-element **broadcasting** is needed.

Broadcasting (1)

- After having applied the broadcasting rules the shape of all arrays must match

$$\underset{(5,6)}{\begin{bmatrix}[0,11,21,3,4,15]\\ [6,17,8,9,10,11]\\ [1,13,4,11,16,1]\\ [18,1,2,21,2,23]\\ [24,2,26,7,28,9]\end{bmatrix}} + \underset{(1,6)\ (5,6)}{\begin{bmatrix}[1,2,3,4,5,10]\\ [1,2,3,4,5,10]\\ [1,2,3,4,5,10]\\ [1,2,3,4,5,10]\\ [1,2,3,4,5,10]\end{bmatrix}}$$

Broadcasting (2)

- Broadcasting allows to deal in a meaningful way with inputs that do not have the same shape.

- broadcasting follows these rules:

  (1) Prepend 1 until all the arrays ndims match

  a.shape (2,2,3,6)   b.shape (3,6) # → b.shape (1,1,3,6)

  a.ndim = 4   b.ndim = 2   # → b.ndim = 4

  (2) Arrays with a size of 1 along a particular dimension act like the array with the **largest size** along that dimension.

  → The **values** of the array are assumed to be **the same along the broadcasted dimension**

Broadcasting (3)

- 1d-ndarrays are always broadcastable

```
a.shape → (3)      b.shape -> (4,3);
a.shape → (1,3)     # first rule, n. of dim matches
a.shape → (4,3)     # second rule
c = a*b     c.shape →  (4,3)    # as expected
```

- Another example

```
a.shape -> (2,1,3)      b.shape -> (2,4,1);
c = a*b     c.shape -> (2,4,3)  # second rule
```

- Arrays not broadcastable

```
a.shape -> (2,5,3)
b.shape -> (2,4,1);        c = a*b     # shape mismatch
```

Broadcasting (4)

- If needed it is possible to add a **trailing dimension** to the shape of a `ndarray`. This is a convenient way of taking the outer product (or any other outer operation) of two arrays

```
a.shape → (3)     b.shape → (4);
c = a[:,np.newaxis]          #  c.shape → (3,1)


c * b    c.shape -> (3,4)
```

Universal functions: performance

- Iterations over array should be avoided because they are not efficient.
- Performance using array arithmetics is better than using python loops

Using ufunc

```
In [1]: x = np.arange(10**7)

In [2]: %timeit y = x*3

10 loops, best of 3: 76 ms per loop
```

Using for loop

```
In [3]: %timeit y = [x*3 for x in xrange (10**7)]

1 loops, best of 3: 1.33 s per loop
```

~ 18x speedup (~ standard across NumPy)

Efficiency note (2)

- The operation

```
>>> b = 2*a + 2
```

can be done with in-place operations

```
>>> b = a      # b is a reference to a
>>> b *= 2
>>> b += 2
```

More efficient and doesn't require storing temp array

- These operations affect array “a” as well; we can avoid this with

```
>>> b = a.copy()
```

- Other in-place operations

```
>>> b += a        >>> b *= a       >>> b **= a
>>> b -= a       >>> b /= a
```

Efficiency note (3):

- Let's consider the function

```
>>> def myfunc(x):      # if x is an array
>>>   if x<0:           # x<0 becomes a bool array
>>>     return 0
>>>   else:
>>>     return sin(x)
```

- "if x<0" results in a boolean array and **cannot** be evaluated by the if statement

Efficiency note (3): Vectorization

- We can vectorize our function using the function `where`

```
>>> def vec_myfunc(x):
>>>    y = np.where(x<0, 0, np.sin(x))
>>>    return y    # now returns an array
```

-
```
np.where(condition, x, y) # condition → bool array
                          # condition is true → x
                          # condition is false → y
```

NumPy universal functions (1)

- There are more than 60 `ufuncs`
- Some `ufuncs` are called automatically: i.e. `np.multiply(x,y)` is called internally when a*b is typed
- NumPy offers trigonometric functions, their inverse counterparts, and hyperbolic versions as well as the exponential and logarithmic functions. Here, a few examples:

```
>>> b = np.sin(a)
>>> b = np.arcsin(a)
>>> b = np.sinh(a)
>>> b = a**2.5  # exponential
>>> b = np.log(a)
>>> b = np.exp(a)
>>> b = np.sqrt(a)
```

NumPy universal functions (2)

- Comparison functions:

  greater, **less**, **equal**, **logical_and/_or/_xor/_nor**, **maximum**, **minimum**, ...

```
>>> a = np.array([2,0,3,5])
>>> b = np.array([1,1,1,6])
>>> np.maximum(a,b)
array([2, 1, 3, 6])
```

- Floating point functions:

  floor, **ceil**, **isreal**, **iscomplex**, ...

Exercise 5: universal functions

- Calculate the molecular center of mass

$$xcm = \frac{1}{MW} \sum_i x_i m_i \qquad ycm = \frac{1}{MW} \sum_i y_i m_i \qquad zcm = \frac{1}{MW} \sum_i z_i m_i$$

- Calculate the moment of inertia tensor

$$I = \begin{bmatrix} I_{11} & I_{12} & I_{13} \\ I_{21} & I_{22} & I_{23} \\ I_{31} & I_{32} & I_{33} \end{bmatrix}$$

$$I_{11} = I_{xx} = \sum_i m_i (y_i^2 + z_i^2)$$

$$I_{22} = I_{yy} = \sum_i m_i (x_i^2 + z_i^2)$$

$$I_{22} = I_{zz} = \sum_i m_i (x_i^2 + y_i^2)$$

$$I_{12} = I_{xy} = -\sum_i m_i x_i y_i$$

$$I_{13} = I_{xz} = -\sum_i m_i x_i z_i$$

$$I_{23} = I_{yz} = -\sum_i m_i y_i z_i$$

Exercise 5: universal functions

- Calculate the molecular center of mass

```
>>> xcm = 1./b['PA'].sum() * (b['PA']*b['x']).sum()
>>> ycm = 1./b['PA'].sum() * (b['PA']*b['y']).sum()
>>> zcm = 1./b['PA'].sum() * (b['PA']*b['z']).sum()
```

- Calculate the moment of inertia tensor

```
>>> Ixx = (b['PA']*(b['y']**2 + b['z']**2)).sum()
>>> Iyy = (b['PA']*(b['x']**2 + b['z']**2)).sum()
>>> Izz = (b['PA']*(b['x']**2 + b['y']**2)).sum()
>>> Ixy = -(b['PA']*b['x']*b['y']).sum()
>>> Ixz = -(b['PA']*b['x']*b['z']).sum()
>>> Iyz = -(b['PA']*b['y']*b['z']).sum()
>>> TI = np.array([[Ixx, Ixy, Ixz],[Ixy, Iyy, Iyz],
[Ixz, Iyz, Izz]])
```

Standard classes inheriting from ndarray

Matrix objects

Matrix objects inherit from ndarray classes

- Matrix can be created using a Matlab-style notation

```
>>> a = np.matrix('1 2; 3 4')
>>> print a
    [[1 2]
     [3 4]]
```

- Matrix are always **two-dimensional** objects
- Matrix objects over-ride multiplication to be **matrix-multiplication**, and over-ride power to be **matrix raised to a power**
- Matrix objects have higher **priority** than ndarrays. Mixed operations result therefore in a matrix object

Matrix objects (2)

- `Matrix` objects have special attributes:

  `.T` returns the transpose of the matrix

  `.H` returns the conjugate transpose of the matrix

  `.I` returns the inverse of the matrix

  `.A` returns a view of the data of the matrix as a 2-d array

Basic modules

Basic modules: linear algebra

- It contains functions to solve **linear systems**, finding the **inverse** and the **determinant** of a matrix, and computing **eigenvalues** and **eigenvectors**

```
A = np.zeros((10,10))   # arrays initialization
x = np.arange(10)/2.0
for i in range(10):
...   for j in range(10):
...      A[i,j] = 2.0 + float(i+1)/float(j+i+1)
b = np.dot(A, x)
y = np.linalg.solve(A, b) # A*y=b → y=x
np.allclose(y,x) # True, mind the tolerance!
```

Basic modules: linear algebra

- Eigenvalues can also be computed:

```
# eigenvalues only:
>>> A_eigenvalues = np.linalg.eigvals(A)

# eigenvalues and eigenvectors:
>>> A_eigenvalues, A_eigenvectors = np.linalg.eig(A)
```

Exercise 6: matrices and linalg

(1) From the array TI of the last exercise build a matrix (mTI), calculate eigenvalues (e) and eigenvectors (**Ev**) and prove that

$$Ev^T\, mTI\, Ev = \begin{bmatrix} e_1 & 0 & 0 \\ 0 & e_2 & 0 \\ 0 & 0 & e_3 \end{bmatrix}$$

(2) Now, for example, you can rotate all the atoms coordinates by multiplying them by the **Ev** matrix

Basic modules: random numbers

- Calling the standard random module of Python in a loop to generate a sequence of random number is inefficient. Instead:

```
>>> np.random.seed(100)

>>> x = np.random.random(4)

array([ 0.89132195,  0.20920212,  0.18532822,
0.10837689])

>>> y = np.random.uniform(-1, 1, n) # n uniform
numbers in interval (-1,1)
```

- This module provides more general distributions like the normal distribution

```
>>> mean = 0.0; stdev = 1.0

>>> u = np.random.normal(mean, stdev, n)
```

Exercise 7: random numbers

- Given a game in which you win back 10 times your bet if the sum of 4 dice is less than 10, determine (brute force, i.e. 1000000 trows) whether it is convenient to play the game or not

hint: use `np.random.radint`

Numpy: good to know

Masked arrays (1)

```
>>> x = np.arange(20).reshape(4,5) # 2d array
>>> x[2:,2:] = 2 # assignment
array([[ 0,  1,  2,  3,  4],
       [ 5,  6,  7,  8,  9],
       [10, 11,  2,  2,  2],
       [15, 16,  2,  2,  2]])
>>> x[x<5]         # x<5 bool array
array([0, 1, 2, 3, 2, 2, 2, 2, 2, 2]) # 1d array
```

- What if we want to maintain the original shape of the array
- We can use masked arrays: the **shape of the array is kept**
- Invalid data can be flagged and ignored in math computations

Masked arrays (2)

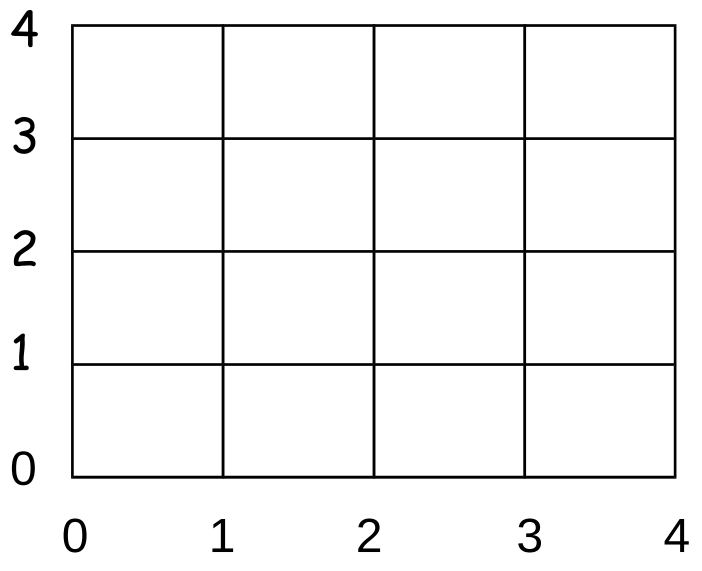
```
>>> import numpy.ma as ma

>>> y = ma.masked_less(x, 4)

>>> masked_array(data =

 [[-- -- -- -- 4]

 [5 6 7 8 9]

 [10 11 -- -- --]

 [15 16 -- -- --]],

            mask =

 [[ True  True  True  True False]

 [False False False False False]

 [False False  True  True  True]

 [False False  True  True  True]],

      fill_value = 999999)

>>> y.sum(axis=0)           # → [30 33 7 8 13]
```

Meshgrids (1)

- Given a two-dimensional grid of points, namely `a`$_{i,j}$`=(x`$_i$`, y`$_j$`)` we want to calculate for each point of the grid the values of a function `f(a`$_{ij}$`)=f(x`$_i$`,y`$_j$`)`
- Suppose `f = x/2 + y`
- `f` is a `ufunc` (implicitly uses `ufuncs: add, divide`) so it operates element-by-element

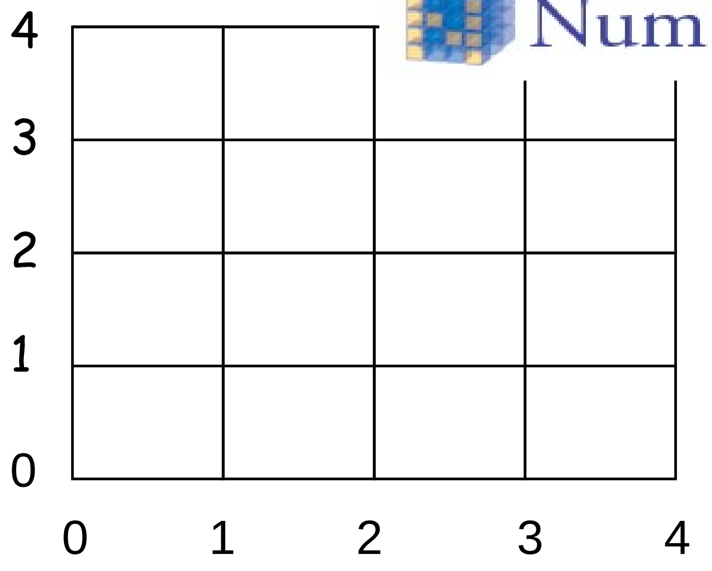
```
>>> x = np.linspace(0,4,5)
array([ 0.,  1.,  2.,  3.,  4.])
>>> y = x.copy()
>>> def f(x,y): return x/2 + y
>>> values = f(x,y)
array([ 0. ,  1.5,  3. ,  4.5,  6. ])
```

WRONG!



Meshgrids (2)

```
>>> x = np.linspace(0,4,5)

>>> y = x.copy()

>>> xv,yv = np.meshgrid(x,y)
```



xv

```
array([[ 0.,  1.,  2.,  3.,  4.],
       [ 0.,  1.,  2.,  3.,  4.],
       [ 0.,  1.,  2.,  3.,  4.],
       [ 0.,  1.,  2.,  3.,  4.],
       [ 0.,  1.,  2.,  3.,  4.]])
```

yv

```
array([[ 0.,  0.,  0.,  0.,  0.],
       [ 1.,  1.,  1.,  1.,  1.],
       [ 2.,  2.,  2.,  2.,  2.],
       [ 3.,  3.,  3.,  3.,  3.],
       [ 4.,  4.,  4.,  4.,  4.]])
```

```
>>> def f(x,y): return x/2 + y  # still operates elementwise

>>> values = f(xv,yv)
```

Bibliography

- http://docs.scipy.org/doc/
- Guide to NumPy (Travis E. Oliphant)
- NumPy User Guide
- Numpy Reference Guide

- Python Scripting for Computational Science (Hans Petter Langtangen)