Python for Data Analysis

Ben Zaitlen
Travis E. Oliphant

PyCon USA
March 13, 2013

Announcements

- Lunch is moved to Exhibit Hall D
- Schedule:
  - 9:00 - 10:50am
  - 20-min break
  - 11:10am - 12:20pm
- Please fill out survey
  - https://www.surveymonkey.com/s/pycon2013_tutorials
  - https://goo.gl/PvHDc
- https://github.com/ContinuumIO/tutorials/
- Volunteering Opportunities Available

PyData

Silicon Valley 2013

http://www.pydata.org/

Changing the way scientists, engineers, and analysts perceive big data

TUTORIALS: March 18 | **MAIN CONFERENCE:** March 19-20

Santa Clara Convention Center
Santa Clara, CA

Sponsorship available. Learn more.

Sponsors

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PyData Beneficiary
NumFOCUS
Open Code, Better Science.

DE Shaw & Co

appnexus

J.P.Morgan

python software foundation

MARINEXPLORE

Python Weekly

Software Developer's Journal

Inside Analysis

O'REILLY

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PyCon 2013 - Volunteering

A great way to meet people

Low-commitment opportunities:

- SWAG bagging: Thur 4-8PM
  - Bag 10! (~1/2 hr)
- Registration Desk
  - 1-2 hrs helps
  - Anytime, but Fri => meet *everyone!*

Current needs

- http://bit.ly/pycon-volunteering-status

- More info:
  - http://bit.ly/pycon2013-volunteer

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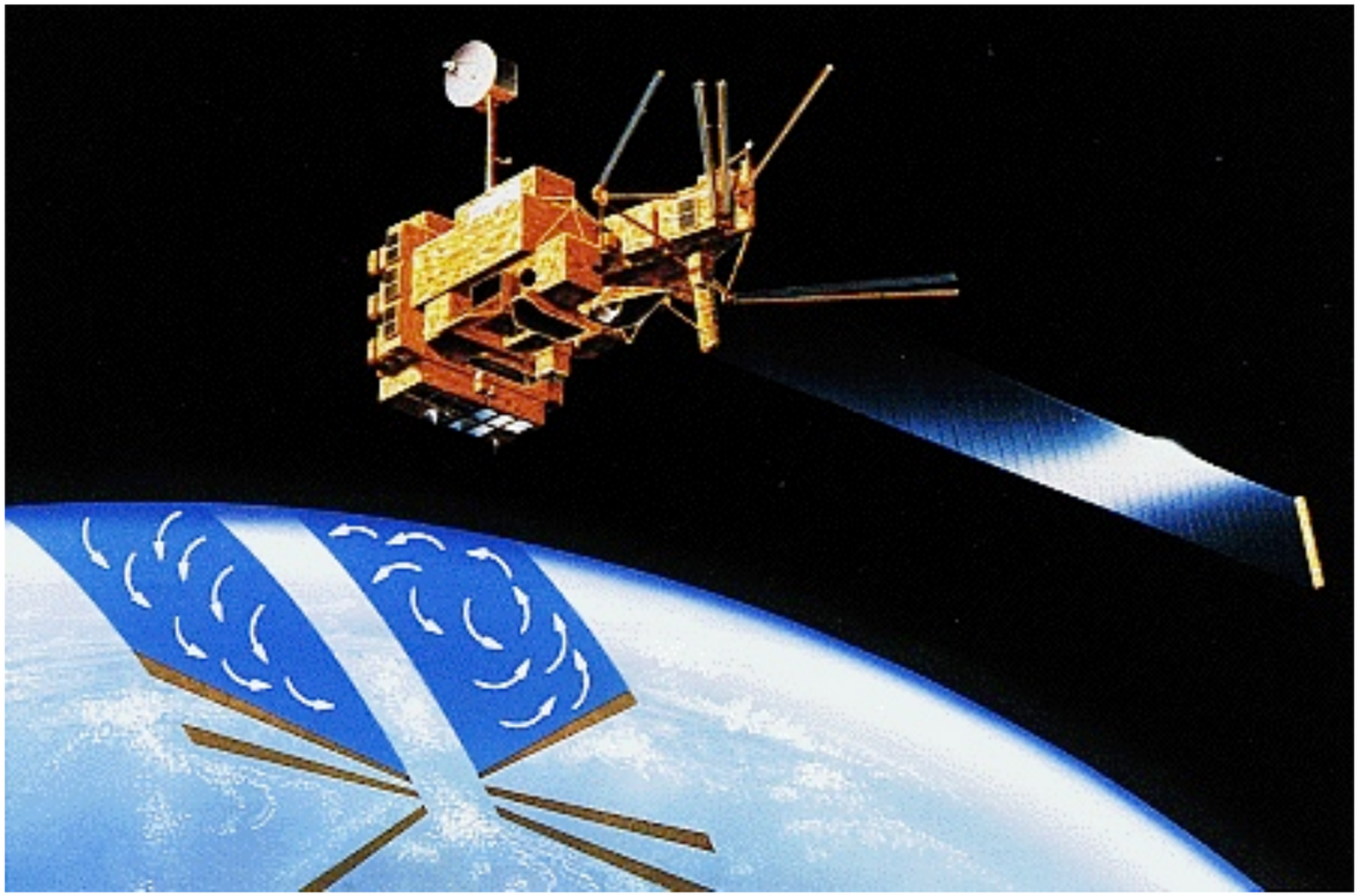
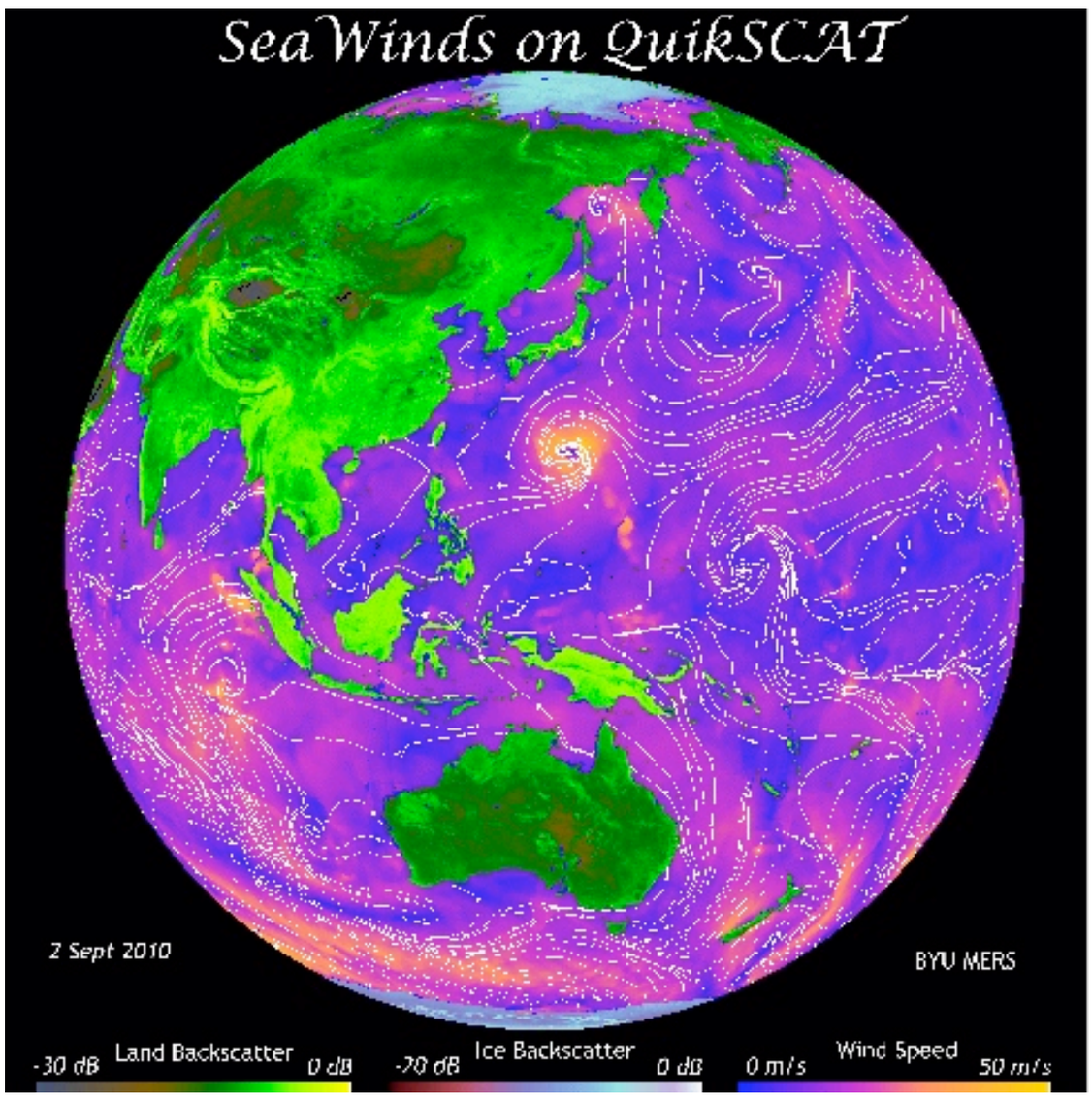
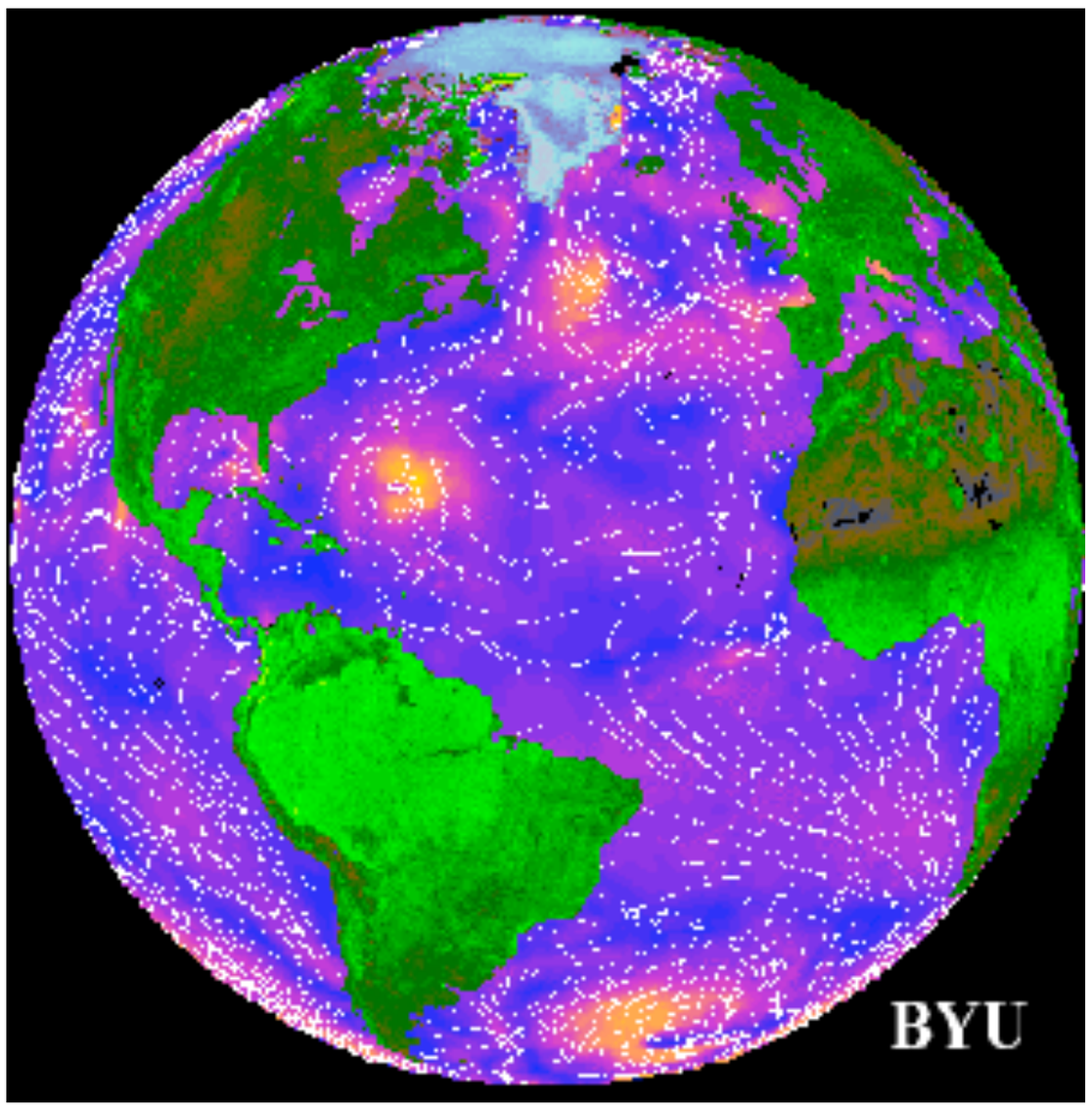
My Roots



My Roots

Images from BYU Mers Lab





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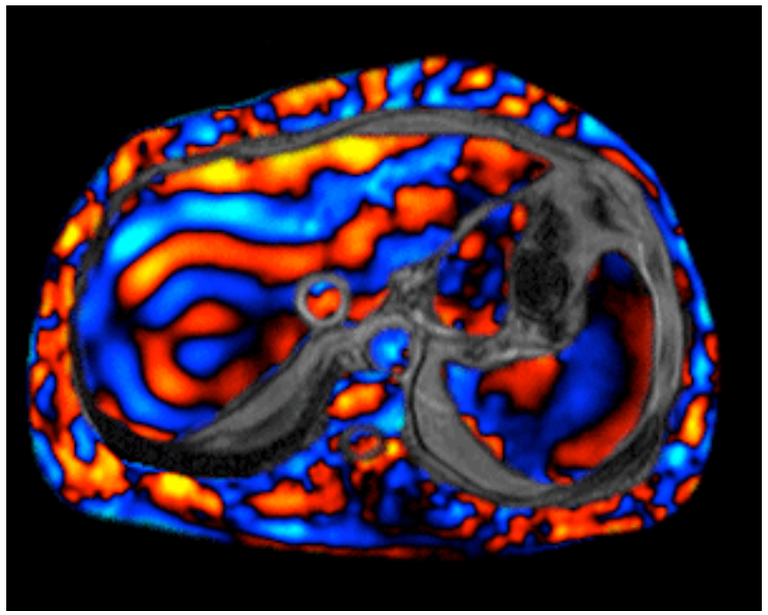
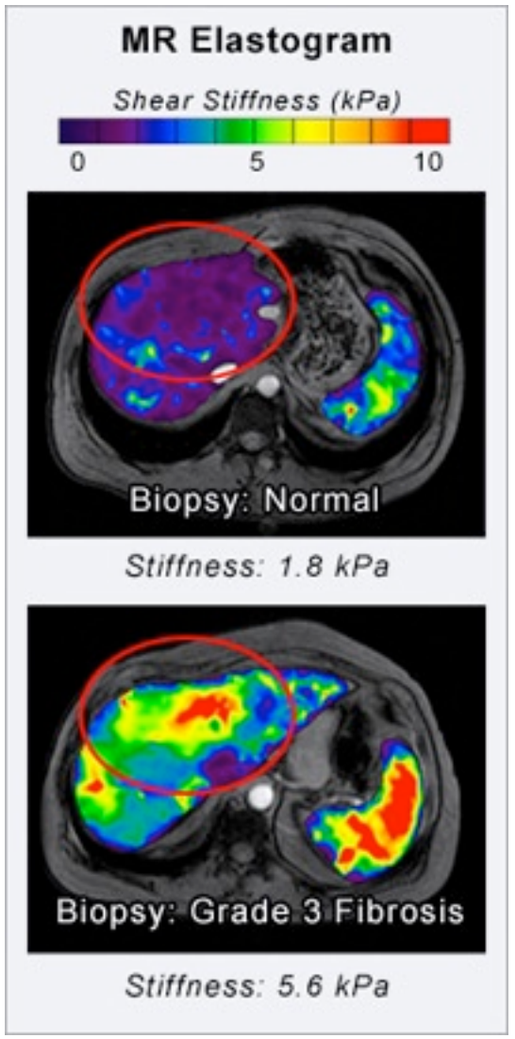
Science led to Python

$$\rho_0 \left(2\pi f\right)^2 U_i \left(\mathbf{a}, f\right) = \left[C_{ijkl} \left(\mathbf{a}, f\right) U_{k,l} \left(\mathbf{a}, f\right)\right]_{,j}$$

Raja Muthupillai



Richard Ehman
1997



Armando Manduca

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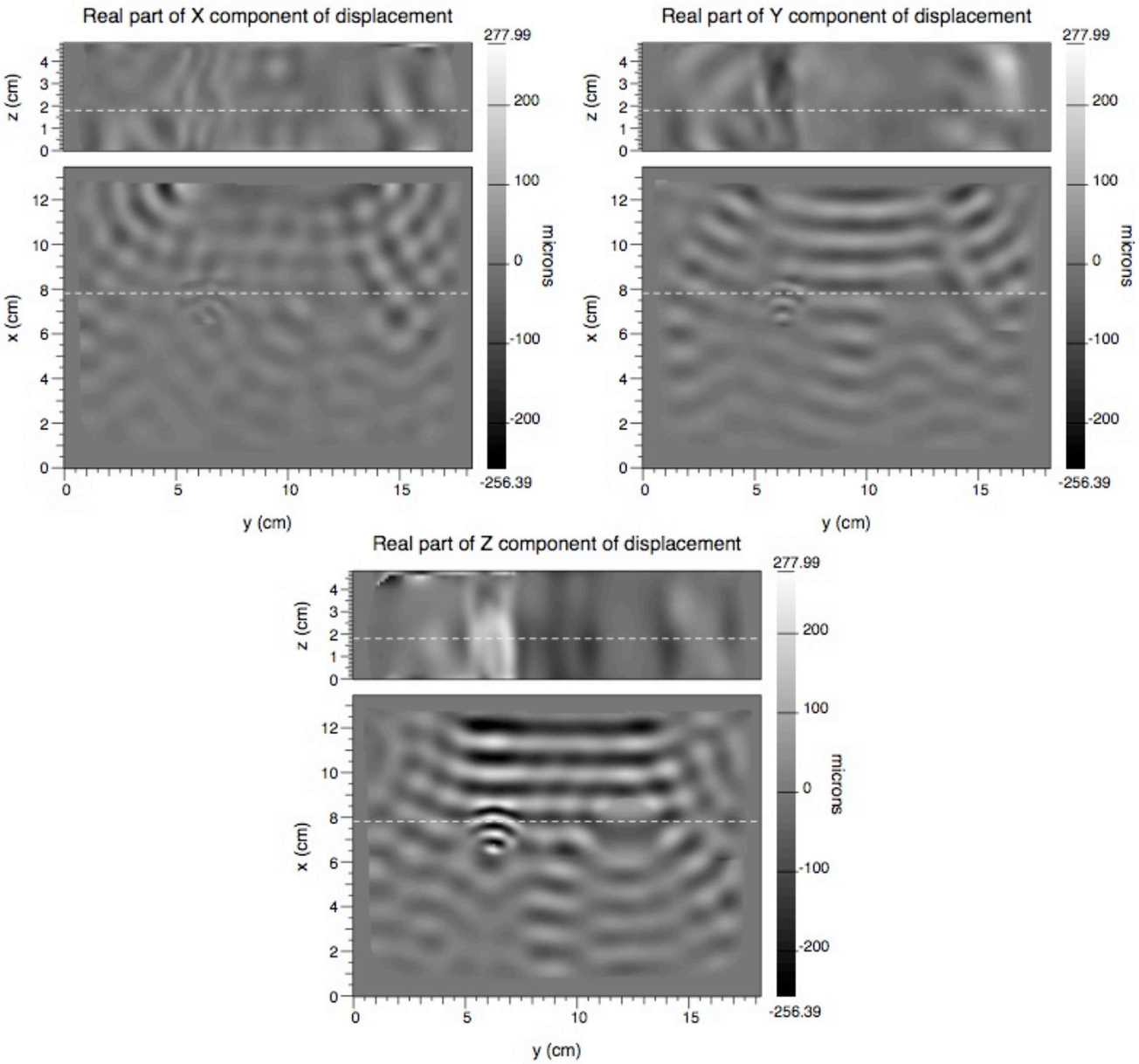
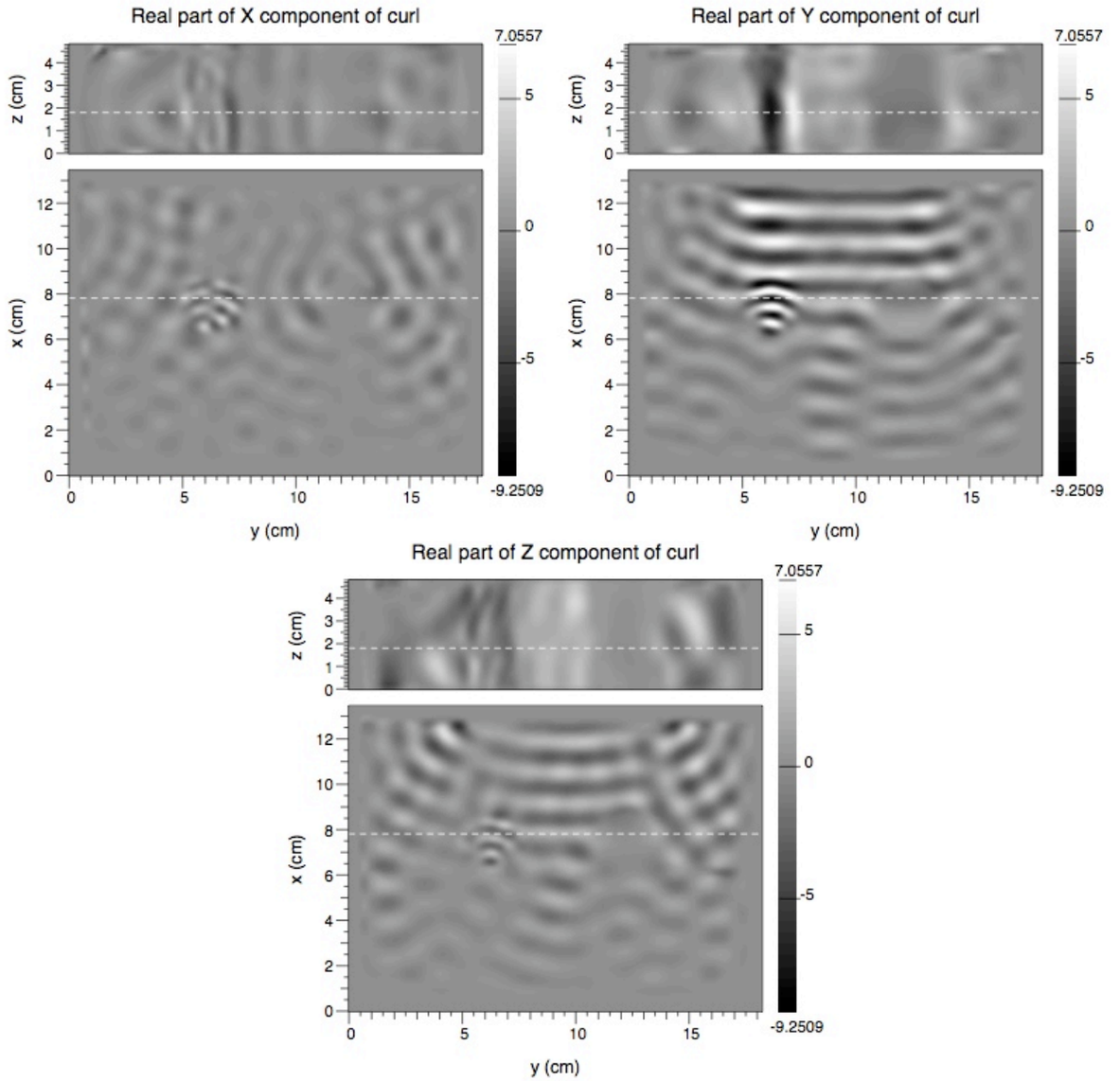
Finding derivatives of 5-d data



$$\Xi = \nabla \times \mathbf{U}$$



Scientist at heart

Python origins

http://python-history.blogspot.com/2009/01/brief-timeline-of-python.html

Version	Date
0.9.0	Feb. 1991
0.9.4	Dec. 1991
0.9.6	Apr. 1992
0.9.8	Jan. 1993
1.0.0	Jan. 1994
1.2	Apr. 1995
1.4	Oct. 1996
1.5.2	Apr. 1999

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Brief History

Person	Package	Year
Jim Fulton	Matrix Object in Python	1994
Jim Hugunin	Numeric	1995
Perry Greenfield, Rick White, Todd Miller	Numarray	2001
Travis Oliphant	NumPy	2005

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1999 : Early SciPy emerges

Discussions on the matrix-sig from 1997 to 1999 wanting a complete data analysis environment: Paul Barrett, Joe Harrington, Perry Greenfield, Paul Dubois, Konrad Hinsen, and others. Activity in 1998, led to increased interest in 1999.

In response on 15 Jan, 1999, I posted to matrix-sig a list of routines I felt needed to be present and began wrapping / writing in earnest. On 6 April 1999, I announced I would be creating this uber-package which eventually became SciPy

Gaussian quadrature	5 Jan 1999
cephes 1.0	30 Jan 1999
sigtools 0.40	23 Feb 1999
Numeric docs	March 1999
cephes 1.1	9 Mar 1999
multipack 0.3	13 Apr 1999
Helper routines	14 Apr 1999
multipack 0.6 (leastsq, ode, fsolve, quad)	29 Apr 1999
sparse plan described	30 May 1999
multipack 0.7	14 Jun 1999
SparsePy 0.1	5 Nov 1999
cephes 1.2 (vectorize)	29 Dec 1999

Plotting??

Gist
XPLOT
DISLIN
Gnuplot

→ Helping with f2py

SciPy 2001

Travis Oliphant
optimize
sparse
interpolate
integrate
special
signal
stats
fftpack
misc

Pearu Peterson
linalg
interpolate
f2py

ENTHOUGHT
SCIENTIFIC COMPUTING SOLUTIONS

Founded in 2001 with Travis Vaught

Eric Jones
weave
cluster
*GA**

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Community effort

- Chuck Harris
- Pauli Virtanen
- David Cournapeau
- Stefan van der Walt
- Dag Sverre Seljebotn
- Robert Kern
- Warren Weckesser
- Ralf Gommers
- Mark Wiebe
- Nathaniel Smith

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Why Python for Data Analysis

- Syntax (it gets out of your way)
- Over-loadable operators
- Complex numbers built-in early
- Just enough language support for arrays
- "Occasional" programmers can grok it
- Supports multiple programming styles
- Expert programmers can also use it effectively
- Has a simple, extensible implementation
- General-purpose language --- can build a system
- Critical mass + Pandas!

What is wrong with Python?

- Packaging is still not solved well (distribute, pip, and distutils2 don't cut it --- but look at conda!)
- Missing anonymous blocks
- The CPython run-time is aged and needs an overhaul (GIL, global variables, lack of dynamic compilation support)
- No approach to language extension (macros) except for "import hooks" (lightweight DSL need) and now IPython cell magics in notebook...
- The distraction of multiple run-times (for most data analysis you should ignore PyPy, IronPython, Jython --- they are cool projects but they don't have the ecosystem)
- Array-oriented and NumPy not used by many Python devs.

Putting Science back in Comp Sci

- Much of the software stack is for systems programming --- C++, Java, .NET, ObjC, web
  - Complex numbers?
  - Vectorized primitives?
- Array-oriented programming has been too often replaced by Object-oriented programming --- and now Hadoop is how people are learning about "vectorization"
- Software stack for scientists is not as helpful as it should be
- Fortran is still where many scientists end up

Array-Oriented Computing

Example 1: Fibonacci Numbers

$$
\begin{aligned}
f_n &= f_{n-1} + f_{n-2} \\
f_0 &= 0 \\
f_1 &= 1
\end{aligned}
$$

$$f = 0, 1, 1, 2, 3, 5, 8, 13, 21, 34, \ldots$$

Common Python approaches

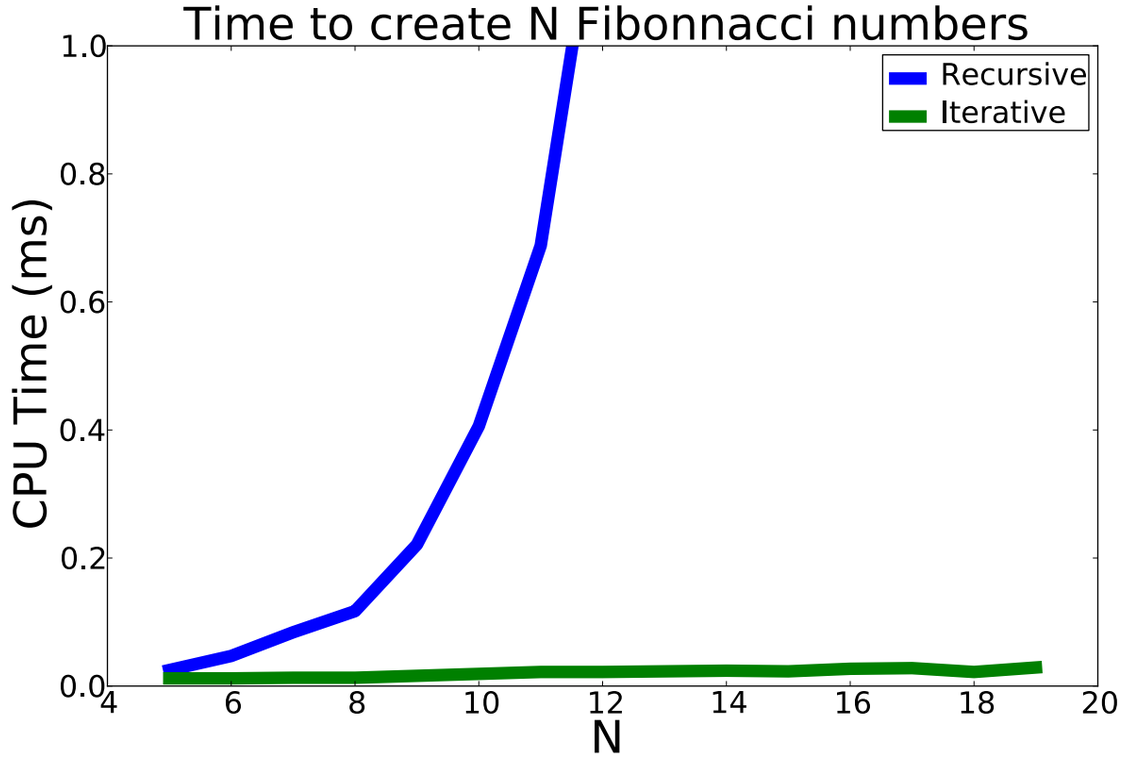
Recursive

```
def _fib(n):
    if n <= 0:
        return 0
    if n == 1:
        return 1
    return fib(n-1) + fib(n-2)

def fib(N):
    return [_fib(n) for n in xrange(N)]
```

Iterative

```
def fib1(N):
    result = [0,1]
    for k in range(2,N):
        result.append(result[k-1] + result[k-2])
    return result
```



Algorithm matters!!

Array-oriented approaches

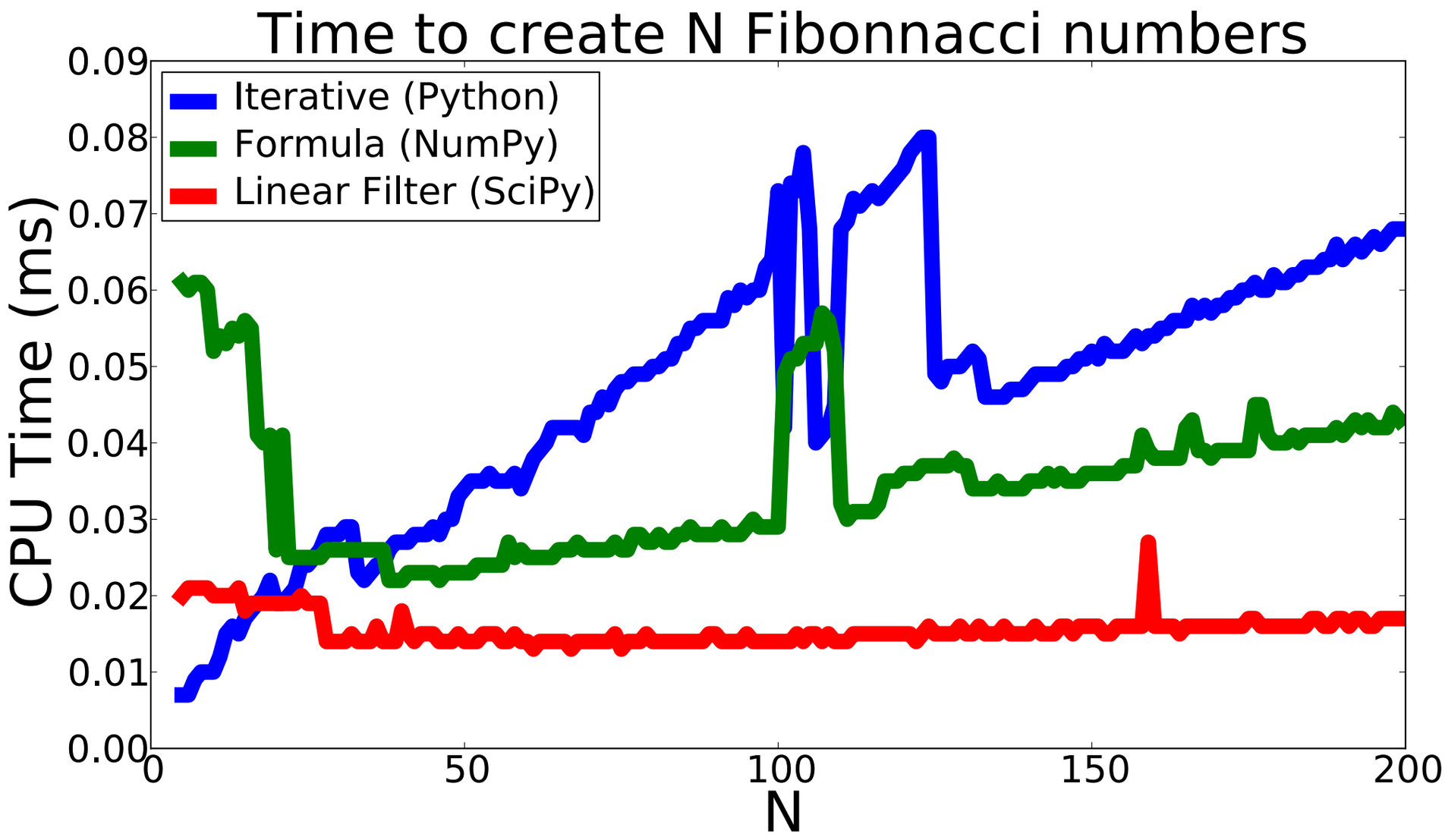
Using LFilter

```
from scipy.signal import lfilter
from numpy import zeros
b = array([1.0])
a = array([1.,-1,-1])
zi = array([0, 1.0])
def fib3a(N):
    y, zf = lfilter(b, a,
                    zeros(N,dtype=float),zi=zi)
    return y
```

Using Formula

```
from numpy import roots, arange
r1, r2 = roots([1,-1,-1])
C = 1.0/(r1-r2)
def fib2a(N):
    n = arange(N,dtype=float)
    return C*(r1**n - r2**n)
```

Array-oriented approaches



NumPy: an Array-Oriented Extension

- Data: the array object
  - slicing and shaping
  - data-type map to Bytes

- Fast Math:
  - vectorization
  - broadcasting
  - aggregations

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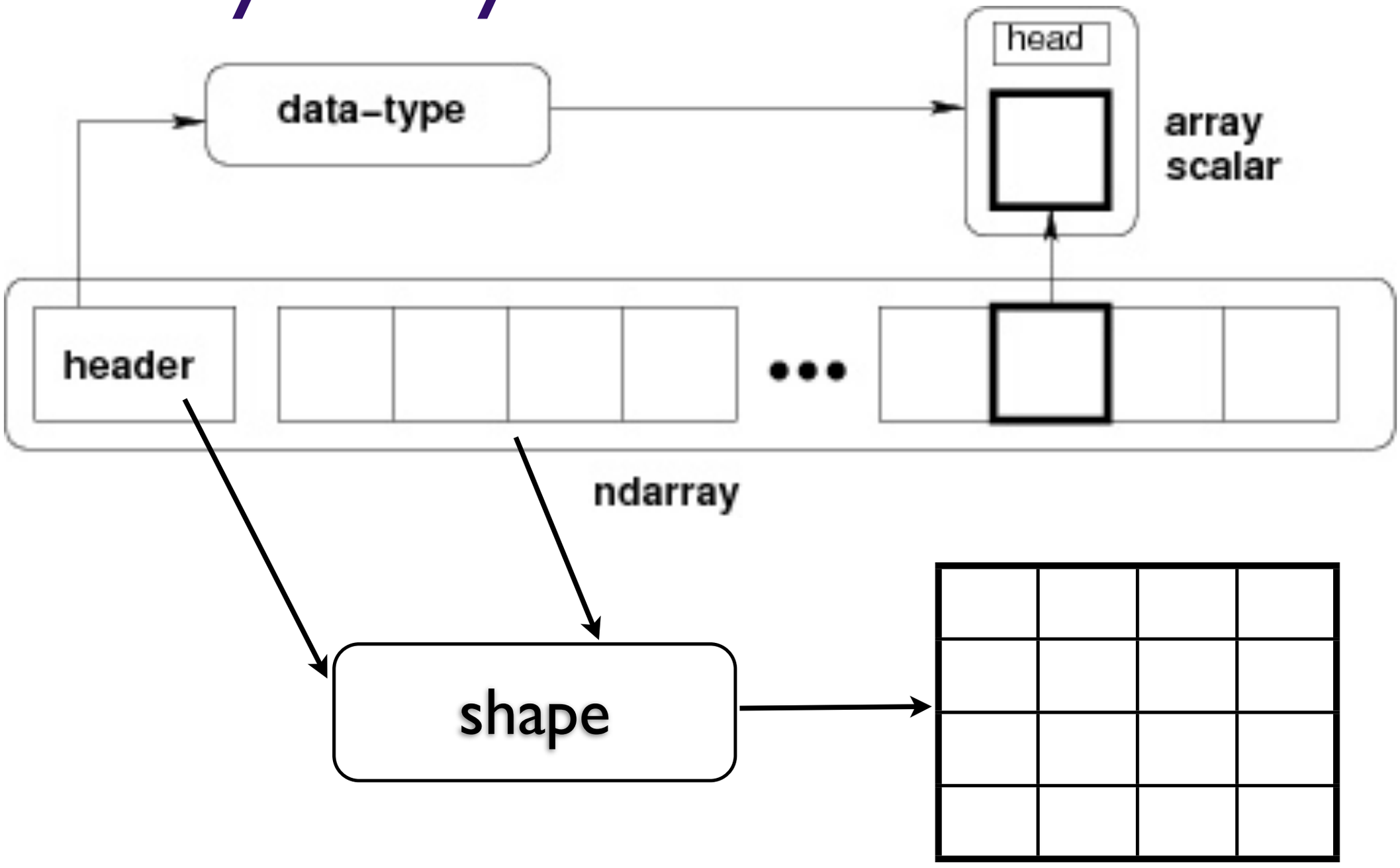
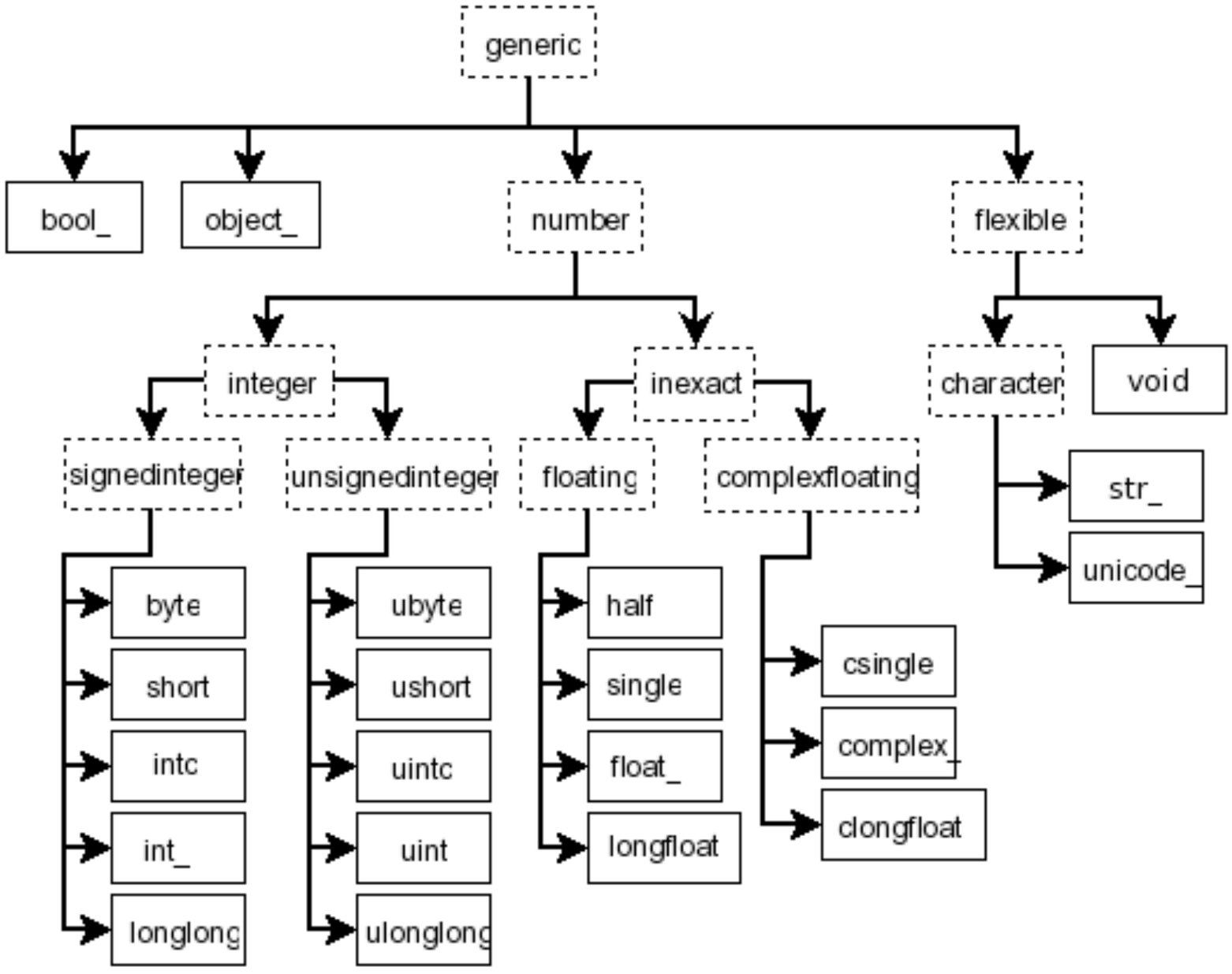
NumPy Array

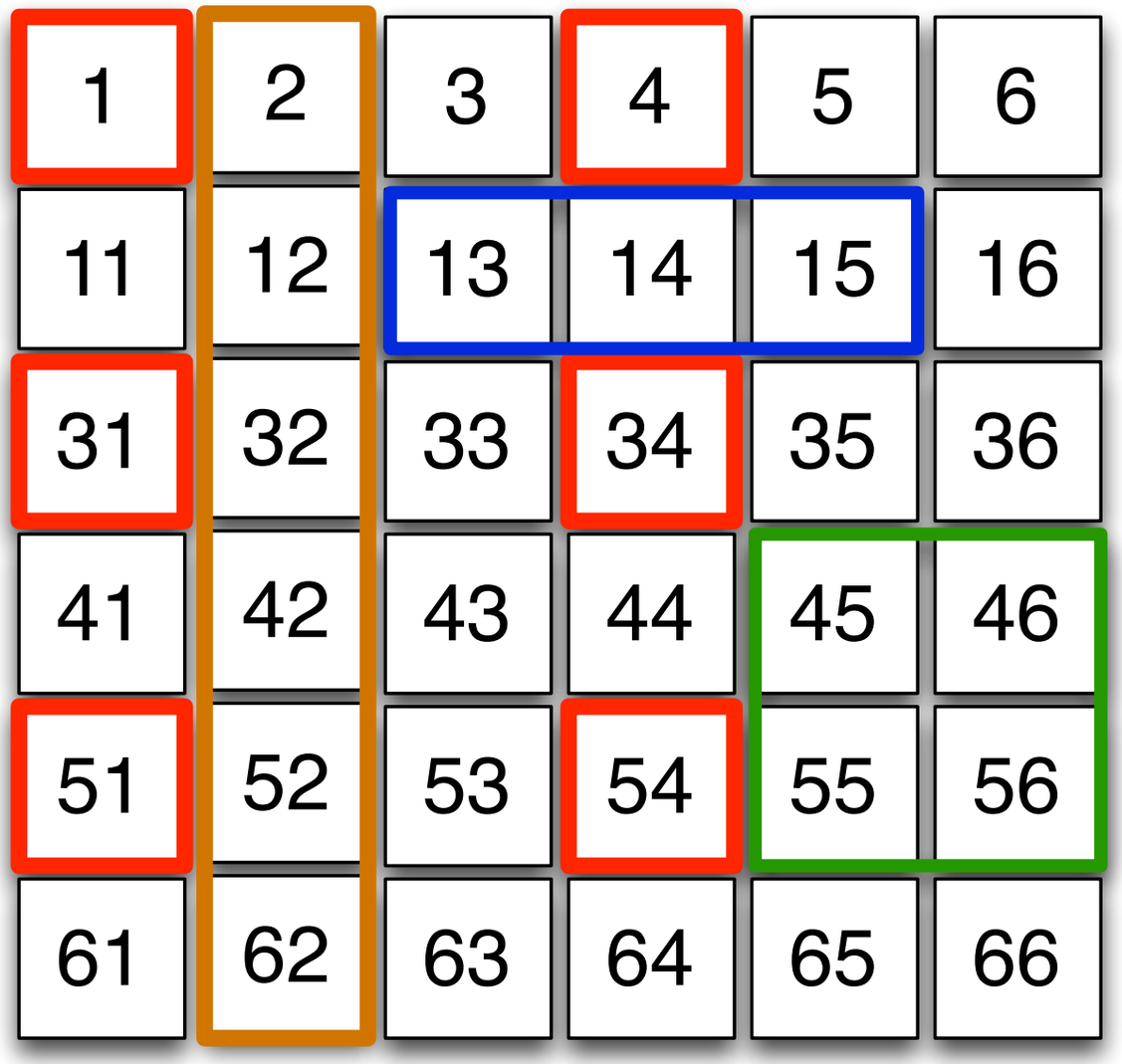


Broad Type Support



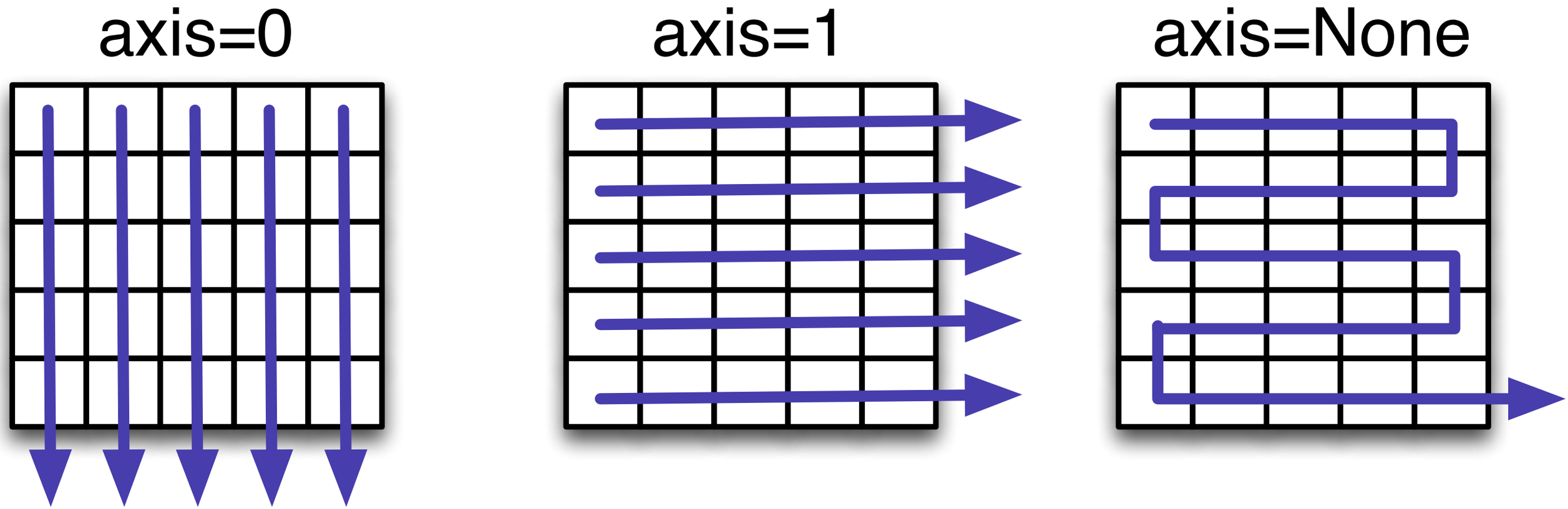
NumPy Slicing

```
>>> a[:,1]

>>> a[::2,::3]

>>> a[1,2:5]

>>> a[3:5,4:6]
```



NumPy axis argument (e.g. reduction)

```
a = rand(10,10)
a.std(axis=0)   --- reduce along 0th dimension
a.std(axis=1)   --- reduce along 1st dimension
a.std()         --- reduce along all dimensions
```



Broadcasting

```
>>> x
array([10, 20])
>>> x.shape
(2,)
```

```
>>> x[np.newaxis,:]
array([[10, 20]])
>>> x[np.newaxis,:].shape
(1, 2)
```

```
>>> y
array([[1],
       [2],
       [3]])
>>> y.shape
(3, 1)
```


```
>>> x+y
array([[11, 21],
       [12, 22],
       [13, 23]])
>>> (x+y).shape
(3, 2)
```

Zen of NumPy

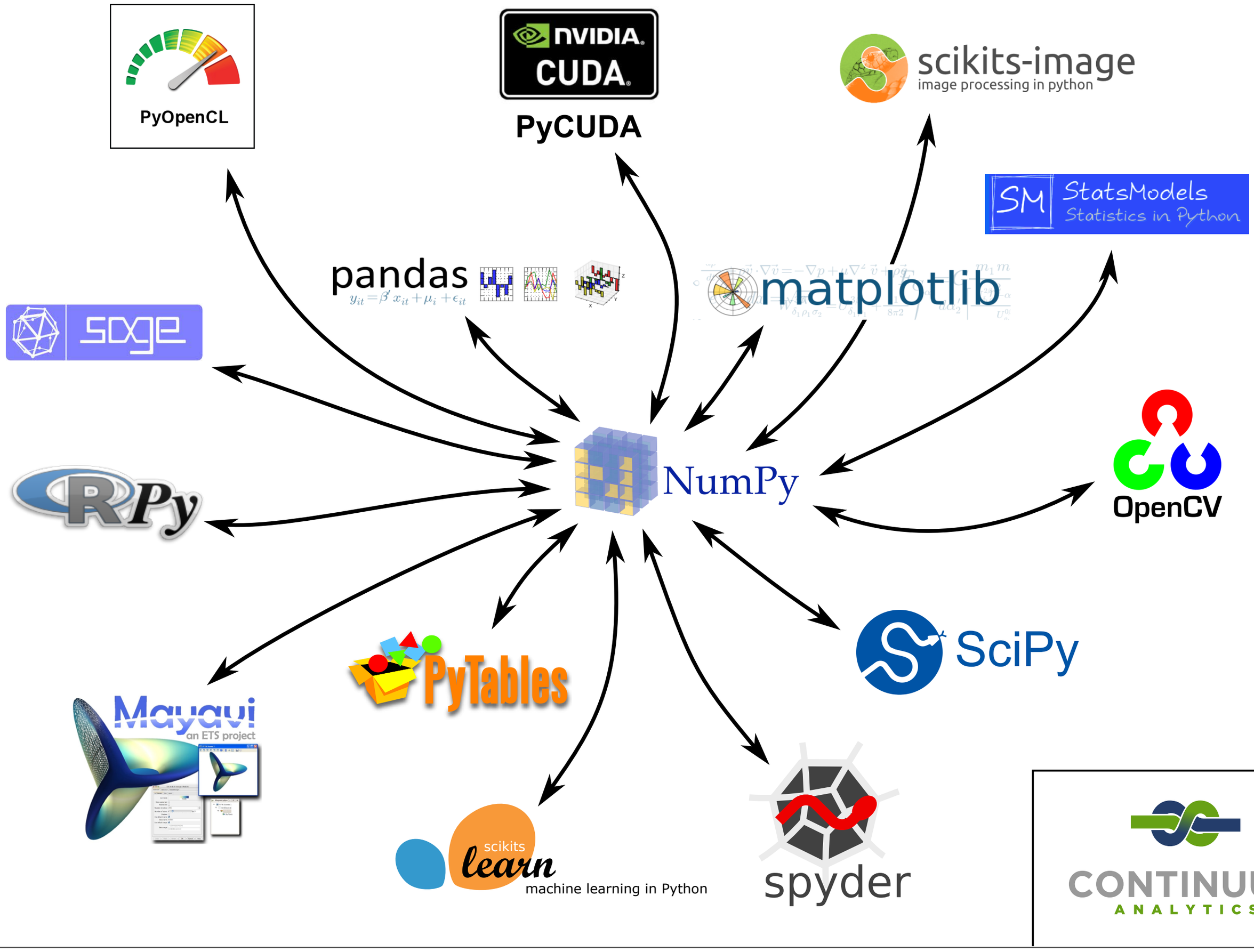
- strided is better than scattered
- contiguous is better than strided
- descriptive is better than imperative
- array-oriented is better than object-oriented
- broadcasting is a great idea
- vectorized is better than an explicit loop
- unless it’s too complicated --- then use Numba
- think in higher dimensions

Benefits of Array-oriented

- Many technical problems are naturally array-oriented (easy to vectorize)
- Algorithms can be expressed at a high-level
- These algorithms can be parallelized more simply (quite often much information is lost in the translation to typical "compiled" languages)
- Array-oriented algorithms map to modern hard-ware caches and pipelines.

What is good about NumPy?

- Array-oriented: slicing and broadcasting
- Extensive Dtype System (including structures)
- C-API
- Simple to understand data-structure
- Memory mapping
- Syntax support from Python
- Large community of users and packages that build on it
- Easy to interface C/C++/Fortran code


PyOpenCL
NVIDIA
CUDA
PyCUDA
scikits-image
image processing in python
StatsModels
Statistics in Python
pandas
matplotlib
sage
NumPy
OpenCV
RPy
PyTables
SciPy
Mayavi
an ETS project
scikits
learn
machine learning in Python
spyder
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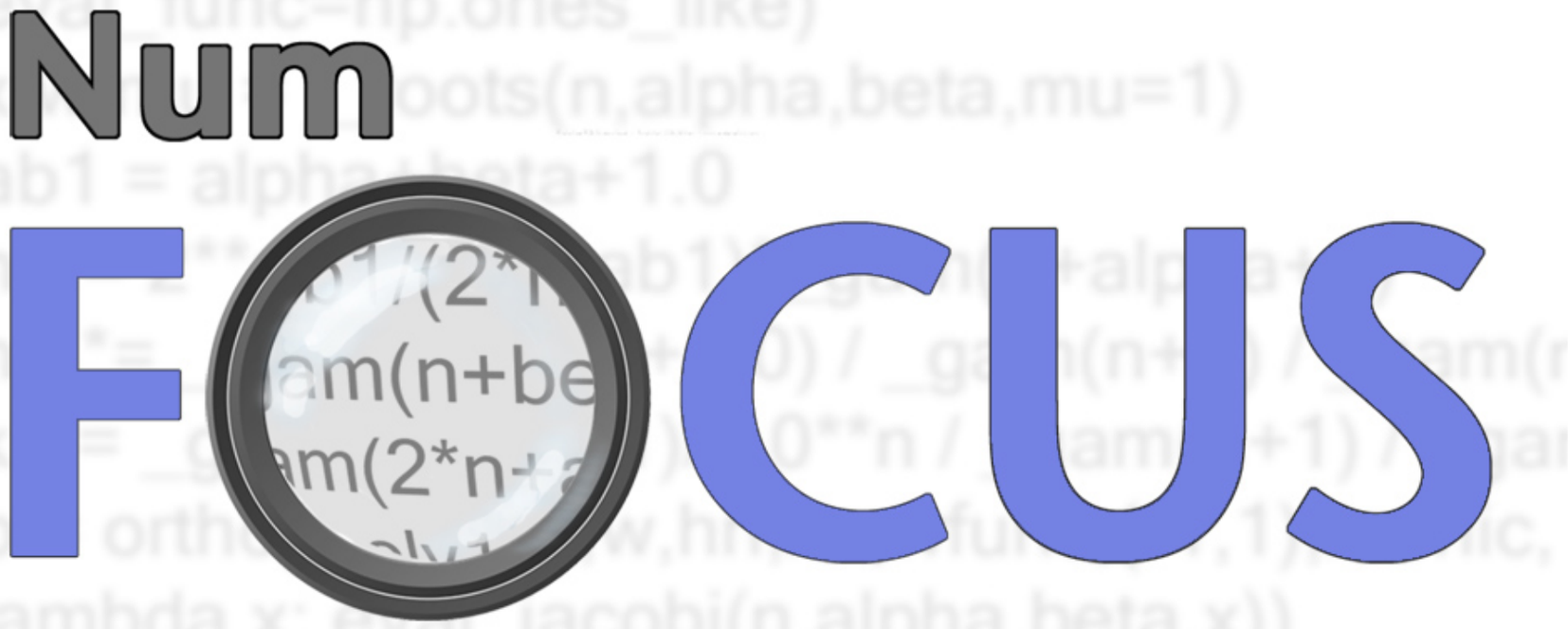
www.numfocus.org

501(c)3 Public Charity



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NumFOCUS

Num FOCUS

Core Projects

NumPy

SciPy

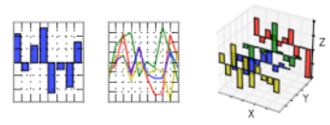
IP[y]:

IPython

Matplotlib

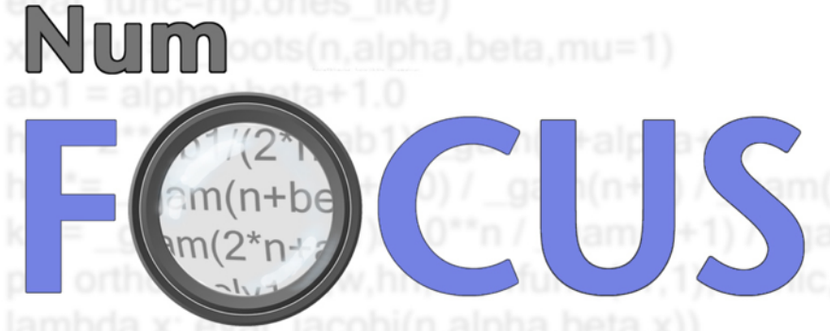
pandas

$y_{it} = \beta' x_{it} + \mu_i + \epsilon_{it}$



Scikits Image

NumFOCUS Mission



- Sponsor development of high-level languages and libraries for science
- Foster teaching of array-oriented and higher-order computational approaches and applied computational science
- Promote the use of open code in science and encourage reproducible and accessible research

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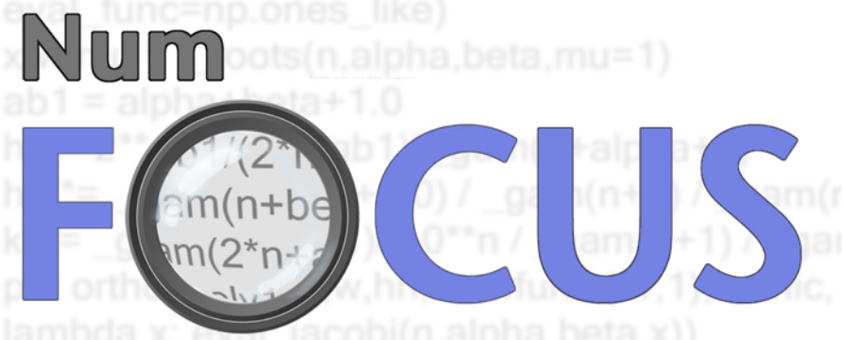
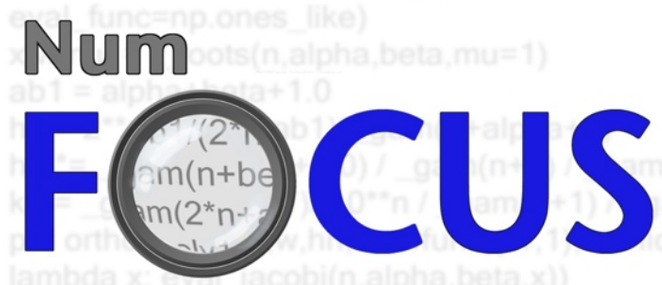
NumFOCUS Activities



- Sponsor sprints and conferences
- Provide scholarships and grants
- Provide bounties and prizes for code development
- Pay for freely-available documentation and basic course development
- Equipment grants
- Sponsor BootCamps
- Raise funds from industries using open source high-level languages

NumFOCUS



- Directors
  - Perry Greenfield
  - Jarrod Millman
  - Travis Oliphant
  - Fernando Perez
  - Andy Terrel
  - Didrik Pinte
  - Rolf Gommers
  - Emanuelle Gouillart

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