“*Quantitative* Naturwissenschaften”
→ Python

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Computerphysik

182bA2.4

20101201 VORLESUNG

Computergestützte Methoden der exakten Naturwissenschaften (Petra Imhof)

Zeit: Di 12:00-14:00, Do 12:00-14:00 (Erster Termin: 17.10.2017)

Ort: Di 1.3.14 Hörsaal A (Arnimallee 14), Do 1.3.14 Hörsaal A (Arnimallee 14)

Ich zeige Euch heute “was ihr eigentlich noch nicht wissen dürft”
(Zitat Ende – frei adaptiert ...)

```
You don't learn programming by learning a programming language.

Languages are tools that allow you to do something you've already
learned - situational analysis, also known as programming.

(Programming isn't typing things into a computer, it's thinking.)
```

Al Klein, 45 years of earning a living developing systems.

Was ist ein Computer ? Was ist ein Compiler ? Was ist “high-level”-Programmierung ?

1. von Neumann Architektur
   a. Eine CPU
   b. Ein Speicher
   c. Ein “Bus”

2. Interpreter vs Compiler
    a. JIT
3. Objekt-Orientiert

https://docs.python.org/3/tutorial

Python ist eine “schöne” Programmiersprache
- keine extra Zeichen … { } ; $
- Dynamische (aber strenge) Typisierung

Python ist strukturiert:
- Module
- Funktionen
- Objekte
    - Methoden

Python ist flexibel
- Einfache Programme: einfach ein paar Kommandos aneinanderreihen....
- Funktionen um Kommandos zu “gruppieren”
- Module um Funktionen zu “gruppieren”
- Objekte um “Daten und Algorithmen” zu kombinieren.
- .
- List-Comprehensions sind sehr praktisch: [x**2 for x in range(10) if x%2 ==0]

Python ist ready-to-go …
- Module für Web, Math, Linear-Alg., GUI, …

Python 1994
Numpy 2005 Numeric 1998? Numarray 2001?
SciPy 2001
AstroPy
Priithon Meins… http://msg.ucsf.edu/sedat/Priithon/PriithonHandbook.html
PyTables
SymPy
http://www.sympy.org/en/index.html
Gamma !
http://www.sympygamma.com/input/?i=integrate%28log%28x%29%2C+%28x%2C+1%2C+a%29%29

5**5**5

There are a few guidelines one has to realize when using Python:

1. A **"variable" is really "just a name"** for something !!
   Every assignment to a variable, like a=5 or a=F.fft(a) throws the old meaning (value) of **a** away and **reassigns a** to whatever is the result of what's on the rights side of = -sign.
   But note: a[:] = F.fft(a) is *NOT* an assignment: there is more than **"just the variable name"** left of the =-sign.
   In other words: is a was a big array, a[:]= 2 would overwrite a's values (each 'pixel' would be set to 2, whereas a=2 would destroy that array and a would from then on refer to the number 2.
2. **Indentation** matters: This must be the strangest "feature" of python:
   - Instead of using curly brackets (like in C/C++/Java)
   - or BEGIN/END (like in PASCAL)
   - or do/done (still others) Python infers the "bracketing" from the way a code-section is indented.
   - This feature seems very strange at first - but it is supposed to make everyone's code look more alike;
     Decide if you want to use tabs or spaces to indent; there are *pros* and *cons* for each choice -- but **stick** with it and don't mix!!
3. Everything is **case-sensitive**
4. Every variable lives inside its **modules**
5. **Importing** a module makes its variables visible - **all code** inside the module's defining file gets **execute**d only the first time it gets imported (by anything - since python started)

Nochmal…

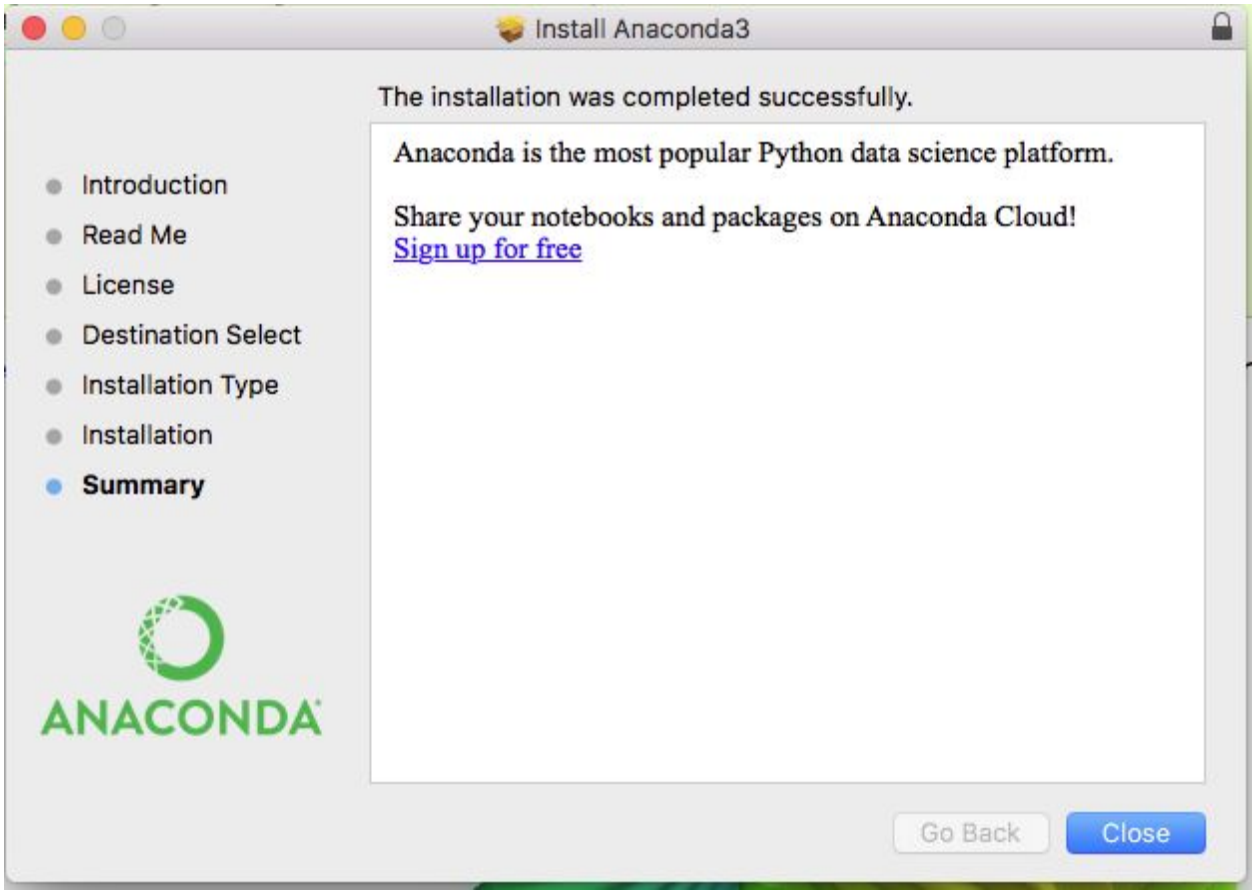
range(5) fängt bei 0 an hört VOR 5 auf also [0,1,2,3,4]
range(0, 5, 2) ? [0, 2, 4]
Argumente können auch als Keyword-Argument übergeben werden …. Macht Code oft lesbarer !!

N.arange(5, step=.5)
array([0. , 0.5, 1. , 1.5, 2. , 2.5, 3. , 3.5, 4. , 4.5])

(Ausnahme: built-in range(10,step=2) → TypeError: range() takes no keyword arguments)

List-Comprehensions sind sehr praktisch: [x**2 for x in range(10 if x%2 ==0]

Praktisches print – bzw. praktische Strings:
"-" * 80
print(3,4,5, sep=' - ') # übrigens ' ist identisch zu " und """ und ''' sind gut für mehrzeilige Strings


Install Anaconda3
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Installation
Summary
Anaconda is the most popular Python data science platform.
Share your notebooks and packages on Anaconda Cloud!
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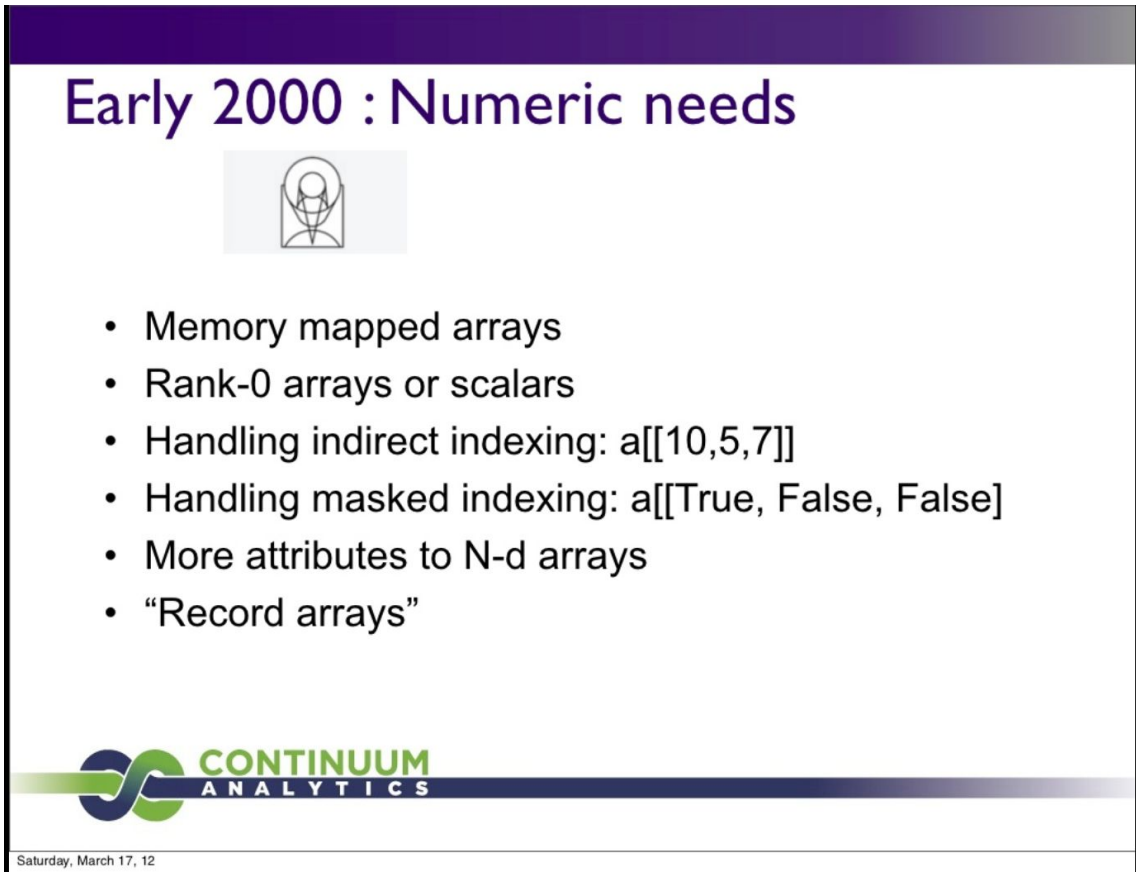
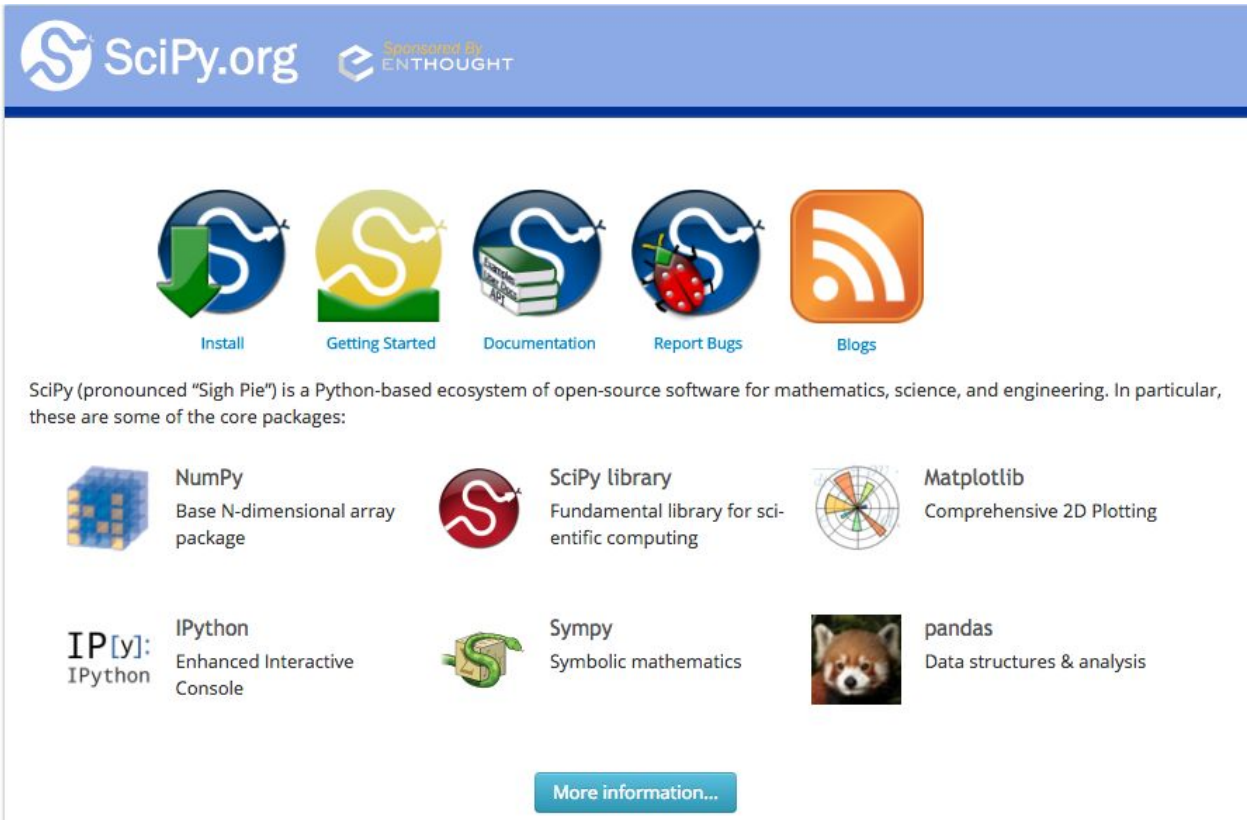


Travis E. Oliphant, "NumPy and SciPy: History and Ideas for the Future"
https://www.slideshare.net/shoheihido/sci-pyhistory

NumPy and SciPy for Data Mining and Data Analysis Including iPython, SciKits, and matplotlib
https://www.slideshare.net/bytemining/numpy-and-scipy-for-data-mining-and-data-analysis-including-ipython-scikits-and-matplotlib

https://www.scipy.org/



http://scipy-cookbook.readthedocs.io/

https://www.dataquest.io/blog/numpy-tutorial-python/

https://jakevdp.github.io/PythonDataScienceHandbook/02.07-fancy-indexing.html

Und nochmal…

Python Assignment != memory-copy / CPU-work
b   = a   # no work !   same object !
b[:] = a # work !

Numpy:
Zeilen-Vektoren   Spalten-Vektoren

Broadcasting ….
a=np.arange(5)
a[[0,0,1,0,1] = 99

%timeit   numpy ….

Jupyter

https://blog.dominodatalab.com/lesser-known-ways-of-using-notebooks/

z.B.

```
%%latex
\begin{align}
\nabla \cdot \vec{\mathbf{E}} & = 4 \pi \rho \\
\nabla \times \vec{\mathbf{E}}\, +\, \frac1c\,
\frac{\partial\vec{\mathbf{B}}}{\partial t} & = \vec{\mathbf{0}} \\
\nabla \cdot \vec{\mathbf{B}} & = 0
\end{align}
```

In [31]:
```
%%latex
\begin{align}
\nabla \cdot \vec{\mathbf{E}} & = 4 \pi \rho \\
\nabla \times \vec{\mathbf{E}}\, +\, \frac1c\, \frac{\partial\vec{\mathbf{B}}}{\partial t} & = \vec{\mathbf{0}} \\
\nabla \cdot \vec{\mathbf{B}} & = 0
\end{align}
```

$$\nabla \cdot \vec{\mathbf{E}} = 4\pi\rho$$

$$\nabla \times \vec{\mathbf{E}} + \frac{1}{c}\frac{\partial \vec{\mathbf{B}}}{\partial t} = \vec{\mathbf{0}}$$

$$\nabla \cdot \vec{\mathbf{B}} = 0$$

https://www.python-course.eu/numpy.php

Swap rows: a[2], a[1] = a[1], a[2].copy() # .copy() weil zwischendurch überschrieben!!

https://stackoverflow.com/questions/14933577/swap-slices-of-numpy-arrays/14933939#14933939

http://jakevdp.github.io/blog/2013/06/15/numba-vs-cython-take-2/

https://stackoverflow.com/questions/36661876/what-is-the-difference-between-importing-matplotlib-and-matplotlib-pyplot

https://github.com/matplotlib/matplotlib/blob/master/lib/matplotlib/__init__.py

Mayavi

A demo

To get you started, here is a pretty example showing a spherical harmonic as a surface:

```
# Create the data.
from numpy import pi, sin, cos, mgrid
dphi, dtheta = pi/250.0, pi/250.0
[phi,theta] = mgrid[0:pi+dphi*1.5:dphi,0:2*pi+dtheta*1.5:dtheta]
m0 = 4; m1 = 3; m2 = 2; m3 = 3; m4 = 6; m5 = 2; m6 = 6; m7 = 4;
r = sin(m0*phi)**m1 + cos(m2*phi)**m3 + sin(m4*theta)**m5 + cos(m6*theta)**m7
x = r*sin(phi)*cos(theta)
y = r*cos(phi)
z = r*sin(phi)*sin(theta)

# View it.
from mayavi import mlab
s = mlab.mesh(x, y, z)
mlab.show()
```

Bulk of the code in the above example is to create the data. One line suffices to visualize it. This produces the following visualization: