Computerphysik II

Python Einführung

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Universität
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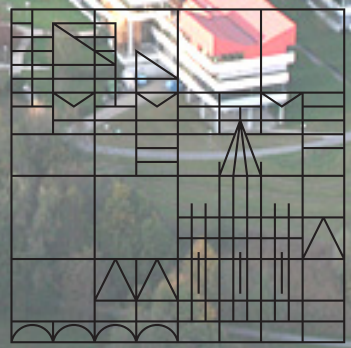
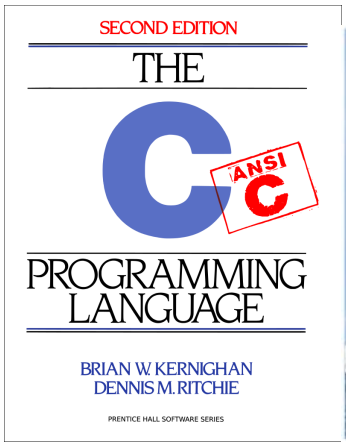
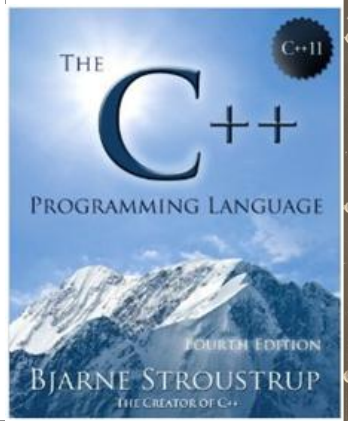
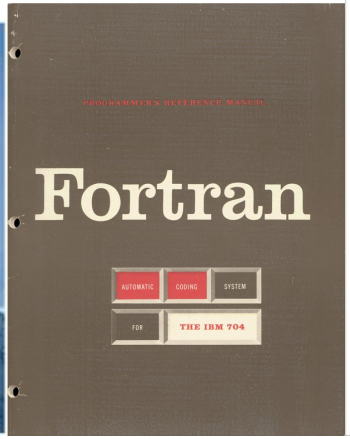


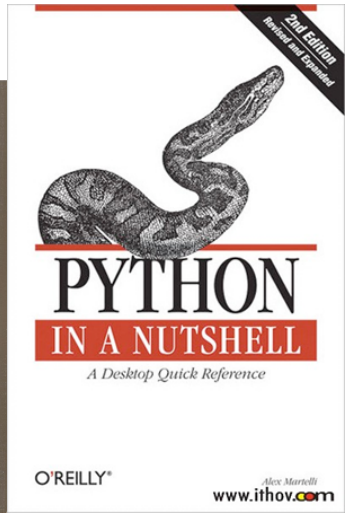
Programmiersprachen

In der Wissenschaft:

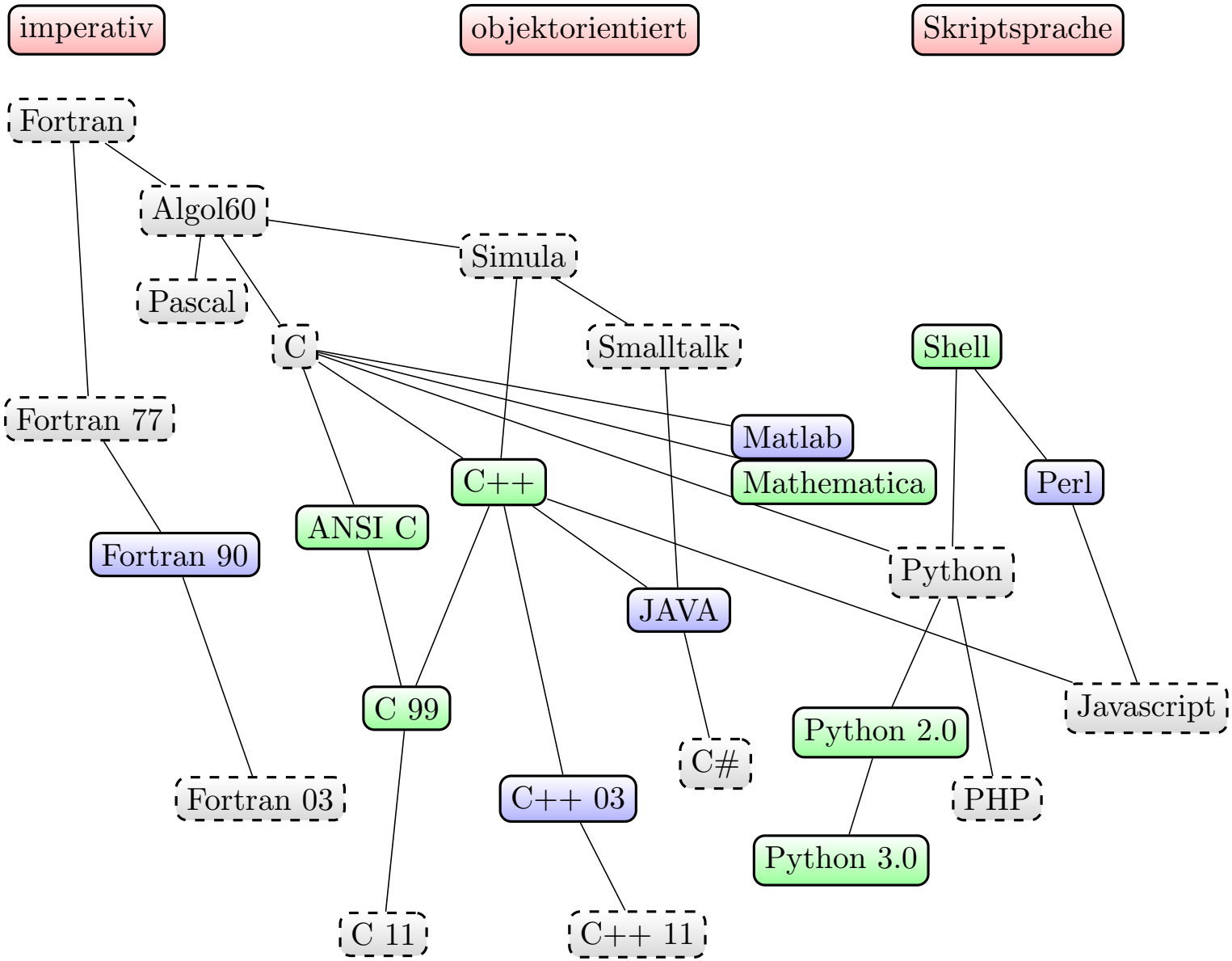








Programmiersprachen in der Wissenschaft



Programmiersprachen - Einteilung

Eigenschaften:

- **Skriptsprachen**: Shell, Python, Perl, ...
- **Kompilierte Sprachen**: C/C++, Fortran, Pascal, ...
- **Objektorientiert**: C++, Java, ...
- **Anwendungssprachen**: R, Mathematica, Matlab, ...

Anwendungen:

- **Skripte, Automatisierung**: Shell, Python, Make, ...
- **Datenauswertung & Tests**: C/C++, Python, Matlab, ...
- **Analytische Rechnungen**: Mathematica, Maple, SAGE, Python (SymPy), ...
- **HPC + Scientific Computing**: C/C++, Fortran, Python (NumPy, Scipy), ...
- **Grafische Darstellung**: gnuplot, Python (matplotlib), Mathematica, ...

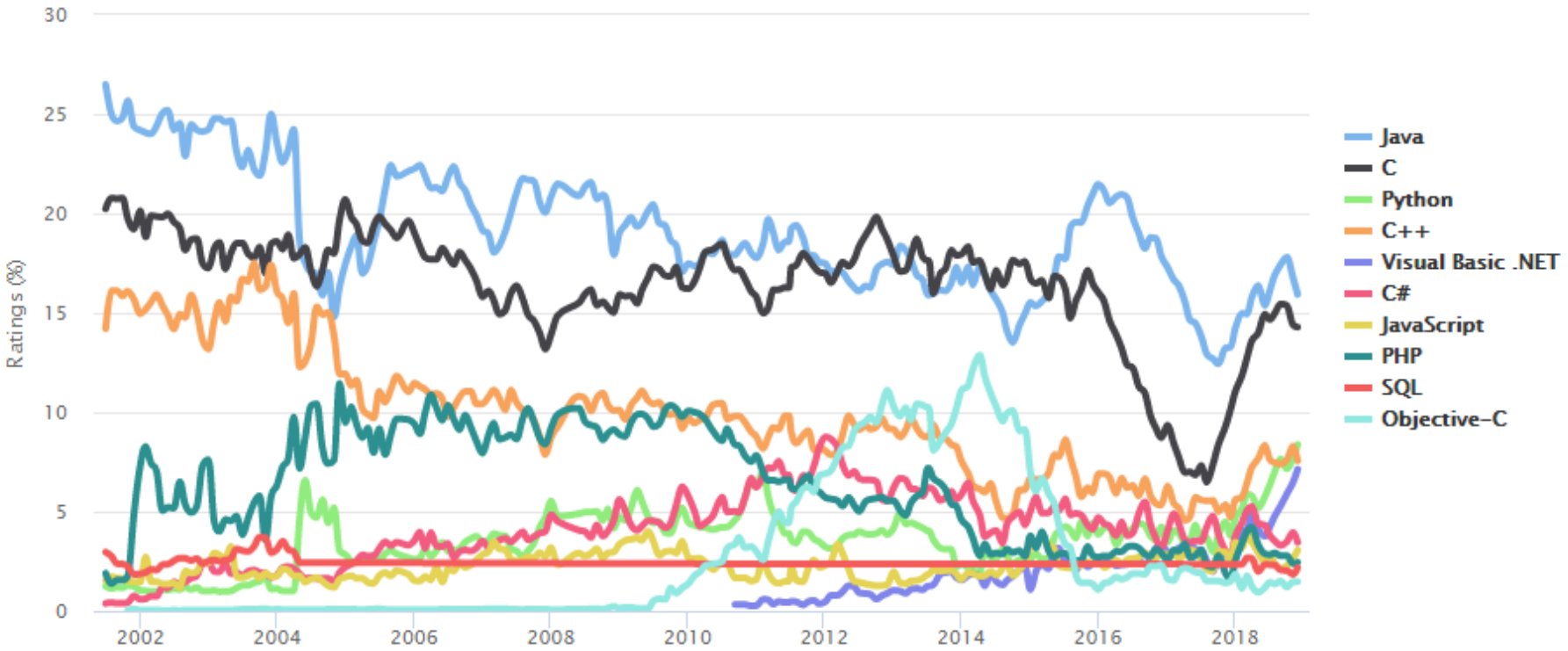
Programmiersprachen - Verbreitung (TIOBE)

Very Long Term History

To see the bigger picture, please find the positions of the top 10 programming languages of many years back. Please note that these are *average* positions for a period of 12 months.

Programming Language	2015	2010	2005	2000	1995	1990	1985
C	1	2	1	1	2	1	1
Java	2	1	2	3	-	-	-
Objective-C	3	23	39	-	-	-	-
C++	4	3	3	2	1	2	12
C#	5	5	8	8	-	-	-
PHP	6	4	4	30	-	-	-
Python	7	6	6	24	22	-	-
JavaScript	8	8	9	7	-	-	-
Perl	9	7	5	4	9	19	-
Visual Basic .NET	10	-	-	-	-	-	-
Pascal	16	13	77	12	3	20	5
Lisp	18	16	12	15	5	3	2
Ada	30	26	15	16	6	4	3

Programmiersprachen - Verbreitung (TIOBE)



Programmiersprache Python

- Hohe **Verbreitung** (gut bekannt, viele Bibliotheken)
- Freie Software
- interaktive Skriptsprache
- **performant** durch Verwendung von optimierten Bibliotheken bzw. Anbindung an C
- Einfach & flexibel (wenige Sprachfeatures, viele Bibliotheken)

aktuell: Python 2.7.17 (bis Ende 2019 gepflegt), Python 3.8.0

`https://en.wikibooks.org/wiki/Python_Programming`
`http://www.scipy-lectures.org/_downloads/ScipyLectures-simple.pdf`

Verwendung - interaktiv

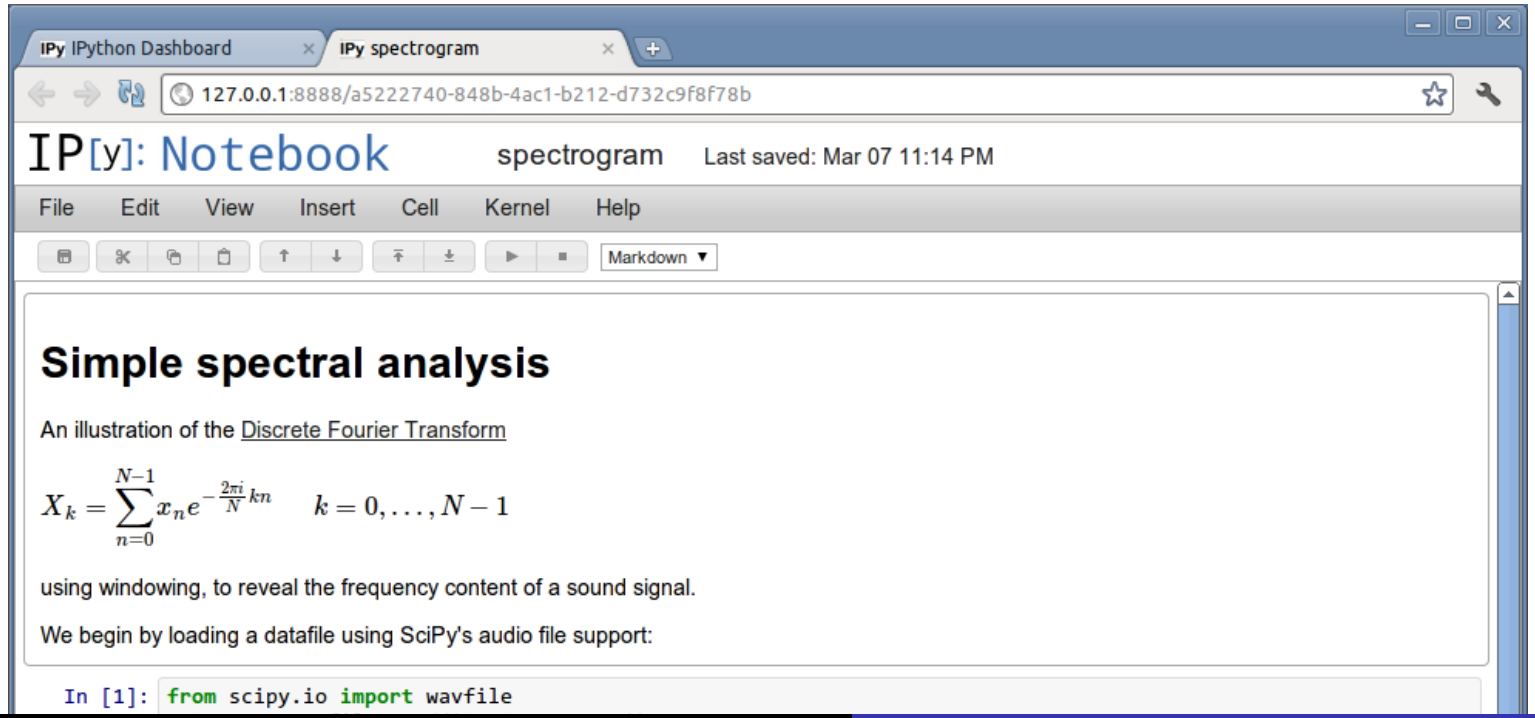
- **Terminal**: `python`, `python3`

  ```
  >>> 1+1
  ```

- **IPython** - opt. Terminal: `ipython3`, `ipython3 qtconsole`

  ```
  In[1]: %hist
  In[2]: hist?
  In[2]: help(abs)
  ```

- **Im Browser** - IPython-Notebook: `ipython3 notebook`



"Hello, World" in Python

A) Interaktiv:

```
>>> print('Hello, World!')
Hello, World!
```

B) Python-Skript:

```
1 print('Hello, World!')
```

```
$ python3 skript.py
```

C) Shell-Skript:

```
1 #!/usr/bin/env python3
2
3 # Kommentar
4 print('Hello, World!')
```

```
$ chmod +x skript.py
$ ./skript.py
Hello, World!
```

Datentypen in Python

- **Integer** (ganzzahlig): `int`

  `>>> 1+2`

```
1 >>> 3/2
2 1.5 (Python 2)
3 1.5 (Python 3)
```

- **Fließkommazahl**: `float`

  `1.5, 2.`

- **Komplexe Zahl**: `complex`

  `1.5+0.4j`

- **Boolean**: `bool`

  `False, True`

Variablen in Python

```
1 a = 4
2 b = 7.
3 c = 1.+2.j
4 d = True
```

→ Datentyp wird automatisch zugewiesen. Keine Deklaration nötig!

```
1 a,b = 1,2
2 a = b = 2.
3 a +=1; a -= 1; a *= 2; a /= 2
4 a,b = b,a
```

Variablenausgabe

```
1 print(a)
2
3 print(a, b)
4
5 print('Ergebnis:', a)
6
7 print('%e' % a)
8 # e - Exponent, f - Floating, g - Automatic
9 # (wie in C)
```

Container

Listen: Sammlung verschiedener Typen

```
1 a = [42, 1+2j, 'blau']
2
3 # Index beginnt bei 0 (wie C)
4 >>> a[0]
5 42
6 >>> a[-1]
7 'blau'
8 >>> a[1:]
9 [1+2j, 'blau']
```

Slicing: `a[start:stop:step]` (*start* <= *i* < *stop*)

`len(a)`

Achtung: `b=a` (gleiches Objekt!), `a[:]=3,4,5` (in place)

Container

String: unveränderbare Liste
Tuples: unveränderbare Listen `a = (1,2,3)`
Mengen: ungeordnete, unique Listen `a = set('a','b','c')`
Wörterbuch: Key-Value-Liste

```
1 tel = {'Stefan':3825, 'Hans': 3815}
2 tel.keys()
3 tel.values()
```

Kontrollstrukturen

if: Vergleich (==, !=, <, <=, > , >=)
(Einrückung!)

```
1  if i < 0:
2      i = 0
3  elif i == 0:
4      i = 1
5  else:
6      print(i)
```

Varianten:

```
1  if 0 < x <= 1:
2      ...
3  if e in a:
4      ...
```

Kontrollstrukturen

for: Schleife mit fester Anzahl an Durchläufen

```
1 for e in a:
2     print(e)
```

(Einrückung!)

```
1 for e in range(10):
2     print(e)
3
4 # range(10) : [0,..,9]
5 # range(6,15,3) : [6,9,12]
```

```
1 for index, item in enumerate(a):
2     print(index, item)
```

Kontrollstrukturen

Funktionale Programmierung:

```
1 zahlen = [1, 2, 3, 4, 5]
2 quadrate = [n**2 for n in zahlen]
3 print(quadrate)
```

while: Schleife mit unbekannter Anzahl an Durchläufen

```
1 b = 0
2 while b < 10:
3     print(b)
4     b += 2
```

Funktionen

```
1 def q(x):
2     return x**2
3
4 # q(2) : 4
5 # default parameter: f(a, b=0)
```

Funktionale Programmierung:

```
1 a = range(10)
2
3 map(q, a)
4 # [0,1,4,9,...,81]
```

Standardbibliotheken

verschiedene Möglichkeiten:

```
1 import bib
2 import bib as alias
3 from bib import *    # schlecht
4 from bib import function
```

Beispiele:

```
1 import numpy
2 numpy.array([1,2,3])
```

```
1 import numpy as np
2 np.array([1,2,3])
```

```
1 from numpy import array
2 array([1,2,3])
```

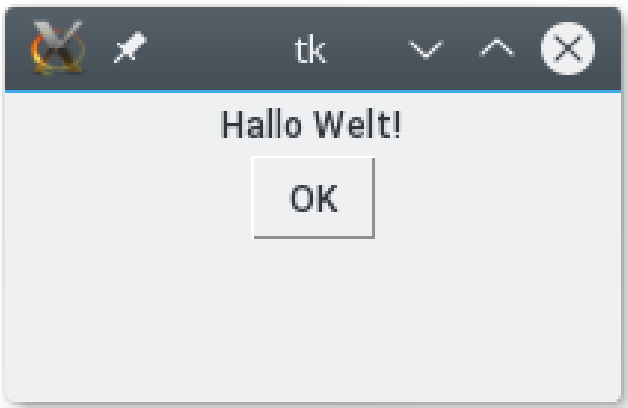
Standardbibliotheken

- **sys**: argv, version, path, ..
- **os**: getcwd(), listdir(), mkdir(), remove(), ..
- **math**: sin(), cos(), log(), exp(), pi, e, ..
- **cmath**: für komplexe Zahlen
- **random**: Zufallszahlen
- **tkinter**: Tk (GUI)
- **numpy**: NumPy (Numerische Methoden)
- **scipy**: SciPy (wissenschaftliche Anwendungen)
- **sympy**: SymPy (symbolisches Rechnen)
- **matplotlib**: Matplotlib (grafische Darstellung)

```
1 In [1]: import math
2 In [2]: help(math)
3 In [3]: print(dir(math))
```

Standardbibliotheken - GUI

```
1  from tkinter import *
2  fenster = Tk()
3  fenster.geometry("200x100")
4  label = Label(fenster, text="Hallo Welt!")
5  label.pack()
6  def befehl():
7      fenster.destroy()
8  button = Button(fenster, text="OK", command=befehl)
9  button.pack()
10 fenster.mainloop()
```



NumPy - NumPy-Arrays

NumPy-Arrays: optimiert für Zahlen (int/float)

```
1  from numpy import array
2  v = array([1,2,3,4])
3  M = array([[1.,2.],[3.,4.]])
4
5  v.shape      # (4,1)
6  M.shape      # (2,2)
7  v.size       # 4
8  M.size       # 4
9  v.dtyp       # int64
10 M.dtype      # float64
11
12 v.reshape(2,2)     # array([[1, 2], [3, 4]])
13 v = array([1,2,3,4], dtype=complex)
```

NumPy - Listen

```
1 from numpy import arange, linspace, diag
2
3 arange(0,1,0.1)      # [0,0.1,...,0.9]
4
5 linspace(0,1,6)      # [0,0.2,0.4,0.6,0.8,1.0]
6
7 diag([1,2])          # [[1,0],[0,2]]
```

```
1 from numpy import sin, cos
2
3 v=array([1,2,3])
4 sin(v)     # [ 0.84147098,  0.90929743,  0.14112001]
5 cos(v)     # ...
6
7 v+1, v*v, 2*x     # elementweise
```

NumPy - Matrix, etc.

```
1 from numpy import dot, matrix
2
3 dot(M, v)          # M.v
4 x=matrix(v).T      # transpose
5 x.T*x              # Skalarprodukt
6 dot(M, M)          # Matrixprodukt
```

- Mathematische Funktionen
- Statistik
- **numpy.polynomial**: Polynome
- **numpy.linalg**: Lineare Algebra
- **numpy.fft**: Fourier-Transformation
- **numpy.random**: Zufallszahlen/-verteilungen
- ...

SciPy - wissenschaftl. Funktionen

- **scipy.constants**: (physik.) Konstanten
- **scipy.special**: Spezielle Funktionen
- **scipy.stats**: Statistik
- **scipy.optimize**: Optimierung
- **scipy.interpolate**: Interpolation
- **scipy.linalg**: Lineare Algebra
- **scipy.integrate**: Numerische Integration
- **scipy.fft**: Fourier-Transformation
- **scipy.signal**: Signalanalyse
- ...

```
1 from scipy.special import binom, j0
2
3 print(binom(4,2))          # 6
4 print(j0(1))               # 0.765..
```

Matplotlib - Darstellung

Im Skript:

```
1 # in "python3":
2 #import matplotlib as mpl
3 #mpl.use("Qt4Agg")
4 import pylab as pl
5
6 x = pl.arange(0,7,0.01)
7 pl.plot(x,x**2)
8 pl.show()
```

Im Notebook:

```
$ ipython3 notebook
In[1]: %pylab inline
In[2]: x=arange(0,10)
In[3]: plot(x**2)
```

Matplotlib - Darstellung

```
1 xlabel("x-Achse")
2 title("$\sin \pi x$")
3 xlim(0,5)
4 plot(x,y,'--r')
```

Legende:

```
1 plot(x,y1,label="sin")
2 plot(x,y2,label="cos")
3 legend(loc='best')
```

SymPy - Symbolisches Rechnen

```
1 import sympy as sp
2
3 e = sp.sqrt(8)      # 2*sqrt(2)
4 e.evalf()          # 2.1828...
5 e.evalf(50)        # 50 Stellen
6 x,y = sp.symbols('x y')
7 e = x**2-2*y
8 e + x**2           # 2*x**2 - 2*y
9 e.subs(x, 1.5)     # Einsetzen
```

```
1 >>> sp.init_printing()    # nette Ausgabe
2       ___
3 2*\/ 2
4 >>> sp.latex(sp.sqrt(x**2))
5 2 \\sqrt{2}
```

SymPy - Algebra

- **expand**`((x+1)**2)`
  `x**2 + 2*x + 1`
- **factor**`(x**3 - x**2 + x - 1)`
  `(x-1)(x**2+1)`
- **collect**`(x*y + x*x + x, x)`
  `x**2 + x(y+1)`
- **cancel**`((x**2+2*x+1)/(x**2+x))`
  `(x+1)/x`
- **apart**`((x**2+2*x)/(x+1))`
  `x+1 - 1/(x+1)`
- **trigsimp**`((sin(x))**2 + (cos(x))**2)`
  `1`
- **expand_trig**`(sin(x+y))`
  `sin(x)*cos(y) + sin(y)*cos(x)`

SymPy - Calculus

- **limit**(sin(x)/x, x, 0)

  1
- **series**(sp.cos(x))

  1 + x**2/2 + ...
- sp.sin(x).series(x,0,10)

  x - x**3/6 + ...
- **diff**(x**2,x)

  2*x
- **solve**(x**2-2, x)

  (-sqrt(2), sqrt(2))
- **summation**(2*i+1,(i,1,n))

  n**2 + 2*n
- **integrate**(x**2,x)

  x**3/3
- **integrate**(sp.sin(x),(x,0,10)).evalf()

  1.8390715...