Scientific Computing using Python

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Guide: Jahfar Ali

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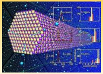


Outline

1 Introduction

2 Python

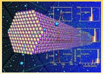
3 NumPy

4 SciPy

5 Matplotlib

6 Advantages

7 Conclusion



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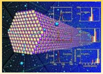

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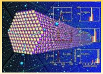

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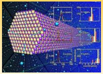

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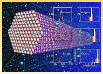

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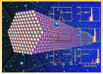

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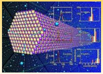
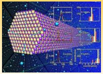
Scientific Computing

The field of study concerned with constructing mathematical models and quantitative analysis techniques and using computers to analyse and solve scientific problems.



Problem Domains

- Numerical simulations
  - Reconstruct and understand known events.
  - Predict future or unobserved situations.
- Model fitting and data analysis
  - Use graph theory to model networks, especially those connecting individuals, organizations, and websites.
- Computational optimization
  - Optimize known scenarios like technical and manufacturing processes, front-end engineering, etc.



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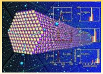

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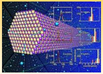
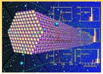


Methods and Algorithms

- Numerical analysis
- Application of Taylor series as convergent and asymptotic series
- Computing derivatives by Automatic differentiation (AD)
- Computing derivatives by finite differences
- Molecular dynamics
- Discrete Fourier transform and applications.
- etc



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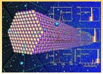

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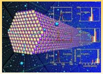

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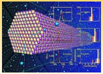

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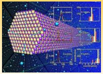

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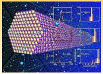

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Python

Python is an interpreted, general-purpose high-level programming language.

Features:

- Cross Platfom
- Clear Syntax
- "batteries included"
  - Has a large library
- Easy to code
- Multi Paradigm
- Useful Built-In Objects
- Functions and Classes
- Ease of Extension

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- Python supports multiple operating systems.
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Clear Syntax

```
def is_digits_even(n):
  if n < 0:
    n = -n
  while n > 0:
    if n % 2 == 1:
      return False
    n /= 10
  return True

a=input()
if is_digits_even(a):
  print "All digits are even!"
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Batteries Included

- Has a vast library.
- New libraries can be easily added.

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Easy to Code

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Useful Built-In Objects

```
>>> type(1), type(1.0), type(1.0j), type('one')
(<type 'int'>, <type 'float'>, <type 'complex'>,
<type 'str'>)
```

Functions & Classes

```
def signum( r ):
    """returns 0 if r is zero
    -1 if r is negative
    +1 if r is positive"""
    if r < 0:
        return -1
    elif r > 0:
        return 1
    else:
        return 0
```

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What is NumPy

- NumPy is a Python Module.
- Supports complex numerical calculations.
- Freely available at http://numpy.org
- It grew out of an original module called Numeric.
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- Current stable version: 1.5.1 (November 21, 2010)

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Data types

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Data types

```
>>> import numpy as N

>>> dt = N.dtype([(id, i4),
(name, S12), (scores, u1, 4)])

>>> a = N.array([(1001, James, [100,98,97,60]),
(1002, Kathy,[100,100,85,98]),
(1003, Michael,[84,75, 98,100]),
(1004, John, [84,76,82,92])], dtype=dt)
```

Data types

```
>>> a[name]
array([James, Kathy, Michael,
John], dtype=S12)

>>> a[scores]
array([[100, 98, 97, 60],
 [100, 100, 85, 98],
 [ 84, 75, 98, 100],
 [ 84, 76, 82, 92], dtype=uint8)
```

Attributes and methods

- All arrays have several attributes and methods.
- Some attributes can be set to alter the array’s characteristics.

```
>>> b = a.take(a[’name’].argsort())

>>> print b
array([(1001, ’James’, [100, 98, 97, 60]),
   (1004, ’John’, [84, 76, 82, 92]),
   (1002, ’Kathy’, [100, 100, 85, 98]),
   (1003, ’Michael’, [84, 75, 98, 100])],
   dtype=[(’id’, ’<i4’), (’name’, ’|S12’),
   (’scores’, ’|u1’, 4)])
```

Indexing

- Supports multiple kinds of indexing.

```
>>> import numpy as n

>>> a = n.random.randn(50,25)

>>> print a.shape, a[10,15]
(50, 25) 0.5295135653
```

Universal Functions

- Simple to define functions that take N inputs and return M outputs.
- Provides universal function objects (ufuncs).
- More than 50 mathematical functions are defined as universal functions.

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Universal Functions - Features

- **Broadcasting**: Specific method for arrays that don't have the same shape to try and act as if they do.
- Provides features to define output arrays explicitly.
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- **Hardware error handling**: Supports querying the result of hardware error flags.

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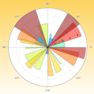

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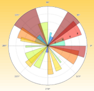

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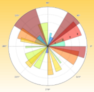

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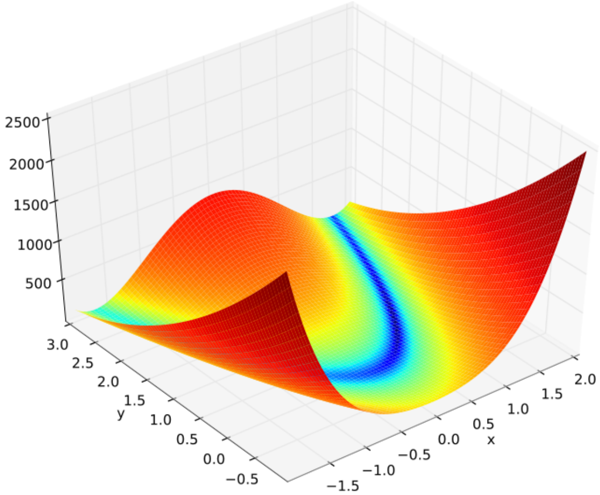
Sample Plot


2500
2000
1500
1000
500
3.0
2.5
2.0
1.5
y
1.0
0.5
0.0
−0.5
−1.5
−1.0
−0.5
0.0
0.5
x
1.0
1.5
2.0

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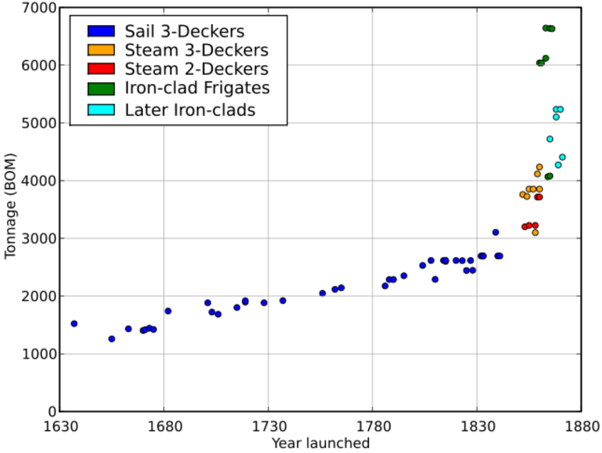
Sail 3-Deckers
Steam 3-Deckers
Steam 2-Deckers
Iron-clad Frigates
Later Iron-clads
Tonnage (BOM)
7000
6000
5000
4000
3000
2000
1000
0
1630
1680
1730
1780
1830
1880
Year launched

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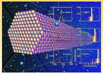

Python + NumPy + Matplotlib

- Based on Python, a full-featured modern OOP language suitable for large-scale software development.
- Suitable for fast scripting, including CGI scripts.
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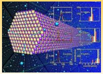

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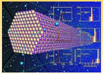

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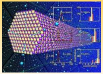
4. SciPy
5. Matplotlib
6. Advantages
7. Conclusion

Conclusion



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Thank You !

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