

# Computing 101 and SciPy

Ivan Girotto (ICTP)  
igirotto@ictp.it





John Von Neumann

# The Basic Model

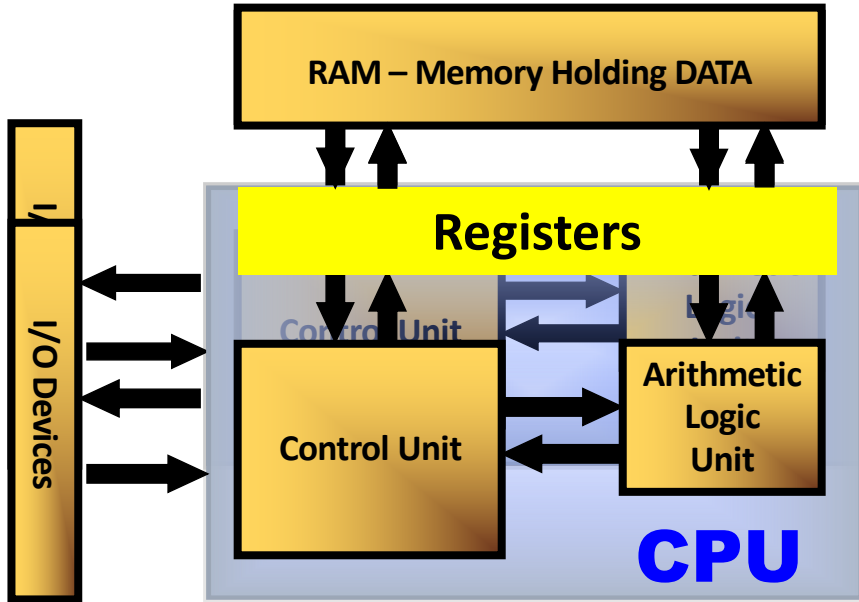
```
int main( ){  
    int c = 0;  
    c = 2 + 3;  
}
```

main.c

```
$gcc main.c -o main.x
```

```
./main.x
```

```
load 2, r1  
load 3, r2  
add r1, r2, r3  
store r3, c
```



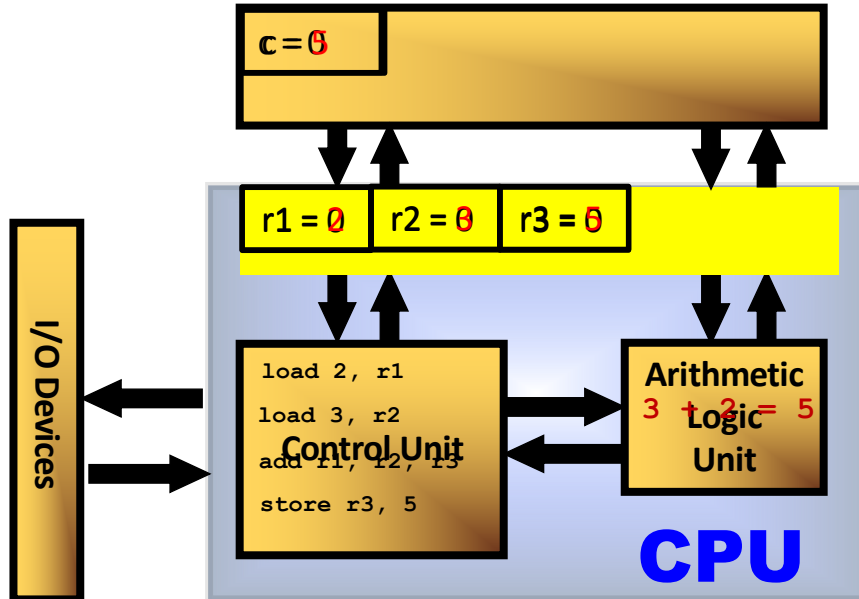


John Von Neumann

# The Basic Model

```
int main( ){
    int c = 0;
    c = 2 + 3;
}
```

main.c



```
$gcc main.c -o main.x
```

```
$/main.x
```

```
load 2, r1 ←
load 3, r2 ←
add r1, r2, r3 ←
store r3, c ←
```



# Performance assesment

- Let's suppose memory data transfer is for free ...
- ... and that our processor runs at  $1 \times 10^9$  hertz ( $1\text{GHz}$ ) => x1 cycle every ns
- ... and that for every clock cycle a single operation is performed
- ... to execute 4 operations, x4 ns ( $10^{-9}$ ) are required!
- Meaning that at full speed, our processor runs our code executing  $10^9$  operations x second (100% efficiency)
- If operations are considered double precision FP (64bits), normally this number is referred as FLOP/s
- Unluckly this is not the case...

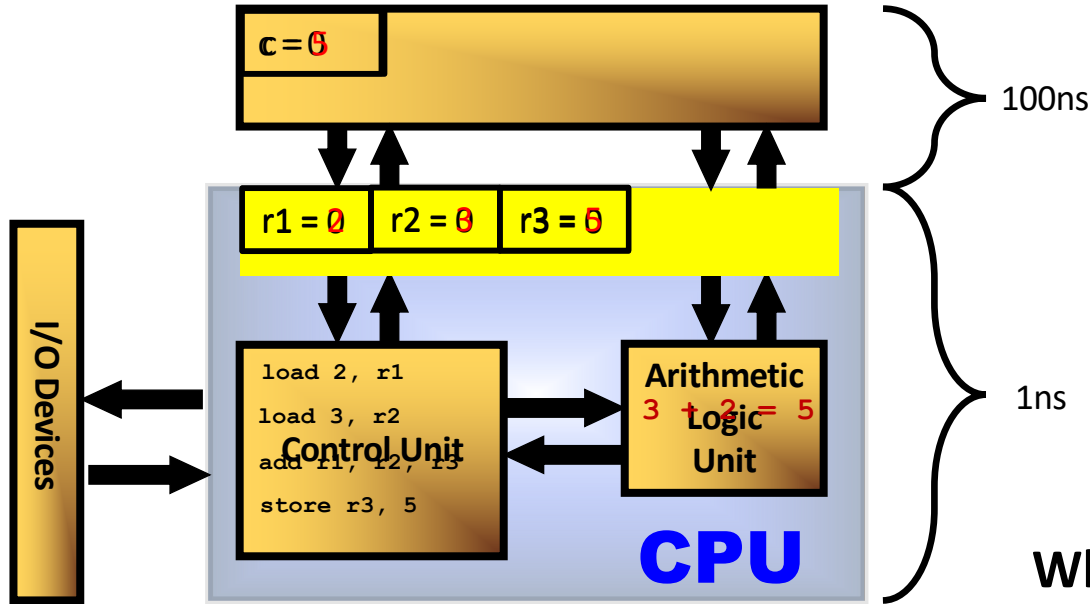


John Von Neumann

# The Basic Model

```
int main( ){
    int c = 0;
    c = 2 + 3;
}
```

main.c



```
$gcc main.c -o main.x
```

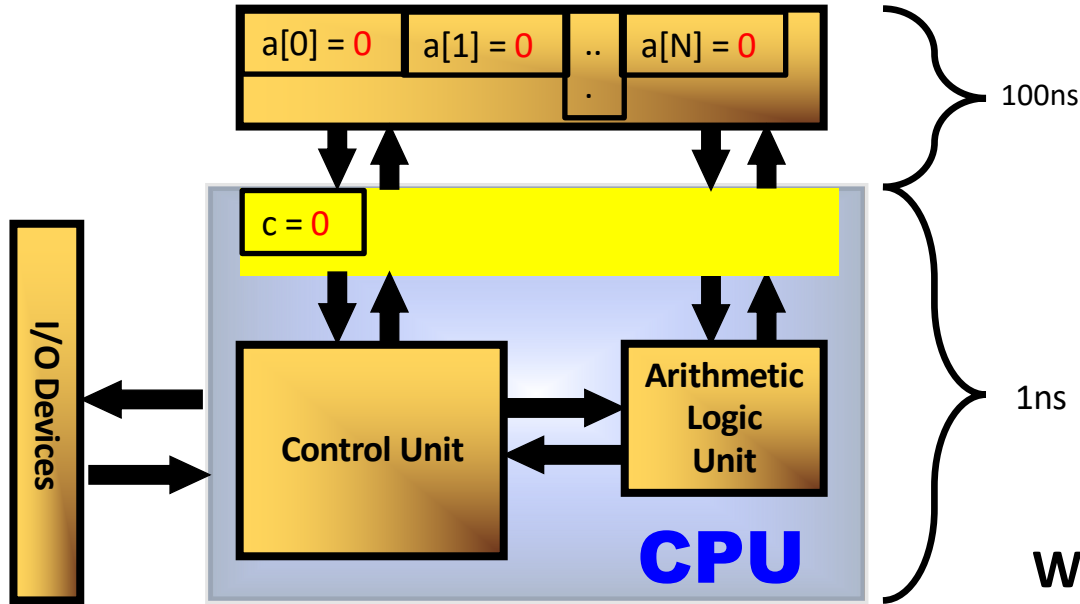
```
$/main.x
```

```
load 2, r1 ←
load 3, r2 ←
add r1, r2, r3 ←
store r3, c ←
```

What is the number of OP/s here?

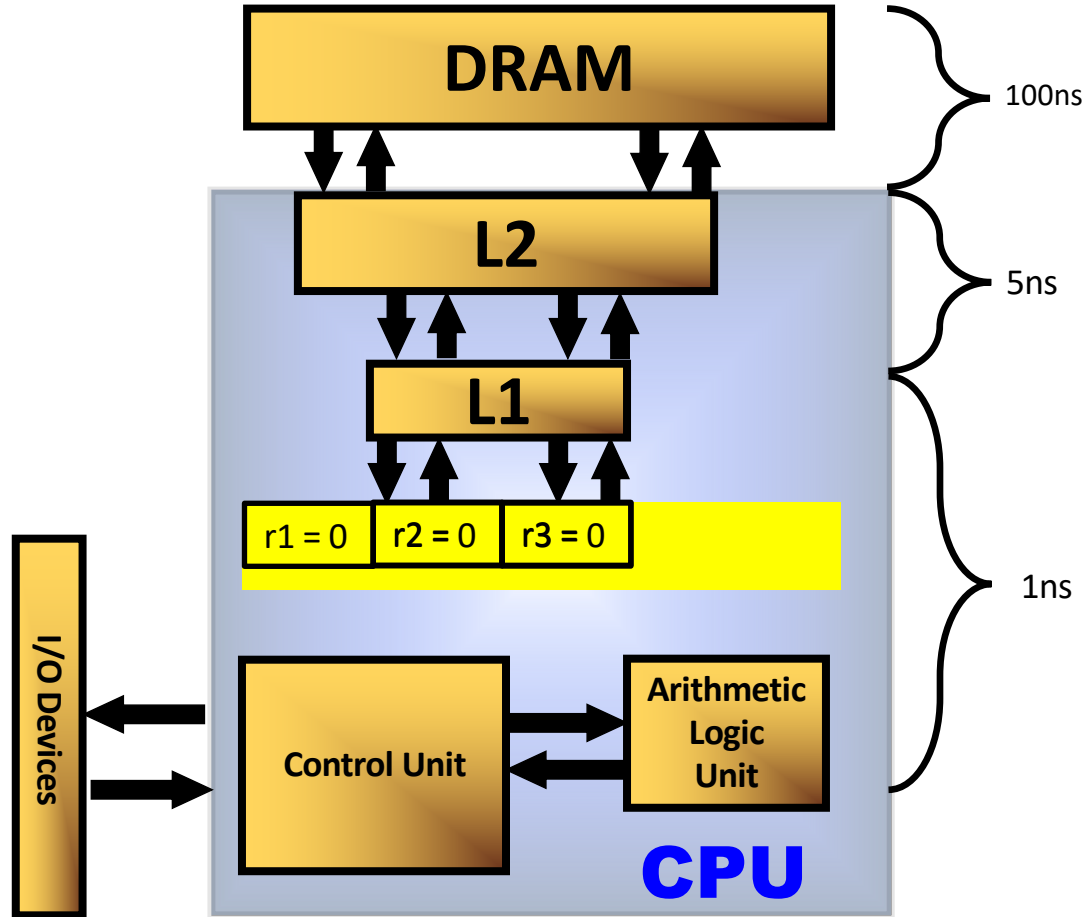
# The Basic Model

```
int main( ){  
    int a[N];  
    for ( c = 0; c < N; c++ )  
        a[c] = c;  
}
```



What is the number of OP/s here?

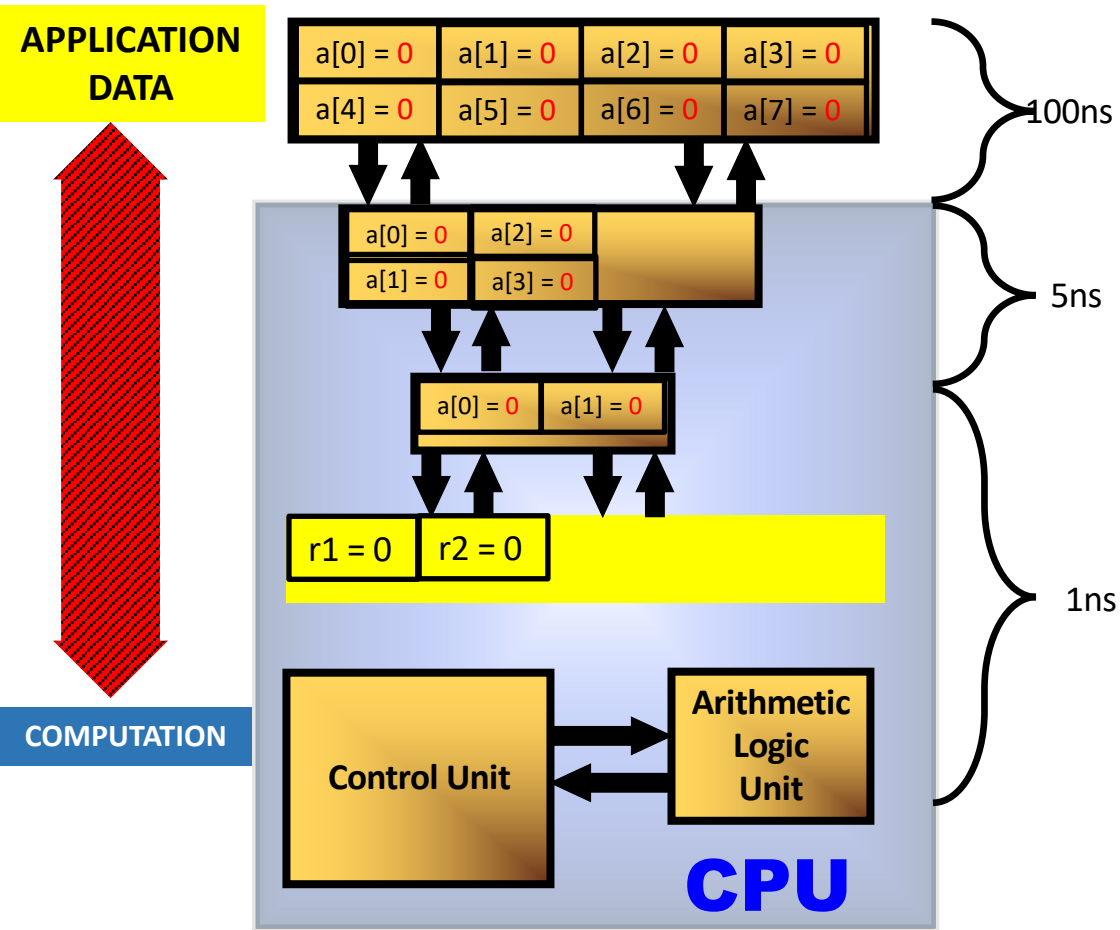
# The Memory Hierarchy



```
int main( ){  
    int a[N];  
    for ( c = 0; c < N; c++ )  
        a[c] = c;  
}
```



# The Memory Hierarchy



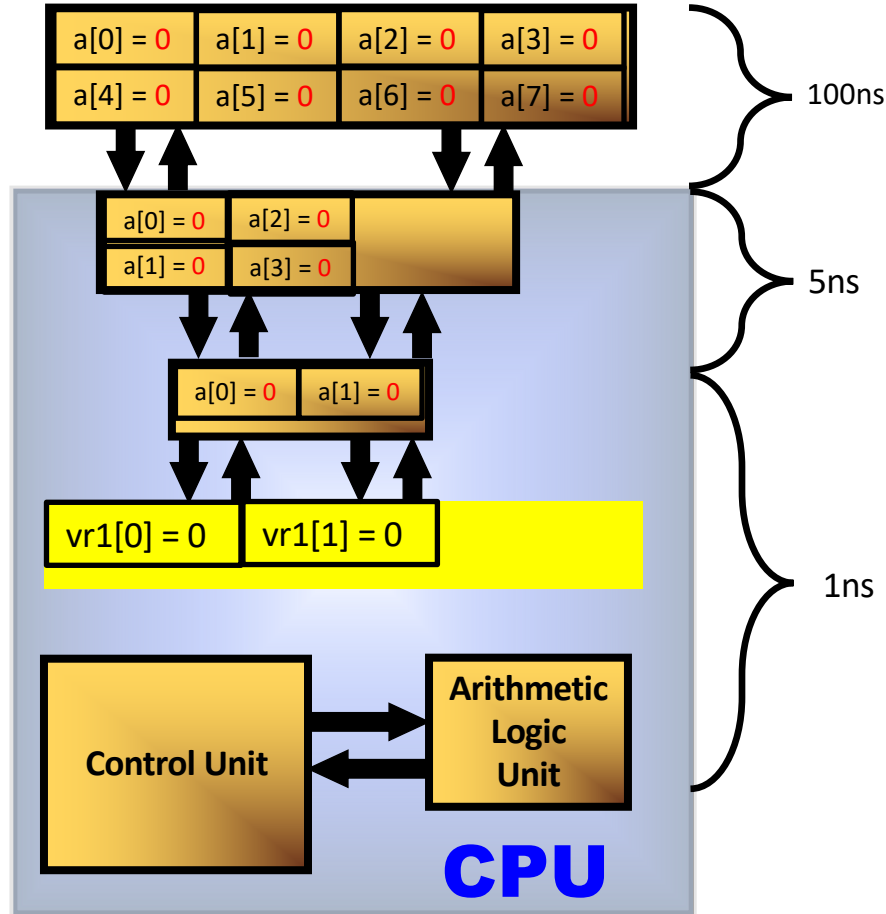
```
int main( ){  
    int a[N];  
    for ( c = 0; c < N; c++ )  
        a[c] = c;  
}
```

- D  
l
- D  
branch => loop

blocks of fixed size, called *cache lines*.

- Operation of LOAD/STORE can lead at two different scenario:
  - *cache hit*
  - *cache miss*

# Vectorization



```
int main( ){  
    int a[N];  
    for ( c = 0; c < N; c++ )  
        a[c] = c;  
}
```

Registers are capable to store more than one primitive type at a time

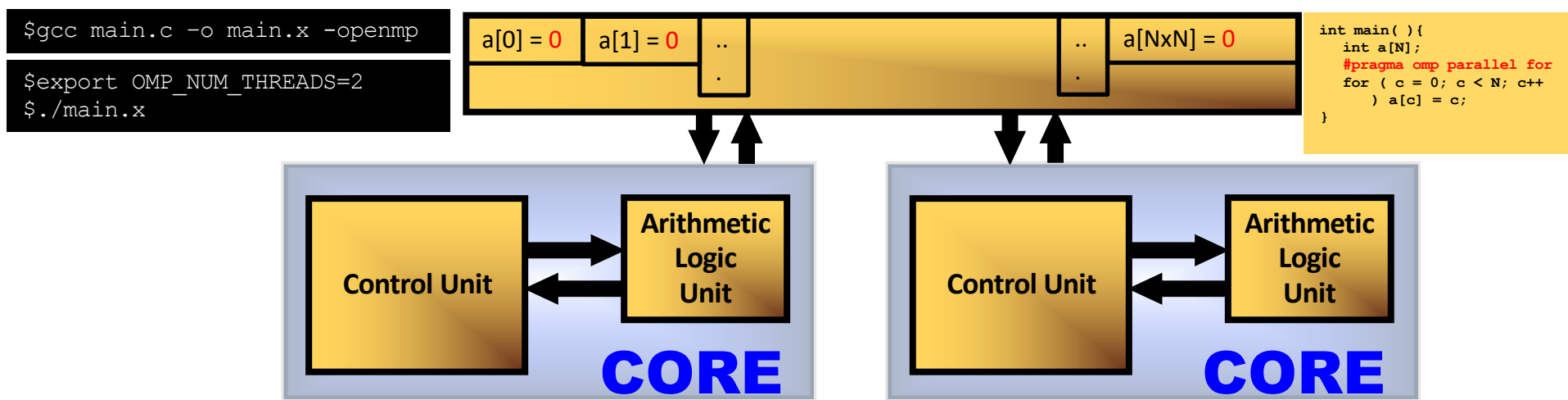
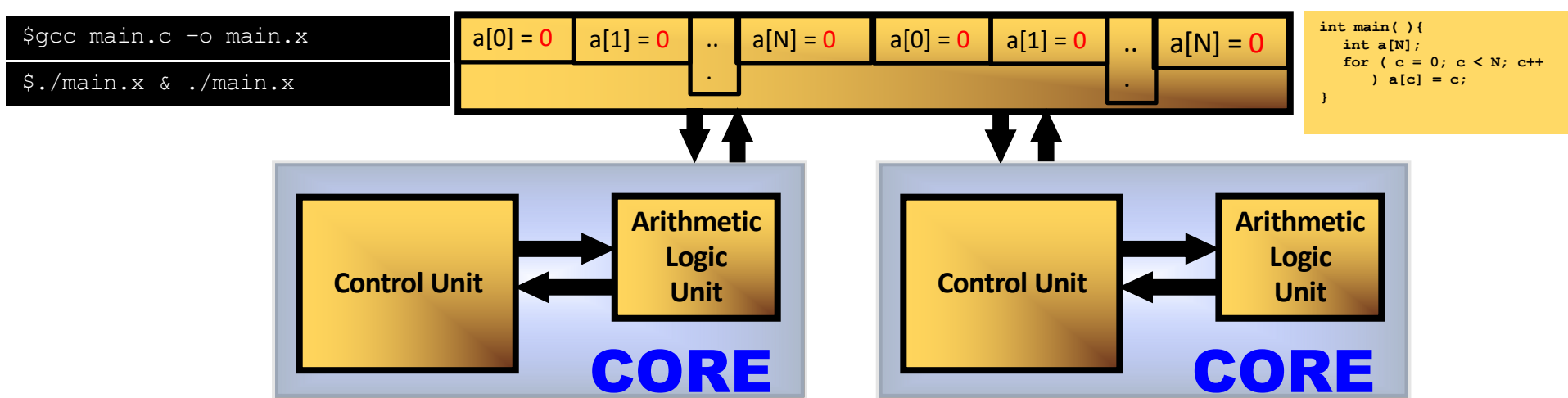
The vectorial ALU is capable to perform the same operation over multiple data of the same kind

## Scalar Mode



# Wrap up on modern computers

- Efficient data memory access patterns are crucial to best performances
  - design and development of computer algorithms that maximize data locality in time and space (data distance)
- Modern CPUs are equipped with vector registers and ALUs capable of multiple concurrent operations on multiple data
  - vectorization is aided by compilers, but requiring design and development of computer codes that maximize simple operations on contiguous data of the same type
- When all CPU component work at maximum speed that is called *peak of performance* (Floating point operations per seconds FLOP/s)
  - Tech-spec normally describe the theoretical peak
  - Benchmarks measure the real peak
  - Applications show the real performance value
- Real performance are also mostly related to the memory bandwidth (GBytes/s)

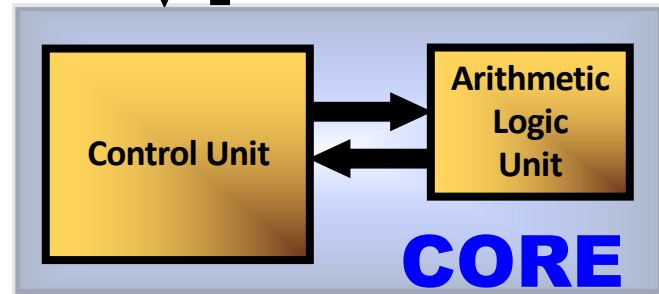
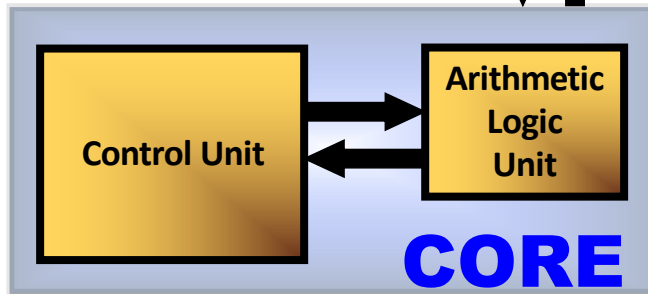




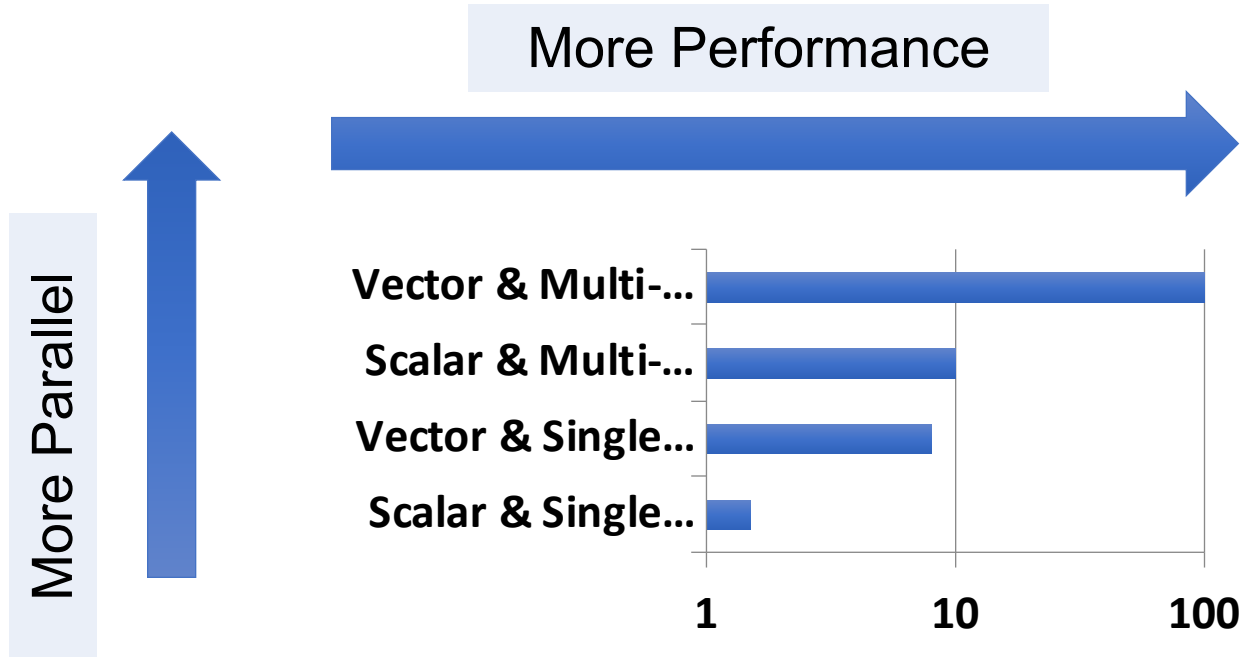
```
int main( ){
  int a[N], sum;
  #pragma omp parallel for
  for ( c = 0; c < N; c++ )
    sum += a[c];
}
```

```
$gcc main.c -o main.x -openmp
```

```
$export OMP_NUM_THREADS=2
$./main.x
```



# Threading and Vectorization



# Three nice reason to use python in scientific programing

NumPy:

<http://www.numpy.org/>

SciPy:

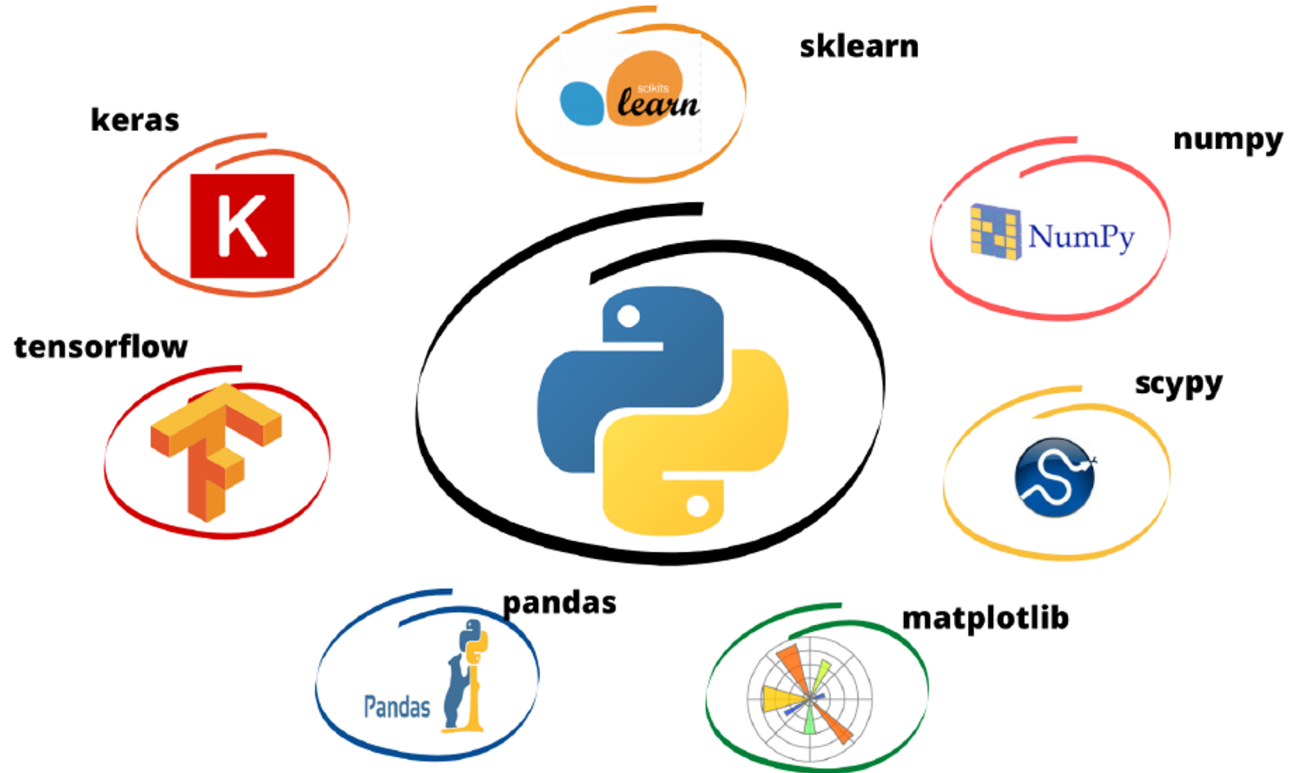
<http://www.scipy.org/>

Matplotlib:

<http://matplotlib.org/>

All are open source!

And more





# Nice reason to use python in scientific programming

**NumPy** provides functionality to create, delete, manage and operate on large arrays of type raw" data (like Fortran and C/C++ arrays).

**SciPy** extends NumPy with a collection of useful algorithms like minimization, Fourier transforms, regression and many other applied mathematical techniques.

Both packages are add-on packages (not part of the Python standard library) containing Python code and compiled with (fftpack, BLAS).

**Matplotlib** is a nice library to plot (but there are others as Seaborn or Bokeh).

# How to import libraries?

```
import numpy as np
import scipy as sp
import matplotlib.pyplot as pp
import matplotlib.pyplot as plt
```



# Numpy

NumPy is the fundamental package for scientific computing in Python.

- A powerful N-dimensional array object.
- Sophisticated (broadcasting) functions.
- Tools for integrating C/C++ and Fortran code.
- Useful linear algebra, Fourier transform, and random number capabilities.
- Operations on matrices and vectors in NumPy are very efficient because they are linked to compiled in BLAS/LAPACK code.



## NumPy functionality:

- Polynomial mathematics.
- Statistical computations.
- Pseudo random number generators.
- Discrete Fourier transforms.
- Size / shape / type testing of arrays.



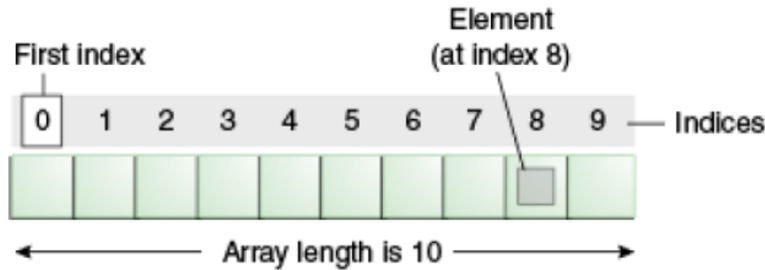


# Fundamental thing from Numpy: `np.array`

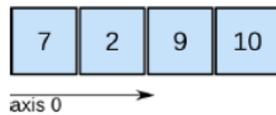
There are 5 general mechanisms for creating arrays:

- Conversion from other Python structures (e.g., lists, tuples).
- Intrinsic numpy array creation objects (e.g., `arange`, `ones`, `zeros`, etc.)
- Reading arrays from disk, either from standard or custom formats.
- Creating arrays from raw bytes through the use of strings or buffers.
- Use of special library functions (e.g., `random`).

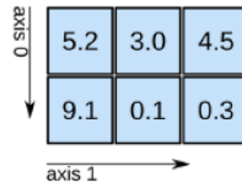
# How is an Array?



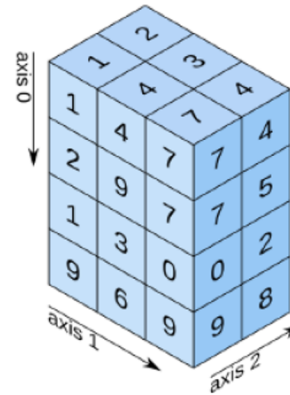
1D array



2D array



3D array





# Examples of how to create arrays

```
x = np.array([2, 3, 1, 0])
```

```
print(x)
```

```
[2 3 1 0]
```

```
np.arange(10)
```

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

```
np.arange(2, 10, dtype=np.float)
```

```
array([2., 3., 4., 5., 6., 7., 8., 9.])
```

```
np.arange(2, 3, 0.1)
```

```
array([2. , 2.1, 2.2, 2.3, 2.4, 2.5, 2.6, 2.7, 2.8, 2.9])
```

# Special Functions

```
a = np.zeros((5, 2))
print(a)
[[0. 0.]
 [0. 0.]
 [0. 0.]
 [0. 0.]
 [0. 0.]]
b = a.reshape((2, 5))
print(b)
[[0. 0. 0. 0. 0.]
 [0. 0. 0. 0. 0.]]
```

# Linear Algebra Operations

```
x = np.array([[1., 2., 3., 4.], [1., 2., 3., 4.]])
print(x)
[[1. 2. 3. 4.]
 [1. 2. 3. 4.]]
b= x.T
print(b)
[[1. 1.]
 [2. 2.]
 [3. 3.]
 [4. 4.]]
```



# Simple Linear Algebra Operations

```
v=np.array([-1, 2,5])
```

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

```
print(v.dot(w))
```

```
18
```

```
print(np.dot(v, w))
```

```
18
```

```
#-----
```

```
v1=np.array([[ -1, 2,5],[1, 3,5]])
```

```
w1=np.array([1,10,3])
```

```
print(v1.dot(w1))
```

```
[34 46]
```

```
print(np.cross(v,w))
```

```
[-4  8 -4]
```

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

```
y=np.array([11, -2,5])
```

```
print(x + y)
```

```
[12  0  8]
```

```
print(np.add(x, y))
```

```
[12  0  8]
```

```
#-----
```

```
print(x - y)
```

```
[-10  4 -2]
```

```
print(np.subtract(x, y))
```

```
[-10  4 -2]
```





# Opening a txt or cvs file

```
import numpy as np

file_name_you_want = np.loadtxt(fname,delimiter=" ")

print "First column element: ",file_name_you_want[0]
#to get the full column:

Transpose_your_file = file_name_you_want.T

print "First column: ", Transpose_your_file[0]
```





# SciPy

One of the core packages. SciPy is built on top of NumPy and implements many specialized scientific computation tools:

- Manly user-friendly.
- Efficient numerical routines such as routines for numerical integration and optimization.
- Clustering.
- Fourier transforms.
- Numerical integration, interpolations. data I/O, LAPACK.

Also:

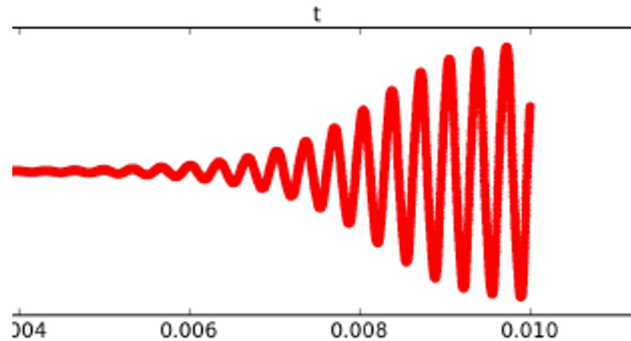
- sparse matrices, linear solvers, optimization.
- signal processing.
- statistical functions





# Nice for numerical integration of equations

```
from scipy.integrate import odeint
dy/dt = func(y, t0, ...)
sol = odeint(func, X0, t)
```



<https://docs.scipy.org/doc/scipy/reference/generated/scipy.integrate.odeint.html>

# Or for example for a simple fit



```
import numpy as np
import matplotlib.pyplot as pp
from scipy.optimize import curve_fit

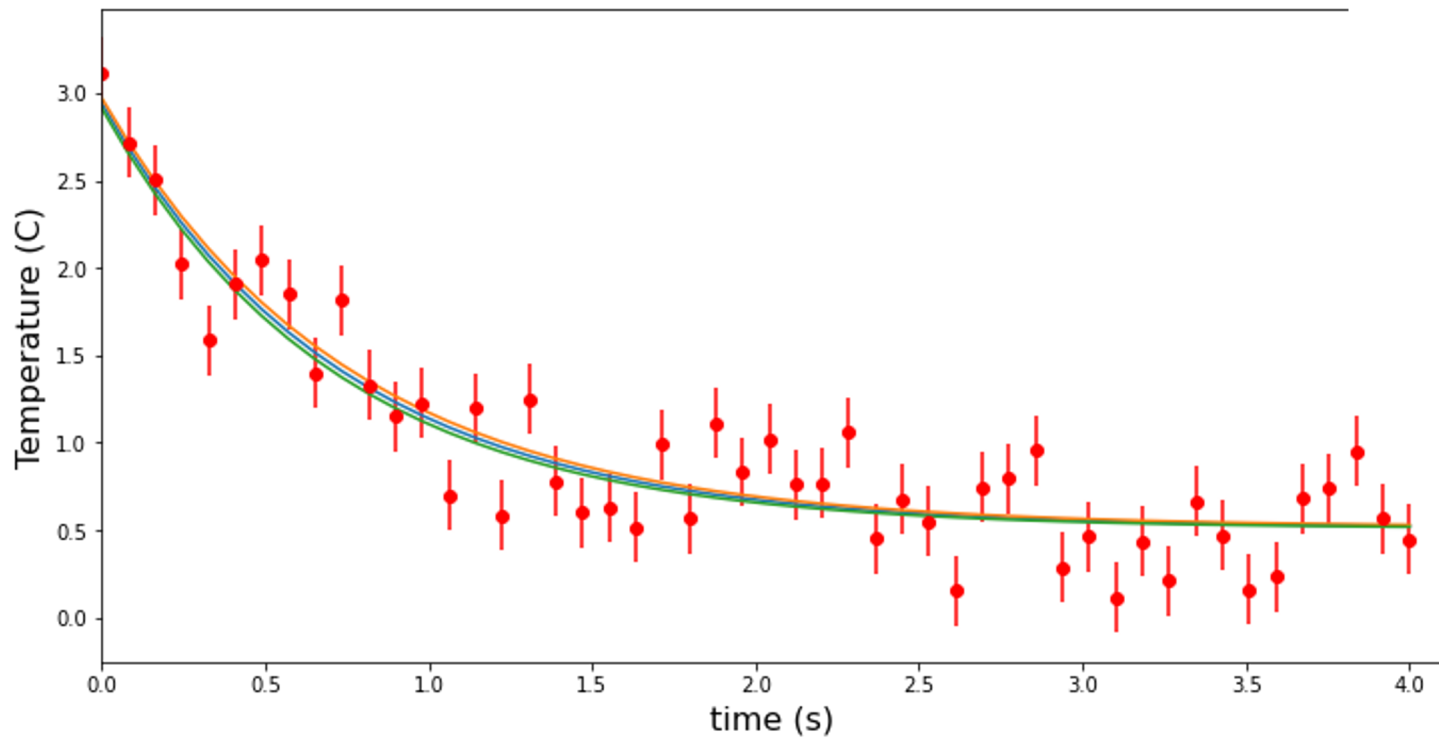
def fitFunc(t, a, b, c):
    return a*np.exp(-b*t) + c

t = np.linspace(0,4,50)
temp = fitFunc(t, 2.5, 1.3, 0.5)
noisy = temp + 0.25*np.random.normal(size=len(temp))
fitParams, fitCovariances = curve_fit(fitFunc, t, noisy)

pp.figure(figsize=(12, 6))
pp.ylabel('Temperature (C)', fontsize = 16)
pp.xlabel('time (s)', fontsize = 16)
pp.xlim(0,4.1)
pp.errorbar(t, noisy, fmt = 'ro', yerr = 0.2)
sigma = [fitCovariances[0,0], fitCovariances[1,1], fitCovariances[2,2] ]
pp.plot(t, fitFunc(t, fitParams[0], fitParams[1], fitParams[2]))
pp.plot(t, fitFunc(t, fitParams[0] + sigma[0], fitParams[1] - sigma[1], fitParams[2] + sigma[2]))
pp.plot(t, fitFunc(t, fitParams[0] - sigma[0], fitParams[1] + sigma[1], fitParams[2] - sigma[2]))
pp.savefig('dataFitted.pdf', bbox_inches=0, dpi=600)
pp.show()
```



And the result!





# With the Fit parameters

[ 2.595658 1.74438726 0.69809511]

**And covariance matrix:**

[[ 0.02506636 0.01490486 -0.00068609]

2 [ 0.01490486 0.04178044 0.00641246]

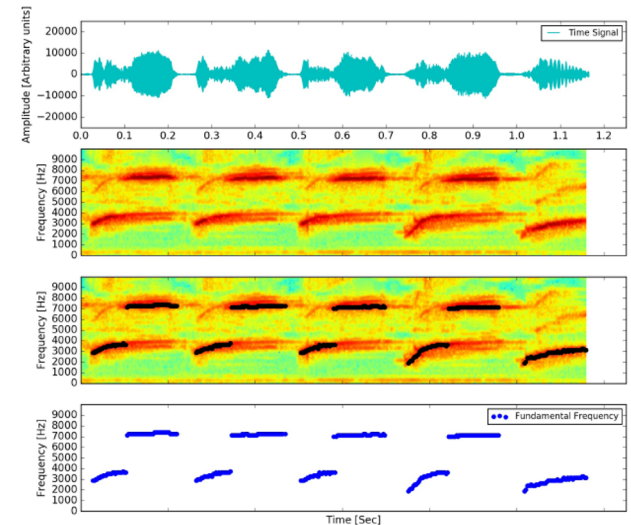
3 [-0.00068609 0.00641246 0.00257799]]

Also possible to apply for signal analysis and time series

DOI:<https://doi.org/10.31527/analesafa.2018.29.2.51>

<https://doi.org/10.1016/j.mex.2018.12.011>

DOI:<https://doi.org/10.31527/analesafa.2019.30.3.68>

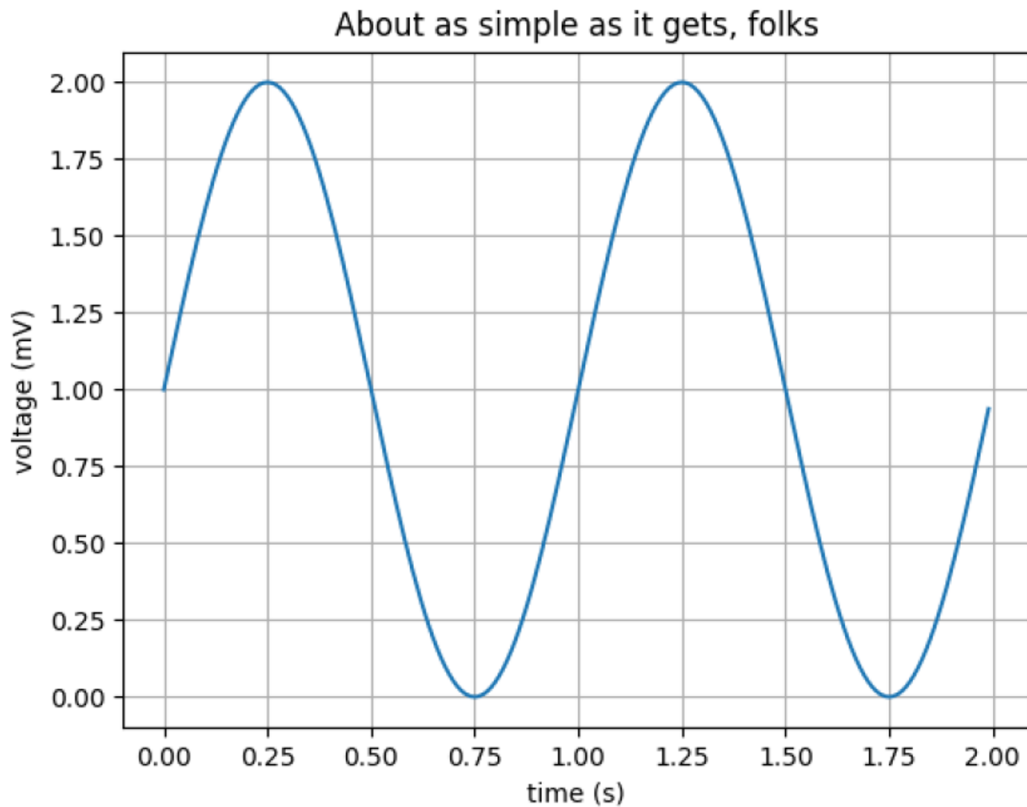


# Matplotlib

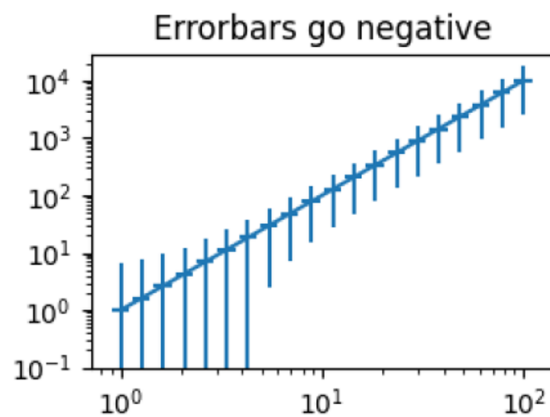
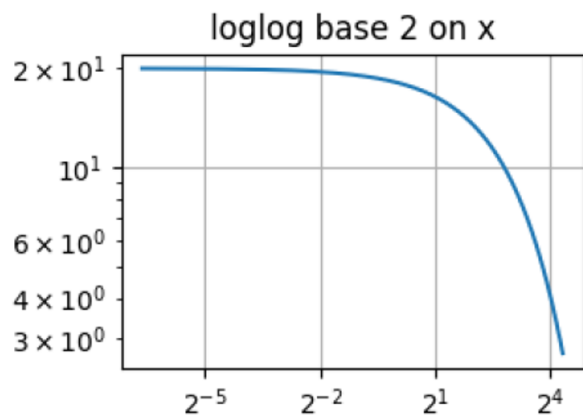
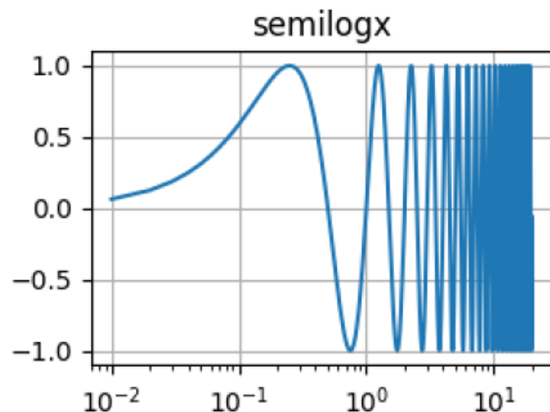
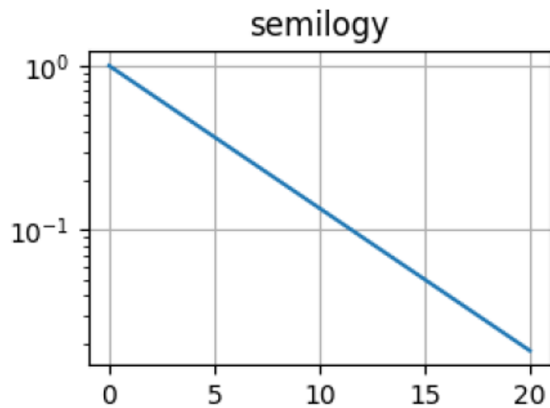
Is a Python 2D plotting library which produces publication quality figures in a variety of hardcopy formats and interactive environments across platforms. Can be used in:

- Python scripts.
- The Python and IPython shell.
- The jupyter notebook.
- Web application servers.
- Graphical user interface toolkits.

# Different kind of plots: y vs. x



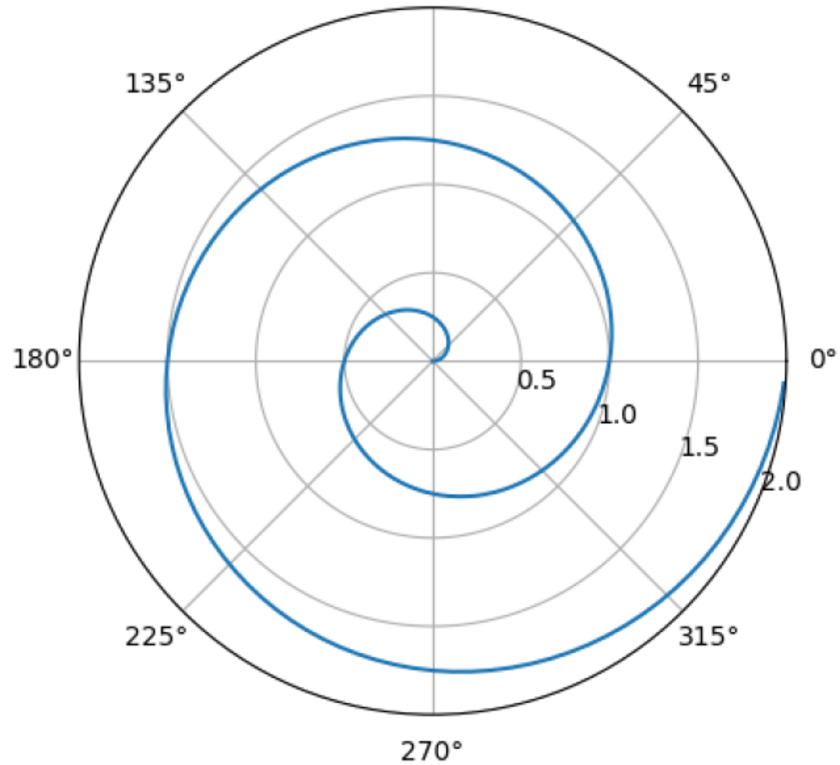
# Different scales:



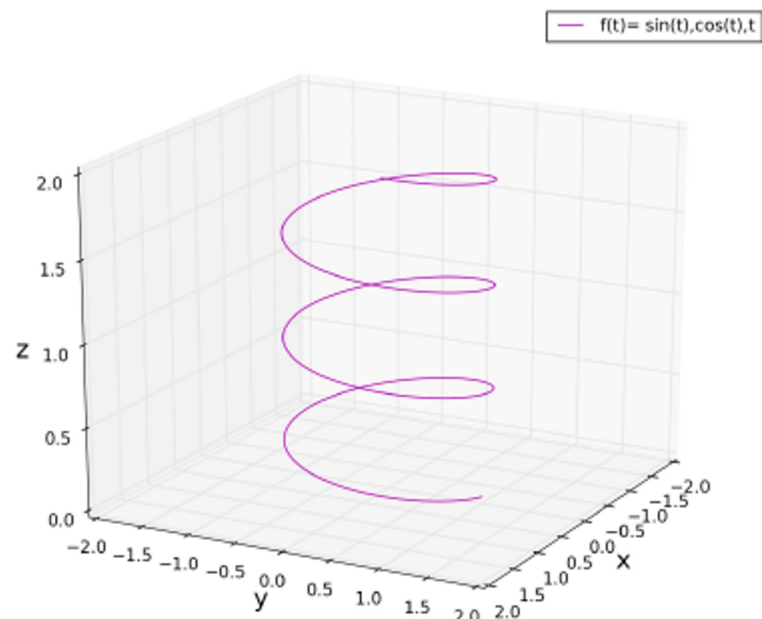
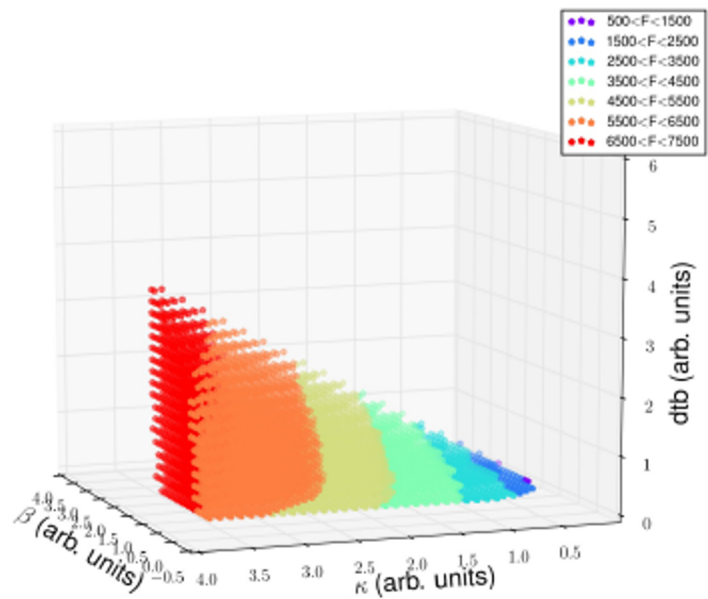


# Different coordinates

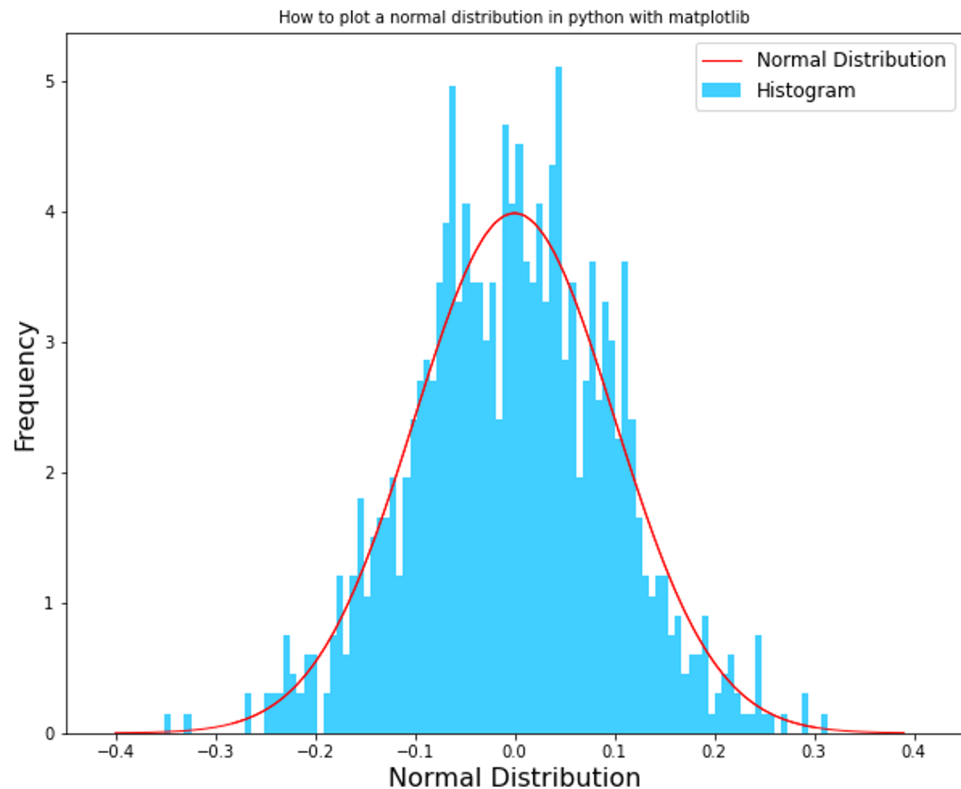
A line plot on a polar axis  
90°



# 3d plots:



# Histograms and distributions





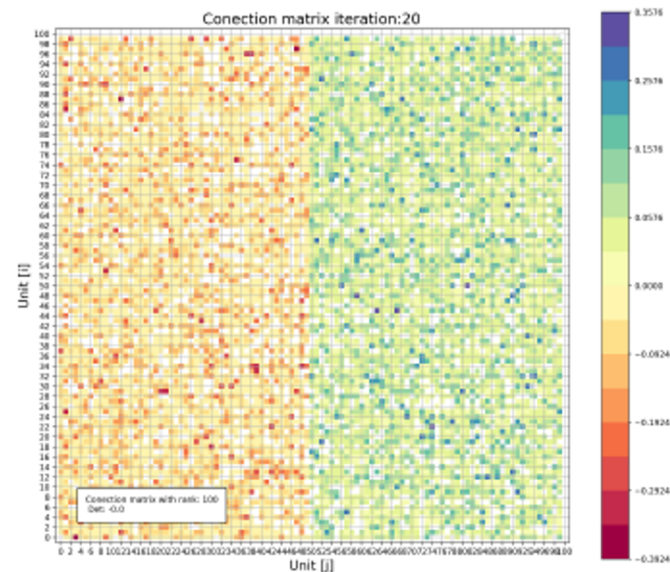
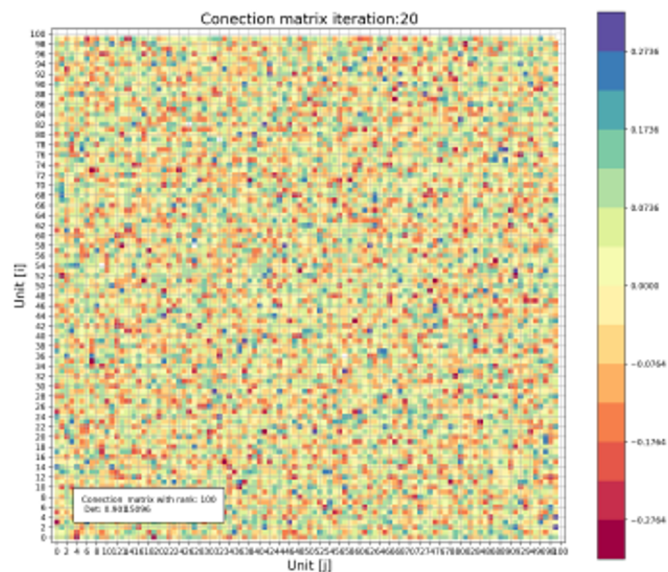
# The code for the histogram:

```
import numpy as np
from scipy.stats import norm
import matplotlib.pyplot as plt
mu, sigma = 0, 0.1 # mean and standard deviation
s = np.random.normal(mu, sigma, 1000)
x_n = np.arange(-0.4,0.4,0.01)
y_n = norm.pdf( x_n, mu, sigma)

fig      = plt.figure(figsize=(10,8))
plt.title('Histogram Normal Distribution', fontsize = 18)
plt.hist(s, 100, density=1, facecolor='deepskyblue',label='Histogram', alpha=0.75)
plt.plot(x_n, y_n, 'r-', linewidth=1,label='Normal Distribution')
plt.show()
```

# Matrices:

## Numpy Scipy Matplotlib





# More on visualization with python

<https://clauswilke.com/dataviz/>

<https://www.python-graph-gallery.com/>



### Matplotlib

Matplotlib is a Python 2D plotting library which produces publication-quality figures in a variety of hardcopy formats and interactive environments across platforms.



### 1 Prepare The Data

Also see Lists & NumPy

#### 1D Data

```
>>> import numpy as np
>>> x = np.linspace(0, 10, 100)
>>> y = np.cos(x)
>>> z = np.sin(x)
```

#### 2D Data or Images

```
>>> data = 2 * np.random.random((10, 10))
>>> data2 = 3 * np.random.random((10, 10))
>>> Y, X = np.mgrid[3:3+100j, -3:3+100j]
>>> U = 1 - X**2 + Y
>>> V = 1 + X - Y**2
>>> from matplotlib.cbook import get_sample_data
>>> img = np.load(get_sample_data('axes_grid/bivariate_normal.npy'))
```

### 2 Create Plot

```
>>> import matplotlib.pyplot as plt
>>> fig = plt.figure()
>>> fig2 = plt.figure(figsize=plt.figaspect(2.0))
```

#### Axes

All plotting is done with respect to an Axes. In most cases, a subplot will fit your needs. A subplot is an axes on a grid system.

```
>>> fig.add_axes()
>>> ax1 = fig.add_subplot(221) # row-col-num
>>> ax3 = fig.add_subplot(212)
>>> fig3, axes = plt.subplots(nrows=2,ncols=2)
>>> fig4, axes2 = plt.subplots(ncols=3)
```

### 3 Plotting Routines

#### 1D Data

```
>>> fig, ax = plt.subplots()
>>> lines = ax.plot(x,y)
>>> ax.scatter(x,y)
>>> axes[0,0].bar([1,2,3],[3,4,5])
>>> axes[1,0].bar([0.5,1.2,5],[0,1,2])
>>> axes[1,1].axhline(0.45)
>>> axes[0,1].axvline(0.65)
>>> ax.fill(x,y,color='blue')
>>> ax.fill_between(x,y,color='yellow')
```

Draw points with lines or markers connecting them  
Draw unconnected points, scaled or colored  
Plot vertical rectangles (constant width)  
Plot horizontal rectangles (constant height)  
Draw a horizontal line across axes  
Draw a vertical line across axes  
Draw filled polygons  
Fill between y-values and o

#### 2D Data or Images

```
>>> fig, ax = plt.subplots()
>>> im = ax.imshow(img,
                  cmap='gist_earth',
                  interpolation='nearest',
                  vmin=-2,
                  vmax=2)
```

Colormapped or RGB arrays

#### Vector Fields

```
>>> axes[0,1].arrow(0,0,0.5,0.5)
>>> axes[1,1].quiver(y,z)
>>> axes[0,1].streamplot(X,Y,U,V)
```

Add an arrow to the axes  
Plot a 2D field of arrows  
Plot a 2D field of arrows

#### Data Distributions

```
>>> ax1.hist(y)
>>> ax3.boxplot(y)
>>> ax3.violinplot(z)
```

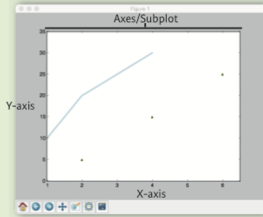
Plot a histogram  
Make a box and whisker plot  
Make a violin plot

```
>>> axes2[0].pcolor(data2)
>>> axes2[0].pcolormesh(data)
>>> CS = plt.contour(Y,X,U)
>>> axes2[2].contour(datal)
>>> axes2[2] = ax.clabel(CS)
```

Pseudocolor plot of 2D array  
Pseudocolor plot of 2D array  
Plot contours  
Plot filled contours  
Label a contour plot

## Plot Anatomy & Workflow

### Plot Anatomy



### Workflow

The basic steps to creating plots with matplotlib are:

- 1 Prepare data
- 2 Create plot
- 3 Plot
- 4 Custom plot
- 5 Save plot
- 6 Show plot

```
>>> import matplotlib.pyplot as plt
>>> x = [1,2,3,4]
>>> y = [10,20,25,30]
>>> fig = plt.figure()
>>> ax = fig.add_subplot(111)
>>> ax.plot(x, y, color='lightblue', linewidth=3)
>>> ax.scatter([2,4,6],
              [5,15,25],
              color='darkgreen',
              marker='^')
>>> ax.set_xlim(1, 6.5)
>>> plt.savefig('foo.png')
>>> plt.show()
```

### 4 Customize Plot

#### Colors, Color Bars & Color Maps

```
>>> plt.plot(x, x, x, x**2, x, x**3)
>>> ax.plot(x, y, alpha = 0.4)
>>> ax.plot(x, y, c='k')
>>> fig.colorbar(im, orientation='horizontal')
>>> im = ax.imshow(img, cmap='seismic')
```

#### Markers

```
>>> fig, ax = plt.subplots()
>>> ax.scatter(x,y,marker=".")
>>> ax.plot(x,y,marker="o")
```

#### Linestyles

```
>>> plt.plot(x,y,linewidth=4.0)
>>> plt.plot(x,y,ls='solid')
>>> plt.plot(x,y,ls='--')
>>> plt.plot(x,y,'--',x**2,y**2,'-.')
>>> plt.setp(lines,color='r',linewidth=4.0)
```

#### Text & Annotations

```
>>> ax.text(1,
          -2.1,
          'Example Graph',
          style='italic')
>>> ax.annotate("Sine",
              xy=(8, 0),
              xycoords='data',
              xytext=(10.5, 0),
              textcoords='data',
              arrowprops=dict(arrowstyle="->",
                              connectionstyle="arc3"),)
```

#### Mathtext

```
>>> plt.title(r'$\sigma_i=15\$', fontsize=20)
```

#### Limits, Legends & Layouts

```
>>> ax.margins(x=0,y=0.1)
>>> ax.axis('equal')
>>> ax.set(xlim=[0,10.5],ylim=[-1.5,1.5])
>>> ax.set_xlim(0,10.5)
```

#### Legends

```
>>> ax.set(title='An Example Axes',
          ylabel='Y-Axis',
          xlabel='X-Axis')
>>> ax.legend(loc='best')
```

#### Ticks

```
>>> ax.xaxis.set(ticks=range(1,5),
               ticklabels=[3,100,-12,'foo'])
>>> ax.tick_params(axis='y',
                  direction='inout',
                  length=10)
```

#### Subplot Spacing

```
>>> fig3.subplots_adjust(wspace=0.5,
                       hspace=0.3,
                       left=0.125,
                       right=0.9,
                       top=0.9,
                       bottom=0.1)
```

#### Axis Spines

```
>>> ax1.spines['top'].set_visible(False)
>>> ax1.spines['bottom'].set_position(('outward', 10))
```

Add padding to a plot  
Set the aspect ratio of the plot to 1  
Set limits for x and y-axis  
Set limits for x-axis

Set a title and x and y-axis labels

No overlapping plot elements

Manually set x-ticks

Make y-ticks longer and go in and out

Adjust the spacing between subplots

Fit subplot(s) in to the figure area

Make the top axis line for a plot invisible  
Move the bottom axis line outward

### 5 Save Plot

#### Save figures

```
>>> plt.savefig('foo.png')
```

#### Save transparent figures

```
>>> plt.savefig('foo.png', transparent=True)
```

### 6 Show Plot

```
>>> plt.show()
```

### Close & Clear

```
>>> plt.cla()
>>> plt.clf()
>>> plt.close()
```

Clear an axis  
Clear the entire figure  
Close a window





<http://pandas.pydata.org/>



# To import library

```
import pandas as pd
```

A unidimensional array with labels:

```
s = pd.Series([3, -5, 7, 4], index=['a', 'b', 'c', 'd'])
```

```
print(s)
```

```
a      3
```

```
b     -5
```

```
c      7
```

```
d      4
```

```
dtype: int64
```

# A bi-dimensional array

```
data = {'Country': ['Belgium', 'India', 'Brazil'], 'Capital': ['Brussels',  
'New Delhi', 'Brasilia'], 'Population': [11190846, 1303171035, 207847528]}
```

```
df = pd.DataFrame(data, columns=['Country', 'Capital', 'Population'])
```

```
print(df)
```

	Country	Capital	Population
0	Belgium	Brussels	11190846
1	India	New Delhi	1303171035
2	Brazil	Brasilia	207847528

# To read a file and write it with pandas

```
pd.read_csv('file.csv', header=None, nrows=5)
```

```
df.to_csv('myDataFrame.csv')
```

# To read multiple sheets of the same file

```
xlsx = pd.ExcelFile('file.xls')
```

```
df = pd.read_excel(xlsx, 'Sheet1')
```

# To request help!

```
help(pd.Series.loc)
```

```
      mark ii      1      4
viper      mark ii      7      1
           mark iii     16     36
```

Single label. Note this returns a DataFrame with a single index.

```
>>> df.loc['cobra']
      max_speed  shield
mark i         12      2
mark ii         0      4
```

Single index tuple. Note this returns a Series.

```
>>> df.loc[('cobra', 'mark ii')]
max_speed    0
shield       4
Name: (cobra, mark ii), dtype: int64
```

Single label for row and column. Similar to passing in a tuple, this returns a Series.

```
>>> df.loc['cobra', 'mark i']....
```

# To select one element

```
s = pd.Series([3, -5, 7, 4], index=['a', 'b', 'c', 'd'])  
s['b']  
-5
```

# To select a subset

```
data = {'Country': ['Belgium', 'India', 'Brazil'], 'Capital': ['Brussels', 'New Delhi', 'Brasilia'],  
        'Population': [11190846, 1303171035, 207847528]}
```

```
df = pd.DataFrame(data, columns=['Country', 'Capital', 'Population'])
```

```
df[1:]
```

	Country	Capital	Population	
1	India	New Delhi	1303171035	
2	Brazil	Brasilia	207847528	

# Retrieving Series/DataFrame Information

```
#(rows, columns)
```

```
df.shape
```

```
#Describe index
```

```
df.index
```

```
#Describe DataFrame columns
```

```
df.columns
```



```
#Info on DataFrame
```

```
df.info()
```

```
#Number of non-NA values
```

```
df.count()
```

```
<class  
'pandas.core.frame.DataFrame'>  
RangeIndex: 3 entries, 0 to 2  
Data columns (total 3 columns):  
#   Column      Non-Null Count  
Dtype  
---  ---  
0   Country    3 non-null  
object  
1   Capital    3 non-null  
object  
2   Population  3 non-null  
int64  
dtypes: int64(1), object(2)  
memory usage: 200.0+ bytes  
Country      3  
Capital      3  
Population    3  
dtype: int64
```

# Applying Functions

```
f = lambda x: x*2
```

```
#Apply function
```

```
df.apply(f)
```

```
#Apply function element-wise
```

```
df.applymap(f)
```