An introduction to Python for Scientific Computation

By Edward Smith

3rd March 2017

Aims for today

- Motivation for using Python.
- Introduction to basic syntax (lists, iterators, etc) and discussion of the differences to other languages.
- Scientific libraries numpy and matplotlib.
- Using python to read files (ASCII, CSV, Binary) and plot.
- Examples of usage for scientific problems.

Overview

- Introduction and Basic Constructs of Python (~30mins)
- Hands on session + break (~20 min)
- Programming in Python (~15 min)
- Hands on Session + break (~20 min)
- Scientific computing and data analysis (~20 min)
- Hands on session (~15 min)

Pros and Cons of Python (vs MATLAB)

Pros

- Free and open-source
- Not just for scientific computing
- Great libraries (One of Google's languages)
- Clear, clever and well designed syntax
- Remote access (ssh)
- Great online documentation

Cons

- No debugging GUI so less user friendly
- Syntax is different with some odd concepts
- No type checking can cause problems
- Not as many scientific toolboxes as MATLAB, inbuilt help not as good
- Slow compared to low level languages

Computing at Imperial

- Aeronautical Engineering – MATLAB in ”Computing” and ”Numerical Analysis”
- Bio-Engineering – MATLAB in ”Modelling for Biology”
- Chemical Engineering – Only MATLAB taught
- Chemistry – Python taught
- Civil Engineering – MATLAB in ”Computational Methods I and II” (some object oriented in second year)
- Computing/Electrical Engineering – low level
- Materials – MATLAB in ”Mathematics and Computing”
- Maths – Python in 2nd term (MATLAB in 1st)
- Mechical Engineering – Only MATLAB taught
- Physics – Start 1st year ”Computing Labs” with Python
- Biology and Medicine – No programming?

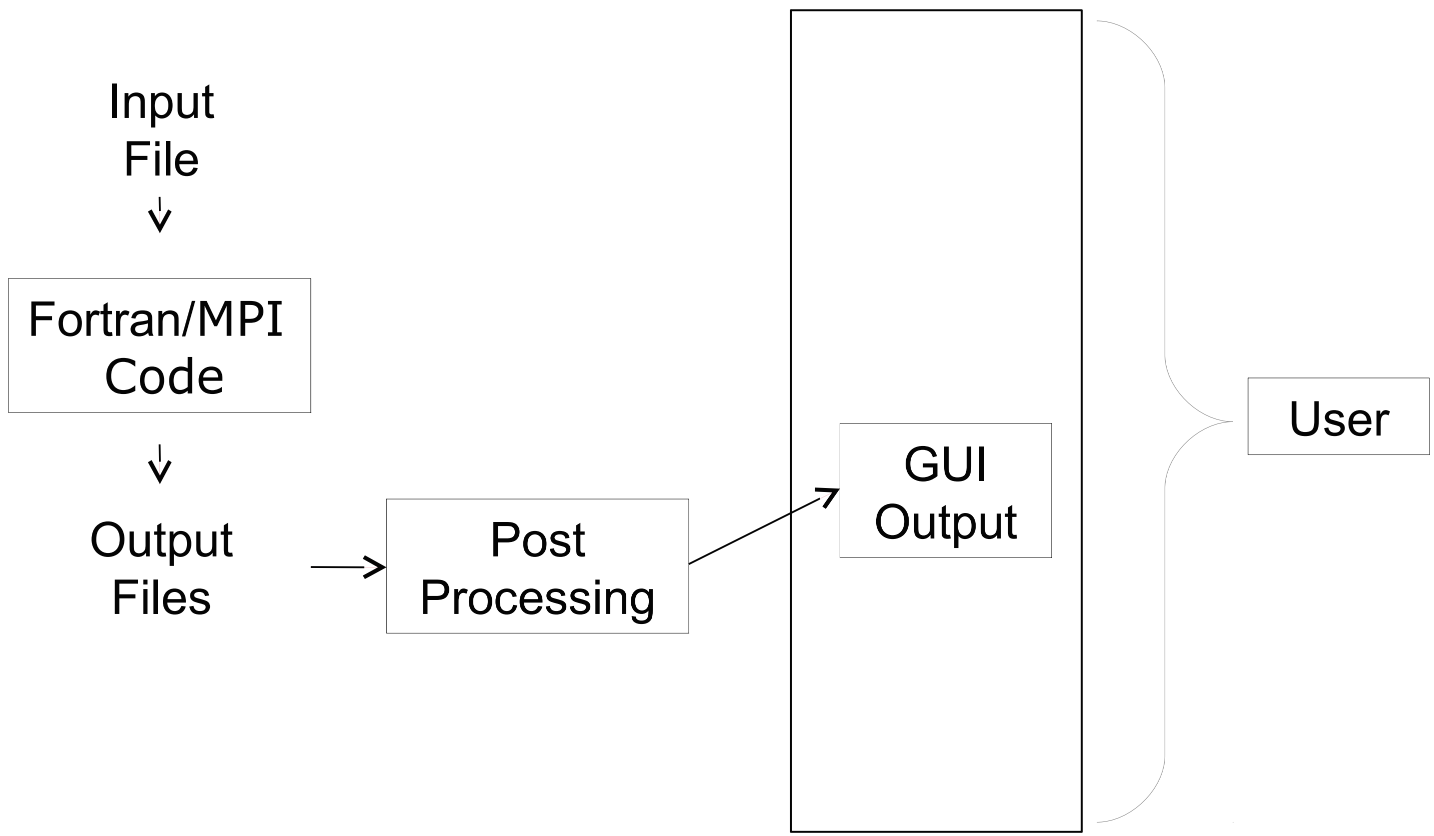
My Background

- Currently a full time software developer/researcher
  - Civil Engineering (Prev Mech & Chem Eng at IC)
  - About 8 years of programming experience
  - Software Sustainability Fellow (www.software.ac.uk)
  - Answer Python questions on Stackoverflow
- Why this course?
  - I learnt MATLAB as undergrad in Mech Eng (also c++ and assembly language but still mainly used excel)
  - Masters project: Lattice Boltzmann solver in MATLAB. PhD: Fortran/MPI Molecular Dynamics, MATLAB post processing
  - Collaborator used Python and too much effort to maintain both but took me a year to kick the MATLAB habit
  - My main incentive for the switch to Python is the long term potential and the ability to write more sustainable code
  - I wish I had learnt Python sooner!

How I use Python in my Work

- Post processing framework
  - Low level data readers for a range of different data formats
  - Higher level field provide standard data manipulation to combine, average and prepare data to be plotted
- Visualiser Graphical User Interface
  - Tried to instantiate all possible field objects in a folder and plot
  - Based on wxpython and inspired by MATLAB sliceomatic
- Batch running framework for compiled code
  - Simple syntax for systematic changes to input files
  - Specifiy resources for multiple jobs on desktop, CX1 or CX2
  - Copies everything needed for repeatability including source code, input files and initial state files

How I use Python in my Work



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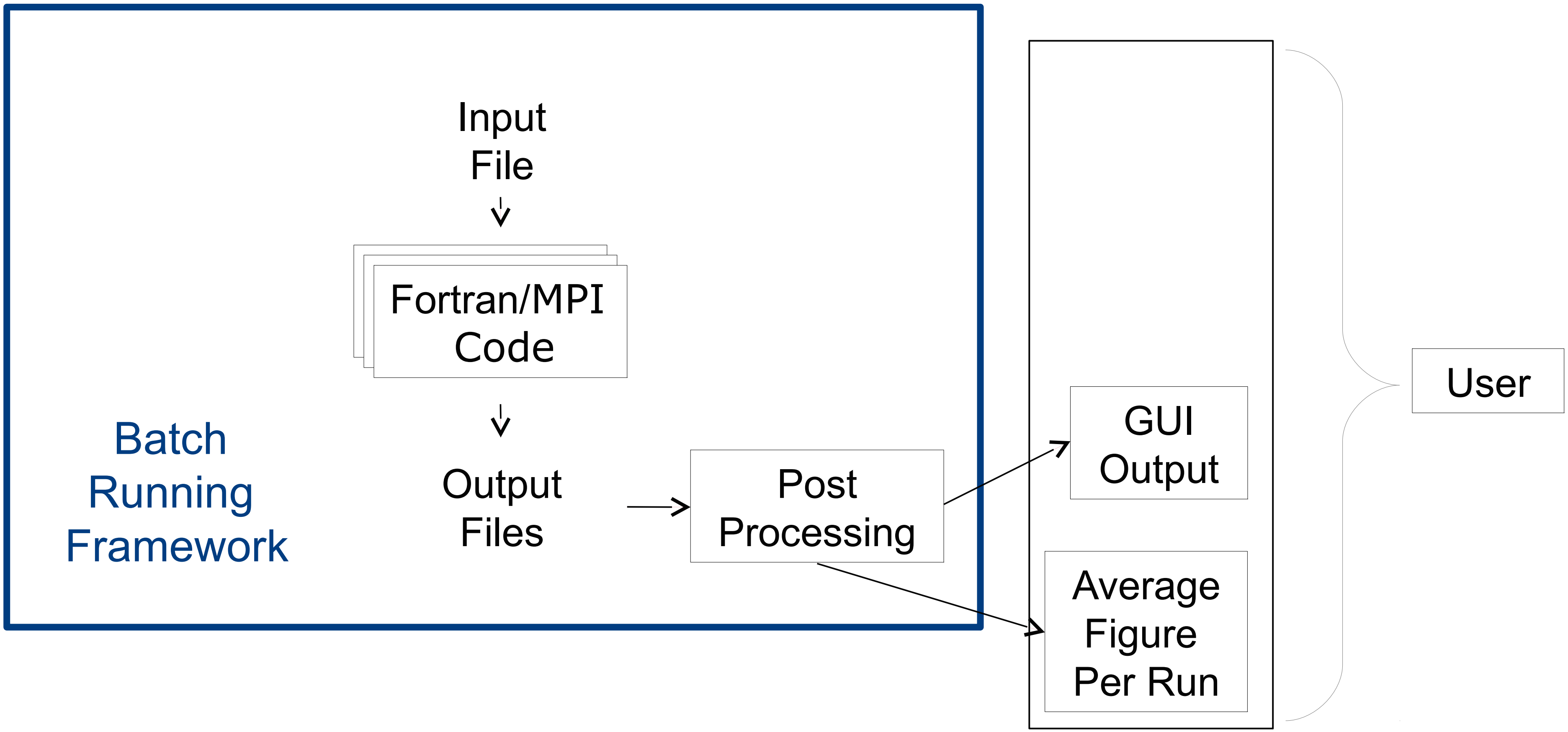

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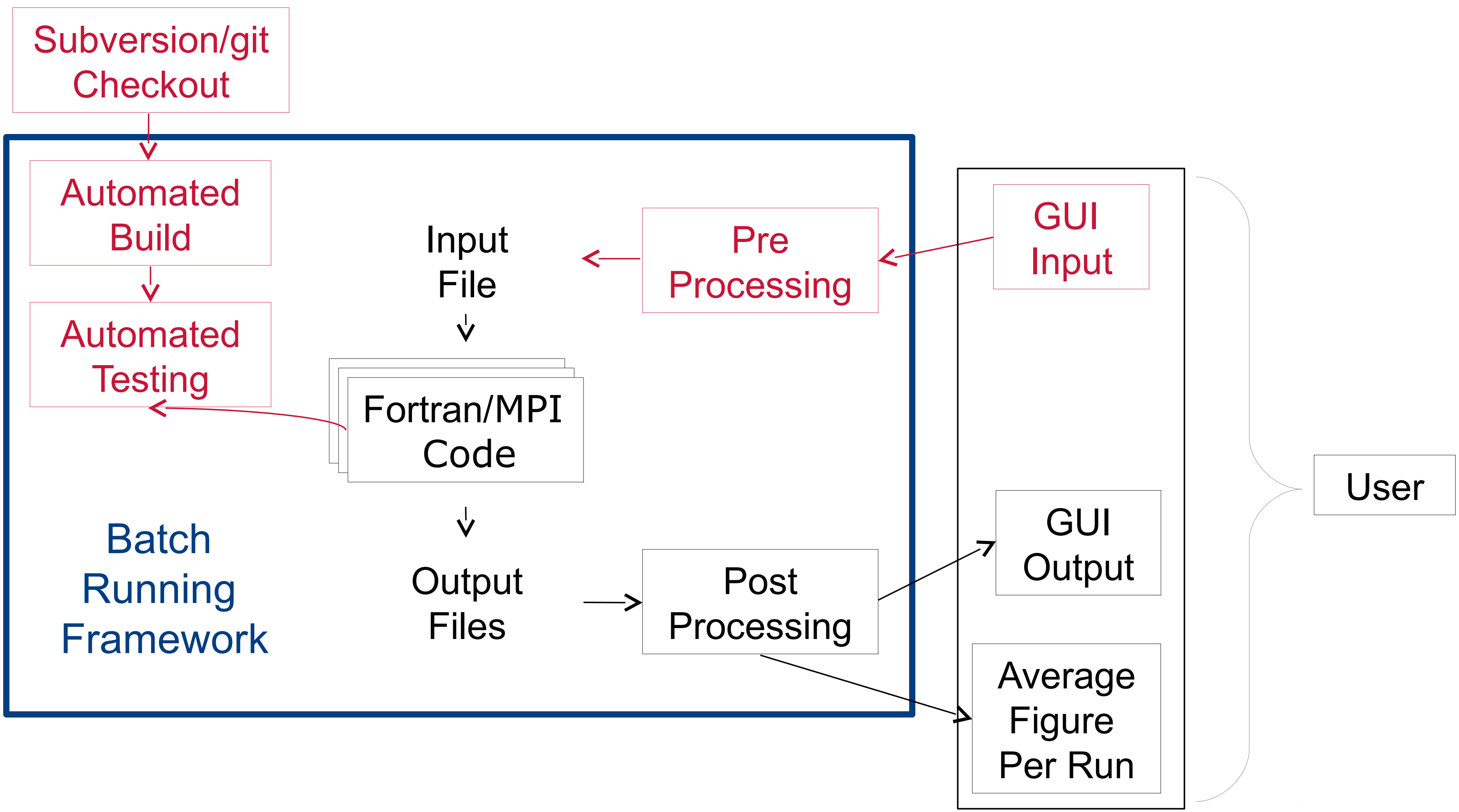
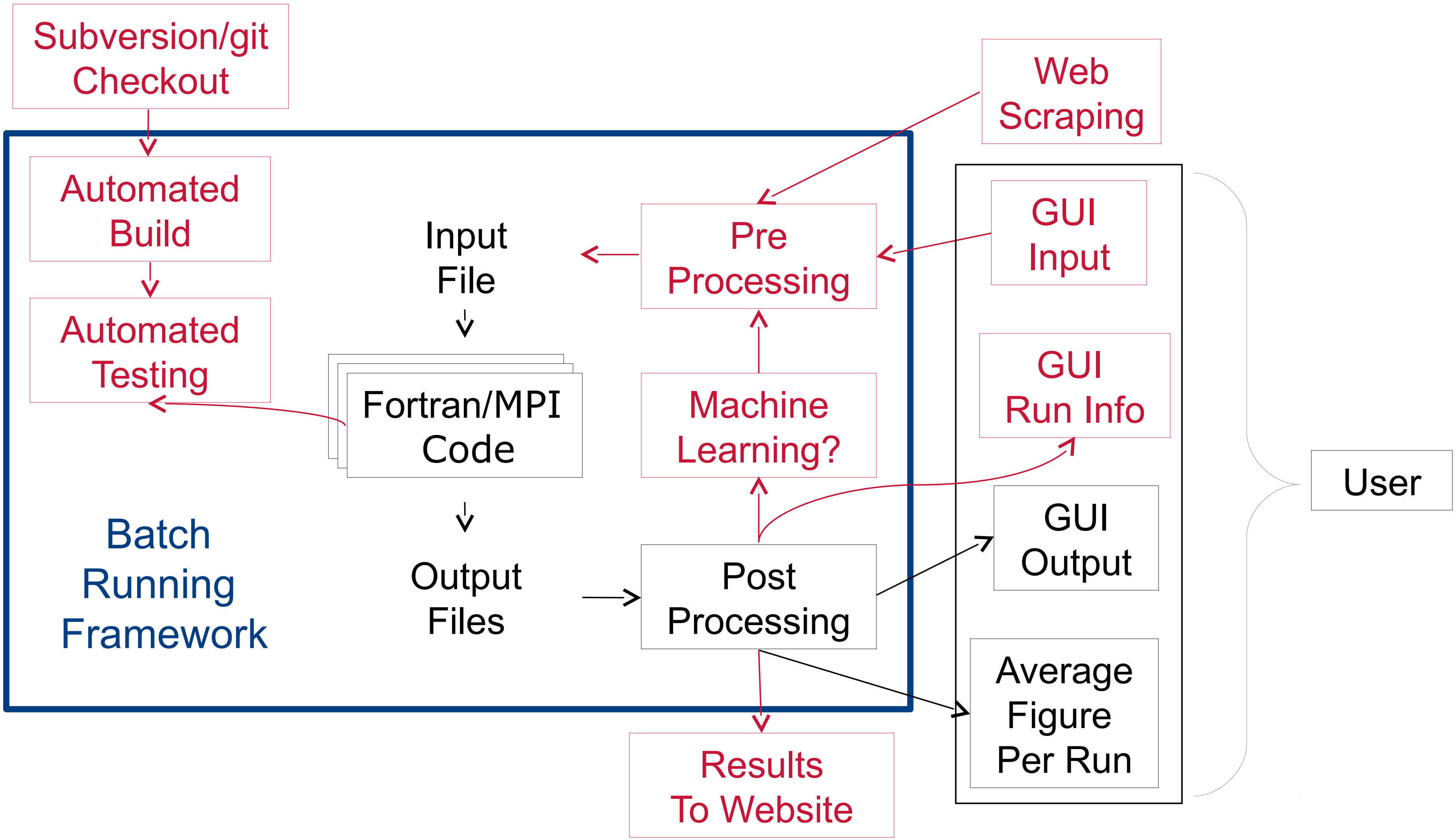
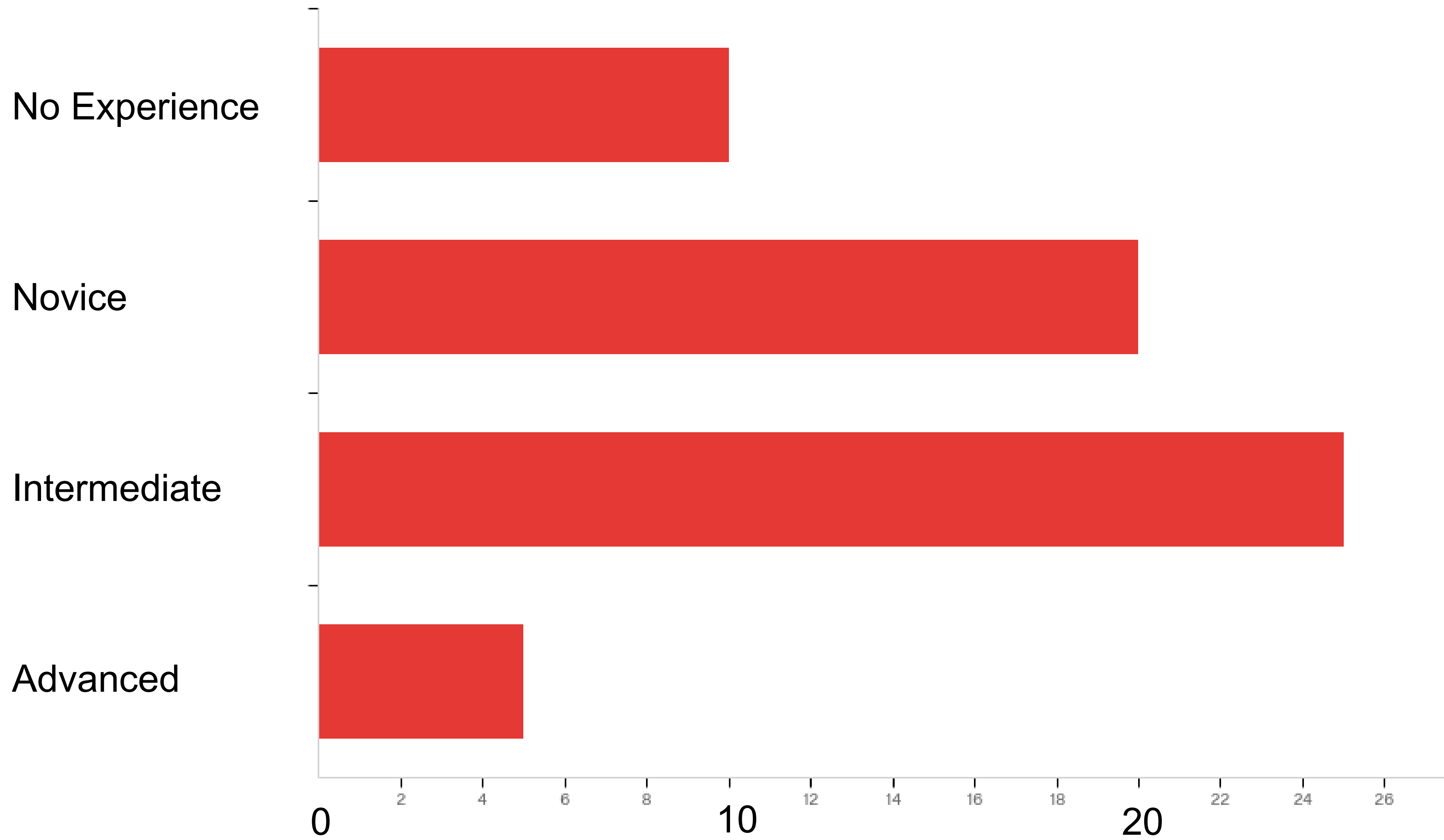


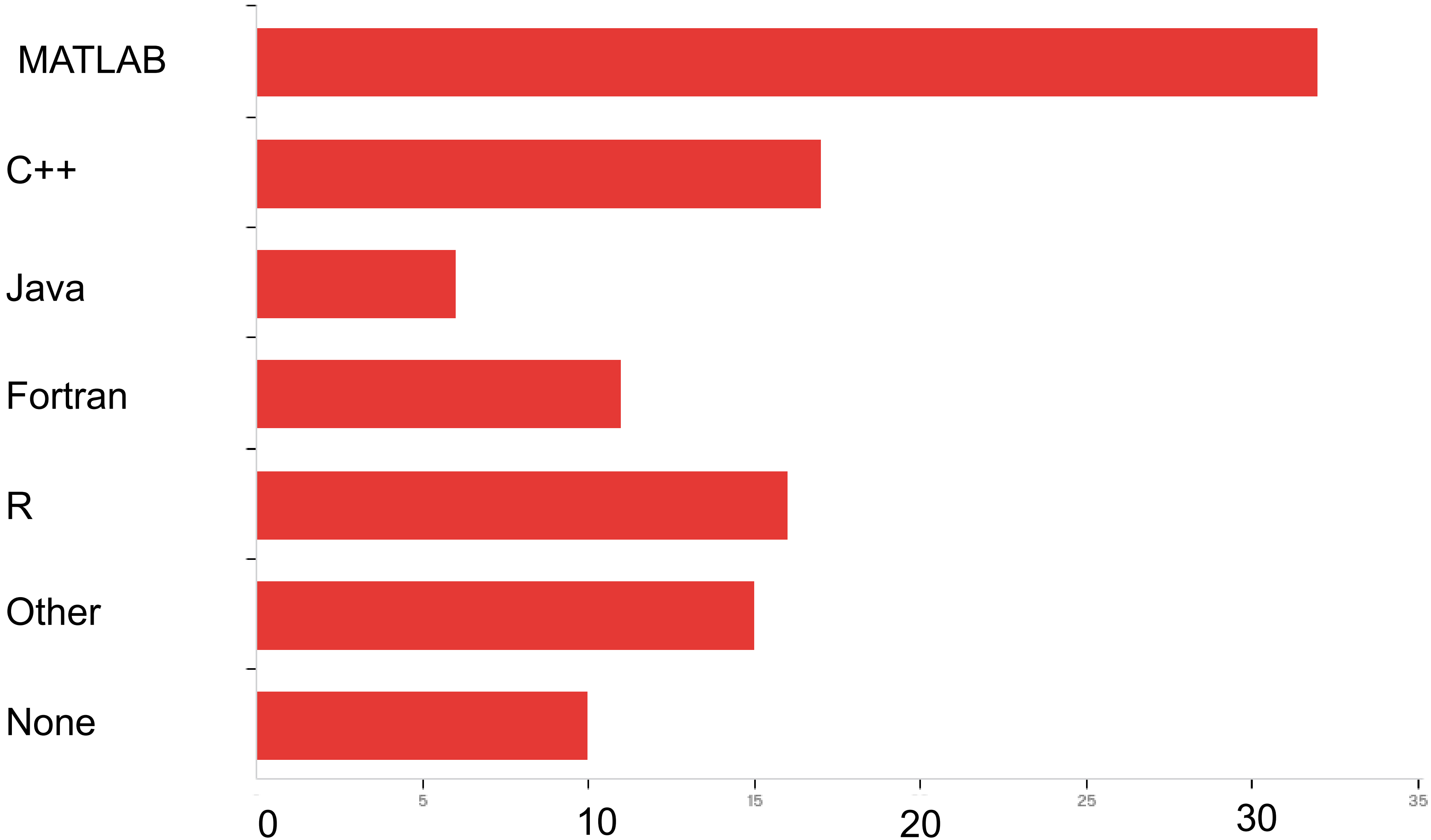
Possible Future Extensions



Your Programming Experience



Your Language Background



Python VS MATLAB (and R?)

VS

An Example

```
%MATLAB
clear all
close all

x = linspace(0,2*pi,100);
y = sin(x);
z = cos(x);
plot(x,y,'-r');
hold all
plot(x,z,'-b')
```

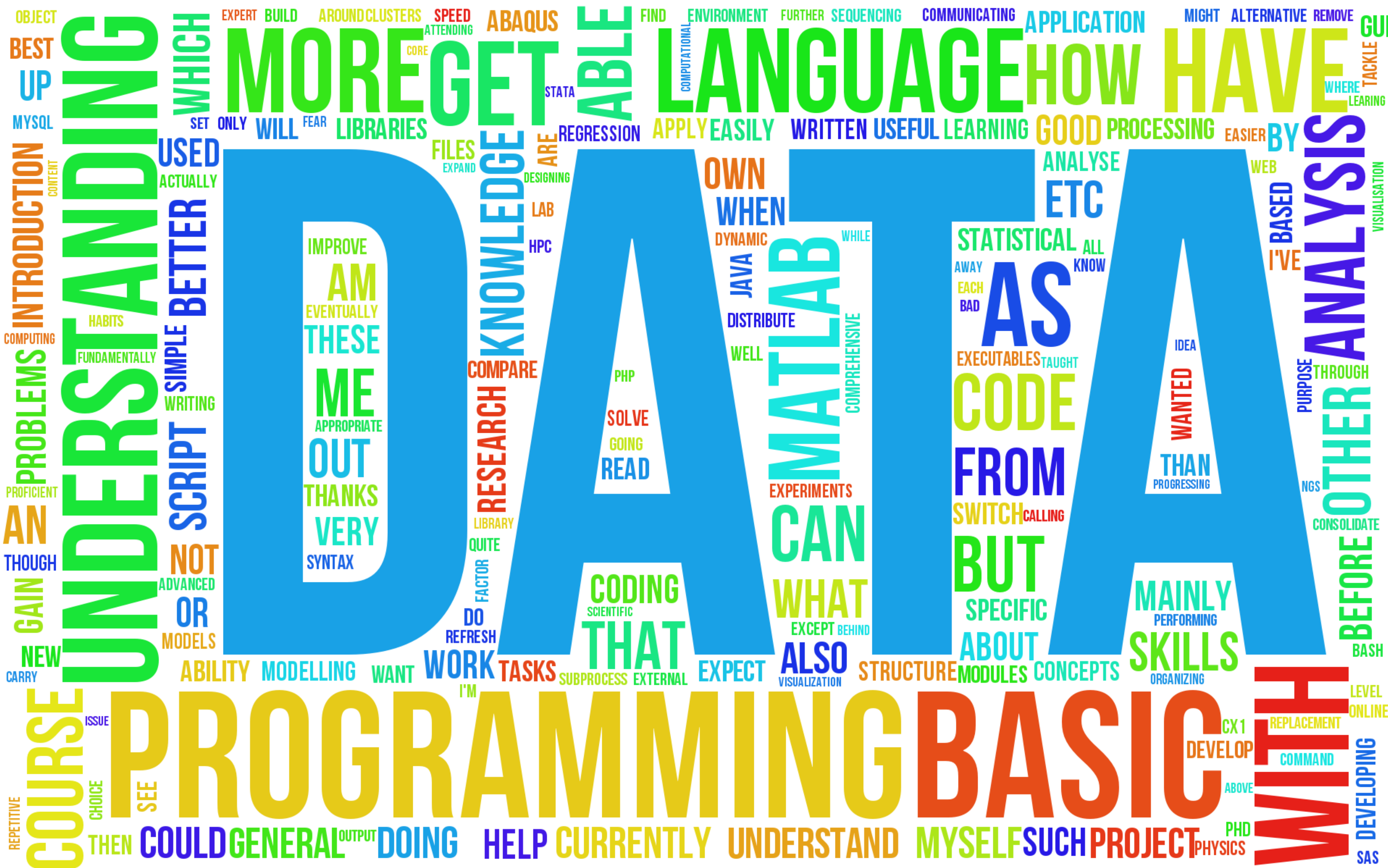
```
#python
import numpy as np
import matplotlib.pyplot as plt

x = np.linspace(0, 2*np.pi, 100)
y = np.sin(x)
z = np.cos(x)
plt.plot(x, y, '-r')
plt.plot(x, z, '-b')
plt.show()
```

Some of your aims for the course

- Learn basics of python, ability to switch away from Matlab …
- Improve my very basic knowledge of Python and understand the advantages of coding in general
- Introduction to Python-specifics (syntax, data types?, ...) rather than general programming concepts.
- Basic understanding of Python so that I can implement it with [PLUG IN] to speed up post-processing of data etc.
- Quite a few scripts that I am using for analysis … are written in Python so I would like to be able to understand better
- See what python could help me while doing research. Get the idea of Object Oriented Programming …
- Using python for Data processing and analysis. A general feel for other uses such as modelling.
- An understanding of a programming language that is currently in high demand.

Some of your aims for the course



My aims for the course

- A focus on the strange or unique features of python as well as common sources of mistakes or confusion
- Help with the initial frustration of learning a new language
- Prevent subtle or undetected errors in later code
- Make sure the course is still useful to the wide range of background experiences

My aims for the course

- Show how to use the command prompt to quickly learn Python
- Introduce a range of data types (Note everything is an object)

```
a = 3.141592653589          # Float
i = 3                       # Integer
s = "some string"           # String
l = [1,2,3]                 # List, note square brackets tuple if ()
d = {”red”:4, ”blue”:5}     # Dictonary
x = np.array([1,2,3])       # Numpy array
```

- Show how to use them in other constructs including conditionals (if statements) iterators (for loops) and functions (def name)
- Introduce external libraries numpy and matplotlib for scientific computing

Key Concepts - Types

- Use the python command prompt as a calculator

```
3.141592653589*3.0     Out: 9.424777961
```

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- Define variables as one of several types

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a = 3.141592653589          # Float
i = 3                       # Integer
```

Variables stay defined (Their "scope") for duration of python session (or script).

Syntax here means: "Define a to be 3.141592653589" and "define i to be 3"

Key Concepts - Types

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- We can then perform the same calculations using variables

```
a * i    Out: 9.42477796076938          # But float*integer
```

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3.141592653589*3.0     Out: 9.424777961
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- We can then perform the same calculations using variables

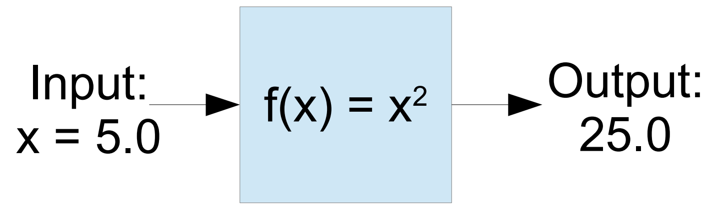
```
a * i     Out: 9.42477796076938         # But float*integer
2 / i     Out: 0                        # WATCH OUT FOR int/int
2./ i     Out: 0.6666666666666          # Use floats for division
2/float(i)  Out: 0.6666666666666        # Explicit conversion
histogram_entry = int(value/binsize) # Integer rounds up/down
```

Key Concepts - Functions

- Check type with

```
type(a)     Out: float
type(i)     Out: int
```

- type(), float() and int() are all examples of functions, i.e.
  - take some input,
  - perform some operation
  - return an output



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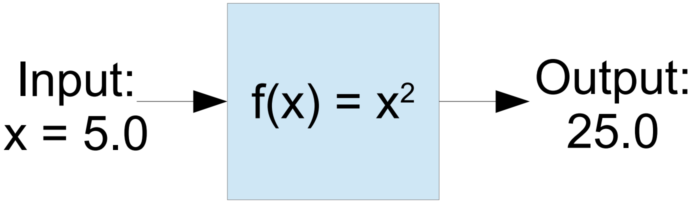


Note: indent whitespace instead of end

```
def square(input):
    """Function to calculate the
       square of a number"""
    output = input*input
    return output
```

```
#Now we can use this
square(5.0) Out: 25.0
```

Key Concepts – Function Syntax

```
#Define a variable
a = 5.0
```

Comment

Function name

Tell Python you are defining a function

Name of input variable to the function

```
#Define Function

def square(input):
    "calculate square"
    output = input*input
    return output
```

Document function here "text" for one line or """ multi-line verbose and descriptive text """

Level of indent determines what is inside the function definition. Variables defined (scope) exists only inside function. Ideally 4 spaces and avoid tabs. See PEP 8

Operation on input variable

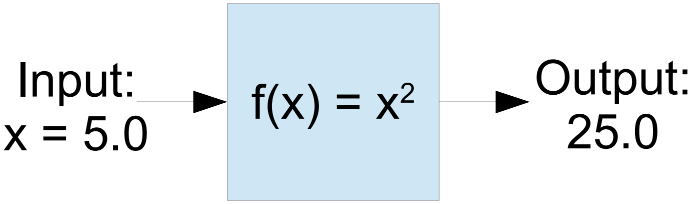
Value to return from function

```
#We call the function like this
square(a) Out: 25.0
```

Key Concepts - Functions

- Note that the input and ouput type are not specified

```
def square(input):
    "calculate square"
    output = input*input
    return output
#Now we can use this
square(5.0) Out: 25.0
square(5)   Out: 25
```



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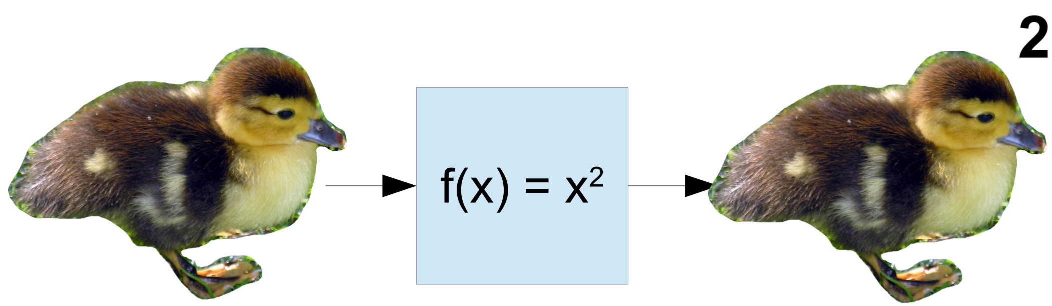


- Python allows "duck typing":
  - "If it looks like a duck and quacks like a duck, it's a duck"
  - Both useful and a possible source of error
  - TypeError: unsupported operand type(s)

Examples of Functions

- take some inputs
- perform some operation
- return outputs

Input → f(a, b, …, z) → Output

```
def divide(a, b):
    output = a/b
    return output
```

```
def do_nothing(a, b):
    a+b
```

```
def get_27():
    return 27
#Call using
get_27()
```

```
def redundant(a, b):
    return b
```

```
def line(m, x, c=3):
    y = m*x + c
    return y
```

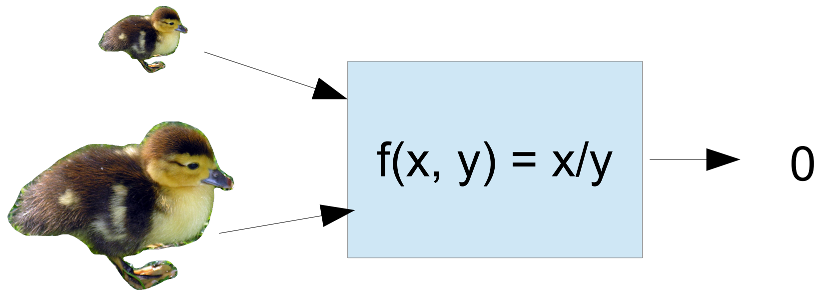
Optional variable. Given a value if not specified

```
def quadratic(a, b, c):
    "Solve: y = ax^2 + bx + c"
    D = b**2 + 4*a*c
    sol1 = (-b + D**0.5)/(2*a)
    sol2 = (-b - D**0.5)/(2*a)
    return sol1, sol2
```

Key Concepts - Functions

- Note that the input and ouput type are not specified

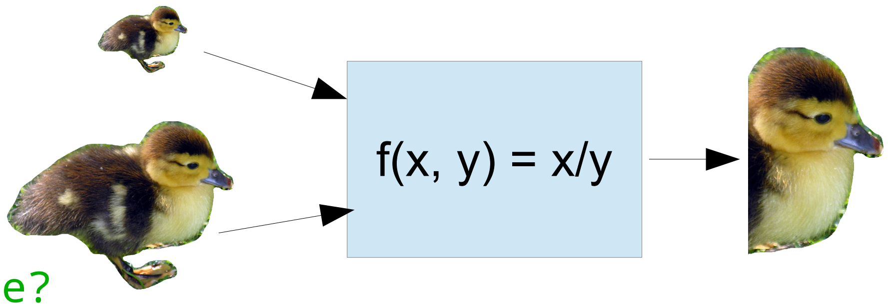
```
#Function to divide one number by another
def divide(a, b):
    output = a/b
    return output
#Which gives us
divide(2,5) Out: 0
```



Key Concepts - Functions

- Note that the input and ouput type are not specified

```
#Function to divide one number by another
def divide(a, b):
    output = a/b
    return output
#Which gives us
divide(2,5) Out: 0
#Maybe more sensible to define?
def divide(a, b):
    output = float(a)/float(b)
    return output
divide(2,5) Out: 0.4
```



You can look at function information with:
help(square) in python
In ipython, also square? Or to see the code: square??

Key Concepts - Conditionals

- Allow logical tests

```python
#Example of an if statement
if a > b:
    print(a)
else:
    print(a, b)
```

Logical test to determine which branch of the code is run

```python
if a < b:
    out = a
elif a == b:
    c = a * b
    out = c
else:
    out = b
```

Indent determine scope
4 spaces here

```python
if type(a) is int:
    a = a + b
else:
    print("Error – a is type ", type(a))
```

Key Concepts - Functions

- Note that the input and ouput type are not specified

```
#Add a check
def divide(a, b):
    if ((type(a) is int) and
        (type(b) is int)):
        raise TypeError
    else:
        return a/b
```

Key Concepts - Functions

- Note that the input and ouput type are not specified

```
#Add a check
def divide(a, b):
    if ((type(a) is int) and
        (type(b) is int)):
        raise TypeError
    else:
        return a/b
```

- Python error Handling – Better to ask forgiveness than seek permission

```
try:
    c = divide(a, b)
    print(c)
except TypeError:
    print("Cannot divide a=", a, " by b=", b)
```

Part 1 Summary

- Two numerical types, floats and Integers

  a = 2.5251

  i = 5

You can look at function information with:
help(type) in python
In ipython, also type? Or to see the code: type??

- Functions allow set operations

```
def divide(a, b):
    output = a/b
    return output
```

Some Functions

type(in) – get type of in

int(in), float(in) – Convert in to int, float

help(in) – Get help on in

- Conditional statement

```
if a > b:
    print(a)
elif a < b
    print(b)
else:
    print(a, b)
```

Design to prevent potential errors caused by Python's duck typing and lack of type checking

Hands on session 1 – Tutors

- Isaac and Edu

- Ask the person next to you – there is a wide range of programming experience in this room and things are only obvious if you've done them before!

Hands on session 1 – Questions

- Introduction
  1) Get Python (ideally ipython) working... Please help each other here.
  2) Play around with basic arithmetic. Does this behave as expected? Note exceptions
  3) What does this do? i=3; i = i + 1
  4) Write a function to add two numbers and always return a float
  5) Use an if statement to print the larger of a or b
  6) Define a function to raise a floating point number to an integer power N. What changes would you need to make to raise to non-integer powers?
- More advanced
  1) Write a function which combines both 4) and 6) above to get the hypotenuse of a triangle from two side lenghts $h^2 = o^2 + a^2$
  2) What does the function here do ==========>
  3) Write a recursive factorial function

```
def add_fn(a, b, fn):
    return fn(a) + fn(b)
```

Key Concepts - Types

Define variables as one of several types

```
a = 3.141592653589        # Float
i = 3                     # Integer
s = "some string"         # String
```

Strings

- String manipulations

```
s = "some string"

t = s + " with more"    Out: "some string with more"

s*3   Out: "some stringsome stringsome string"

s[3]                               Out: e

s[0:4]                             Out: some
```

Strings

- String manipulations

```
s = "some string"
t = s + " with more"     Out: "some string with more"
s*3   Out: "some stringsome stringsome string"
s[3]                            Out: e
s[0:4]                          Out: some
s.title()                       Out: 'Some String'
s.capitalize()                  Out: "Some string"
s.find("x")                     Out: -1    #Not found
s.find("o")                     Out: 1
t = s.replace("some", "a")      Out: t="a string"
```

Note object oriented use of a function here. Instead of title(s) we have s.title(). The object s is automatically passed to the title function. A function in this form is called a method (c.f. c++ member function)

- In ipython, use tab to check what functions (methods) are avaliable

Strings

- Useful for opening and reading files (Saved as a string)

```
#Get data from file
fdir = "C:/path/to/file/"
f = open(fdir + './log')
filestr = f.read()

w = "keyword"
if w in filestr:
    indx = filestr.find(w)
    print(int(filestr[indx+len(w)+1]))
Out: 4
```

Note object oriented use of a function (method). Instead of read(f) we have f.read(). The object f is automatically passed to the read function.

All the contents of the file are read in as a string. This can be manipulated. E.g. if filestr = "contents of the file with some keyword=4 hidden inside"

Key Concepts - Types

Define variables as one of several types

```
a = 3.141592653589      # Float
i = 3                   # Integer
s = "some string"       # String
l = [1,2,3]             # List, note square brackets tuple if ()
```

Lists

- Lists of integers

```
l = [1,2,3]

l = l + [4]     #Note l.append(4) is an alternative

Out: [1,2,3,4]
```

- We can make lists of any type

```
m = ["another string", 3, 3.141592653589793, [5,6]]

print(m[0], m[3][0])     #Note indexing starts from zero

Out: ("another string“, 5)
```

- But, these don't work in the same way as arrays

```
l * 2  Out: [1, 2, 3, 4, 1, 2, 3, 4]

l * 2.0 Out: TypeError: can't multiply sequence by non-int of type 'float'
```

Loops or iterators

- Iterators – loop through the contents of a list

```
m = ["another string", 3, 3.141592653589793, [5,6]]

for item in m:

    print(type(item), " with value ", item)
```

Loops or iterators

- Iterators – loop through the contents of a list

```
m = ["another string", 3, 3.141592653589793, [5,6]]
for item in m:
    print(type(item), " with value ", item)
```

- Slightly more cumbersome for indexing

```
l = [1,2,3,4]
for i in range(4):
    print("element", i, " is ", l[i] )
```

len(l) returns 4
range(4) returns a list with 4: [0,1,2,3]

Loops or iterators

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len(l) returns 4
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- To add one to every element we could use

```
for i in range(len(l)):
    l[i] = l[i] + 1
```

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```
for i in range(len(l)):
    l[i] = l[i] + 1
```

Note: will not work:

```
for i in l:
    i = i + 1
```

List comprehension
l = [i+1 for i in l]

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Define variables as one of several types

```
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i = 3                     # Integer
s = "some string"         # String
l = [1,2,3]               # List, note square brackets tuple if ()
d = {"red":4, "blue":5}   # Dictonary
```

Dictionaries

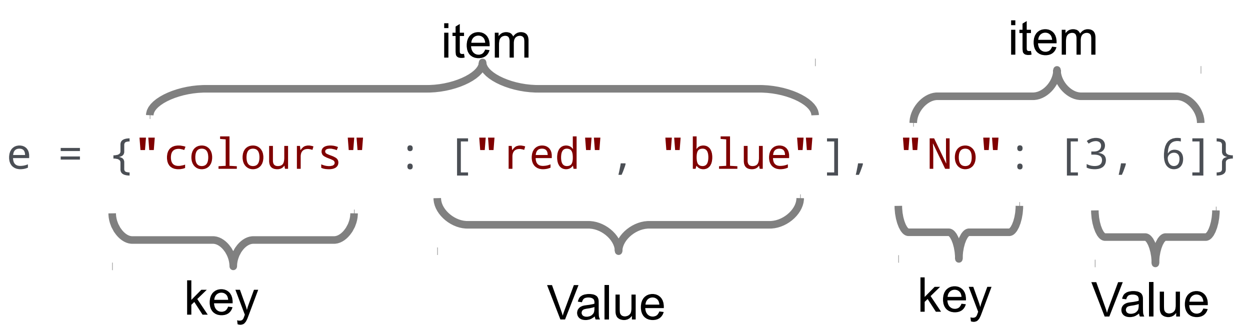
- Dictonaries for more complex data storage

```
d = {"red":4, "blue":5}     #Dictonary
d["green"] = 6              #Adds an entry
print(d)
```

- Instead of numerical index, use a word to access elements

```
print(d["red"])
```

- Useful for building more complex data storage




```
e.items()

e.keys()
e.values()
```

Dictionaries

- Dictonaries are for more complex data storage

```
e = {"colours" : ["red", "blue"], "No": [3, 6]} #Dictonary
e["colours"]    out: ["red", "blue"]
```

- Elements can also be accessed using key iterators

```
for key in e.keys():
    print(key, e[key])
```

```
Out: ("colours", ["red", "blue"])
     ("No", [3, 6])
```

Dictionaries

- Could be used instead of variables, consider F=ma

```
Newton = {}

Newton["F"] = 2.

Newton["m"] = 0.5

Newton["a"] = Newton["F"]/Newton["m"]
```

- More importantly, variables do not need to be know in advance

```
Newton = {}
f = open('./log')
for l in f.readlines():
    key, value = l.split()
    Newton[key] = float(value)
```

```
### log file ###
Nsteps 1000
domain_x 10.0
domain_y 20.0
timestep 0.5
Nx       100
Ny       200
```

Part 2 Summary

- Strings

```
s = "some string"
t = s + " with more"
```

- Lists and dictonaries

```
m = ["another string", 3, 3.141592653589793, [5,6]] #List
d = {"red":4, "blue":5}     #Dictonary
```

- Iterators (loops)

```
 for item in m:
     print(type(item), " with value ", item)
#Loop with numbers
 for i in range(10):
     print(i)
```

Hands on session 2 – Questions

- Introduction
  1) Build a sentence s by defining and adding the 4 strings ”is” ,”a”, ”this” and ”sentence” in the right order. Capitalise the first letter of each of the words. Print the first letter of each word. (note no unique way to do these).
  2) Write a loop to print 10 strings with names: "filename0", "filename1", … "filename9" (note str(i) converts an int to a string)
  3) Define two lists, one for odd and one for even numbers less than 10. Combine them to form a list of all numbers in the order [1,2,3,4,5,6,7,8,9].
  4) Using keys ”even”, ”odd” and ”combined” put lists from 3) in a single dictonary.
  5) Using l = [1,2,3], write a loop to add a number to all elements giving [2,3,4]. Write a function to take in a list l and number N, which adds N to all elements of l.
- More advanced
  1) For the string s=”test” and the list l = [”t”,”e”,”s”,”t”], we see s[0] == l[0], s[1] == l[1]. Are they equal? Can you convert the string to a list? What about list to string?
  2) Define a = [1,2,3]; b = a; b.append(4). Why does a = [1,2,3,4]?

     what about if you use b = b + [4] instead of append?

Numerical and Plotting Libraries

- Numpy – The basis for all other numerical packages to allow arrays instead of lists (implemented in c so more efficient)
  - `x = np.array([[1,2,3],[4,5,6],[7,8,9]])`
  - `mean, std, linspace, sin, cos, pi, etc`
- Matplotlib – similar plotting functionality to MATLAB
  - `plot, scatter, hist, bar, contourf, imagesc (imshow), etc`
- Scipy
  - Replaces lots of the MATLAB toolboxes with optimisation, curve fitting, regression, etc
- Pandas
  - Dataframes to organise, perform statistics and plot data

NOTE: Downloading and installing packages is trivial with “pip” or conda

Importing Numerical and Plotting Libraries

- Numpy – The basis for all other numerical packages to allow arrays instead of lists (implemented in c so more efficient)

```
import numpy as np
x = np.array([[1,2,3],[4,5,6],[7,8,9]])
```

$$x = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{pmatrix}$$

Import module numpy and name np
Similar to:
- c++ #include
- Fortran use
- R source()
- java import (I think...)
- MATLAB adding code to path

Dot means use array from module numpy.
The numpy module is just a big collection of Python code where array (and many other things) are defined.

Use tab in ipython to see what code is available (or look online)

Key Concepts - Types

Define variables as one of several types

```
a = 3.141592653589        # Float
i = 3                     # Integer
s = "some string"         # String
l = [1,2,3]               # List, note square brackets tuple if ()
d = {"red":4, "blue":5}   # Dictonary
x = np.array([1,2,3])     # Numpy array
```

Key Concepts – Arrays of data

- Lists of lists seem similar to matrices or arrays.

```
m = [[1,2,3],[4,5,6],[7,8,9]]
m[0][1]     Out: 2
m[1][2]     Out: 6
```

$$m = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{pmatrix}$$

Key Concepts – Arrays of data

- Lists of lists seem similar to matrices or arrays.They are not!

```
m = [[1,2,3],[4,5,6],[7,8,9]]

m[0][1]    Out: 2

m[1][2]    Out: 6
```

m =

- Lists are dynamic, you can add values and mix datatypes

Key Concepts – Arrays of data

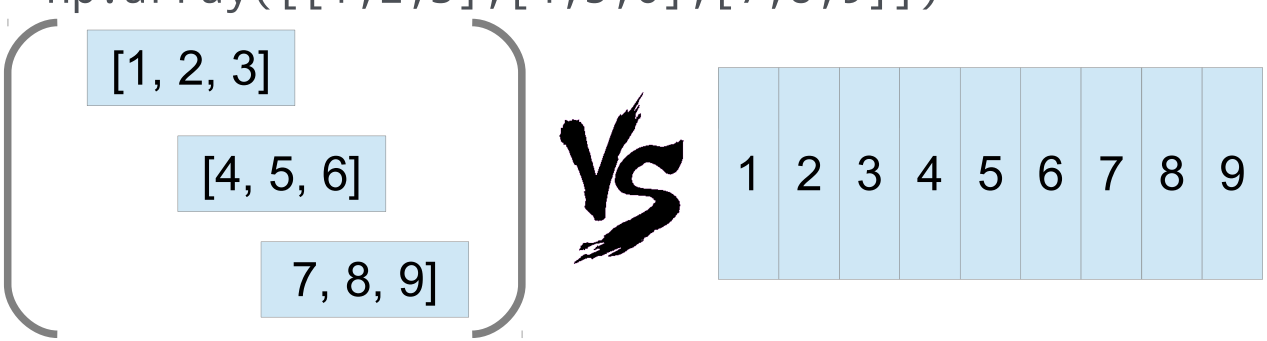
- Lists of lists seem similar to matrices or arrays. They are not!

```
m = [[1,2,3],[4,5,6],[7,8,9]]
m[0][1]     Out: 2
m[1][2]     Out: 6
```

m = 

- Lists are dynamic, you can add values and mix datatypes
- For numerics, use Numpy arrays which are contigous memory implemented in c (more efficient)

```
import numpy as np
x = np.array([[1,2,3],[4,5,6],[7,8,9]])
```



Key Concepts – Arrays of data

- Numpy – the basis for most numerical work (implemented in c so more efficient). Should be all the same type

$$x = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{pmatrix}$$

```
import numpy as np
x = np.array([[1,2,3],[4,5,6],[7,8,9]])
y = x * 2     #Array operations
x.T           #Transpose array
x * y         #Elementwise (eqiv to MATLAB x .* y)
np.dot(x,y)   #Matrix multiply
# Invert matrix using linera algebra submodule of numpy
invy = np.linalg.inv(y)
```

- Numpy has a wide range of functions. As it is written in c, it is often faster to perform operations with numpy instead of loops

Key Concepts – Arrays of data

- Numpy arrays similar to MATLAB, Fortran, C++ std::array, R, Java?

```
import numpy as np
x = np.array([[1,2,3],[4,5,6],[7,8,9]])
print(x[:,0])   #Out: Array([1, 4, 7])
print(x[1,:])   #Out: Array([4, 5, 6])
for i in range(x.shape[0]):
    for j in range(x.shape[1]):
        print(x[i,j])
```

$$x = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{pmatrix}$$

Method to get shape returns 2 elements for a 2D array, accessed by index

- Numpy allows statistical operations

```
x.mean()        Out: 5.0       (Note np.mean(x) equivalent)
x.std()          Out: 2.5819888974716112  (Also np.std(x))
np.median(x)    Out: 5.0  (But x.median doesn't work!!)
np.gradient(x)  Out: Numerical diff x_{i+1} - x_i (No x.gradient either)
```

Importing Numerical and Plotting Libraries

- matplotlib – similar plotting functionality to MATLAB

```
import matplotlib.pyplot as plt
plt.plot(x)
plt.show()
```

We need the pyplot submodule of matplotlib for most things. Dot uses plot/show from matplotlib.pyplot

Use tab in ipython to see what is available (or look online)

An Example vs MATLAB

Import Plotting module matplotlib as plt

```
%MATLAB
clear all
close all

x = linspace(0,2*pi,100);
y = sin(x);
z = cos(x);
plot(x,y,'-r');
hold all
plot(x,z,'-b')
```

```
#python
import numpy as np
import matplotlib.pyplot as plt

x = np.linspace(0,2*np.pi,100)
y = np.sin(x)
z = np.cos(x)
plt.plot(x,y,"-r")
plt.plot(x,z,"-b")
plt.show()
```

Use plot function from plt module

Plotting syntax based on MATLAB

An Example vs MATLAB

```
%MATLAB
clear all
close all

x = linspace(0,2*pi,100);
y = sin(x);
z = cos(x);
plot(x,y,'-r');
hold all
plot(x,z,'-b')
```

```
#python
from numpy import *
from matplotlib.pyplot import *

x = linspace(0,2*pi,100)
y = sin(x)
z = cos(x)
plot(x,y,"-r")
plot(x,z,"-b")
show()
```

Import all

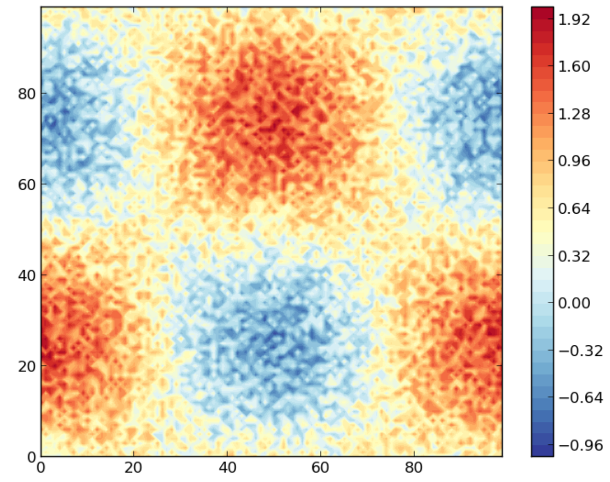
plot function has been imported

Better not to do this to avoid nameclashes

An Example plotting a histogram

```
import numpy as np
import matplotlib.pyplot as plt


#10,000 Uniform random numbers
x = np.random.random(10000)
#10,000 Normally distributed random numbers
y = np.random.randn(10000)
#Plot both on a histogram with 50 bins
plt.hist(y, 50)
plt.hist(x, 50)
plt.show()
```

An Example plotting a 2D field (matrix)

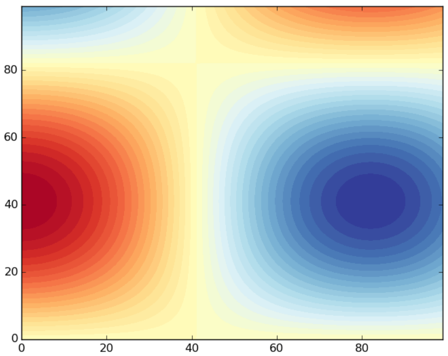


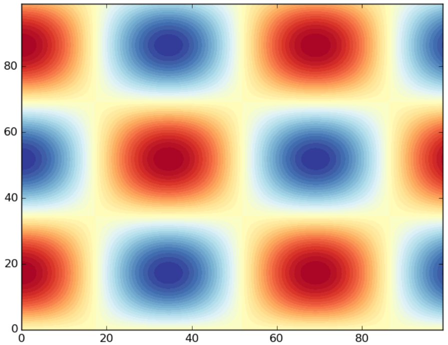

```python
import numpy as np
import matplotlib.pyplot as plt


N = 100
x = np.linspace(0,2*np.pi,N)
y = np.sin(x); z = np.cos(x)
#Create 2D field from outer product of previous 1D functions
u = np.outer(y,z) + np.random.random([N,N])
plt.contourf(u, 40, cmap=plt.cm.RdYlBu_r)
plt.colorbar()
plt.show()
```

Don't use Jet colormap

An Example plotting a 2D field + function + loop

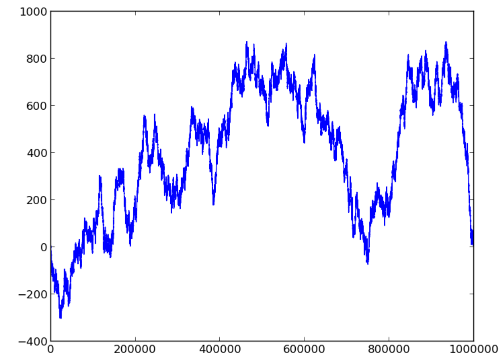
```
import numpy as np
import matplotlib.pyplot as plt
def get_field(a, N = 100):
    x = a*np.linspace(0,2*np.pi,N)
    y = np.sin(x); z = np.cos(x)
    return np.outer(y,z)
plt.ion(); plt.show()   #Interactive plot
for i in np.linspace(0., 5., 200):
    u = get_field(i)    #Call function with new
    plt.contourf(u, 40, cmap=plt.cm.RdYlBu_r)
    plt.pause(0.01)   #Pause to allow redraw
    plt.cla()   #Clear axis for next plot
```

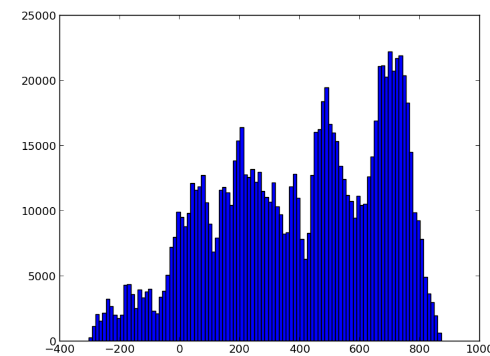


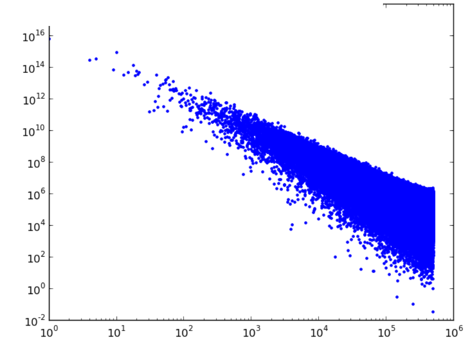


An Example using time series

```
plt.ioff()
import numpy as np
import matplotlib.pyplot as plt


N = 1000000
signal = np.cumsum(np.random.randn(N))
plt.plot(signal); plt.show()
plt.hist(signal, 100); plt.show()
Fs = np.fft.fft(signal)**2
plt.plot(Fs.real[:N/2], ".")
plt.xscale("log"); plt.yscale("log")
plt.show()
```







An Example using data from a csv file

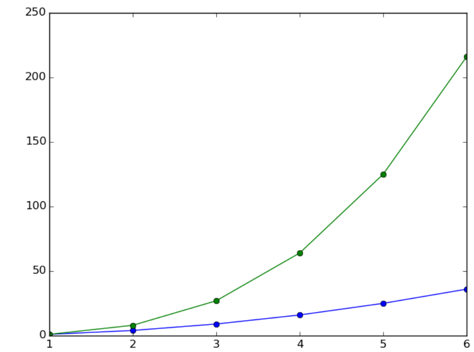
```
import numpy as np
import matplotlib.pyplot as plt

#Read data from comma seperated variable file
data = np.genfromtxt("./file.csv", delimiter=',')

#Store columns as new variables x and y
x = data[:,0]
y = data[:,1]
plt.plot(x,y,"-or")
plt.show()
```

file.csv

```
x,    y
1.0, 1.0
2.0, 4.0
3.0, 9.0
4.0, 16.0
5.0, 25.0
6.0, 36.0
```

An Example using data from a csv file + function

```
import numpy as np
import matplotlib.pyplot as plt


def read_file(filename):
    data = np.genfromtxt(filename, delimiter=',')
    x = data[:,0]; y = data[:,1]
    return x, y


for filename in ["sqr.csv", "cube.csv"]:
    x, y = read_file(filename)
    plt.plot(x, y, "-o")
plt.show()
```



sqr.csv

```
x,   y
1.0, 1.0
2.0, 4.0
3.0, 9.0
4.0, 16.0
5.0, 25.0
6.0, 36.0
```

cube.csv

```
x,   y
1.0, 1.0
2.0, 8.0
3.0, 27.0
4.0, 64.0
5.0, 125.0
6.0, 216.0
```

Reading from files

- Opening and finding keywords in file

```
#Find a keyword in file and read numbers to the left
with open('./log') as f:
    for l in f.readlines():
        if l.find("timestep") != -1:
            dt = float(l.strip('timestep'))
            break
```

```
### log file ###
Nsteps 1000
domain_x 10.0
domain_y 20.0
timestep 0.5
Nx      100
Ny      200
```

- Reading binary data (see e.g. stackoverflow)

```
with open('./log.bin', 'rb') as f:
    filecontent = f.read()
struct.unpack("iii", filecontent)  #Need to import struct
```

Overview

- Show how to use the command prompt to quickly learn Python
- Introduce a range of data types (Note everything is an object)

```
a = 3.141592653589          # Float
i = 3                       # Integer
s = "some string"           # String
l = [1,2,3]                 # List, note square brackets tuple if ()
d = {”red”:4, ”blue”:5}     # Dictonary
x = np.array([1,2,3])       # Numpy array
```

- Show how to use them in other constructs including conditionals (if statements) iterators (for loops) and functions (def name)
- Introduce external libraries numpy and matplotlib for scientific computing

Other libraries

- Graphical User Interfaces (GUI) e.g. Tkinter, wxpython, pyGTK, pyQT
- Multi-threading and parallel e.g. Subprocess, MPI
- Image and video manipulation e.g. pyCV, PIL
- Machine learning e.g. Scikit-learn, Pybrain
- Build system e.g. scons, make using os/system
- Differential equations solvers e.g. FEniCS, Firedrake
- Databasing and file storage e.g. h5py, pysqlite
- Web and networking e.g. HTTPLib2, twisted, django, flask
- Web scraping – e.g. scrapy, beautiful soup
- Any many others, e.g. PyGame, maps, audio, cryptography, etc, etc
- Wrappers/Glue for accelerated code e.g. HOOMD, PyFR (CUDA)
- It is also possible to roll your own

Summary

- Background and motivations for this talk
  - MATLAB is the main programming language taught at Imperial
  - Python provides similar plotting, numerical analysis and more
- Some key concepts
  - Data types, lists/arrays, conditionals, iterators and functions
  - Modules for scientific computing: numpy and matplotlib
  - Clean syntax, ease of use but no checking!
- Advantages of learning Python
  - General programming (better both in academia and outside)
  - Allows an integrated framework and can be bundled with code
  - Open source libraries with tutorials and excellent help online

What to do next?

- Find a project
  - Use Python instead of your desktop calculator
  - Ideally something at work and outside
- Use search engines for help, Python is ubiquitous so often you can find sample code and tutorials for exactly your problem
  - Stackoverflow is often the best source of explanation
  - Official documentation is okay as a reference but not introductory, look for many excellent tutorials, guides and videos
  - help(function) in python. Tab, ? or ?? in ipython
- Be prepared for initial frustration!
  - Worth the effort to learn

Next Week

- Next Friday 10th March, 2017 14:15-16:15 SAF 120
- Further details of the Python language

  a) More on Python data structures.

  b) Use of functions and design of interfaces.

  c) Introduction to classes and objects.

  d) Structuring a project, importing modules and writing tests.

  e) Examples of usage for scientific problems.

- Please provide feedback on the quadratics form (link on your email) to help tailor the course

Hands on session 3 – Questions

- Introduction
  1) Import numpy and matplotlib. These may not be installed so you will need to use conda, pip, easy_install or some other means of getting them.
  2) Setup a 3 by 3 identity matrix I (ones on the diagonal, zeros off diagonal). Create a 3 by 3 array of random numbers r. Check np.dot(I,r) is as expected
  3) Plot a tanh function in the range -2 p to 2 pi using linspace and matplotlib plot.
  4) Create a 1D array of 10,000 normally distributed random numbers t. Plot as a time history and zoom in to see the detail.
  5) Plot a histrogram of the array t from question 4) with 50 bins.
  6) Convert array t to a 2D array using t.reshape(100,100) and plot using contourf.
  7) Create a comma seperated variable file (e.g. 2 columns in excel). Import into Python using `np.genfromtxt("./file.csv", delimiter=',')` and plot. Check against the plot from excel or other software.
- More Advanced/open ended
  - Apply python to read some data from your research. Use numpy to perform basic statistical tests (results as expected). Plot using matplotlib