Introduction to High Performance Scientific Computing

Autumn, 2016

Lecture 4

Imperial College London

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Functions

Basic idea: input → function → output

```
def function_name(input1,input2,inputN):
            #Code with operations involving input variables
            #that assigns values to output variables

            return output1,output2,outputM
```

- Again: extent of function "block" set by colon and indentation

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Functions: an example

Add three numbers:

```
In [5]: def sum3(x,y,z):
   ...:     #return sum of three numbers, x,y,z
   ...:     return x+y+z
   ...:

In [6]: sum3(1,2,3)
Out[6]: 6
```

- Function name is sum3 and can be called from command line
- Typically include functions in scripts and *import* them into command line (or other scripts)

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Functions: a few details

```
def example(x,y,z):
    '''Example of a python function,
    returns twice the first input variable
    and the product of the 2nd and 3rd input
    variables'''

    x2 = 2*x

    return x2,y*z

In [45]: from function_example import example

In [46]: example(1,2,3)
Out[46]: (2, 6)
```

- Here, we have *imported* the function into the terminal and called it with input 1,2,3 generating output 2,6
- *x2* is a *local* variable and cannot be accessed from the terminal…

Functions: a few details

```
In [45]: from function_example import example

In [46]: example(1,2,3)
Out[46]: (2, 6)

In [47]: x2
---------------------------------------------------------------------------
NameError                                 Traceback (most recent call
last)
<ipython-input-47-e2ee9ad17fdf> in <module>()
----> 1 x2

NameError: name 'x2' is not defined
```

- Here, we have *imported* the function into the terminal and called it with input 1,2,3 generating output 2,6
- *x2* is a *local* variable and cannot be accessed from the terminal…

Functions: a few details

- Be careful when sending a mutable object (*e.g.* a list) into a function: it can change!

```
def example2(x,y,z):
    '''Another example of a python function which
    returns twice the first input variable
    and the product of the 2nd and 3rd input
    variables, but now we assume that x is a list and
    only double its 1st element.'''

    x[0] = x[0]+1

    return x,y*z

In [98]: a=[1,2,3]

In [99]: example2(a,2,3)
Out[99]: ([2, 2, 3], 6)

In [100]: a
Out[100]: [2, 2, 3]
```

Functions: keyword arguments

- Can easily set default values for optional input arguments

```
def example3(x,y,z=1):
    '''Example of a python function,
    returns twice the first input variable
    and the product of the 2nd and 3rd input
    variables, and z has a default value of 1'''

    return 2*x,y*z

In [105]: example3(1,2,3)
Out[105]: (2, 6)

In [106]: example3(1,2)
Out[106]: (2, 2)
```

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Demo: computing sqrt with Newton's method

Newton's method: solve $f(x)=0$

1. guess solution x_1
2. compute $f(x_1)$
3. Is $f(x_1)$ sufficiently close to zero?
4. If not, compute df/dx and use Newton's formula to generate new guess, x_2
5. Repeat steps 2-4

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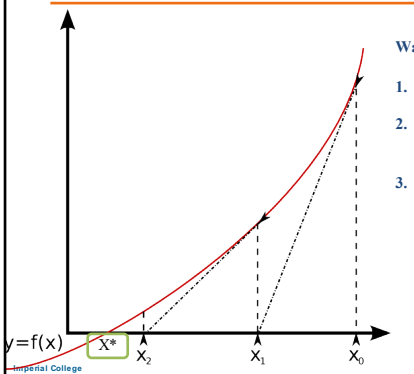
Demo: computing sqrt with Newton's method



Want to find x*:

1. Guess x0
2. Estimate x* based on tangent at x0
3. Repeat

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Demo: computing sqrt with Newton's method

We want to solve: $x = \sqrt{a}$

Or: $x^2 - a = 0$

with $\frac{df}{dx} = 2x$

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General Newton's method: $x_1 = -f_0 / \frac{df}{dx}|_{x_0} + x_0$

Here, x_0 is the initial guess

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For our function, Newton's method becomes:

$x_1 = \frac{a}{2x_0} + \frac{x_0}{2}$

Let's code this!

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Let's code this!: see *mysqrt.py for details*

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