# Introduction to Python Part 1

v0.2

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### **About You**

- Working with Python already?
- Have you used any other programming languages?
- Why do you want to learn Python?



# Running Python for the Tutorial

- If you have an SCC account, log into it and use Python there.
  - Run:

module load anaconda3 spyder &



### Links on the Rm 107 Terminals

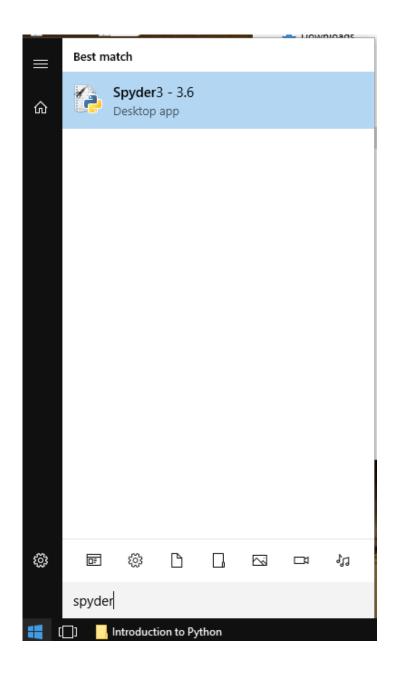
- On the Desktop open the folders:
   Tutorial Files → RCS\_Tutorials → Tutorial Files → Introduction to Python
- Copy the whole Introduction to Python folder to the desktop or to a flash drive.
  - When you log out the desktop copy will be deleted!





# Run Spyder

- Click on the Start Menu in the bottom left corner and type: spyder
- After a second or two it will be found. Click to run it.





# Running Python: Installing it yourself

- There are many ways to install Python on your laptop/PC/etc.
- https://www.python.org/downloads/
- https://www.anaconda.com/download/
- https://www.enthought.com/product/enthought-python-distribution/
- https://python-xy.github.io/





# BU's most popular option: Anaconda

- https://www.anaconda.com/download/
- Anaconda is a packaged set of programs including the Python language, a huge number of libraries, and several tools.
- These include the Spyder development environment and Jupyter notebooks.
- Anaconda can be used on the SCC, with some caveats.



# Python 2 vs. 3

- Python 2: released in 2000, Python 3 released in 2008
  - Python 2 is in "maintenance mode" no new features are expected
- Py3 is not completely compatible with Py2
  - For learning Python these differences are almost negligible
- Which one to learn?
  - If your research group / advisor / boss / friends all use one version that's probably the best one for you to choose.
  - If you have a compelling reason to focus on one vs the other
  - Otherwise just choose Py3. This is where the language development is happening!



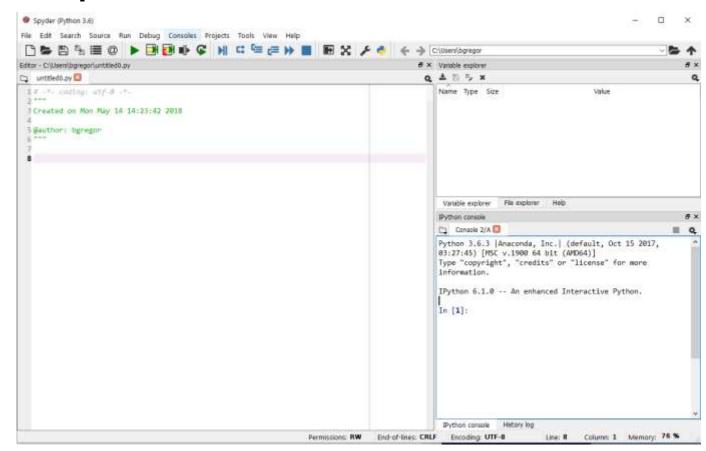
# Spyder – a Python development environment

#### Pros:

- Faster development
- Easier debugging!
- Helps organize code
- Increased efficiency

#### Cons

- Learning curve
- Can add complexity to smaller problems





- What is Python?
- Operators
- Variables
- Functions
- Classes
- If / Else
- Lists



- Loops
- Tuples and dictionaries
- Modules
- numpy and matplotlib modules
- Script setup
- Debugging



- What is Python?
- Operators
- Variables
- If / Else
- Lists
- Loops
- Functions



# What is Python?

- Python...
  - ...is a general purpose interpreted programming language.
  - ...is a language that supports multiple approaches to software design, principally structured and object-oriented programming.
  - ...provides automatic memory management and garbage collection
  - ...is extensible
  - ...is dynamically typed.
- By the end of the tutorial you will understand all of these terms!



### Some History

"Over six years ago, in December 1989, I was looking for a "hobby" programming project that would keep me occupied during the week around Christmas...I chose Python as a working title for the project, being in a slightly irreverent mood (and a big fan of Monty Python's Flying Circus)."

–Python creator Guido Van Rossum, from the foreward to *Programming Python* (1<sup>st</sup> ed.)

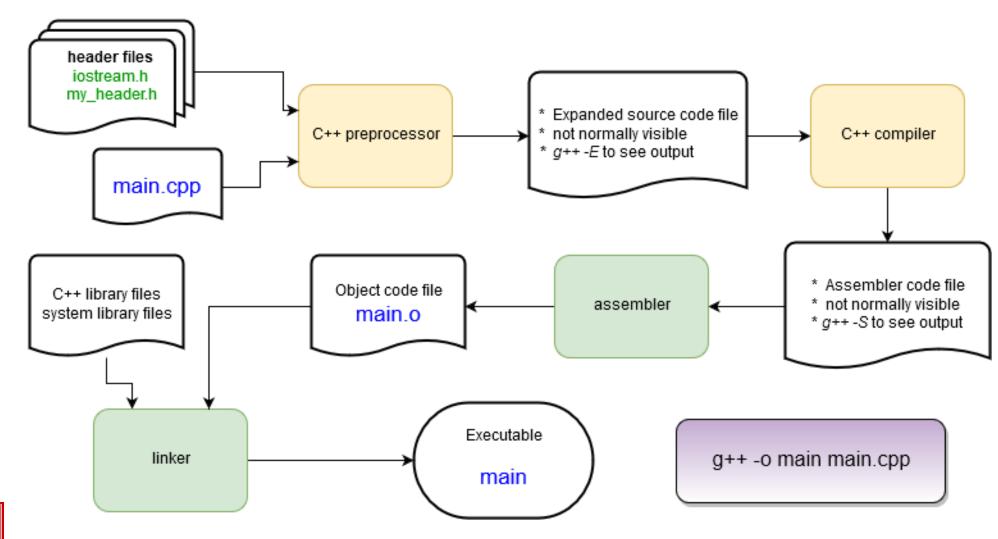
#### Goals:

- An easy and intuitive language just as powerful as major competitors
- Open source, so anyone can contribute to its development
- Code that is as understandable as plain English
- Suitability for everyday tasks, allowing for short development times



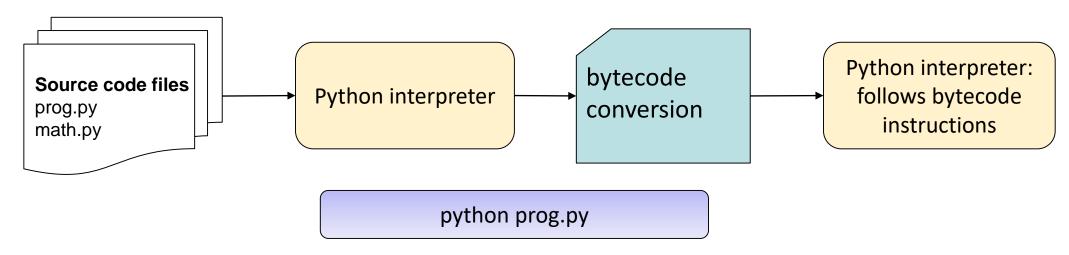


# Compiled Languages (ex. C++ or Fortran)





### Interpreted Languages (ex. Python or R)



- Clearly, a lot less work is done to get a program to start running compared with compiled languages!
- Bytecodes are an internal representation of the text program that can be efficiently run by the Python interpreter.
- The interpreter itself is written in C and is a compiled program.



# Comparison

#### Interpreted

- Faster development
- Easier debugging
  - Debugging can stop anywhere, swap in new code, more control over state of program
- (almost always) takes less code to get things done
- Slower programs
  - Sometimes as fast as compiled, rarely faster
- Less control over program behavior



#### Compiled

- Longer development
  - Edit / compile / test cycle is longer!
- Harder to debug
  - Usually requires a special compilation
- (almost always) takes more code to get things done
- Faster
  - Compiled code runs directly on CPU
  - Can communicate directly with hardware
- More control over program behavior

# The Python Prompt

The standard Python prompt looks like this:

```
[bgregor@scc2 bg]$ python
Python 3.6.2 (default, Aug 30 2017, 15:46:55)
[GCC 4.4.7 20120313 (Red Hat 4.4.7-3)] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>>
```

The IPython prompt in Spyder looks like this:

```
Python 3.6.3 | Anaconda, Inc. | (default, Oct 15 2017, 03:27:45) [MSC v.1900 64 bit (AMD64)] Type "copyright", "credits" or "license" for more information.

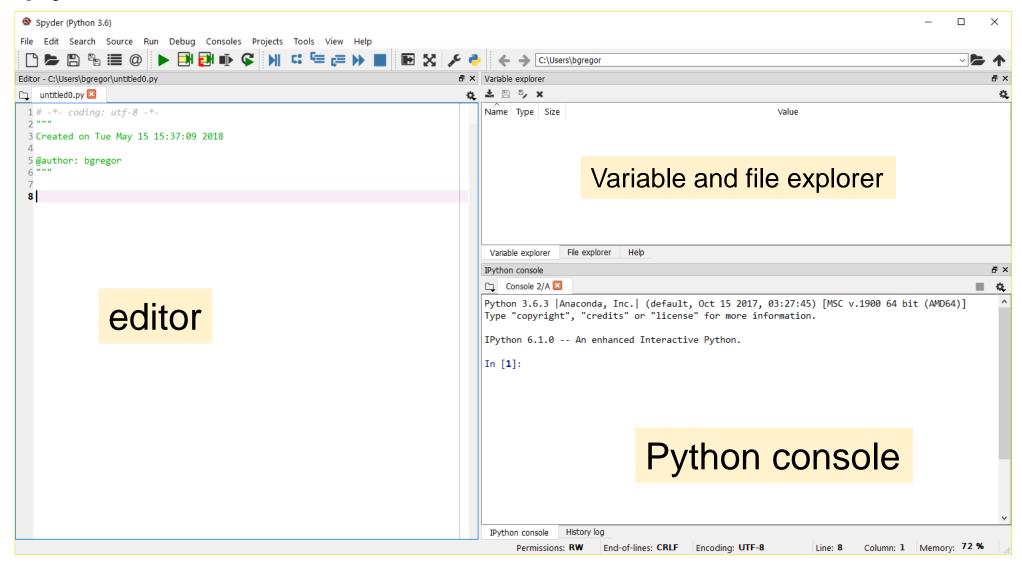
IPython 6.1.0 -- An enhanced Interactive Python.

In [1]:
```



IPython adds some handy behavior around the standard Python prompt.

# The Spyder IDE





- What is Python?
- Operators
- Variables
- If / Else
- Lists
- Loops
- Functions



### **Operators**

Python supports a wide variety of operators which act like functions, i.e. they do something and return a value:



# Try Python as a calculator

Python 3.6.3 |Anaconda, Inc.| (default, Oct 15 2017, 03:27:45)
Type "copyright", "credits" or "license" for more information.

IPython 6.1.0 -- An enhanced Interactive Python.

In [1]: 1 + 3
Out[1]: 4

In [2]: 4\*2
Out[2]: 8

In [3]: |

- Go to the Python prompt.
- Try out some arithmetic operators:

```
+ - * / % ** == (
```

Can you identify what they all do?



# Try Python as a calculator

- Go to the Python prompt.
- Try out some arithmetic operators:

Operator	Function
+	Addition
-	Subtraction
*	Multiplication
/	Division (Note: 3 / 4 is 0.75!)
%	Remainder (aka modulus)
**	Exponentiation
==	Equals



### More Operators

 Try some comparisons and Boolean operators. True and False are the keywords indicating those values:

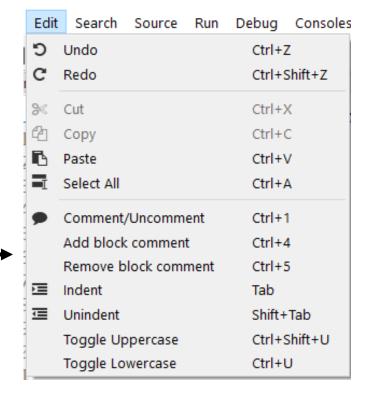
```
In [15]: 4 > 5
Out[15]: False
In [16]: 6 > 3 and 3 > 0
Out[16]: True
In [17]: not False
Out[17]: True
In [18]: True and (False or not False)
Out[18]: True
In [19]:
```



### Comments

- # is the Python comment character. On any line everything after the # character is ignored by Python.
- There is no multi-line comment character as in C or C++.
- An editor like Spyder makes it very easy to comment blocks of code or viceversa. Check the *Edit* menu

```
a=1
b=2
# this is a comment
c=3 # this is also a comment
# this is a
# multiline comment
```





- What is Python?
- Operators
- Variables
- If / Else
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- Loops
- Functions



### Variables

- Variables are assigned values using the = operator
- In the Python console, typing the name of a variable prints its value
  - Not true in a script!
- Variables can be reassigned at any time
- Variable type is not specified
- Types can be changed with a reassignment

```
In [1]: a=1
In [2]: b=2
In [3]: a
Out[3]: 1
In [4]: b
Out[4]: 2
In [5]: a=b
In [6]: a
Out[6]: 2
In [7]: b=-0.15
```



### Variables cont'd

- Variables refer to a value stored in memory and are created when first assigned
- Variable names:
  - Must begin with a letter (a z, A B) or underscore \_
  - Other characters can be letters, numbers or \_
  - Are case sensitive: capitalization counts!
  - Can be any reasonable length
- Assignment can be done en masse:

$$x = y = z = 1$$

Multiple assignments can be done on one line:

$$x, y, z = 1, 2.39, 'cat'$$

Try these out!



### Variable Data Types

- Python determines data types for variables based on the context
- The type is identified when the program runs, called dynamic typing
  - Compare with compiled languages like C++ or Fortran, where types are identified by the programmer and by the compiler **before** the program is run.
- Run-time typing is very convenient and helps with rapid code development...but requires the programmer to do more code testing for reliability.
  - The larger the program, the more significant the burden this is!!



### Variable Data Types

- Available basic types:
  - Numbers: Integers and floating point (64-bit)
  - Complex numbers: x = complex(3,1) or x = 3+1j
  - Strings, using double or single quotes: "cat" 'dog'
  - Boolean: True and False
  - Lists, dictionaries, and tuples
    - These hold collections of variables
  - Specialty types: files, network connections, objects
- Custom types can be defined. This will be covered in Part 2.



# Variable modifying operators

Some additional arithmetic operators that modify variable values:

Operator	Effect	Equivalent to
x += y	Add the value of y to x	x = x + y
x -= y	Subtract the value of <i>y</i> from <i>x</i>	x = x - y
x *= y	Multiply the value of <i>x</i> by <i>y</i>	x = x * y
x /= y	Divide the value of x by y	x = x / y

The += operator is by far the most commonly used of these!



# Check a type

- A built-in function, type(), returns the type of the data assigned to a variable.
  - It's unusual to need to use this in a program, but it's available if you need it!
- Try this out in Python do some assignments and reassignments and see what type() returns.

```
In [1]: a=1.0
In [2]: b=3
In [3]: c='Hello!'
In [4]: type(a)
Out[4]: float
In [5]: type(b)
Out[5]: int
In [6]: type(c)
Out[6]: str
```



# Strings

Strings are a basic data type in Python.

- Indicated using pairs of single " or double "" quotes.
- Multiline strings use a triple set of quotes (single or double) to start and end them.

Strings have many built-in functions...

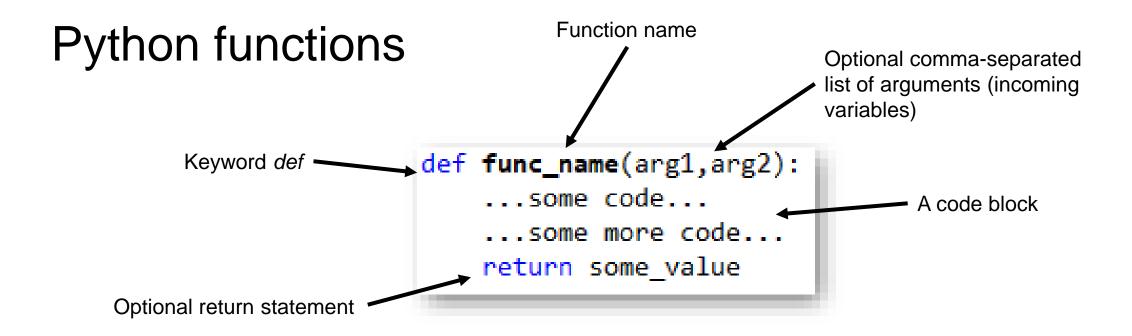
```
BOSTON
UNIVERSITY
```

```
'cat'
"dog"
"What's that?"
'They said "hello"'
    This is
    a multiline
    string
```

### **Functions**

- Functions are used to create code that can be used in a program or in other programs.
- The use of functions to logically separate the program into discrete computational steps.
- Programs that make heavy use of function definitions tend to be easier to develop, debug, maintain, and understand.





- The return value can be any Python type
- If the return statement is omitted a special None value is still returned.
- The arguments are optional but the parentheses are required!
- Functions must be defined before they can be called.

#### **Function Return Values**

- A function can return any Python value.
- Function call syntax:

```
A = some_func()  # return a value
Another_func()  # ignore return value or nothing returned
b,c = multiple_vals(x,y,z)  # return multiple values
```

Open function\_calls.py for some examples



### Function arguments

- Function arguments can be required or optional.
- Optional arguments are given a default value

```
def my_func(a,b,c=10,d=-1):
    ...some code...
```

- To call a function with optional arguments:
- Optional arguments can be used in the order they're declared or out of order if their name is used.

```
my_func(x,y,z)  # a=x, b=y, c=z, d=-1
my_func(x,y)  # a=x, b=y, c=10, d=-1
my_func(x,y,d=w,c=z)  # a=x, b=y, c=z, d=w
```



### Function arguments

Remember the list assignment?

```
x = ['a', [], 'c', 3.14]

y=x # y points to the same list as x
```

This applies in function calls too.

```
def my_func(a_list):
    # modifies the list in the calling routine!
    a_list.append(1)
```

Then call it:

```
my_func(x) # x and a_list inside the function are the same list!

TON

'a' [] 'c' 3.14
```

### Garbage collection

- Variables defined in a function (or in any code block) no longer have any "live" references to them once the function returns.
- These variables become garbage, and garbage collection operates to remove them from the computer's memory, freeing up the memory to be re-used.
- There is no need to explicitly destroy or release most variables.
  - Some complex data types provide .close(), .clean(), etc. type functions. Use these where available.
  - Simple data types (int, string, lists) will be taken care of automatically.



### When does garbage collection occur?

- That's hard to say. It happens when Python thinks it should.
- For the great majority of programs this is not an issue.
- Programs using very large quantities of memory or allocating large chunks of memory in repeated function calls can run into trouble.

```
def my_func(N):
    # make a large list
    tmp = [1]*N
    # get its sum
    sum tmp = sum(tmp)
    return sum tmp
# What happens to the list created for tmp?
# It gets garbage collected.
# when? ????
# Call my_func with a large N repeatedly
sums = []
for i in range(1000):
    sums.append(my func(100000))
```



### Memory usage in functions

- If possible, pre-allocate a list or other large data structures and re-use it.
  - i.e. allocate outside the function call and send it as a function argument. Remember function arguments are just references so they don't copy large data structures.
- There are numerous tools to profile a program, which means exam the CPU and memory usage of different parts of the program.
- Need to control memory cleanup? Python <u>provides</u> <u>a library</u> for this.

```
BOSTON
```

```
my_lst = 1000*[0]
for i in range(1000):
    my_lst[i] = some_func()

# that's better than:
my_lst = []
for i in range(1000):
    my_lst.append(some_func())
```

### Tutorial Outline – Part 1

- What is Python?
- Operators
- Variables
- Functions
- Classes
- If / Else
- Lists



#### Classes

- In OOP a class is a data structure that combines data with functions that operate on that data.
- An object is a variable whose type is a class
  - Also called an instance of a class
- Classes provide a lot of power to help organize a program and can improve your ability to re-use your own code.



## Object-oriented programming

- Python is a fully object oriented programming (OOP) language.
- Object-oriented programming (OOP) seeks to define a program in terms of the *things* in the problem (files, molecules, buildings, cars, people, etc.), what they need, and what they can do.

#### class GasMolecule

- Data:
  - molecular weight, structure, common names, etc.
- Methods:
  - IR(wavenumStart, wavenumEnd): return IR emission spectrum in range



#### Objects (instances of a class)

```
GasMolecule ch4
GasMolecule co2
```

```
spectrum = ch4.IR(1000,3500)
```

Name = co2.common name



'pseudo-code'

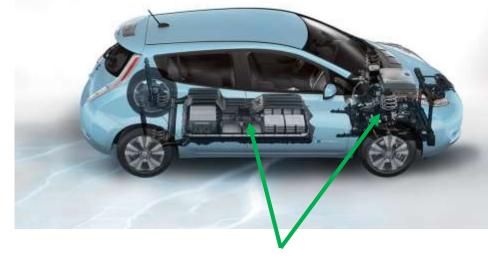
# Object-oriented programming

- OOP defines classes to represent the parts of the program.
- Classes can contain data and methods (internal functions).
  - Bundling these together is called encapsulation.
- Classes can inherit from one another
  - A class (the subclass) can use all of the data and methods from another class (the superclass) and add its own.
- This is a highly effective way of modeling real world problems inside of a computer program.



public interface







### **Encapsulation in Action**

In Python, calculate the area of some shapes after defining some functions.

```
# assume radius and width_square are assigned
# already
a1 = AreaOfCircle(radius)  # ok
a2 = AreaOfSquare(width_square)  # ok
a3 = AreaOfCircle(width square)  # !! OOPS
```

• If we defined Circle and Rectangle classes with their own area() methods...it is not possible to miscalculate.

```
c1 = Circle(radius)
r1 = Square(width_square)
a1 = c1.area()
a2 = r1.area()
```



# Strings in Python

- Python defines a string class all strings in Python are objects.
- This means:
  - Strings have their own internal management to handle storage of the characters



## String functions

 In the Python console, create a string variable called mystr

type: dir(mystr)

Try out some functions: -

Need help? Try: help(mystr.title) len(mystr)

mystr.upper()

mystr.title()

mystr.isdecimal()

help(mystr.isdecimal)



### The len() function

The len() function is not a string specific function.

 It'll return the length of any Python variable that contains some sort of countable thing.

 In the case of strings it is the number of characters in the string.



### String operators

 Try using the + and += operators with strings in the Python console.

- + concatenates strings.
- += appends strings.

```
a="Hello BU!"
print(a[4])
```

Index strings using square brackets, starting at 0.



### String operators

Changing elements of a string by an index is **not allowed**:

```
In [79]: a='Hello BU!'
In [80]: a[4] = '0'
Traceback (most recent call last):

File "<ipython-input-80-7c5733c2cb67>", line 1, in <module>
    a[4] = '0'

TypeError: 'str' object does not support item assignment
```

Python strings are immutable, i.e. they can't be changed.



# String Substitutions

 Python provides an easy way to stick variable values into strings called substitutions %s means sub in value

variable name comes after a %

Syntax for one variable:

'string with a %s' % <u>variable</u>

For more than one:

```
'x: %s y: %s z: %s' % (xval,yval,zval)
```

Variables are listed in the substitution order inside ()



### Variables with operators

- Operators can be combined freely with variables and variable assignment.
- Try some out again!
- This time type them into the editor. Click the green triangle to run the file. Save the file and it will run.

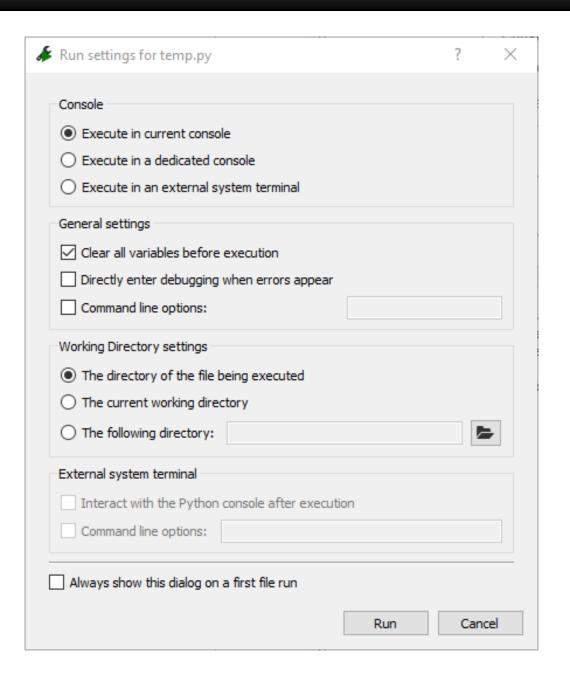


```
Spyder (Python 3.6)
    Edit Search Source Run Debug Consoles Projects
    Editor - C:\Users\bgregor\untitled0.py
   untitled0.py* 🖾
  1# -*- coding: utf-8 -*-
  3 Created on Tue May 15 15:37:09 2018
  5 @author: bgregor
 10 c = a * 3 - 11
 11 d = c / 0.5 + b**3
 12
 13 a
 14 b
 15 c
 16 d
 18 print(a,b,c,d)
```

# Spyder setup

The first time you run a script Spyder will prompt you with a setup dialog:

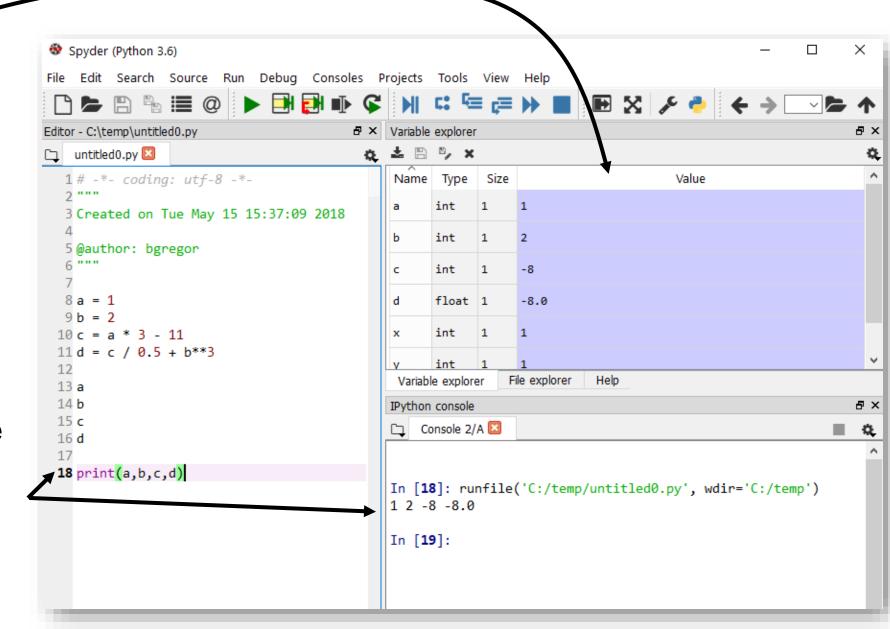
 Just click "Run" to run the script. This will only appear once.





 The Variable Explorer window is displaying variables and types defined in the console.

- Only the *print* function printed values from the script.
  - Key difference between scripts and the console!





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### If / Else

 If, elif, and else statements are used to implement conditional program behavior

```
• Syntax:

if Boolean_value:
    ...some code
elif Boolean_value:
    ...some other code
else:
    ...more code
```

 elif and else are not required – used to chain together multiple conditional statements or provide a default case.



- Try out something like this in the Spyder editor.
- Do you get any error messages in the console?
- Try using an *elif* or *else* statement by itself without a preceding *if*. What error message comes up?

```
untitled0.py* 🔼
 1 if True:
      print('true!')
 4a = 1
 5b = 2
 7 if a > b:
 9 elif b > a:
10 c = b
11 else:
12   c = 'Equal!'
13
14 print(c)
```



# Indentation of code...easier on the eyes!

• C:

```
int x ;
if (3 > 4) {
x = 5 ;
} else {
x = 6 ;
}
```

or

Matlab:

```
if (3 > 4)
x = 5
else
x = 6
end
```

or

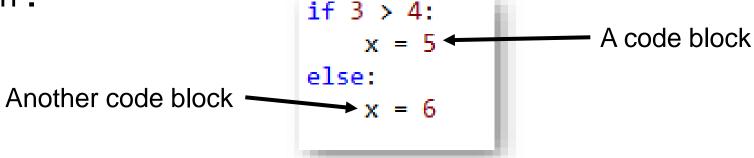


#### The Use of Indentation

Python uses whitespace (spaces or tabs) to define code blocks.

Code blocks are logical groupings of commands. They are always

preceded by a colon:



- This is due to an emphasis on code readability.
  - Fewer characters to type and easier on the eyes!
- Spaces or tabs can be mixed in a file but not within a code block.



#### If / Else code blocks

 Python knows a code block has ended when the indentation is removed.

 Code blocks can be nested inside others therefore if-elif-else statements can be freely nested within others.

```
a = 1
b = 2
if a <= b:
    c = a
    print('a <= b')
    if c == 1:
        print('c is 1')
print('out of the if statement')</pre>
```

 Note the lack of "end if", "end", curly braces, etc.



#### File vs. Console Code Blocks

 Python knows a code block has ended when the indentation is removed.

 EXCEPT when typing code into the Python console. There an empty line indicates the end of a code block. Let's try this out in Spyder

 This sometimes causes problems when pasting code into the console.

 This issue is something the IPython console helps with.



### Tutorial Outline – Part 1

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### Lists

- A Python list is a general purpose 1-dimensional container for variables.
  - i.e. it is a row, column, or vector of things
- Lots of things in Python act like lists or use list-style notation.
- Variables in a list can be of any type at any location, including other lists.
- Lists can change in size: elements can be added or removed
- Lists are not meant for high performance numerical computing!
  - We'll cover a library for that in Part 2
  - Please don't implement your own linear algebra with Python lists unless it's for your
     own educational interests.

### Making a list and checking it twice...

- Make a list with [] brackets.
- Append with the append() function
- Create a list with some initial elements
- Create a list with N repeated elements

Try these out yourself!
Edit the file in Spyder and run it.
Add some print() calls to see the lists.

```
list 1 = []
list 1.append(1)
list 1.append('A string!')
list 1.append([])
list 2 = [4, 5, -23.0+4.1j, 'cat']
list 3 = 10 * [42]
```



### List functions

- Try dir(list\_1)
- Like strings, lists have a number of built-in functions
- Let's try out a few...
- Also try the len() function to see how many things are in the list: len(list\_1)

```
'append',
'clear',
'copy',
'count',
'extend',
'index',
'insert',
'pop',
'remove',
'reverse',
'sort']
```



## Accessing List Elements

- Lists are accessed by index.
  - All of this applies to accessing strings by index as well!
- Index #'s start at 0.
- List: x=['a', 'b', 'c', 'd', 'e']
- First element: x[0]
- Nth element: x [2]
- Last element: x[-1]
- Next-to-last: x [-2]



### List Indexing

- Elements in a list are accessed by an index number.
- Index #'s start at 0.
- List: x=['a', 'b', 'c', 'd', 'e']
- First element:  $x[0] \rightarrow 'a'$
- Nth element:  $x[2] \rightarrow 'c'$
- Last element:  $x[-1] \rightarrow 'e'$
- Next-to-last:  $x[-2] \rightarrow 'd'$



### List Slicing

- List: x=['a', 'b', 'c', 'd', 'e']
- Slice syntax: x[start:end:step]
  - The start value is inclusive, the end value is exclusive.
  - Step is optional and defaults to 1.
  - Leaving out the end value means "go to the end"
  - Slicing always returns a new list copied from the existing list
- $\bullet x[0:1] \rightarrow ['a']$
- $x[0:2] \rightarrow ['a', 'b']$
- $\mathbf{x}[-3:] \rightarrow ['c', 'd', 'e'] + Third from the end to the end$
- $x[2:5:2] \rightarrow ['c', 'e']$



### List assignments and deletions

Lists can have their elements overwritten or deleted (with the del) command.

```
List: x=['a', 'b', 'c', 'd', 'e']
```

• 
$$x[0] = -3.14$$
  $\rightarrow$  x is now [-3.14, 'b', 'c', 'd', 'e']

• del x[-1]  $\rightarrow$  x is now [-3.14, 'b', 'c', 'd']



### **DIY Lists**

- Go to the menu File → New File
- Enter your list commands there
- Give the file a name when you save it
- Use print() to print out results
- In the Spyder editor try the following things:
- Assign some lists to some variables.
  - Try an empty list, repeated elements, initial set of elements
- Add two lists: a + b What happens?
- Try list indexing, deletion, functions from dir(my\_list)
- Try assigning the result of a list slice to a new variable



#### More on Lists and Variables

Open the sample file list\_variables.py but don't run it yet!

What do you think will be printed?

Now run it...were you right?

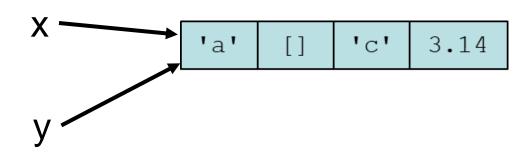
```
x = ['a',[],'c',3.14]
v = x
# id() returns a unique identifier for a variable
print('x: %s addr of x: %s' % (x,id(x)))
print('y: %s addr of y: %s' % (y,id(y)))
x[0] = -100
print('x: %s' % x)
print('v: %s' % y)
```



### Variables and Memory Locations

- Variables refer to a value stored in memory.
- y = x does not mean "make a copy of the list x and assign it to y" it means "make a copy of the memory location in x and assign it to y"
- x is not the list it's just a reference to it.

```
x = ['a',[],'c',3.14]
y = x
```





# Copying Lists

```
z=x[:]
z[0] = 'frog'
print('x: %s addr of x: %s' % (x,id(x)))
print('z: %s addr of z: %s' % (z,id(z)))
```

How to copy (2 ways...there are more!):

```
• y = x[:] or y=list(x)
```

- In list\_variables.py uncomment the code at the bottom and run it.
- This behavior seems weird at first. It will make more sense when calling functions.



### Tutorial Outline – Part 1

- What is Python?
- Operators
- Variables
- If / Else
- Lists
- Loops
- Functions



### While Loops

- While loops have a condition and a code block.
  - the indentation indicates what's in the while loop.
  - The loop runs until the condition is false.
- The break keyword will stop a while loop running.
- In the Spyder edit enter in some loops like these. Save and run them one at a time. What happens with the 1<sup>st</sup> loop?

```
while True:
    print("looping!")
a = 10
while a > 0:
    print(a)
    a -= 1
my list=['a','b','c','d','e']
i=0
while i < len(my_list):</pre>
    print( my_list[i] )
    i += 1
    if i==3:
        break
```

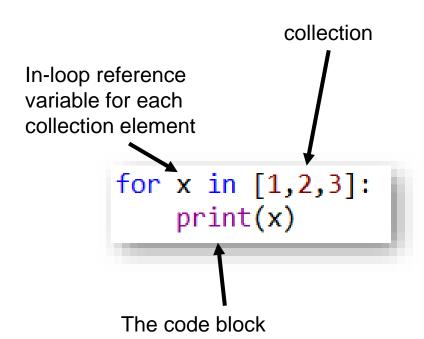


## For loops

- for loops are a little different. They loop through a collection of things.
- The for loop syntax has a collection and a code block.
  - Each element in the collection is accessed in order by a reference variable
  - Each element can be used in the code block.

 The break keyword can be used in for loops too.





### Processing lists element-by-element

A for loop is a convenient way to process every element in a list.

- There are several ways:
  - Loop over the list elements
  - Loop over a list of index values and access the list by index
  - Do both at the same time
  - Use a shorthand syntax called a list comprehension
- Open the file looping\_lists.py
- Let's look at code samples for each of these.



# The range() function

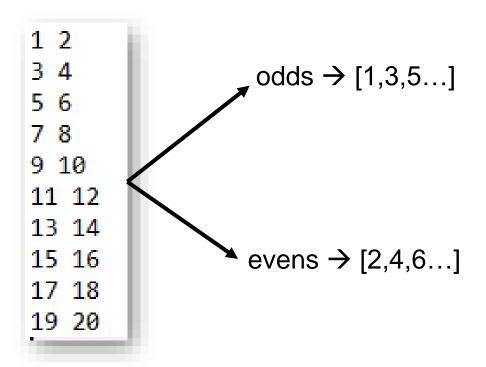
- The range() function auto-generates sequences of numbers that can be used for indexing into lists.
- Syntax: range(start, exclusive end, increment)
- range $(0,4) \rightarrow$  produces the sequence of numbers 0,1,2,3
- range(-3,15,3)  $\rightarrow$  -3,0,3,6,9,12
- range $(4,-3,2) \rightarrow 4,2,0,-2$
- Try this: print(range(4))



## Lists With Loops

- Open the file read\_a\_file.py
- This is an example of reading a file into a list. The file is shown to the right, numbers.txt
- We want to read the lines in the file into a list of strings (1 string for each line), then extract separate lists of the odd and even numbers.





- Edit *read\_a\_file.py* and try to figure this out.
- A solution is available in read\_a\_file\_solved.py
- Use the editor and run the code frequently after small changes!